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EL EFECTO AHARONOV-BOHM

T E S I S

QUE PARA OBTENER EL GRADO ACADÉMICO DE

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P R E S E N T A

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Capítulo 1

Introducción

En la teoría de la física clásica el movimiento de las partículas está determinado por las fuerzas que actúan sobre ellas. Para conocer su comportamiento es suficiente determinar las fuerzas que son aplicadas. Es, por lo tanto, un aspecto fundamental en la física clásica el determinar las fuerzas que actúan sobre las partículas.

En el caso de la teoría clásica del electromagnetismo, la fuerza se determina a través de los campos electromagnéticos. Por ende, los campos son las cantidades físicas fundamentales. De hecho, la teoría misma del electromagnetismo es construida a través del concepto del campo electromagnético.

Sin embargo, la realidad no se comporta siempre como lo predice el modelo teórico de la física clásica. No es suficiente conocer las fuerzas que actúan sobre una partícula para determinar su comportamiento. Experimentos hechos con electrones en 1982 y 1986 por Tonomura et al. [63, 64] (ver también [66]) dan fuerte evidencia de la existencia de cantidades físicas, diferentes a las fuerzas, que influyen sobre el comportamiento de dichos electrones. Recientemente en [9] se hizo un nuevo experimento que fundamenta la ausencia de efectos debidos a algún tipo de fuerza en los resultados de Tonomura et. al. [63, 64]. Esto último es discutido por Tonomura y Nori en un artículo publicado en 2008 en Nature [67].

Por medio de la física cuántica se pueden predecir los resultados experimentales de Tonomura et al. [63, 64] y también los resultados obtenidos en [9] , además, se pueden definir las cantidades electromagnéticas fundamentales. El concepto de la física a través del cual se determinan las cantidades electromagnéticas fundamentales en la física cuántica es llamado el efecto Aharonov-Bohm. El efecto Aharonov-Bohm es un concepto fundamental en la física, no sólo porque describe las cantidades electromagnéticas fundamentales en la física cuántica sino también porque, al predecir comportamientos que no se pueden deducir a través de la física clásica, constituye en si mismo una prueba para la teoría misma de la mecánica cuántica. El efecto Aharonov-Bohm es también importante por ser la única evidencia experimental de que los campos de norma (gauge fields) producen observables físicos (ver [66, 87]). Los campos de norma se convirtieron a finales de la década de 1970 en los candidatos más probables para la construcción de una teoría de gran unificación que involucre todas las fuerzas en la naturaleza (ver [66]). En [87] se describe la relación entre el efecto Aharonov-Bohm y los campos de norma. Por su importancia, el efecto Aharonov-Bohm es estudiado en la mayoría de los libros de texto de física cuántica.

El efecto Aharonov-Bohm toma su nombre a partir del trabajo fundamental de Aharonov y Bohm en 1959 [2]. En dicho trabajo se propone una fórmula (el Ansatz de Aharonov-Bohm) para describir el comportamiento de los electrones sobre regiones en donde el campo electromagnético es nulo. En los experimentos fundamentales de Tonomura et al. [63, 64] y el experimento descrito en [9] (ver también [67]) se verifica el Ansatz de Aharonov-Bohm. Estos experimentos se consideran como la evidencia más importante sobre la existencia de este fenómeno.

En los experimentos de Tonomura el al. [63, 64] se utiliza un magneto en forma toroidal que contiene un campo magnético confinado. Se envían electrones que pasan por el centro del magneto y por fuera del agujero, y se hacen coincidir los electrones en una misma región produciendo un patrón de interferencia. El patrón de interferencia obtenido coincide con las predicciones descritas por el Ansatz de Aharonov y Bohm.

En la configuración experimental en [63, 64], no hay campo magnético en el exterior del obstáculo, sin embargo, algunos autores argumentan [8, 88, 24] que el patrón de interferencia se debe a la acción del campo electromagnético que acelera de manera diferente a los electrones que pasan por el centro del magneto y los que pasan por fuera. En [8] se hace un cálculo que muestra que en el caso en el que en lugar del magneto de forma toroidal se utilice un solenoide recto de longitud infinita, el patrón de interferencia se puede explicar por medio de la acción de cierta fuerza. Esto último implicaría (en el caso de que fuera cierto) que los resultados en los experimentos de Tonomura et al. [63, 64] no son un efecto puramente cuántico y por lo tanto que el efecto Aharonov-Bohm no existiría.

Para demostrar que los electrones no se aceleran y, por ende, que no existe ninguna fuerza que afecte su comportamiento, en [9] se hace un experimento en donde se calcula el tiempo en el que los electrones pasan por el agujero del magneto y se demuestra que no se aceleran. El Ansatz de Aharonov-Bohm predice que la posición de los electrones evoluciona de manera libre (no se aceleran), lo que es verificado en el experimento [9]. Esto último es una evidencia convincente de que los resultados en los experimentos de Tonomura et al. [63, 64] son puramente cuánticos, lo que muestra que el efecto Aharonov-Bohm existe.

La existencia del efecto Aharonov Bohm es un tema controvertido, existen más de 300 artículos relacionados con esta controversia. En [56, 9, 67] y sus referencias, se pueden encontrar los artículos involucrados en esta discusión.

En este trabajo de tesis doctoral se demuestra por primera vez de manera rigurosa que el Ansatz de Aharonov-Bohm es una consecuencia de la física cuántica, además, utilizando los datos en los experimentos de Tonomura et al., se demuestra también por primera vez de manera cuantitativa que la mecánica cuántica predice los resultados experimentales de Tonomura et al. y los resultados del experimento descrito en [9] (ver también [67]).

La ecuación de Schrödinger es la ecuación fundamental de la física cuántica. La solución de la ecuación de Schrödinger es la función de onda que describe las funciones de probabilidad en la posición y el momento de los electrones en cada instante. El Ansatz de Aharonov-Bohm es una solución aproximada de la ecuación de Schrödinger para todo tiempo, cuando el electrón viaja en regiones en donde no hay campo electromagnético. En el artículo fundamental de Aharonov y Bohm de 1959 [2], en donde se introduce el Ansatz, se resuelve explicitamente la ecuación de Schrödinger en el caso ideal de un solenoide infinito, reduciendo el problema a dos dimensiones. Sin embargo, en el caso que corresponde a la realidad física, en tres dimensiones, y para un magneto acotado, no se demuestra que esta fórmula sea una aproximación de la solución exacta de la ecuación de Schrödinger, de hecho, simplemente se enuncia sin dar ninguna justificación matemática de su aplicabilidad. No es sino hasta el año 2009, en este trabajo doctoral, que se da por primera vez una justificación rigurosa de que el Ansatz de Aharonov Bohm es una aproximación de la solución exacta de la ecuación de Schrödinger en el caso tridimensional y para magnetos acotados. Se estima la diferencia entre la solución exacta de la ecuación de Schrödinger y el Ansatz de Aharonov-Bohm y se encuentra una fórmula explícita y simple para la cota de error que mide esta diferencia. La fórmula para la cota de error es uniforme en el tiempo y tiene una interpretación física en términos de la probabilidad que tiene el electrón de estar fuera de la región donde el campo electromagnético es cero; cuando esta probabilidad es pequeña la cota de error puede ser extremadamente reducida, menor a 10^{-99}, en norma. Lo que es muy relevante, pues en este caso conocemos prácticamente de manera exacta la solución de la ecuación de Schrödinger y demostramos que los electrones no se aceleran (contrariamente a lo que se muestra en [8], dando fundamento teórico casi exacto a los resultados en [9] y los argumentos en [67]); además, también se demuestra de manera muy precisa que los resultados en los experimentos de Tonomura et al. [63, 64] son una consecuencia de la mecánica cuántica.

En este trabajo se estudia también la teoría de dispersión de electrones en presencia de un obstáculo que es la unión de cuerpos con asas y suponemos además que fuera del obstáculo existen campos eléctrico y magnético. A partir del operador de dispersión recuperamos los campos eléctrico y magnético en cierta región y adicionalmente reconstruimos el flujo del campo magnético módulo 2π sobre determinadas superficies dentro del obstáculo. Esto es muy relevante, pues recuperamos información del campo magnético dentro del obstáculo a partir de dispersión de partículas que no tienen acceso al interior del mismo (esto es una evidencia del efecto Aharonov-Bohm). Adicionalmente, caracterizamos las cantidades electromagnéticas que son fundamentales para la física cuántica, a saber: el campo magnético fuera del obstáculo y el flujo del mismo módulo 2π sobre ciertas superficies dentro del obstáculo que proporcionamos explícitamente (ver la parte final de la sección 2.1.1, asi como la definición 3.9 y el teorema 4.1 de [4]).

Como se apuntó antes, el Ansatz de Aharonov-Bohm es una fórmula creada en 1959 y su justificación rigurosa se establece hasta el año 2009, en este trabajo. Esto se debe a las siguientes dos razones:

- El método que introducimos para estimar la solución de la ecuación de Schrödinger con campos magnéticos uniformemente en el tiempo es original. Nos basamos en el método dependiente del tiempo de Enss y Weder [16]. Esta forma de proceder para estimar soluciones a ecuaciones diferenciales es muy diferente a otros métodos. Para intervalos de tiempo acotados, en la región de interacción, utilizamos el límite de alta velocidad de los operadores de onda y de dispersión para estimar la solución de la ecuación de Schrödinger con cotas de error que crecen con el tamaño del intervalo. Para intervalos de tiempo no acotados, en las regiones entrante y saliente, usamos teoría de dispersión. De esta manera obtenemos estimaciones de la solución de la ecuación de

Schrödinger uniformes en el tiempo. En el artículo [16] se obtuvieron estimaciones de la solución de la ecuación de Schrödinger uniformes en el tiempo en el caso con potencial eléctrico y sin campo magnético. El método que utilizamos nos permite estimar la solución uniformemente para todo tiempo y de manera muy precisa, lo que es muy difícil de obtener con otros métodos.

- Como ya hemos dicho, el método dependiente del tiempo que utilizamos fué introducido por Enss y Weder [16] y fué utilizado por Weder [76] para estudiar el efecto Aharonov-Bohm en el caso de un flujo magnético contenido en un cilindro infinito y con sección transversal arbitraria. Este caso se reduce a dos dimensiones, pero no tiene solución explícita. Este método nos permite estudiar el límite de altas velocidades del operador de dispersión utilizando las propiedades de propagación de funciones de onda localizadas en el espacio, lo que nos permite estimar la solución de la ecuación de Schrödinger uniformemente para todo tiempo. Esto no se puede hacer con los métodos estándar en la teoría de dispersión, que utilizan la formulación estacionaria con soluciones periódicas en el tiempo, lo que implica que se pierde tanto la localización de la solución en el espacio, como la propagación temporal de la misma.

  Las ondas planas perturbadas que se usan en los métodos estacionarios son periódicas en el tiempo y se extienden por todo el espacio, de modo que es imposible suponer que los electrones, que son representados por estas funciones de onda, se propagan sobre regiones del espacio en las que no hay campo electromagnético, como lo exige el Ansatz Aharonov-Bohm, a menos que el campo electromagnético sea cero en todo el espacio. Esto implica que el Ansatz de Aharonov-Bohm no es en realidad una buena aproximación de las ondas planas perturbadas de la teoría estacionaria. Con el método dependiente del tiempo de [16, 76] podemos considerar paquetes de onda de energía finita cuya localización en el espacio podemos controlar de manera que se propagen en regiones localizadas del espacio adonde no hay campos electromagnéticos, o son muy pequeños.

Esta tesis está organizada de la siguiente forma: en el capítulo de antecedentes (capítulo 2) se presenta primeramente un resumen de la historia y el concepto del efecto Aharonov-Bohm (secciones 2.1.1 y 2.1.2) y posteriormente (sección 2.2) se hace una breve recapitulación de la historia de los problemas inversos. En el capítulo 3 se estudia el efecto Aharonov-Bohm bajo las condiciones de los experimentos de Tonomura et al. [63, 64]. Se demuestra que el Ansatz de Aharonov y Bohm es válido, se establece una fórmula para la cota de error que estima la diferencia entre la solución exacta de la ecuación de Schrödinger y el Ansatz y, finalmente, se interpretan los términos que aparecen en la cota de error. Este capítulo presenta los resultados del artículo [5] que es el contenido del capítulo 7.

En el capítulo 4 se estudia el operador de dispersión en el complemento de un obstáculo que es una unión finita de cuerpos con asas y se demuestra que a partir de éste se puede recuperar el campo electromagnético en cierta región. También recuperamos a partir del operador de dispersión, en el caso en el que el campo magnético en el exterior del obstáculo sea cero, ciertos flujos del campo magnético sobre determinadas secciones transversales del obstáculo. Podemos conocer también a partir del operador de dispersión cierta información de la clase de cohomología de de Rham del potencial magnético. En este mismo capítulo introducimos una definición matemática que describe cuándo los electrones pasan por algún agujero del obstáculo. Finalmente, demostramos que, en el límite de altas energías, el operador de dispersión, en ausencia de campo magnético exterior al obstáculo, actúa sobre los electrones que viajan por un determinado hoyo como un operador de multiplicación por un número complejo unitario cuya fase está dada por un flujo del campo magnético sobre cierta sección transversal del obstáculo asociada al hoyo. Este capítulo presenta los resultados del artículo [4], que es el contenido del capítulo 8.

El capítulo 5 contiene las conclusiones del trabajo. En el capítulo 6 se presentan los proyectos futuros relacionados con esta tesis, en los que ya estoy trabajando con el doctor Ricardo Weder y de los cuales tenemos resultados parciales. En el capítulo 7 se presenta el artículo [5] cuyo resumen esta contenido en el capítulo 3. Por último, en el capítulo 8 se presenta el artículo [4], del cual se hace una síntesis en el capítulo 4.

Capítulo 2

Antecedentes

2.1. Efecto Aharonov-Bohm

2.1.1. El Concepto del Efecto Aharonov-Bohm

La teoría de la física clásica encuentra su fundamento en la noción de fuerza. La posición ($\mathbf{X}(t)$) de una partícula clásica de masa m para todo tiempo t está determinada por las fuerzas ($\mathbf{F}$) que actúan sobre ella y las condiciones iniciales en velocidad y posición a través de la segunda ley de Newton:

$$\mathbf{F} = m\frac{d^2}{dt^2}\mathbf{X}(t), \tag{2.1}$$

es, por lo tanto, un aspecto fundamental en la física clásica el determinar las fuerzas que actúan sobre las partículas.

En la teoría de la electrodinámica clásica, la fuerza es producida por los campos electromagnéticos; esta fuerza es llamada la fuerza de Lorentz:

$$\mathbf{F} = q[E + \mathbf{V}(t) \times B], \qquad \mathbf{V}(t) := \frac{\partial \mathbf{X}(t)}{\partial t}, \tag{2.2}$$

en donde q es la carga del electrón, E es el campo eléctrico y B es el campo magnético. Los campos son las cantidades físicas fundamentales, ya que a través de ellos se obtiene la fuerza, la cual determina el comportamiento de las partículas cargadas que se desplazan bajo su influencia. De hecho, la teoría misma del electromagnetismo es construida a través del concepto mismo de campo electromagnético.

En el estudio del electromagnetismo clásico, se define el concepto de potencial magnético. El potencial magnético (A) es una función tal que su rotacional es el campo magnético ($\nabla \times A = B$). El potencial magnético resulta ser muy útil en el manejo de las ecuaciones de Maxwell, así como en la formulación hamiltoniana del electromagnetismo.

La ecuación $\nabla \times A = B$ no tiene una solución única; si un potencial magnético A satisface esa ecuación, entonces, sumándole el gradiente de una función escalar λ, obtenemos un potencial magnético $A + \nabla\lambda$ que satisface la misma ecuación. En general, la cantidad de potenciales magnéticos asociados a un mismo campo magnético depende de la topología del espacio en el que están definidos los campos, sin embargo, la elección del potencial magnético no cambia las predicciones físicas que se puedan hacer con la teoría. De hecho, el potencial magnético en la física clásica resulta ser solamente un concepto matemático que no tiene ninguna realidad física; esto se debe a que la fuerza que actúa sobre las partículas (la fuerza de Lorentz, (2.2)) depende sólo del campo magnético.

En términos de la velocidad ($\mathbf{V}(t) := \frac{\partial \mathbf{X}(t)}{\partial t}$) de la partícula, la segunda ley de newton toma la siguiente forma:

$$\mathbf{F} = m\frac{d}{dt}\mathbf{V}(t), \tag{2.3}$$

si la fuerza es cero en la ecuación (2.3) entonces la velocidad ($\mathbf{V}(t)$) es constante, es decir, una partícula tiene velocidad constante (o bien, evoluciona de manera libre) a menos que exista una fuerza actuando sobre ella.

Si tiramos una canica sobre el agujero de un aro, el movimiento de la canica no es modificado por la existencia del aro. De manera similar, consideremos un magneto en forma toroidal (o en forma de aro) que contiene un campo electromagnético confinado dentro de él (es decir, el campo electromagnético es cero fuera del magneto). Si enviamos un electrón por el agujero del magneto, entonces, como el campo electromagnético es cero en cada punto de la trayectoria del electrón, no hay fuerzas que actúen sobre el electrón, y, por lo tanto, debería clásicamente seguir una trayectoria libre, como en el caso de la canica. En otras palabras, el magneto no debería influir sobre el comportamiento del electrón y el electrón debería seguir la misma trayectoria que seguiría si no estuviera el magneto. Sin embargo, esto no ocurre;

en el mundo real, el magneto sí tiene cierta influencia sobre el electrón. Este fenómeno es llamado el efecto Aharonov-Bohm y fue descrito por primera vez por Franz [20], después por Eherenberg y Siday [13] y Aharonov y Bohm [2]. La verificación experimental fue realizada por Tonomura et al. [63], [64], quienes implementaron básicamente la experiencia con magnetos en forma toroidal descrita anteriormente en la introducción de este texto.

Como se explicó anteriormente en la introducción, el efecto Aharonov-Bohm no puede ser modelado por medio de la física clásica. Es en el contexto de la física cuántica que este fenómeno puede ser explicado. La ecuación fundamental de la física cuántica es la de Schrödinger, que en ausencia del campo eléctrico toma la siguiente forma:

$$i\hbar \frac{\partial}{\partial t}\phi(x,t) = H\phi(x,t), \tag{2.4}$$

en donde,

$$H := \frac{1}{2M}(\mathbf{P} - \frac{q}{c}\tilde{A})^2 \tag{2.5}$$

es el hamiltoniano, $\hbar$ es la constante de Planck, $\mathbf{P} := -i\hbar\nabla$ es el operador de momento, c es la velocidad de la luz, M y q son, respectivamente, la masa y la carga del electrón y $\tilde{A}$ es un potencial magnético tal que $\nabla \times \tilde{A} = \tilde{B}$ ($\tilde{B}$ el campo magnético). En la ecuación (2.4), ϕ es una función a valores complejos que es llamada la función de onda del electrón. A través de la función de onda se obtienen las funciones de probabilidad en posición y momento del electrón. La función $|\phi|^2$ representa densidad de probabilidad en posición. Denotamos por $\hat{\phi}$ la transformada de Fourier de ϕ,

$$\mathcal{F}(\phi) := \hat{\phi}(p) := \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} e^{-i\frac{p}{\hbar}\cdot x}\phi(x)dx, \tag{2.6}$$

en donde $\hbar$ es la constante de Planck. La función $|\hat{\phi}|^2$ representa la probabilidad en momento del electrón.

De la ecuación de Schrödinger misma (2.4) se puede ver la dependencia del potencial magnético y no del campo magnético, de manera que pudiéramos esperar que el potencial magnético fuera la cantidad física importante y no el campo magnético como en la física clásica. Sin embargo, este argumento simple está muy lejos de ser satisfactorio.

Desde mucho antes del descubrimiento del efecto Aharonov-Bohm, la comunidad de física ya había notado el hecho evidente de que el potencial magnético aparece en la ecuación de Schrödinger. No obstante, para concluir de este hecho que el potencial magnético tiene una realidad física, es necesario mostrar efectos físicos medibles que pongan en evidencia la influencia del potencial magnético. Esto último no es trivial y es motivo de una controversia que involucra más de 300 artículos en el periodo de 1959 (fecha de publicación del artículo de Aharonov y Bohm [2]) a 1986 (fecha de publicación de los resultados del experimento de Tonomura et al. [64], que dió fuerte evidencia de la existencia de este fenómeno). En [56] se encuentra una revisión bibliográfica de la controversia hasta 1989. La controversia sobre la existencia de este fenómeno tiene plena vigencia, en [88], [8], [24], [9], [67] y sus referencias se pueden encontrar los detalles de esta discusión hasta la fecha.

En la mecánica cuántica los potenciales magnéticos están definidos en todo el espacio ($\mathbb{R}^3$). Dados dos potenciales magnéticos (A^1 y A^2) asociados al mismo campo magnético (es decir, $\nabla \times A^1 = \nabla \times A^2$) existe una función escalar λ tal que $A^2 = A^1 + \nabla\lambda$. La selección de un potencial magnético es llamada también selección de la norma y la fórmula

$$A^2 = A^1 + \nabla\lambda \tag{2.7}$$

es la fórmula cambio de norma (o transformación de norma).

Denotemos por

$$D_{(i)} = \mathbf{P} - \frac{q}{c}A^i, \quad i \in 1, 2. \tag{2.8}$$

Si ϕ_1 es solución de la ecuación de Schrödinger (2.4)

$$i\hbar\frac{\partial}{\partial t}\phi_1(x,t) = \frac{1}{2M}D_{(1)}^2\phi_1(x,t), \tag{2.9}$$

entonces $\phi_2 := e^{-i\lambda}\phi$ es solución de la ecuación de Schrödinger (2.4)

$$i\hbar\frac{\partial}{\partial t}\phi_2(x,t) = \frac{1}{2M}D_{(2)}^2\phi_2(x,t), \tag{2.10}$$

La ecuación (2.9) se transforma en la ecuación (2.10) bajo las reglas de transformación que son llamadas transformaciones de norma,

$$\phi_2 = e^{-i\lambda}\phi_1, \quad D_{(2)} = e^{i\lambda}D_{(1)}e^{-i\lambda}. \tag{2.11}$$

En la ecuación de Schrödinger la función de onda no es observable físicamente; cuando se elige un potencial magnético y una función de onda para representar un estado físico, se está eligiendo una representación entre muchas posibles. Una vez que se elige una representación, es posible cambiar de representación por medio de las fórmulas (2.11). Todas las representaciones son equivalentes y describen la misma física; esto quiere decir que la física cuántica es covariante ante cambios de norma. Como para dos potenciales magnéticos, cualesquiera que sean, existe una transformación de norma que los relaciona, entonces la física cuántica no depende de la elección de potencial magnético y, por lo tanto, depende sólo del campo magnético.

En efecto, el campo magnético definido en todo el espacio (en ausencia del campo eléctrico) determina el comportamiento de los electrones, pero el campo magnético en la física cuántica no actúa de la misma forma que en la mecánica clásica. El campo magnético en la mecánica cuántica actúa también a distancia, es decir, puede tener influencia sobre un electrón que nunca está en contacto con él. Pero entonces, ¿cuál es la cantidad física que está en contacto con electrón?. La respuesta es el potencial magnético. Para explicar este concepto pensemos en la configuración de los experimentos de Tonomura et al. [64].

Consideremos un magneto en forma toroidal impenetrable que tiene confinado un campo magnético dentro de él (el campo magnético es cero fuera de él). Al enviar un electrón por el centro del magneto, éste siente la influencia del campo magnético aun cuando el electrón nunca está en contacto con el campo. Empero, no es posible construir un potencial magnético que se anule también en el exterior del magneto. Podemos suponer, sin pérdida de generalidad, que el potencial magnético que elegimos tiene soporte en el casco convexo del magneto (ya que cualquier otro describe la misma física a través de un cambio de norma). Cuando el electrón viaja por el centro del magneto, el potencial magnético no es cero aunque el campo magnético sea cero; es entonces el potencial magnético el que influye en el comportamiento de electrón cuando éste pasa por el centro del magneto. Este hecho se evidencia por el Ansatz de Aharonov-Bohm [2], el cual describe una solución aproximada de la ecuación de Schrödinger en la cual el potencial magnético aparece de forma explícita (ver [4], fórmula (7.17)). En el artículo fundamental de Aharonov y Bohm de 1959 [2], en donde se introduce el Ansatz, se resuelve explícitamente la ecuación de Schrödinger en el caso ideal de un solenoide infinito, reduciendo el problema a dos dimensiones. Sin embargo, en el caso que corresponde a la realidad física, en tres dimensiones, y para un magneto acotado, no se demuestra que esta fórmula sea una aproximación de la solución exacta de la ecuación de Schrödinger, de hecho, simplemente se enuncia sin dar ninguna justificación matemática de su aplicabilidad. Los experimentos de Tonomura et al. [63, 64] y [9] dieron una fuerte evidencia de la validez de esta fórmula. No es sino hasta el año 2009, en este trabajo doctoral, que se da por primera vez una justificación rigurosa de que el Ansatz de Aharonov Bohm es una aproximación de la solución exacta de la ecuación de Schrödinger en el caso tridimensional y para magnetos acotados. Concluimos, entonces, como fue dicho por primera vez por Aharonov y Bohm, que el potencial magnético tiene una interpretación física en la mecánica cuántica. De hecho, es a través de él que el campo magnético puede actuar sobre un electrón sin tener contacto directo.

Como se mencionó antes, en la mecánica cuántica la función de onda está definida en todo el espacio ($\mathbb{R}^3$), ya que los electrones viven en el mundo físico real tridimensional. En el caso de que exista una región inaccesible para los electrones (o un obstáculo), se debería modelar estrictamente la misma en términos de campos electromagnéticos que limiten las regiones en las que los electrones pueden estar. No obstante, podemos considerar simplemente que el obstáculo no forma parte del espacio, restringiendo el dominio de las funciones de onda al exterior del obstáculo que denotamos por Λ. En este contexto, podemos considerar que el campo magnético y los potenciales magnéticos están definidos en el exterior del obstáculo (aunque estrictamente son restricciones de distribuciones definidas en todo el espacio). En el caso de que Λ tenga una topología no trivial, entonces, dados dos potenciales magnéticos (A^1 y A^2) asociados al mismo campo magnético ($\nabla \times A^1 = \nabla \times A^2$), no existe necesariamente una transformación de norma que los relacione (ver [4], Sección 3).

Supongamos que el obstáculo es una unión finita de cuerpos con asas (como se hace en [4]) y sea $\{\hat{\gamma}_i\}_{i\in\{1,\cdots,l\}}$ una base del primer grupo de homología singular de Λ con coeficientes en los enteros. Si las integrales de los potenciales A^1 y A^2 sobre las curvas $\{\hat{\gamma}_i\}_{i\in\{1,\cdots,l\}}$ difieren en múltiplos enteros de 2π, entonces, se puede definir una especie de transformación de norma, llamado factor no integrable (ver [4], fórmula (3.45) y [87]), entre los potenciales A^1 y A^2, lo que implica que ambos potenciales representan la misma física. Esto último es equivalente, por el teorema de Stokes, a fijar los flujos del campo magnético sobre superficies S_i cuya frontera sea $\hat{\gamma}_i$. De la argumentación anterior, podemos concluir que las cantidades electromagnéticas fundamentales en la mecánica cuántica son el campo electromagnético en Λ

y los flujos del potencial magnético módulo 2π sobre las curvas $\{\hat{\gamma}_i\}_{i\in\{1,\cdots,l\}}$. Concluimos que los potenciales magnéticos tienen un verdadero significado físico pero, además, especificamos cuáles son las cantidades asociadas a éstos que tienen efecto sobre la física, que son las circulaciones de esos mismos potenciales sobre las curvas $\{\hat{\gamma}_i\}_{i\in\{1,\cdots,l\}}$ módulo 2π. Esto no contradice la covarianza de la mecánica cuántica ante transformaciones de norma, porque fijar las circulaciones del potencial magnético es equivalente a fijar los flujos del campo magnético sobre ciertas superficies contenidas en el obstáculo, lo que, por supuesto, es invariante de norma.

2.1.2. Resumen Histórico

La cantidad de trabajos relacionados con el efecto Aharonov-Bohm es muy extensa. Es imposible referirnos a todo lo que se ha hecho con respecto a este tema en este texto. En esta sección nos limitamos a describir los trabajos más importantes. En el libro de Peshkin y Tonomura [56] (ver también [57]) se presenta una revisión histórica detallada hasta el año de 1989. En particular, en [56] se discute de manera detallada la controversia que involucra más de 300 artículos sobre la existencia del efecto Aharonov-Bohm. El efecto Aharonov-Bohm es a la fecha un tema de investigación activo.

El primer trabajo que describe el efecto Aharonov-Bohm, fue hecho por Franz en 1939 [20]. En este trabajo se predice la influencia del campo magnético sobre electrones que no están en contacto con el mismo. Posteriormente, Ehrenberg y Siday en 1949 [13] describen el mismo fenómeno. No fue sino hasta 1959 a partir del trabajo de Aharonov y Bohm [2], que el efecto Aharonov-Bohm obtuvo reconocimiento en la comunidad científica como un fenómeno fundamental en la física. Aunque el fenómeno fue descrito primeramente por Franz, Aharonov y Bohm son los primeros que atribuyen este efecto a la influencia del potencial magnético sobre los electrones.

En el trabajo original de Aharonov y Bohm se propone un experimento para verificar el efecto que lleva su nombre. Ellos sugieren utilizar un solenoide recto muy largo para confinar un campo magnético dentro de él. En esta configuración es imposible que el campo magnético sea cero fuera del solenoide, sin embargo, Aharonov y Bohm suponen que el solenoide es suficientemente largo de forma que se pueda considerar infinito, en cuyo caso se puede considerar que el campo magnético es cero fuera del solenoide. El experimento consiste en enviar un haz coherente de electrones que se separa en dos partes, una de ellas se dirige hacia un lado del solenoide y la otra hacia el otro lado. Después de cruzar el solenoide, se hacen converger ambas partes en una sola región formando un patrón de interferencia. Aharonov y Bohm proponen una fórmula (el Ansatz Aharonov-Bohm) que describe de manera separada cada una de las partes del haz; por medio de esta fórmula predicen el patrón de interferencia, el cual depende de manera explícita del potencial magnético (o bien el flujo del campo magnético en el solenoide).

El caso del solenoide ha sido ampliamente estudiado, desde el punto de vista teórico y experimental. El análisis teórico se reduce al caso de dos dimensiones una vez que se supone que el solenoide es de longitud infinita. No obstante, es imposible construir un solenoide de longitud infinita y, por lo tanto, el campo magnético no puede estar confinado en el solenoide. La existencia de campo magnético fuera del solenoide fue un tema muy controversial, se argumentaba que el patrón de interferencia se debía al campo magnético fuera del magneto. Las evidencias experimentales no fueron aceptadas por la comunidad científica como verificación de este fenómeno. Era necesario construir magnetos con otra geometría que permitiera la existencia de un campo magnético enteramente confinado en ellos. Los magnetos de forma toroidal daban respuesta a este problema. En 1982 y 1986, Tonomura et al. [63, 64] instrumentaron un experimento con magnetos de forma toroidal. En estos notables experimentos, fueron capaces de superponer detrás del magneto un paquete de ondas de electrones que viajaba por dentro del agujero del magneto con otro que viajaba fuera del agujero formando un patrón de interferencia. A través del patrón de interferencia midieron el cambio de fase producido por el campo magnético en el interior del magneto, dando una evidencia fuerte a la existencia del efecto Aharonov-Bohm. Sin embargo, algunos autores [8, 88] (ver tambien [67, 9]) argumentan que el cambio de fase se puede deber a la acción de fuerzas electromagnéticas clásicas que aceleren de manera diferente a los electrones que pasan por dentro del agujero del magneto y los que pasan por fuera. En [8] se hace un cálculo que muestra que el cambio de fase se debe a fuerzas electromagnéticas que actúan sobre los electrones, en el caso del solenoide recto infinito propuesto por Aharonov y Bohm. Este cálculo es criticado por Tonomura y Nori [67], quienes argumentan que no existe campo electromagnético fuera del magneto. En [9] se hace un experimento que confirma que los electrones no son acelerados por ninguna fuerza en el caso de la configuración de los experimentos de Tonomura et al. [63, 64]; este experimento es descrito también en [67], en donde se argumenta que los resultados del mismo proporcionan una evidencia convincente de la ausencia de fuerzas sobre los electrones y, por lo tanto, sobre la existencia del efecto Aharonov-Bohm.

En el caso de magnetos toroidales, se han propuesto muchas fórmulas (o Ansätse) para la solución de la ecuación de Schrödinger. La mayoría de estos trabajos son cualitativos, aunque algunos dan valores numéricos para los Ansätse. Métodos como la difracción de Fraunhöfer, aproximaciones de Born en primer orden y a grandes energías, integrales de trayectoria de Feynman y el método de Kirchoff en óptica fueron utilizados para proponer los Ansätse. Sin embargo, ninguno de esos trabajos demuestra de manera rigurosa que los Ansätse son válidos. En [76, 51] se hace un estudio riguroso del efecto Aharonov-Bohm en el caso del solenoide de longitud infinita (en dos dimensiones). En [27] se hace un análisis semiclásico para el efecto Aharonov-Bohm en dos dimensiones para estados ligados.

2.2. Historia de los Problemas Inversos en la Física Cuántica

Cuando pensamos en un problema de la física, normalmente tratamos de predecir el comportamiento de un objeto o de cierta variable física al interactuar con un medio, de manera que necesitamos conocer cómo es la interacción (o cómo es la fuerza que se imprime al objeto) para predecir cómo evoluciona el objeto en el tiempo; a ésto lo llamamos un problema directo.

En nuestra experiencia cotidiana, lo que conocemos normalmente es el movimiento de las cosas, mas no las fuerzas que lo producen. Inferimos, por ejemplo, la forma, textura y tamaño de un objeto por medio de la luz que absorbe y dispersa.

De modo que es natural pensar en describir la fuerza ejercida sobre un objeto por medio del movimiento del mismo. Ésto último se conoce como un problema inverso. Naturalmente, en el problema descrito anteriormente entendemos de forma implícita que conocemos la ley de movimiento (es decir, por ejemplo, la segunda ley de Newton: F = m a); en realidad, lo que queremos es encontrar el parámetro F de la ecuación a partir del conocimiento de las soluciones. Resolver la ecuación si conocemos la fuerza F, significa resolver el problema directo.

De modo más general, describimos a continuación lo que entendemos por problemas inversos y directos.

La modelación matemática de un problema físico es un mapeo M de un conjunto de funciones C (llamado parámetros), en un conjunto de funciones E (llamado resultados), de forma que para cada parámetro c de C existe un único resultado e en E (es decir e = M(c)). Encontrar el resultado M(c) a partir de un parámetro c de C, es resolver el problema directo. Obtener el subconjunto de C que corresponde a un elemento dado de E significa resolver el problema inverso.

Los elementos de E deben ser expresiones matemáticas que representan variables físicas que se pueden calcular a partir de los resultados de los experimentos.

La primera persona que estudió problemas inversos de la clase que consideramos fue Lord Rayleigh (1877)[59], quien discutió la posibilidad de inferir la densidad de una cuerda por medio de sus frecuencias de vibración.

Más recientemente, una generalización fue expuesta por Marc Kac (1966) [35] en su famosa lección titulada: "Can one hear the shape of a drum ?".

Con la invención de la ecuación de Schrödinger se incrementó en gran medida la aplicabilidad de los problemas espectrales en ecuaciones diferenciales parciales a los problema de la física: el tipo de ecuaciones que anteriormente tenían solamente aplicaciones a problemas de vibraciones mecánicas, se utilizarían ahora para la descripción de átomos y moléculas.

Fröberg (1947) [21] comenzó una nueva línea de investigación, en donde se parte de la ecuación radial de Schrödinger con potencial central y se trata de reconstruirlo a partir del conocimiento del cambio de fase para ciertas soluciones estacionarias de la ecuación de Schrödinger, dejando fijo el momento angular y sin usar el método WKB. Este método fue desarrollado por Hylleran, Bargman y Levinson. Marčenko, V. M. (1950) [41] inició una serie de estudios para resolver el problema de unicidad del potencial radial a partir del cambio de fase y del conocimiento de los estados acotados; estos estudios fueron culminados en el famoso artículo de Gel'fand y Levitan (1951) [22].

La invención de la matriz de dispersión fue hecha por Wheeler (1937) [86] y Heisenberg (1943 [25], 1944 [26]). Heisenberg tenía la conjetura de que la matriz de dispersión tenía toda la información del problema físico. Aunque posteriormente se descubrió que los estados acotados no se podían recuperar a partir del cambio de fase cuando se deja fijo el momento angular de las soluciones. Faddeev (1956) [18] demuestra que si la amplitud de dispersión es conocida para todos los ángulos y energías, entonces el potencial está determinado de manera unívoca.

Los resultados de Gel'fand y Levitan (1951) [22] fueron desarrollados por Jost y Kohn (1953) [33] y por Levinson (1955) [40]. Posteriormente Krein (1953 [36], 1955 [37]) y Marčenko (1955) [42] descubrieron nuevas alternativas y extensiones.

Esta aproximación al problema estaba basada en 2 ecuaciones integrales, una debida a Gel'fand y Levitan y la otra a Marčenko.

Sin embargo, los métodos basados en la ecuación de Gel'fand-Levitan o en la de Marčenko se basaban en el conocimiento de la dispersión a todas las energías.

Un método alternativo debería utilizar la amplitud de dispersión (o todos los cambios de fase) a una energía fija para recuperar el potencial.

Un método a energía fija, análogo a los métodos que utilizan la ecuación de Gel'fand-Levitan, fue aportado por Newton (1962) [46], quien mostró que los potenciales no podían ser inferidos de manera única.

Sabatier (1971)[60] creó un nuevo método que permitió la solución completa del problema inverso a energía fija.

Hasta ahora, los problemas que se han mencionado consideran que el potencial tiene simetría esférica, es decir, dependen sólo de la distancia al origen. El problema de determinar a partir del la matriz de dispersión de manera única el potencial eléctrico fue resuelto por primera vez por Faddev (1956) [19] y fue estudiado después por Berezanskii (1958) [7] y Saito (1984)[61]; éste último determinó la unicidad para potenciales eléctricos que cumplen la condición $|V(y)| \leqq C(1+|y|)^{-1-\epsilon}$. Para generalizar el método de Gel'fand-Levitan o el de Marčenko para potenciales en dimensión 3 sin simetría esférica; Faddeev (1966)[19] introdujo aportaciones muy importantes. El problema inverso fue estudiado por Fadeev (1966) [19] y Newton (1973 [47], 1974[48], 1977[49]) y posteriormente por Lavine y Nachman (1987) [38, 39], por Novikov y Henkin (1987) [53] y por Henkin y Novikov (1988) [28].

El problema de determinar condiciones necesarias y suficientes para que el operador de dispersión sea operador de dispersión de algún potencial en cierta clase, fue estudiado usando el método $\bar{\partial}$ en la teoría de las funciones complejas en varias dimensiones por Beals y Coifman (1985) [6] y después por Nachman y Ablowitz (1984) [43, 44], y por Henkin y Novikov (1988) [28]. Este problema también fue estudiado por Weder (1991) ([70], [71]) de una manera diferente, utilizando el principio del límite de absorción. En particular para el caso de potenciales $C_0^\infty(\mathbb{R}^n)$ y en espacios de Sobolev con peso.

La unicidad del potencial eléctrico a energía fija a partir de la matriz de dispersión fue demostrada por Ramm (1987) [58], Novikov (1988)[54] y por

Nakamura, Sun y Uhlmann (1995) [45] para potenciales de soporte compacto.

Aunque es sabido que, en general, el potencial eléctrico no se puede recuperar a partir del operador de dispersión a energía fija [10, 23], se demuestra en Weder (1991) [72] que la unicidad es cierta si se conoce el potencial eléctrico fuera de una bola. La unicidad a energías fijas para potenciales que decaen de manera exponencial fue estudiada en Novikov (1994) [55], Eskin y Ralston (1995)[30], Isozaki (1997)[17], y Uhlmann y Vasy (2002) [69]. En Weder (2004) [77], se demuestra que la matriz de dispersión a cuasi-energía fija determina de manera única a potenciales periódicos en el tiempo que decaen de forma exponencial en las coordenadas espaciales en infinito. En Weder y Yafaev (2005) [79], se consideran potenciales eléctricos y magnéticos que son sumas asintóticas de términos homogéneos; se demuestra que a partir de la matriz de dispersión a energía fija se pueden recuperar los términos de la suma; usando esto y los resultados de Weder (1991) [72], se demuestra la unicidad en el caso de que el potencial magnético sea cero y que el potencial eléctrico sea una suma finita de términos homogéneos (o bien, suma asintótica de términos homogéneos que converge al potencial eléctrico). Este último resultado fue generalizado por Weder (2006) [80], en donde considera potenciales eléctricos y magnéticos.

Isozaki y Kitada (1986) [29] estudian el problema para potenciales de rango largo en el límite de grandes energías. Recientemente Weder y Yafaev (2007) [87] estudiaron el problema de dispersión inversa a energía fija en dimensiones mayores o iguales a tres para potenciales de rango largo.

Todas las contribuciones a los problemas inversos en la física cuántica mencionados en las líneas anteriores, utilizan métodos estacionarios, es decir, la solución física es idealizada como periódica en el tiempo, con energía infinita. Haciendo esto, las propiedades físicas de propagación en las soluciones se pierden (ya que la función de onda en realidad no evoluciona en el tiempo, sino permanece en un estado estacionario). Esta carencia de intuición física implica que la herramienta matemática que se utiliza para resolver los problemas dé poca información acerca de la física del problema.

Además, en los métodos estacionarios se utiliza una transformación de Fourier generalizada que integra sobre espacios de medida infinita las funciones de onda, que son periódicas en el tiempo. Otro problema de los métodos estacionarios es que utilizan de manera fundamental la linealidad del problema directo, siendo difícil pensar en generalizar el método para resolver problemas no lineales.

Introdujeron V. Enss y R. Weder (1993 [14], 1994 [15], 1995 [16]) un nuevo método dependiente del tiempo para reconstruir univocamente los potenciales de sistemas cuánticos de N-cuerpos, en donde se aplican fundamentalmente las propiedades físicas de propagación de las funciones de onda de energía finita para resolver los problemas inversos en mecánica cuántica, utilizando más clara y sencillamente la herramienta matemática, la cual está muy relacionada con la intuición física del problema. Además, a diferencia de los métodos estacionarios, este método puede aplicarse para la solución de problemas de dispersión inversa para ecuaciones no lineales [75, 81, 82, 83, 84, 85, 62].

En los últimos años, el método dependiente del tiempo ha tenido numerosas aplicaciones, por ejemplo: para estudiar hamiltonianos con campo eléctrico y magnético [3]; en la ecuación de Dirac [34]; en el caso de N cuerpos [16, 14]; en el efecto Aharonov-Bohm [4, 5, 76]; en el efecto Stark [73, 51, 1]; en potenciales dependientes del tiempo para la ecuación de Schrödinger [74, 52] y para la ecuación de Dirac [31, 32], para reconstruir parámetros físicos de agujeros negros [11, 12], entre otras.

El estudio de los problemas inversos ha sido de gran interés en la comunidad de físicos y matemáticos; tan solo el libro de K.Chadan y C. Sabatier (1989) [10] tiene cerca de 1000 referencias; por lo tanto, es imposible presentar en este texto una exposición completa del trabajo que se ha realizado hasta la fecha en los temas relacionados con problemas inversos en la física cuántica. En la presente introducción se mencionan sólo los trabajos más importantes y las tendencias principales que ha tomado el estudio de los problemas inversos. Para más referencias, se puede consultar el libro: K.Chadan and C. Sabatier (1989)[10], en el que me he basado para presentar los datos anteriores a 1989 en esta introducción, y el libro: Newton (1989) [50].

Capítulo 3

Efecto Aharonov-Bohm y los Experimentos de Tonomura et al.

En este capítulo se explica de manera resumida los resultados del artículo [5].

3.1. Resumen

En este capítulo se muestra de manera rigurosa que el Ansatz clásico de Aharonov y Bohm es una buena aproximación a la solución exacta de la ecuación de Schrödinger. Se da por primera vez un análisis matemático cuantitativo del efecto Aharonov-Bohm con magnetos en forma toroidal bajo las condiciones experimentales de Tonomura et al. [63, 64]. Suponemos que el electrón incidente libre está representado por un paquete de ondas gaussiano, lo que es razonable desde el punto de vista de la física. Las ventajas técnicas de usar un paquete de onda gaussiano para el electrón libre incidente es que en este caso conocemos de manera explicíta la evolución libre y podemos hacer estimaciones de manera precisa. Damos una fórmula rigurosa simple y cuantitativa para la cota de error que estima la diferencia entre la solución exacta de la ecuación de Schrödinger y la solución aproximada dada por el Ansatz de Aharonov y Bohm. La cota de error es uniforme en el tiempo. También probamos que el operador de dispersión aplicado al estado gaussiano está dado por un operador de multiplicación por $e^{i\frac{q}{\hbar c}\Phi}$ (donde q es la carga del electrón, c es la velocidad de la luz, $\hbar$ es la constante de Planck, y Φ es el flujo del campo magnético en una sección transversal del magneto), salvo una cota de error que se proporciona de manera explícita. De hecho, la cota de error es la misma para los casos de la estimación del Ansatz de Aharonov-Bohm y el operador de dispersión.

Aharonov y Bohm y Tonomura et al. sugirieron dividir el paquete de ondas electrónico en la parte que pasa por el agujero del magneto y la parte que pasa por fuera. Tonomura et al. observaron que la imagen que se produce detrás del magneto muestra de forma clara la sombra del magneto, así como el agujero y el exterior del mismo. Concluyen [63] que esto indica que no hay interferencia entre la parte del paquete de ondas que va por el agujero y la parte que choca con el magneto o viaja por fuera. La parte del paquete de ondas que viaja por fuera del agujero del magneto y que no choca, se puede tomar como el paquete de ondas de referencia. Entonces podemos modelar sólo la parte que atraviesa el agujero del magneto. Usando los datos experimentales de Tonomura et al. [63, 64], proporcionamos cotas inferiores y superiores en la varianza de la gausiana para que el paquete de ondas viaje por el interior del agujero. También demostramos de manera rigurosa que los resultados experimentales de Tonomura et al. [63, 64], que fueron predichos por Aharonov y Bohm [2], son una consecuencia de la mecánica cuántica.

Si tomamos la varianza del paquete de ondas incidente en un cierto intervalo, cuyos extremos damos de manera explicíta, el Ansatz de Aharonov-Bohm difiere, en norma, de la solución exacta por un número menor a 10^{-99} para todo tiempo; llamamos a este tipo de paquetes de onda paquetes de onda de tamaño intermedio. Si utilizamos paquetes de onda de tamaño intermedio, la probabilidad de que el electrón choque con el magneto es menor que 10^{-199}, de modo que los electrones representados por este tipo de funciones de onda no interactúan con ningún campo en su trayectoria y, sin embargo, son afectados por la presencia del potencial magnético. Nuestros resultados sugieren que sería muy interesante llevar a cabo un experimento con paquetes de onda de tamaño intermedio.

Nuestra cota de error tiene una interpretación física. Para varianzas chicas, ésta se debe al principio de incertidumbre de Heisenberg: cuando la varianza en posición es chica, la varianza en momento es grande, por lo tanto, el ángulo de apertura del paquete de ondas es grande y la interacción con el magneto también lo es, lo que provoca que la cota de error lo sea igualmente. Cuando la varianza es grande, entonces el paquete de ondas también lo es y, por lo tanto, el electrón interactúa con el magneto, lo que provoca de nuevo que la cota de error sea grande.

3.2. Experimentos de Tonomura et al.

Tonomura et al. [63, 64] construyeron pequeños magnetos de forma toroidal, de tal forma que el campo magnético que generan es prácticamente cero fuera de ellos. En [64] los magnetos son impenetrables y, además, están cubiertos por una capa superconductora que impide que el campo magnético salga del magneto. Denotamos al magneto por,

$$\tilde{K} := \{(x_1, x_2, x_3) \in \mathbb{R}^3 : 0 < \tilde{r}_1 \leq (x_1^2 + x_2^2)^{1/2} \leq \tilde{r}_2, |x_3| \leq \tilde{h}\}, \tag{3.1}$$

y por $\tilde{B}$ al campo magnético. Suponemos que $\tilde{B}(x)$ es cero para x fuera del magneto.
Utilizamos el símbolo Λ para denotar el complemento del magneto,

$$\Lambda := \mathbb{R}^3 \setminus \tilde{K}. \tag{3.2}$$

Tonomura et al. [63, 64] utilizan un paquete de ondas electrónico que es dirigido hacia el magneto, el paquete se divide en 2 paquetes, uno de los cuales sigue su camino hacia el magneto y el otro pasa por afuera del mismo. Posteriormente, se hacen converger los paquetes de ondas en una única región, de manera que se forma un patrón de interferencia. En la parte posterior del magneto se produce una imagen que muestra claramente la sombra del magneto así como el agujero del magneto. El patrón de interferencia en el agujero es diferente del correspondiente en el exterior, esto es debido al flujo del campo magnético en el interior del magneto.

El paquete de ondas electrónico era mucho más grande que el magneto. Este paquete tenía simetría cilíndrica con respecto al eje a través del cual se propaga la onda. El tamaño del paquete de ondas era de 3 micrómetros en la dirección de propagación y tenía un radio de 10 micrómetros en cualquier dirección perpendicular al eje de propagación [68]. El paquete de ondas cubría completamente al magneto. Como se mencionó anteriormente, se observa una imagen detrás del magneto que muestra de manera clara la sombra del magneto así como el agujero del mismo y también la parte del paquete de ondas que no choca con el magneto ni atraviesa el agujero [63, 64]. Tonomura et al. [63] indicaron que esto implica que no hay interferencia entre la parte del paquete de ondas que atraviesa el agujero y las otras partes del mismo, por lo que podemos estudiar de forma separada esta parte del paquete de ondas. Nos concentraremos en el análisis de la parte del paquete de ondas que atraviesa el agujero y tomaremos a ésta como el paquete de ondas electrónico mismo. Nuestro paquete de ondas se puede interpretar como la parte del paquete de ondas que pasa por el agujero o bien como un paquete de ondas más chico que el que se utiliza en los experimentos, que pasa verdaderamente por el agujero del magneto.

3.2.1. El Paquete de Ondas

En el tiempo de emisión (cuando el tiempo tiende a menos infinito) el paquete de ondas electrónico está lejos del magneto, de manera que no interactúa con este último, podemos suponer, por ende, que evoluciona libremente (más adelante se explica de manera precisa el significado de este concepto). Representaremos al paquete de ondas (en el tiempo de emisión) por la evolución libre de una función gaussiana de varianza σ:

$$\varphi_{\mathbf{v}} := e^{im\mathbf{v}\cdot x}\varphi, \tag{3.3}$$

adonde

$$\varphi := \left(\frac{1}{\sigma^2\pi}\right)^{3/4} e^{-\frac{x^2}{2\sigma^2}}, \tag{3.4}$$

lo cual es físicamente razonable. En las ecuaciones anteriores $m = \frac{M}{\hbar}$, donde M es la masa del electrón $\hbar$ es la constante de Planck; $\mathbf{v} \in \mathbb{R}^3$ es un vector fijo que representa la velocidad de propagación y $x \in \mathbb{R}^3$.

Denotamos por $v = |\mathbf{v}|$ y por $\hat{\mathbf{v}} = \frac{\mathbf{v}}{|\mathbf{v}|}$. Suponemos en este texto que $\hat{\mathbf{v}}$ tiene la misma dirección que el eje vertical. Esto quiere decir que los electrones se propagan en la dirección positiva del eje vertical.

La función de onda (3.3) en el espacio de momentos está dada por su transformación de Fourier (ver (2.6)). El efecto que tiene el factor $e^{i\frac{M}{\hbar}\mathbf{v}\cdot x}$ en la representación de momentos es el de trasladar la función de onda por el vector $M\mathbf{v}$ (que representa el momento clásico del electrón), lo que implica que la función de onda (3.3) en el espacio de momentos está centrada en el momento clásico, $M\mathbf{v}$,

$$\hat{\varphi}_{\mathbf{v}}(p) = \hat{\varphi}(p - M\mathbf{v}). \tag{3.5}$$

En los experimentos de Tonomura et al. la varianza en la dirección de propagación es diferente de la varianza en la dirección transversal a la dirección de propagación. El suponer que estas dos varianzas son diferentes complica la notación y no agrega ningún elemento nuevo a nuestro análisis, de modo que por simplicidad suponemos que son iguales. Resultados análogos se pueden obtener suponiendo que son diferentes. La varianza σ es menor que el radio interior del Magneto $\tilde{r}_1$ (ver (3.1)) puesto que estamos modelando la parte del paquete de ondas que atraviesa el agujero.

3.3. Solución Exacta de la Ecuación de Schrödinger con Condiciones Iniciales en $-\infty$

3.3.1. La Ecuación de Schrödinger

El electrón satisface la ecuación de Schrödinger,

$$i\hbar \frac{\partial}{\partial t}\phi(x,t) = H\phi(x,t), x \in \Lambda, t \in \mathbb{R}, \tag{3.6}$$

en donde

$$H := \frac{1}{2M}(\mathbf{P} - \frac{q}{c}\tilde{A})^2 \tag{3.7}$$

es el hamiltoniano, $\hbar$ es la constante de Planck, $\mathbf{P} := -i\hbar\nabla$ es el operador de momento, c es la velocidad de la luz, M y q son, respectivamente, la masa y la carga del electrón y $\tilde{A}$ es un potencial magnético tal que $\nabla \times \tilde{A} = \tilde{B}$, en donde $\tilde{B}$ es el campo magnético, recordemos además que $\Lambda := \mathbb{R}^3 \setminus \tilde{K}$. Definimos el hamiltoniano (3.7) en $L^2(\Lambda)$ con condiciones de Dirichlet en $\partial\Lambda$, es decir, $\phi(x) = 0$ para $x \in \partial\Lambda$ (en el sentido de traza). Estas condiciones a la frontera corresponden a un magneto impenetrable en donde la existencia del efecto Aharonov Bohm es más clara, porque de esta forma no hay interacción del electrón con el campo magnético que se encuentra en el interior del magneto. Sin embargo, nuestros resultados también funcionan cuando la ecuación de Schrödinger (3.6) está definida en todo el espacio (caso penetrable), de hecho, el análisis es un poco más simple en ese caso.

En ausencia del magneto, el hamiltoniano (hamiltoniano libre) está dado por,

$$H_0 := \frac{1}{2M}\mathbf{P}^2, \tag{3.8}$$

El electrón libre satisface la ecuación de Schrödinger libre,

$$i\hbar\frac{\partial}{\partial t}\phi(x,t) = H_0\phi(x,t), x \in \mathbb{R}^3, t \in \mathbb{R}. \tag{3.9}$$

Al tiempo de emisión (cuando el tiempo tiende a menos infinito) la función de onda del electrón ($\psi_{\mathbf{v}}(x,t)$) satisface (ver la sección 3.2.1),

$$\psi_{\mathbf{v}}(x,t) \approx e^{-i\frac{tH_0}{\hbar}}\varphi_{\mathbf{v}}(x), \qquad (t \to -\infty). \tag{3.10}$$

El hamiltoniano libre (H_0) es auto-adjunto definido en $L^2(\mathbb{R}^3)$ con dominio el espacio de Sobolev $\mathcal{H}^2(\mathbb{R}^3)$, lo que nos permite usar cálculo funcional para definir la exponencial en la fórmula anterior.

Finalmente, concluimos que la función de onda del electrón $\psi_{\mathbf{v}}(x,t)$ es la única solución de la ecuación de Schrödinger (3.6) que satisface (3.10).

3.3.2. Operadores de Onda

Haciendo uso de los operadores de onda, podemos resolver la ecuación (3.6) con condiciones iniciales en menos infinito dadas por (3.10) en términos de la solución de (3.6) con condiciones iniciales en cero.

Sea J el operador de multiplicación por la función característica de $\mathbb{R}^3\setminus\tilde{K}$. Los operadores de onda se definen como sigue,

$$W_{\pm} := \text{s-}\lim_{t\to\pm\infty} e^{i\frac{t}{\hbar}H}\, J\, e^{-i\frac{t}{\hbar}H_0}. \tag{3.11}$$

En la anterior fórmula las exponenciales se definen por cálculo funcional, ya que eligiendo los dominios de los hamiltonianos H y H_0 de manera adecuada, éstos son auto-adjuntos.

Los límites (3.11) existen y podemos usar una función de corte χ infinitamente diferenciable en lugar de J. Elegimos la función de corte χ de forma que el soporte de $1-\chi$ está contenido en el conjunto

$$K := \{(x_1,x_2,x_3) \in \mathbb{R}^3 : 0 < r_1 \leq (x_1^2+x_2^2)^{1/2} \leq r_2, |x_3| \leq h\}, \tag{3.12}$$

tal que $\tilde{K} \subset K$ y

$$r_1 = \frac{49}{50}\tilde{r}_1, \quad r_2 := \tilde{r}_2 - \frac{1}{50}\tilde{r}_1. \tag{3.13}$$

3.3.3. Condiciones Iniciales en $-\infty$

La solución de la ecuación de Schrodinger $\psi_{\mathbf{v}}(x,t)$ (3.6) que satisface,

$$\psi_{\mathbf{v}}(x,t) \approx e^{-i\frac{tH_0}{\hbar}} \varphi_v(x), \quad (t \to -\infty), \tag{3.14}$$

está dada por

$$\psi_{\mathbf{v}}(x,t) := e^{-i\frac{t}{\hbar}H} W_- \varphi_{\mathbf{v}}. \tag{3.15}$$

La funcion de onda $\psi_{\mathbf{v}}(x,t)$ satisface,

$$\lim_{t \to -\infty} \|\psi_{\mathbf{v}}(x,t) - Je^{-i\frac{tH_0}{\hbar}} \varphi_v(x)\|_{L^2(\Lambda)} = 0. \tag{3.16}$$

3.3.4. El Operador de Dispersión

El operador de dispersión está dado por,

$$S := W_+^* W_-. \tag{3.17}$$

Para tiempos positivos largos, cuando el paquete de ondas está fuera del magneto, éste se puede aproximar por una función de onda saliente que es solución de la ecuación libre de Schrödinger,

$$\psi_{+,\mathbf{v}} := e^{-i\frac{t}{\hbar}H_0} \varphi_{+,\mathbf{v}},$$

tal que

$$\lim_{t \to \infty} \|\psi_{\mathbf{v}} - J\psi_{+,\mathbf{v}}\| = 0.$$

Los datos iniciales (a tiempo $t = 0$) de la función de onda entrante ($e^{-i\frac{tH_0}{\hbar}} \varphi_{\mathbf{v}}(x)$) y la función de onda saliente ($e^{-i\frac{t}{\hbar}H_0}\phi_{+,\mathbf{v}}$) están relacionados por el operador de dispersión.

$$\varphi_{+,\mathbf{v}} = S\varphi_v.$$

3.4. Ansatz de Aharonov-Bohm

Aharonov y Bohm [2] proponen una solución aproximada de la ecuación de Schrödinger sobre regiones simplemente conexas en donde el campo electromagnético es cero, por medio de un cambio de norma a partir del potencial vectorial cero (ver (2.7)). En el caso de los experimentos de Tonomura et al., elegimos esta región como,

$$\mathcal{H} = \Lambda \setminus S,$$

en donde (ver (3.1)),

$$\mathcal{S} := \{(x_1, x_2, x_3) \in \mathbb{R}^3 : (x_1^2 + x_2^2)^{1/2} > \tilde{r}_2^2, x_3 = 0\}.$$

Podemos suponer, sin pérdida de generalidad, que el soporte de $\tilde{A}$ está contenido en el casco convexo de $\tilde{K}$ (ver seccion 7.1 de [4]). Para todo $x \in \mathcal{H}$ y un vector fijo $x_0 = (x_{0,1}, x_{0,2}, x_{0,3})$ en $\mathcal{H}$ tal que $x_{0,3} \leq -\tilde{h}$ (ver (3.1)), definimos,

$$\lambda_{A,0}(x) := \int_{x_0}^{x} \frac{q}{\hbar c}\tilde{A}, \quad A = \frac{q}{\hbar c}\tilde{A}. \tag{3.18}$$

en donde la integral se toma sobre una curva en $\mathcal{H}$.
Claramente la transformación de norma (3.18) no puede estar definida en todo Λ, pues esto implicaría que el flujo del campo magnético en cualquier sección transversal del magneto fuera cero, de manera que la transformación de norma tiene que ser discontinua en algún lugar. En nuestro caso $\mathcal{S}$ es la superficie de discontinuidad.

Para toda $x \in \mathcal{H}$, $\lambda_{A,0}(x)$ satisface la siguiente fórmula de cambio de norma entre el potencial magnético cero y A (ver (2.7)),

$$A(x) = 0 + \nabla\lambda_{A,0}(x).$$

Dada una función de onda ϕ cuya evolución permanece todo el tiempo en $\mathcal{H}$ y que no choca con el magneto, Aharonov y Bohm sugirieron una fórmula para la solución de la ecuación de Schrödinger dada por el cambio de norma siguiente,

$$\phi(x,t) \approx e^{i\lambda_{A,0}} e^{-i\frac{t}{\hbar}H_0} e^{-i\lambda_{A,0}} \phi(x,0). \tag{3.19}$$

La fórmula (3.19) sería una igualdad estricta si H_0 estuviera definido en Λ y el potencial magnético estuviera definido y fuera regular en todo Λ (ver

(2.9)-(2.11)), sin embargo, en este caso no puede ser una igualdad, porque $\lambda_{A,0}(x)$ es discontinuo en $\mathcal{S}$ y H_0 está definido en $\mathbb{R}^3$. Además, tampoco podemos suponer que la evolución de la función de onda permanece todo el tiempo en $\mathcal{H}$, pues la ecuación de Schrödinger es dispersiva. No obstante, es de esperarse que si es muy chica la probabilidad de que el electrón esté cerca de la superficie de discontinuidad al igual que la probabilidad de que choque con el magneto, entonces la ecuación (3.19) define une buena aproximación a la solución de la ecuación de Schrödinger.

La ecuación (3.19) es el Ansatz de Aharonov-Bohm para la solución de la ecuación de Schrödinger a valores iniciales al tiempo $t = 0$ dados por $\phi(x, 0)$. A partir de esta ecuación, se puede deducir el Ansatz a valores iniciales cuando el tiempo tiende a menos infinito dados por (3.14). Esta fórmula está dada por lo siguiente,

Aharonov-Bohm Ansatz 3.4.1. *La solución de la ecuación de Schrödinger (3.6) $\psi_{\mathbf{v}}(x,t)$ que satisface (3.14) se puede aproximar por,*

$$\psi_{\mathbf{v}}(x,t) \approx e^{i\lambda_{A,0}} e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}} := \psi_{AB}(x,t), \tag{3.20}$$

siempre y cuando el electrón no choque con el magneto y permanezca lejos de la superficie de discontinuidad.

La solución propuesta por Aharonov y Bohm (ψ_{AB}) es lo que se puede ver en los experimentos de Tonomura et al. Como el soporte del potencial magnético $\tilde{A}$ está contenido en el casco convexo de $\tilde{K}$, para toda x cuya componente vertical sea mayor que $\tilde{h}$, $\lambda_{A,0}(x)$ es igual a la constante $\frac{q}{\hbar c}\tilde{\Phi}$, en donde $\tilde{\Phi}$ es el flujo del campo magnético sobre cualquier sección transversal del magneto. La función de onda saliente de Aharonov y Bohm (ver sección 3.3.4) está dada por (recordar que los electrones se propagan en la dirección positiva del eje vertical, ver la sección 3.2.1),

$$e^{i\frac{q}{\hbar c}\tilde{\Phi}} e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}},$$

esto es exactamente lo que se puede ver en los experimentos de Tonomura et al..

Se sigue de esto último y de la sección 3.3.4 que el Ansatz de Aharonov-Bohm para el operador de dispersión, actuando en los datos iniciales (al tiempo $t = 0$) de la función de onda incidente, es:

$$S\varphi_{\mathbf{v}} = e^{i\frac{q}{\hbar c}\tilde{\Phi}}\varphi_{\mathbf{v}},$$

es decir, el operador de dispersión actuando en el estado gaussiano $\varphi_{\mathbf{v}}$ está dado, en una buena aproximación, por el operador de multiplicación por $e^{i\frac{q}{\hbar c}\tilde{\Phi}}$. Esto mismo es lo que se observa en los experimentos de Tonomura et al. [63, 64].

3.5. Resultados Principales

La evolución libre del paquete electrónico está centrada en la trayectoria clásica, pero se dispersa con el tiempo. Si el paquete de ondas está en el tiempo $t = 0$ en el centro del magneto, de tal forma que la probabilidad de que el electrón esté cerca del magneto sea muy baja, al transcurrir el tiempo, este paquete de ondas se dispersa al mismo tiempo que el centro del paquete de ondas se aleja del magneto siguiendo la trayectoria clásica. La relación entre la distancia que hay entre el centro del paquete de ondas al centro del magneto y la dispersión (o el ensanchamiento del paquete de ondas) se puede entender en términos del ángulo de apertura en la propagación del electrón (más adelante se define este concepto de manera precisa). La probabilidad de que el electrón choque con el magneto crece cuando crece la varianza σ de paquete de ondas (pues entonces la probabilidad de que el electrón esté cerca del magneto crece). Esta probabilidad también crece cuando aumenta el ángulo de apertura, pues si el ángulo de apertura es grande, en poco tiempo el electrón se dispersa mucho y choca con el magneto. El ángulo de apertura crece al decrecer la varianza σ, ya que por el principio de incertidumbre de Heisenberg, al decrecer la varianza en posición σ crece la varianza en momento. Si la varianza en momento es grande, entonces el electrón evoluciona en todas direcciones y choca con el magneto. De lo anterior se sigue que para asegurar que la probabilidad de que electrón choque sea chica (o bien que el electrón pase por el agujero del magneto), es necesario imponer cotas inferiores y superiores para la varianza σ . Estas mismas cotas también aseguran que el electrón permanezca fuera de la superficie de discontinuidad $\mathcal{S}$ (ver el Ansatz de Aharonov-Bohm 3.4.1).

En el siguiente teorema proporcionamos de forma explícita las cotas inferiores para la varianza que aseguran que electrón pase por el agujero del magneto y estimamos la diferencia entre el Ansatz de Aharonov-Bohm 3.4.1 y la solución exacta de la ecuación de Schrödinger.

Teorema 3.5.1. *Bajo las condiciones experimentales de Tonomura et al., para cada función de onda gaussiana con varianza* $\sigma \in [1.3 \times 10^{-6} r_1, \frac{r_1}{2}]$

y para todo tiempo $t \in \mathbb{R}$, la solución de la ecuación de Schrödinger que se comporta como ($e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}}$) cuando el tiempo tiende a menos infinito está dada por

$$\psi_{AB} := e^{i\lambda_{A,0}} e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}}, \tag{3.21}$$

salvo un error acotado por

$$\begin{aligned} &\|e^{-i\frac{t}{\hbar}H} W_-(A)\varphi_{\mathbf{v}} - \psi_{AB}\| \leq \\ &7e^{-\frac{r_1^2}{2\sigma^2}} + 177 \times 10^3 e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} + 10^{-100}. \end{aligned} \tag{3.22}$$

Teorema 3.5.2. *Bajo las condiciones del teorema anterior,*

$$\|S\varphi_{\mathbf{v}} - e^{i\frac{q}{\hbar c}\tilde{\Phi}}\varphi_v\| \leq 7e^{-\frac{r_1^2}{2\sigma^2}} + 177 \times 10^3 e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} + 10^{-100}.$$

en donde $\tilde{\Phi}$ es el flujo del campo magnético sobre cualquier sección transversal del magneto.

Los términos principales que aparecen en la cota de error (3.22) son los siguientes,

- Factor del tamaño del electrón.

$$e^{-\frac{r_1^2}{2\sigma^2}} \tag{3.23}$$

- Factor del ángulo de apertura.

$$e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} \tag{3.24}$$

Cuando la varianza σ es cercana al radio interior del magneto (el paquete de ondas electrónico es grande), (3.23) es cercano a 1 y (3.24) es extremadamente chico (porque $\sigma m v$ es grande). Entonces cuando el paquete de ondas es grande comparado con el radio interior del magneto, (3.23) es el término importante (lo que justifica el nombre). Cuando la varianza es pequeña (de forma que $\sigma m v$ es cercano a 1) el factor (3.24) es cercano a 1 y (3.23) es extremadamente reducido ($\frac{r_1}{\sigma}$ es grande) y, por lo tanto, el factor importante en la cota de error es (3.24). Notemos que cuando la varianza en posición, σ, es chica, por el principio de incertidumbre de Heisenberg la varianza en momento es grande, lo que implica que el ángulo de apertura sea grande. Esto justifica el nombre del término (3.24). Cuando σ no es grande ni pequeño (o bien es intermedio) la cota de error (3.22) es extremadamente chica.

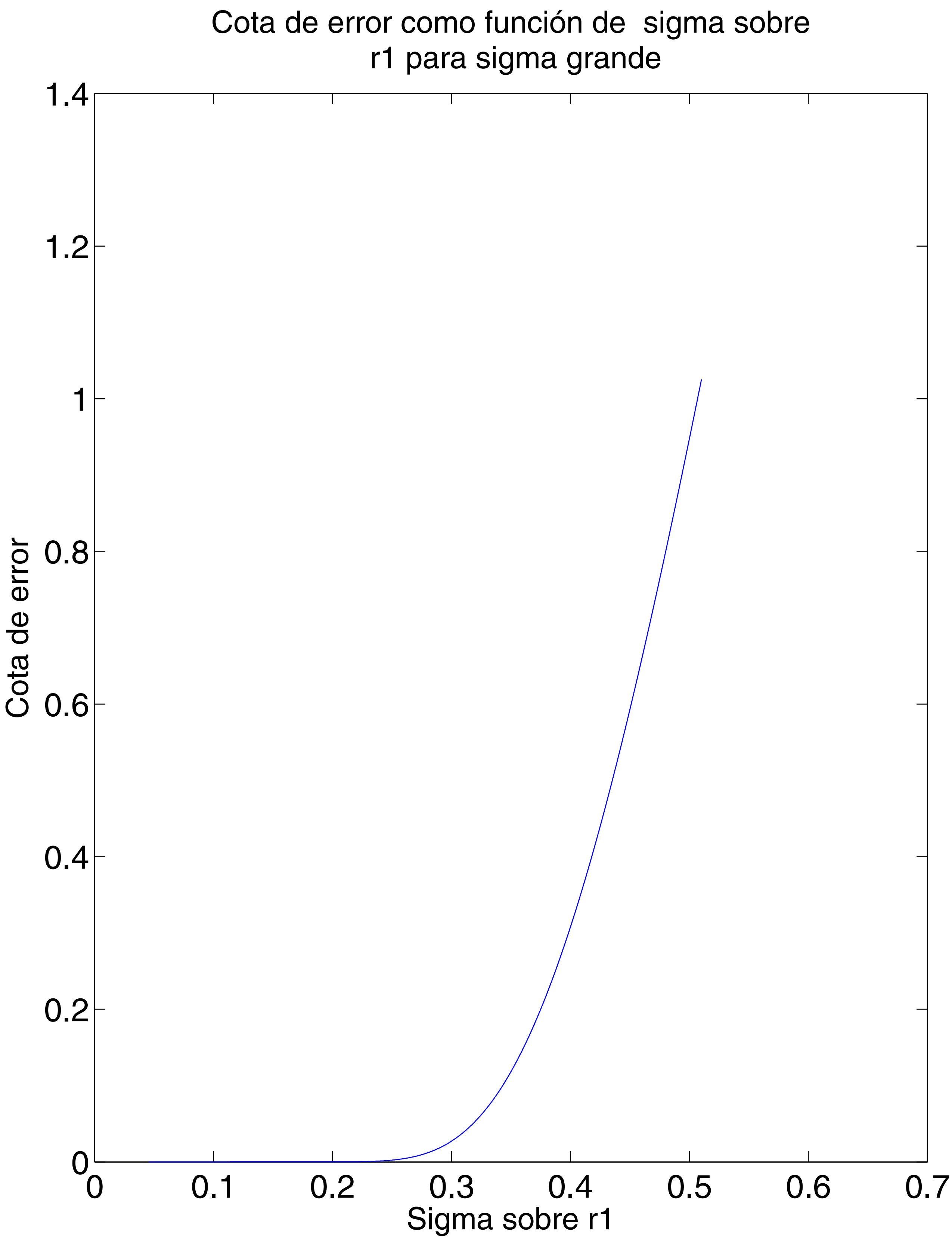
3.5.1. Sigma Grande, $\sigma \in [\frac{r_1}{22}, \frac{\tilde{r}_1}{2}]$

Tomamos el radio interior del magneto $\tilde{r}_1$ que fue utilizado en los experimentos de Tonomura et al. [65] $\tilde{r}_1 = 1.75 \times 10^{-4} cm$. Entonces, en términos absolutos, los valores de sigma grande varían en el $[7.7955 \times 10^{-6}, 8.7500 \times 10^{-5}]$.

En seguida mostramos algunos datos del comportamiento de la cota de error como función de $\frac{\sigma}{r_1}$.

Cota de error como función de sigma sobre r_1 para sigma grande.	
Sigma sobre r_1	***Cota de error***
.34305	10^{-1}
.27626	10^{-2}
.23764	10^{-3}
.21170	10^{-4}
.19274	10^{-5}
.17811	10^{-6}
.16637	10^{-7}
.15668	10^{-8}
.14851	10^{-9}
.14150	10^{-10}

En la siguiente figura mostramos la gráfica de la cota de error en términos de $\frac{\sigma}{r_1}$, para sigma grande.


Cota de error como función de sigma sobre
r1 para sigma grande
Cota de error
Sigma sobre r1
0
0.2
0.4
0.6
0.8
1
1.2
1.4
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7

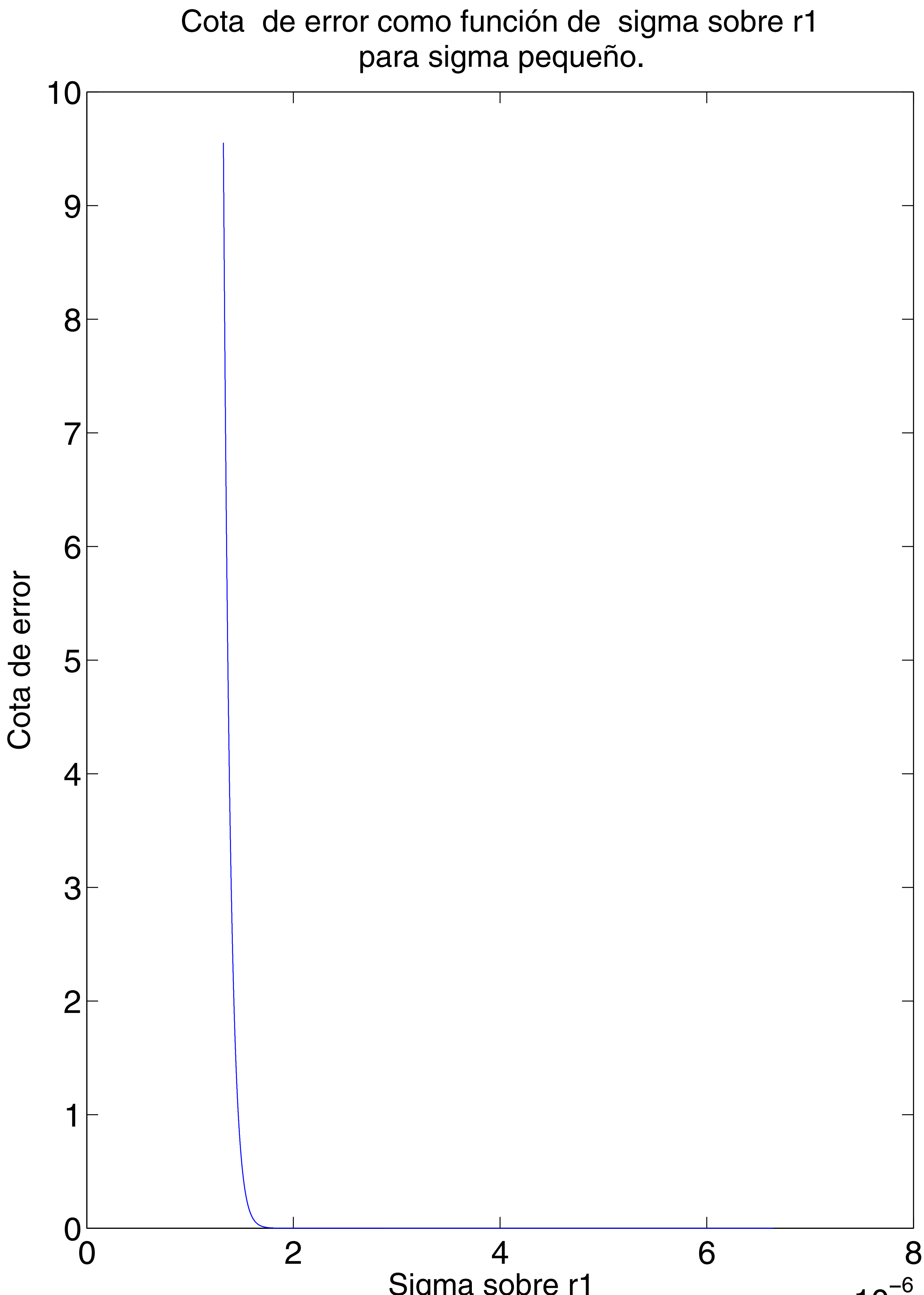
3.5.2. Sigma Pequeño, $\sigma \in [1.\,3224 \times 10^{-6} r_1, 6.\,7591 \times 10^{-6} r_1]$, o $\sigma \in [\frac{4.5}{mv}, \frac{23}{mv}]$

Tomamos el radio interior del magneto $\tilde{r}_1$ que fue utilizado en los experimentos de Tonomura et al. [65] $\tilde{r}_1 = 1.\,75 \times 10^{-4} cm$. En términos absolutos, los valores de sigma grande varían en el intervalo $[2.\,2679 \times 10^{-10}, 1.\,1592 \times 10^{-9}]$.

En seguida mostramos algunos datos del comportamiento de la cota de error como función de $\frac{\sigma}{r_1}$.

Cota de error como función de sigma sobre r_1 para sigma pequeño.	
Sigma sobre r_1	***Cota de error***
1.6001 $\times 10^{-6}$	10^{-1}
1.7234 $\times 10^{-6}$	10^{-2}
1.8384 $\times 10^{-6}$	10^{-3}
1.9467 $\times 10^{-6}$	10^{-4}
2.0492 $\times 10^{-6}$	10^{-5}
2.1469 $\times 10^{-6}$	10^{-6}
2.2403 $\times 10^{-6}$	10^{-7}
2.3299e $\times 10^{-6}$	10^{-8}
2.4162 $\times 10^{-6}$	10^{-9}
2.4996 $\times 10^{-6}$	10^{-10}

En la siguiente figura mostramos la gráfica de la cota de error en términos de $\frac{\sigma}{r_1}$, para sigma pequeño.


Cota de error como función de sigma sobre r1
para sigma pequeño.
Cota de error
Sigma sobre r1
x 10^{-6}
0
1
2
3
4
5
6
7
8
9
10
0
2
4
6
8

3.5.3. Sigma Intermedio, $\sigma \in [6.7591 \times 10^{-6} r_1, \frac{r_1}{22}]$, o $\sigma \in [\frac{23}{mv}, \frac{154678}{mv}]$

Tomamos el valor de mv que fue utilizado en los experimentos de Tonomura et al. [65], $mv = 1.9842 \times 10^{10}$. En términos absolutos, los valores de sigma grande varían en el intervalo $[1.1592 \times 10^{-9}, 7.7955 \times 10^{-6}]$.

Para valores de σ intermedio, la probabilidad de que el electrón choque con el magneto es menor a 10^{-199} (ver el Remark 8.12 y la sección 9.2 de [5]). De manera que para estos valores de sigma no hay ninguna interacción del electrón con algún campo electromagnético y el electrón debería seguir una trayectoria libre, sin embargo, la función de onda del electrón está dada por el Ansatz de Aharonov Bohm 3.4.1, en el cual el potencial magnético influye de manera directa. Por la precisión de nuestros resultados en el caso de σ intermedio, sería muy interesante realizar experimentos con estos valores de σ.

A continuación definimos de manera formal el ángulo de apertura y el radio del paquete de ondas. Las cotas de error (3.22) pueden ser expresadas en términos de estos conceptos, lo que ayuda a entender de manera físicamente apropiada el origen de las cotas de error.

3.5.4. El Radio del Paquete de Ondas

Denotamos por $\mathcal{C}$ al cilindro $\{(x, y, z) \in \mathbb{R}^3 : \sqrt{x^2 + y^2} \leq r_1\}$. $\mathcal{C}$ es básicamente el agujero del magneto. El factor $e^{-\frac{r_1^2}{2\sigma^2}}$ es prácticamente la raíz cuadrada de la probabilidad de que la partícula libre esté en el agujero del magneto a tiempo cero:

$$e^{-\frac{r_1^2}{2\sigma^2}} = \left\| \chi_{\mathbb{R}\setminus\mathcal{C}} (\frac{1}{\sigma^2 \pi})^{3/4} e^{-\frac{x^2}{2\sigma^2}} \right\|. \tag{3.25}$$

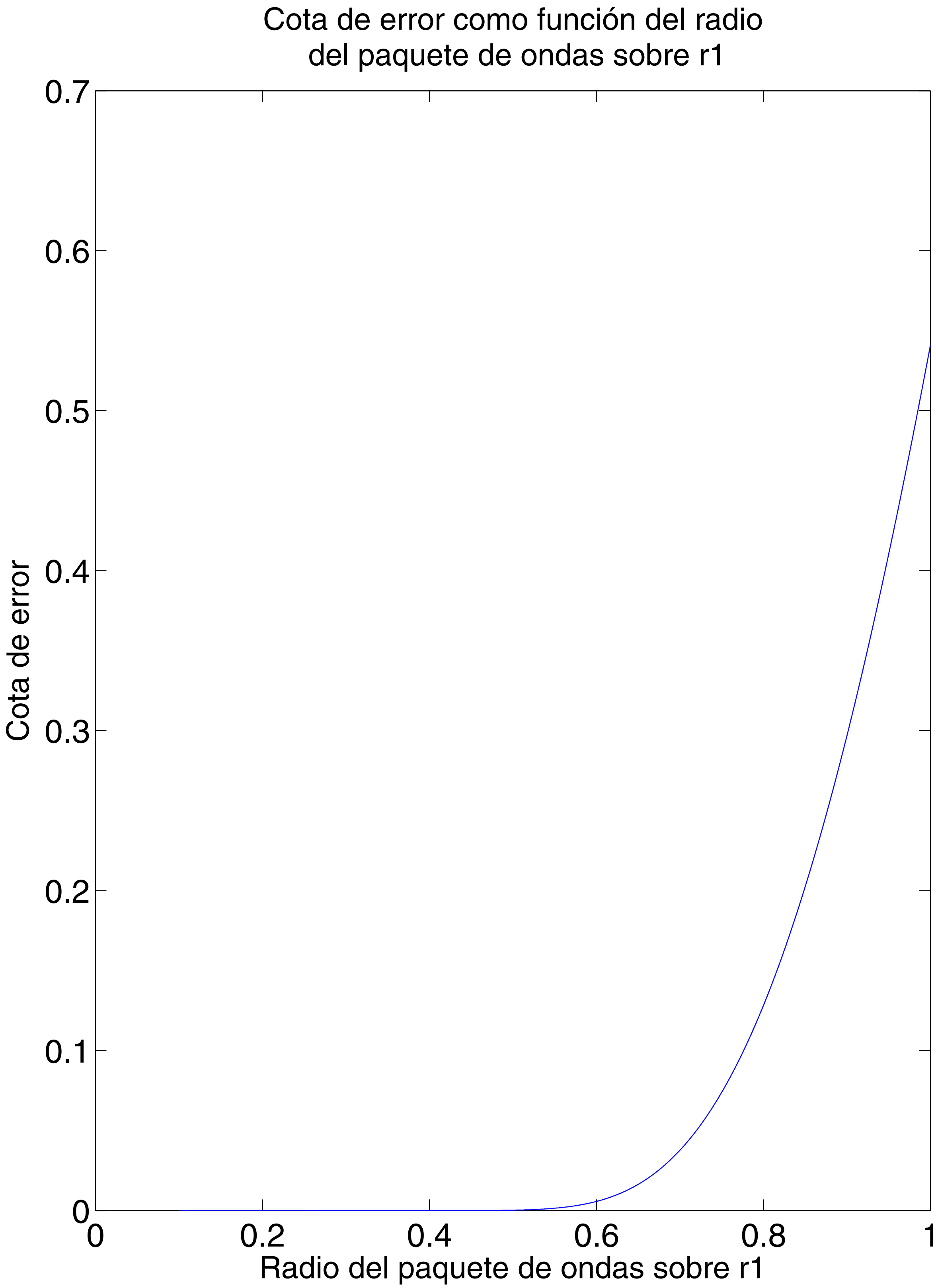
Tomamos la convención de que el electrón esté realmente localizado en el espacio de configuración en una bola centrada en la posición clásica $\mathbf{v}t$ de radio (R) elegido, de tal forma que la probabilidad de encontrar el electrón en esa bola sea del 99 %. Se obtiene que,

$$R := R(\sigma) = 2.263\sigma.$$

En seguida mostramos algunos datos del comportamiento de la cota de error como función de del radio del paquete de ondas sobre r_1 para sigma grande (ver la sección 3.5.1).

Cota de error como función del radio del paquete de ondas sobre r_1 para sigma grande.	
Radio del paquete de ondas sobre r_1	***Cota de error***
.81716	10^{-1}
.65806	10^{-2}
.56606	10^{-3}
.50427	10^{-4}
.45911	10^{-5}
.42425	10^{-6}
.39629	10^{-7}
.37322	10^{-8}
.35376	10^{-9}
.33703	10^{-10}

En la siguiente figura mostramos la gráfica para la cota de error (3.22) en términos del radio del paquete de ondas sobre r_1 para sigma grande (ver 3.5.1), en este caso el limite inferior del radio del paquete de ondas es $0.\,182r_1$. Tomamos el radio interior del magneto $\tilde{r}_1$ que fue utilizado en los experimentos de Tonomura et al. [65] $\tilde{r}_1 = 1.\,75 \times 10^{-4}cm$ (ver también (3.13)).



Cota de error como función del radio
del paquete de ondas sobre r1
Cota de error
Radio del paquete de ondas sobre r1
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
0.2
0.4
0.6
0.8
1

3.5.5. Ángulo de Apertura

Tomamos la convención de que el electrón libre (en la representación de momentos) está localizado en la bola, $B_P(M\mathbf{v})$ centrada en el momento clásico ($M\mathbf{v}$) y de radio P tal que existe un 99 % de probabilidad para que el electrón tenga su momento en esa bola. Entonces definimos el ángulo de apertura, $\omega(\sigma)$ como sigue,

$$\sin(\frac{\omega(\sigma)}{2}) := \frac{P}{Mv} = \frac{2.\,263}{\sigma mv}.$$

El factor $e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}$ dentro de la cota de error en (3.22) tiene la siguiente interpretación en términos del ángulo de apertura:

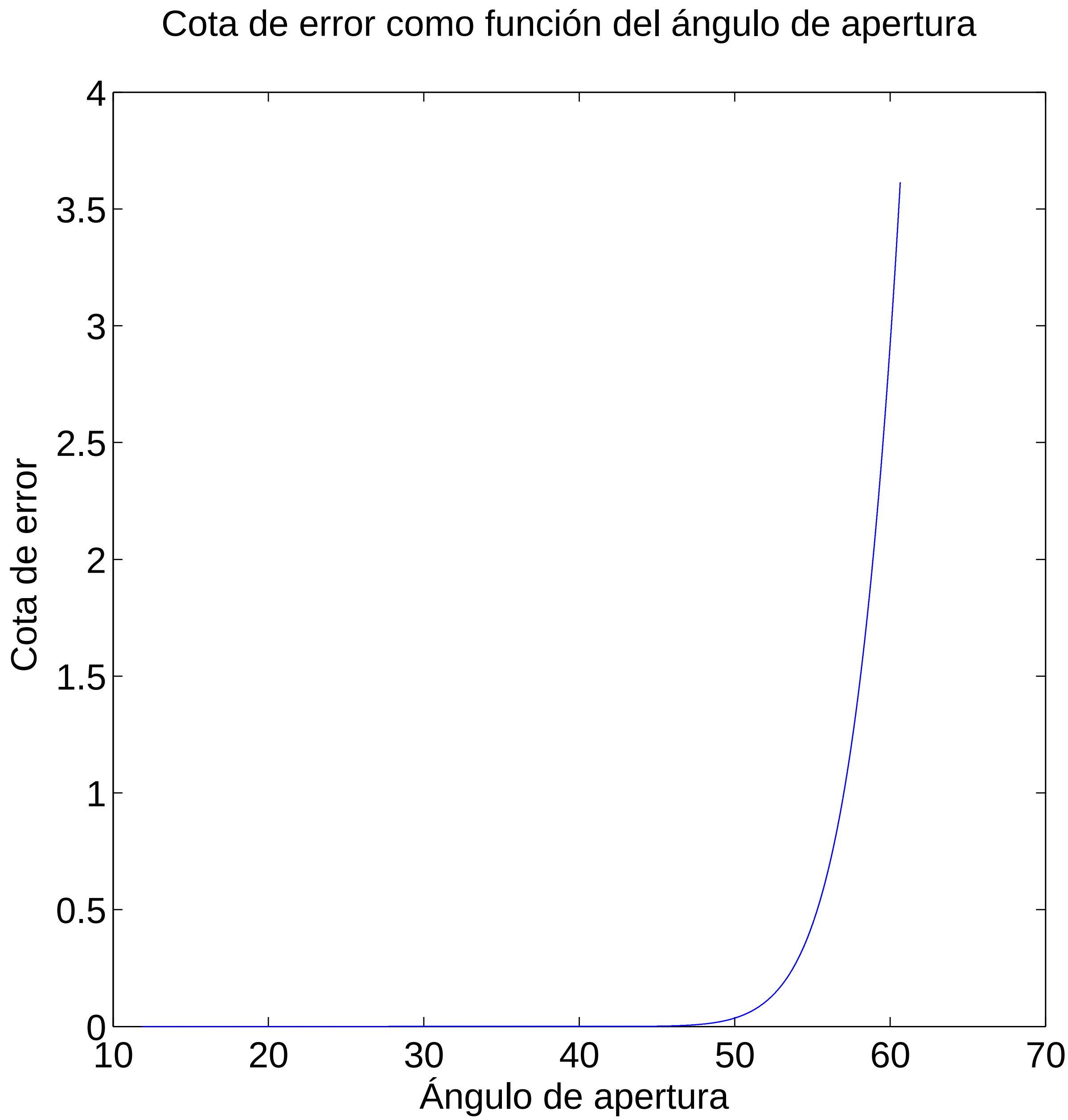
$$e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}} = e^{-2.48(\frac{1}{\sin(\omega(\sigma)/2)})^2}.$$

Este factor es prácticamente cero (menor que 10^{-100}) cuando $\omega \leq 11.\,8$ grados ($\sigma \geq 1.\,1592\times 10^{-9}$ o $\sigma mv \geq 23$), después crece conforme crece ω (σ decrece).

En seguida mostramos algunos datos del comportamiento de la cota de error como función del ángulo de apertura para sigma pequeño (ver la sección 3.5.2).

Cota de error como función del ángulo de apertura para sigma pequeño.	
Ángulo de apertura (grados)	***Cota de error***
51.8407	10^{-1}
47.8885	10^{-2}
44.7231	10^{-3}
42.1135	10^{-4}
39.9137	10^{-5}
38.0265	10^{-6}
36.3842	10^{-7}
34.9380	10^{-8}
33.6517	10^{-9}
32.4979	10^{-10}

En la siguiente gráfica se presenta la cota de error (3.22) en términos del ángulo de apertura para sigma pequeño (ver la sección 3.5.2).



Capítulo 4

Estimaciones a Grandes Energías del Operador de Dispersión y el Efecto de Aharonov-Bohm

En este capítulo se explica de manera resumida el contenido del artículo [4].

4.1. Resumen

Obtenemos estimaciones, con cotas de error, a velocidades altas del operador de dispersión para la ecuación de Schrödinger en tres dimensiones con campos electromagnéticos en el exterior de un obstáculo que suponemos es la unión finita de cuerpos con asas. Consideramos estimaciones a velocidades altas cuando la dirección de la velocidad permanece fija, mientras que la norma tiende a infinito. En el caso del toro, nuestros resultados proporcionan una prueba rigurosa cualitativa de que la física cuántica predice los patrones de interferencia observados en los fundamentales experimentos de Tonomura et al. que mostraron una evidencia concluyente de la existencia del efecto Aharonov-Bohm, usando un magneto en forma toroidal. En particular, esto muestra que la forma particular del toro utilizada en [5] para obtener los resultados cuantitativos no es importante. Damos además un método para la reconstrucción del flujo del campo magnético sobre una sección transversal del toro módulo 2π. De manera equivalente, determinamos módulo 2π la diferencia en la fase entre un electrón que viaja por el centro del magneto y otro que viaja por fuera del agujero del magneto. Para este propósito, necesitamos el límite de grandes velocidades del operador de dispersión en una sola dirección de la velocidad de los electrones incidentes. Cuando el obstáculo está compuesto de varios toros (o de manera más general, cuerpos con asas), la información sobre los flujos que podemos recuperar depende de la posición de los cuerpos con asas y de la dirección de la velocidad del electrón incidente. Para ciertas posiciones de los toros, podemos recuperar todos los flujos módulo 2π, tomando el límite a altas velocidades del operador de dispersión en una sola dirección. Damos también un método de reconstrucción del campo eléctrico y el campo magnético a partir del operador de dispersión.

Definimos de forma rigurosa cuándo los electrones pasan por algún agujero del obstáculo y demostramos, en el caso de que el campo magnético sea cero fuera del obstáculo, que el límite a altas energías del operador de dispersión es constante al actuar sobre electrones que pasan por un mismo agujero; de hecho, está dado por un operador de multiplicación por un número complejo unitario cuya fase está determinada por el flujo del campo magnético en cierta superficie dentro del obstáculo.

Obtenemos, en el caso de que el campo magnético sea cero fuera del obstáculo, cierta información de la clase de cohomología de de Rham del potencial magnético. En ciertos casos, podemos determinar módulo 2π los coeficientes de esta clase de cohomología, en cierta base que definimos explícitamente.

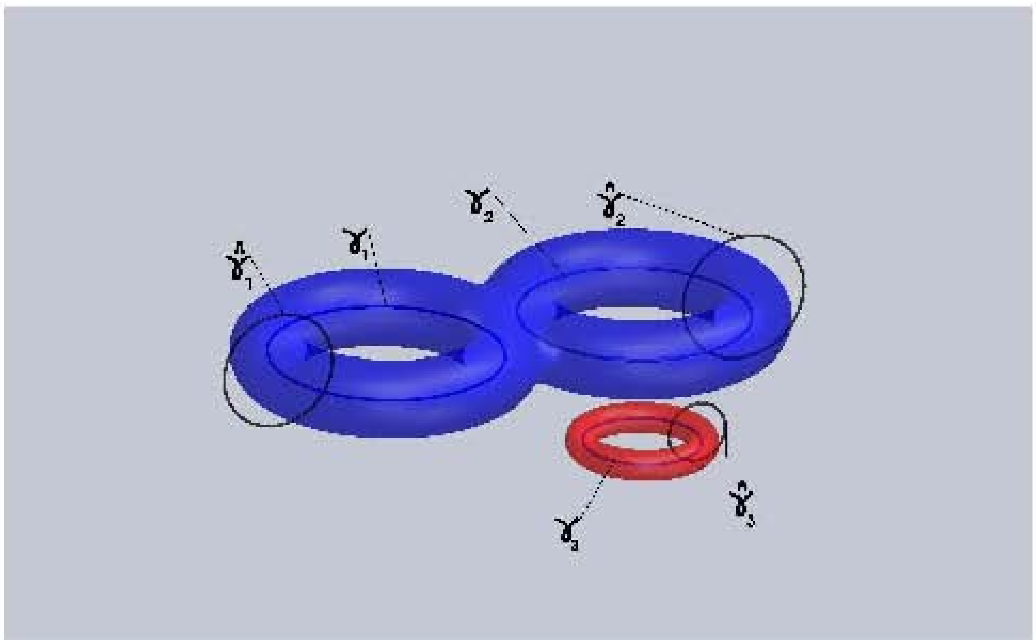
4.2. El Obstáculo

Estudiaremos un caso más general que el planteado en los experimentos de Tonomura el. al. [63, 64]. En nuestro caso, el magneto (o bien el obstáculo) es una unión finita disjunta de cuerpos con asas o handlebodies:

$$K = \cup_{j=1}^{L} K_j \quad \subset \mathbb{R}^3,$$

en donde K_j es un cuerpo con asas para toda j.
Definimos el dominio exterior como $\Lambda := \mathbb{R}^3 \setminus K$.
En la siguiente figura se muestra un caso particular del obstáculo K. Las clases de homología de las curvas $\{\gamma_i\}_1^m$ forman una base de la 1-homología

singular de K y las clases de homología de las curvas $\{\hat{\gamma}_i\}_{i=1}^{m}$ forman una base de la 1-homología de singular Λ.



Para toda $x \in \mathbb{R}^3 \setminus \{0\}$ denotamos por $\hat{x} := \frac{x}{|x|}$. Definimos además para toda $r > 0$, $B_r^{\mathbb{R}^3} := \{x \in \mathbb{R}^3 : |x| < r\}$.

Definición 4.2.1. *Sea $B \in L^p\Omega^2(\overline{\Lambda}), p > 3$, una $2-$ forma cerrada continua en una vecindad de ∂K. Suponemos que no hay monopolos magnéticos en K:*

$$\int_{\partial K_j} B = 0,\ j \in \{1, 2, \cdots, L\}.$$

Definimos el flujo, Φ, como una función $\Phi : \{\hat{\gamma}_j\}_{j=1}^m \to \mathbb{R}$. Denotamos por $\mathcal{A}_\Phi(B)$ al conjunto de $1-$ formas continuas en $\overline{\Lambda}$ que satisfacen.

1.
$$|A(x)| \leq C\frac{1}{1+|x|},\ a(r) := \max_{x\in\Lambda,|x|\geq r}\{|A(x)\cdot\hat{x}|\} \in L^1(0,\infty).$$

2.
$$\int_{\hat{\gamma}_j} A = \Phi(\hat{\gamma}_j),\ j \in \{1, 2, \cdots, m\}.$$

3.
$$dA|_\Lambda = B|_\Lambda.$$

4.3. Potencial de Coulomb

Teorema 4.3.1. *[4] Sea B como en la Definición 4.2.1. Supongamos que existe r tal que $K \subset B_r^{\mathbb{R}^3}(0)$ y*

$$|B(x)| \leq C(1+|x|)^{-\mu}, |x| \geq r, \mu > 2. \tag{4.1}$$

entonces, para todo flujo , Φ, existe un potencial $A_C \in \mathcal{A}_\Phi(B)$ tal que $A_C = A_{(C,1)} + A_{(C,2)}$, en donde $A_{(C,1)}$ es continuo en $\overline{\Lambda}$, $A_{(C,2)}$ es C^∞ en $\overline{\Lambda}$, y $\delta A_{(C,j)} = -\operatorname{div} A_{(C,j)} = 0$, $j = 1, 2$. Asimismo,

$$|A_{(C,1)}(x)| \leq C(1+|x|)^{-\min(2-\varepsilon,\mu-1)}, \forall\varepsilon > 0,$$

$$|A_{(C,2)}(x)| \leq C(1+|x|)^{-2}.$$

Además, se puede encontrar una forma explícita para los potenciales $A_{(C,1)}$ y $A_{(C,2)}$ del teorema anterior:

$$A_{(C,1)} := -\frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{x-y}{|x-y|^3} \times \overline{B}(y)\, dy,$$

en donde $\overline{B}$ es una extensión de B a $\mathbb{R}^3$, ver el Teorema 3.2 de [4].

$$A_{(C,2)} := \sum_{j=1}^{m} \left(\Phi(\hat{\gamma}_j) - \int_{\hat{\gamma}_j} A_{(C,1)} \right) G^{(j)},$$

en donde $G^{(j)}, j = 1, 2, \cdots, m$ están dadas por

$$G^{(j)}(x) := \ \operatorname{curl} \frac{1}{4\pi} \int \frac{1}{|x-\gamma_j(t)|}\, \dot{\gamma}_j(t)\, dt.$$

Se puede demostrar que $\operatorname{curl} G^{(j)}(x) = 0,\ x \in \mathbb{R}^3 \setminus \gamma_j$ y que

$$\int_{\hat{\gamma}_k} G^{(j)} = \delta_{k,j}, j, k = 1, 2, \cdots, m.$$

A partir de lo anterior, se encuentra que $\left\{ \left[G^{(j)}\right]_{H^1_{\text{de R}}}(\Lambda) \right\}_{j=1}^{m}$

es una base del grupo de homología de de Rham $H^1_{\text{de R}}(\Lambda)$.
El problema divergencia-rotacional en dominios exteriores en el caso de campos vectoriales de clase C^1 con primeras derivadas Hölder-continuas fue estudiado por Neudert y Von Wahl (2001).

4.4. Condición para el Flujo Módulo 2π

Lema 4.4.1 (Transformaciones de norma). *Supongamos que $A, \tilde{A} \in \mathcal{A}_\Phi(B)$. Entonces existe una $0-$ forma de clase C^1 λ en $\overline{\Lambda}$ tal que, $\tilde{A} - A = d\lambda$. Podemos elegir $\lambda(x) := \int_{C(x_0,x)}(\tilde{A} - A)$ en donde x_0 es un punto fijo en Λ y $C(x_0, x)$ es una curva que conecta x_0 con x. Además, $\lambda_\infty(x) := \lim_{r\to\infty} \lambda(rx)$ existe, es continuo en $\mathbb{R}^3 \setminus \{0\}$ y es una función homogénea de orden cero, es decir, $\lambda_\infty(rx) = \lambda_\infty(x), r > 0, x \in \mathbb{R}^3 \setminus \{0\}$.*

Definición 4.4.1. *Denotamos por $\mathcal{A}_{\Phi,2\pi}(B)$ al conjunto de $1-$ formas continuas en $\overline{\Lambda}$ que satisfacen, $dA = B$ y*

$$|A(x)| \leq C\frac{1}{1+|x|},\ a(r) := \max_{x\in\Lambda,|x|\geq r} \{|A(x)\cdot\hat{x}|\} \in L^1(0,\infty).$$

$$\int_{\hat{\gamma}_j} A = \Phi(\hat{\gamma}_j) + 2\pi n_j(A), n_j(A) \in \mathbb{Z},\ j \in \{1, 2, \cdots, m\}.$$

Para toda $A \in \mathcal{A}_{\Phi,2\pi}(B)$ definimos,

$$A_\Phi := A - \sum_{j=1}^{m} 2\pi n_j(A)\, G^{(j)} \in \mathcal{A}_\Phi(B).$$

Suponemos que $A, \tilde{A} \in \mathcal{A}_{\Phi,2\pi}(B)$. Entonces, $A_\Phi, \tilde{A}_\Phi \in \mathcal{A}_\Phi(B)$, y

$$\tilde{A}_\phi - A_\Phi = d\lambda.$$

Se sigue que,

$$\tilde{A} - A = d\lambda + A_{\mathbb{Z}},$$

en donde

$$A_{\mathbb{Z}} := \sum_{j=1}^{m} 2\pi(n_j(\tilde{A}) - n_j(A))\, G^{(j)}.$$

Sea C una curva cerrada en Λ. Se obtiene que,

$$\int_C (\tilde{A} - A) = 2\pi N, \text{ para alguna } N \in \mathbb{Z}.$$

Por lo tanto, podemos definir los factores no integrables,

$$U_{\tilde{A},A}(x) := e^{i \int_{C(x_0,x)} (\tilde{A}-A)} = e^{i(\lambda(x) + \int_{C(x_0,x)} A_{\mathbb{Z}})},$$

en donde x_0 es un punto fijo en Λ y $C(x_0, x)$ es una curva en Λ que conecta x_0 con x.

Para toda $x \neq 0$ existe un número real $C_{\tilde{A},A}$ independiente de x tal que,

$$\lim_{r\to\infty} U_{\tilde{A},A}(rx) = e^{i(\lambda_\infty(x) + C_{\tilde{A},A})},$$

4.5. El Operador de Dispersión

Suponemos que el campo magnético, B, es una $2-$ forma acotada a valores reales definida en $\overline{\Lambda}$, continua en una vecindad de ∂K y

1. B is cerrada : $dB|_\Lambda \equiv \text{div}B = 0$.

2. No hay monopolos magnéticos en K:

$$\int_{\partial K_j} B = 0,\ j \in \{1, 2, \cdots, L\}.$$

3. $$|B(x)| \leq C(1 + |x|)^{-\mu}, \text{ para alguna } \mu > 2.$$

4. $d * B|_\Lambda \equiv \text{curl}\, B$ es acotado y

$$|\text{curl}\, B| \leq C(1 + |x|)^{-\mu}.$$

5. El potencial eléctrico V es una función a valores reales, $\Delta-$acotada, y

$$\left\| F(|x| \geq r) V(-\Delta + I)^{-1} \right\| \leq C(1 + |r|)^{-\alpha}, \text{ para alguna } \alpha > 1.$$

Denotamos por H al Hamiltoniano con condiciones a la frontera de Dirichlet en $\partial\Lambda$,

$$H := \frac{1}{2m}(\mathbf{p} - A)^2 + V, A \in \mathcal{A}_{\Phi,2\pi}(B).$$

Los operadores de onda

$$W_\pm(A, V) := \text{s-}\lim_{t\to\pm\infty} e^{itH(A,V)}\, J\, e^{-itH_0},$$

existen y son isométricos,

$$W_\pm(\tilde{A}, V) = e^{-iC_{\tilde{A},A}}\, U_{\tilde{A},A}\, W_\pm(A, V)\, e^{-i\lambda_\infty(\pm\mathbf{p})}, \tilde{A}, A \in \mathcal{A}_{\Phi,2\pi}(B).$$

El operador de dispersión,

$$S(A, V) := W_+^*(A, V)\, W_-(A, V),$$

se transforma de la siguiente manera,

$$S(\tilde{A}, V) = e^{i\lambda_\infty(\mathbf{p})}\, S(A, V)\, e^{-i\lambda_\infty(-\mathbf{p})},\ \tilde{A}, A \in \mathcal{A}_{\Phi,2\pi}(B).$$

Definición 4.5.1. *Decimos que* $A \in \mathcal{A}_{\Phi,2\pi}(B)$ *es de rango corto si*

$$|A(x)| \leq C(1+|x|)^{-1-\varepsilon}, \text{ para alguna } \varepsilon > 0. \tag{4.2}$$

Denotamos por $\mathcal{A}_{\Phi,2\pi,\mathrm{SR}}(B)$ *al conjunto de potenciales de rango corto en* $\mathcal{A}_{\Phi,2\pi}(B)$.

Notemos que si $\tilde{A}, A \in \mathcal{A}_{\Phi,2\pi}(B)$ y $\tilde{A} - A$ satisface (4.2), λ_∞ es constante y

$$S(\tilde{A}, V) = S(A, V).$$

esto se cumple en particular cuando $\tilde{A}, A \in \mathcal{A}_{\Phi,2\pi,\mathrm{SR}}(B)$.

Además, dado $A \in \mathcal{A}_{\Phi,2\pi}(B)$ existe $\tilde{A} \in \mathcal{A}_{\Phi}(B)$ tal que,

$$S(\tilde{A}, V) = S(A, V).$$

Podemos elegir por ejemplo, $\tilde{A} = A_\Phi$ (recordemos que cambiamos los flujos sumando potenciales de rango corto).

4.6. Reconstrucción del Campo Magnético

Denotamos por

$$\Lambda_{\hat{\mathbf{v}}} := \{x \in \Lambda : x + \tau\hat{\mathbf{v}} \in \Lambda,\ \forall \tau \in \mathbb{R}\}, \text{ para } \mathbf{v} \neq 0,$$

$$a(\hat{\mathbf{v}}, x) := \int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(x + \tau\hat{\mathbf{v}})\, d\tau,$$

recordemos que $\hat{\mathbf{v}} := \frac{\mathbf{v}}{|\mathbf{v}|}$.

Teorema 4.6.1. (Fórmula de reconstrucción I)*[4] Sea* Λ_0 *un subconjunto compacto de* $\Lambda_{\hat{\mathbf{v}}}$, *para* $\mathbf{v} \in \mathbb{R} \setminus \{0\}$. *Para toda* Φ *y toda* $A \in \mathcal{A}_{\Phi,2\pi}(B)$ *existe una constante* C *tal que,*

$$\left\| \left(e^{-im\mathbf{v}\cdot x}\, S(A,V)\, e^{im\mathbf{v}\cdot x} - e^{ia(\hat{\mathbf{v}},x)} \right) \phi \right\|_{L^2(\mathbb{R}^3)} \leq$$

$$\tfrac{C}{v} \|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)},$$

para toda $\phi \in \mathcal{H}_2(\mathbb{R}^3)$ *tal que* soporte $\phi \subset \Lambda_0$.

4.7. Fórmula de Reconstrucción del Potencial Eléctrico

Denotemos por

$$\Xi_\eta(x,t) := \frac{1}{2m}\chi(x)\left[-\mathbf{p}\cdot\eta(x,t) - \eta(x,t)\cdot\mathbf{p} + (\eta(x,t))^2\right],$$

$$\eta(x,t) := \int_0^t (\hat{\mathbf{v}}\times B)(x+\tau\hat{\mathbf{v}})d\tau.$$

Teorema 4.7.1. *[4]* **(Fórmula de reconstrucción II)** *Sea Λ_0 un subconjunto compacto de $\Lambda_{\hat{\mathbf{v}}}$, para $\mathbf{v}\in\mathbb{R}\backslash\{0\}$. Para toda Φ y toda $A\in\mathcal{A}_{\Phi,2\pi,\mathrm{SR}}(B)$*

$$\begin{aligned}
&v\left(\left[e^{-im\mathbf{v}\cdot x}S(A,V)e^{im\mathbf{v}\cdot x} - e^{ia(\hat{\mathbf{v}},x)}\right]\phi,\psi\right) = \\
&\left(-ie^{ia(\hat{\mathbf{v}},x)}\int_{-\infty}^{\infty} V(x+\tau\hat{\mathbf{v}})\,d\tau\,\phi,\,\psi\right) \\
&+\left(-ie^{ia(\hat{\mathbf{v}},x)}\int_{-\infty}^{0}\Xi_\eta(x+\tau\hat{\mathbf{v}},-\infty)\,d\tau\,\phi,\psi\right) + \\
&\left(-i\int_0^\infty \Xi_\eta(x+\tau\hat{\mathbf{v}},\infty)\,d\tau\,e^{ia(\hat{\mathbf{v}},x)}\phi,\psi\right) + R(\mathbf{v},\phi,\psi),
\end{aligned}$$

en donde,

$$\begin{aligned}
&|R(\mathbf{v},\phi,\psi)| \\
&\leq C\|\phi\|_{\mathcal{H}_6(\mathbb{R}^3)}\|\psi\|_{\mathcal{H}_6(\mathbb{R}^3)}\begin{cases}
\frac{1}{v^{\text{mín}(\mu-2,\alpha-1)}}, \text{ si mín}(\mu-3,\alpha-2)<0, \\
\frac{|\ln v|}{v}, \text{ si mín}(\mu-3,\alpha-2)=0, \\
\frac{1}{v}, \text{ si mín}(\mu-3,\alpha-2)>0,
\end{cases}
\end{aligned}$$

Para alguna constante C y todo $\phi_0,\psi_0\in\mathcal{H}_6(\mathbb{R}^3)$ de soporte compacto en Λ_0.

4.8. Problema Inverso

Definición 4.8.1. *Denotamos por Λ_{rec} al conjunto de puntos $x\in\Lambda$ tales que existe un plano bidimensional P_x con $x+P_x\subset\Lambda$.*

Teorema 4.8.1. *[4] Para todo flujo, Φ, y toda $A\in\mathcal{A}_{\Phi,2\pi}(B)$, el límite a grandes velocidades de $S(A,V)$ conocido para toda Λ_0, todo vector unitario $\hat{\mathbf{v}}$ y todo $\phi_0\in\mathcal{H}_2(\mathbb{R}^3)$ con soporte contenido en Λ_0, determina de manera única $B(x)$ y $V(x)$ para casi toda $x\in\Lambda_{\mathrm{rec}}$.*

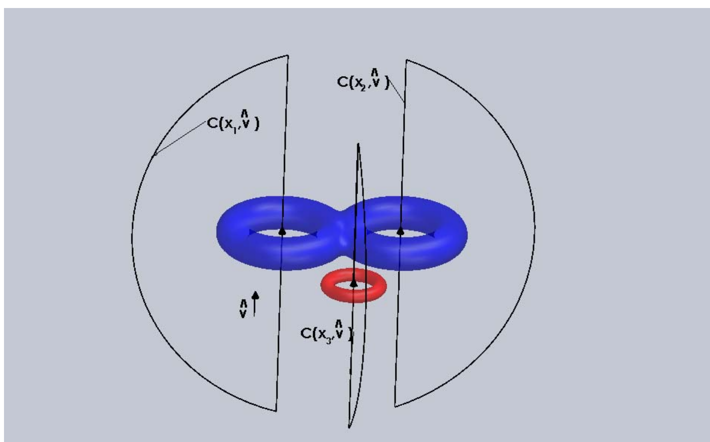
4.9. Efecto Aharonov-Bohm

Suponemos que $B \equiv 0$, es decir, que no hay campo magnético en Λ. El potencial eléctrico, V, no tiene que ser cero, es decir, estudiamos el efecto Aharonov-Bohm bajo la influencia de un campo eléctrico.

Para toda $x \in \mathbb{R}^3$ y todo vector unitario $\hat{\mathbf{v}} \in \mathbb{S}^2$ denotamos por

$$L(x, \hat{\mathbf{v}}) := x + \mathbb{R}\hat{\mathbf{v}}.$$

Damos ahora una definición precisa de cuándo una línea $L(x, \hat{\mathbf{v}})$ pasa por un agujero de K. Sea $r > 0$ tal que $K \subset B_r^{\mathbb{R}^3}(0)$. Supongamos que $L(x, \hat{\mathbf{v}}) \subset \Lambda$, y $L(x, \hat{\mathbf{v}}) \cap B_r^{\mathbb{R}^3}(0) \neq \emptyset$. Denotamos por $c(x, \hat{\mathbf{v}})$ a la curva que consiste del segmento de línea $L(x, \hat{\mathbf{v}}) \cap \overline{B_r^{\mathbb{R}^3}(0)}$ y un arco sobre $\partial \overline{B_r^{\mathbb{R}^3}(0)}$ que conecta los puntos $L(x, \hat{\mathbf{v}}) \cap \partial \overline{B_r^{\mathbb{R}^3}(0)}$. Orientamos a la curva, de tal forma que el segmento de recta siga la dirección $\hat{v}$.



Definición 4.9.1. *Una línea $L(x,\hat{\mathbf{v}}) \subset \Lambda$ pasa por un agujero de K si $L(x,\hat{\mathbf{v}}) \cap B_r^{\mathbb{R}^3}(0) \neq \emptyset$ y $[c(x,\hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} \neq 0$. De lo contrario, $L(x,\hat{\mathbf{v}})$ no pasa por algún agujero de K.*

Definición 4.9.2. *Dos líneas $L(x,\hat{\mathbf{v}}), L(y,\hat{\mathbf{v}})$ pasan por el mismo agujero en el mismo sentido si $[c(x,\hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} = [c(y,\hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})}$.*

Definición 4.9.3. *Definimos la siguiente relación de equivalencia en $\Lambda_{\hat{\mathbf{v}}}$. Dadas $x, y \in \Lambda_{\hat{\mathbf{v}}}$, x está relacionada con y si $L(x,\hat{\mathbf{v}})$ y $L(y,\hat{\mathbf{v}})$ pasan por el mismo agujero en la misma dirección o bien ambas no pasan por algún a agujero.*
Denotamos por $\{\Lambda_h\}_{h\in\mathcal{I}} \cup \{\Lambda_{out}\}$ a la partición inducida por la anterior relación de equivalencia. Λ_{out} es la clase de las x tales que $L(x,\hat{\mathbf{v}})$ no pasa por algún agujero de K. Intuitivamente entendemos a los conjuntos Λ_h como los agujeros de K en la dirección $\hat{\mathbf{v}}$.

Para toda Φ, $A \in \mathcal{A}_\Phi(0)$, $\hat{\mathbf{v}} \in \mathbb{S}^2$, y $h \in \mathcal{I}$ definimos,

$$F_h := \int_{c(x,\hat{\mathbf{v}})} A,$$

Denotamos por $\mathcal{H}_2(\mathbb{R}^3)$ al espacio de Sobolev de funciones con dominio $\mathbb{R}^3$ a valores complejos cuyo modulo al cuadrado es integrable y cuyas derivadas distribucionales de primer orden son funciones de cuadrado integrable.

Sea $\phi_0 \in \mathcal{H}_2(\mathbb{R}^3)$ con soporte compacto contenido en $\Lambda_{\hat{\mathbf{v}}}$. Entonces,

$$\phi_0 = \sum_{h\in\mathcal{I}} \varphi_h + \varphi_{\text{out}},$$

en donde *soporte*$(\phi_h) \subset \Lambda_h$ y *soporte*$(\phi_{out}) \subset \Lambda_{out}$.
Denotamos por

$$\phi_{\mathbf{v}} := e^{im\mathbf{v}\cdot x}\phi_0,\ \varphi_{h,\mathbf{v}} := e^{im\mathbf{v}\cdot x}\varphi_h,\ \varphi_{\text{out},\mathbf{v}} := e^{im\mathbf{v}\cdot x}\varphi_{\text{out}}.$$

Teorema 4.9.1. *[4] Supongamos que $B \equiv 0$. Entonces para toda Φ y toda $A \in \mathcal{A}_\Phi(0)$,*

$$S(A,V)\,\phi_{\mathbf{v}} = e^{-i(\lambda_\infty(\hat{\mathbf{v}})-\lambda_\infty(-\hat{\mathbf{v}}))}\left(\sum_{h\in\mathcal{I}} e^{iF_h}\varphi_{\mathbf{v},h} + \varphi_{\text{out},\mathbf{v}}\right) + O\left(\frac{1}{v}\right).$$

Teorema 4.9.2. *Además, el límite a grandes velocidades de $S(A,V)$ en la dirección $\hat{\mathbf{v}}$ determina $\lambda_\infty(\hat{\mathbf{v}}) - \lambda_\infty(-\hat{\mathbf{v}})$ y los flujos $F_h, h \in \mathcal{I}$, módulo 2π.*

Recordemos que siempre podemos elegir $A \in \mathcal{A}_{\Phi,\text{SR}}(0)$ en donde $\lambda_\infty(\hat{\mathbf{v}}) - \lambda_\infty(-\hat{\mathbf{v}}) = 0$.

4.9.1. Efectos Topológicos Sobre La Dispersión de los Electrones

Sean x, y vectores en $\mathbb{R}^3$ tales que

$$L(x, \hat{\mathbf{v}}) \cup L(y, \hat{\mathbf{w}}) \subset \Lambda.$$

Sea $\rho > 0$ tal que

$$\begin{aligned}\text{convex}\left((x + (-\infty, -\rho]\hat{\mathbf{v}}) \cup (y + (-\infty, -\rho]\hat{\mathbf{w}})\right) \cup \\ \text{convex}\left((x + [\rho, \infty)\hat{\mathbf{v}}) \cup (y + [\rho, \infty,)\hat{\mathbf{w}})\right) \subset B_r^{\mathbb{R}^3}(0)^c,\end{aligned} \tag{4.3}$$

en donde r es un número fijo tal que $K \subset B_r(0)$, $B_r(0)^c$ es el complemento de $B_r(0)$ y el símbolo *convex*$(\cdot)$ denota el casco convexo del conjunto indicado. Denotamos por $\gamma(x, y, \hat{\mathbf{v}}, \hat{\mathbf{w}})$ la curva cerrada simple continua y orientada con lados $x + [-\rho, \rho]\hat{\mathbf{v}}$ (orientado en la dirección de $\hat{\mathbf{v}}$),

$x + [-\rho, \rho]\hat{\mathbf{w}}$ (orientado en la dirección de $-\hat{\mathbf{w}}$) y las rectas que unen los puntos $x + \rho\hat{\mathbf{v}}$ con $y + \rho\hat{\mathbf{w}}$ y $y - \rho\hat{\mathbf{w}}$ con $x - \rho\hat{\mathbf{v}}$.

Supongamos que A es de rango corto (ver definición 4.5.1). Denotamos por $x_{\perp,\hat{\mathbf{v}}} := x - (x, \hat{\mathbf{v}})\hat{\mathbf{v}}$. Se sigue del teorema de Stokes que si $|x_{\perp,\hat{\mathbf{v}}}| \geq r$,

$$\int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(x + \tau\hat{\mathbf{v}})\, d\tau = \int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(x_\perp + \tau\hat{\mathbf{v}})\, d\tau = \lim_{s\to\infty} \int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(sx_\perp + \tau\hat{\mathbf{v}})\, d\tau = 0. \tag{4.4}$$

Usamos de nuevo el teorema de Stokes para obtener,

$$\int_{\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})} A = \int_{L(x,\hat{\mathbf{v}})} A - \int_{L(y,\hat{\mathbf{w}})} A. \tag{4.5}$$

Para toda $z \in \mathbb{R}^3$ tal que $|(x+z)_{\perp,\hat{\mathbf{v}}}| \geq r$, $|(y+z)_{\perp,\hat{\mathbf{w}}}| \geq r$, se obtiene también por el teorema de Stokes,

$$\int_{L(x+z,\hat{\mathbf{v}})} A = \int_{L(y+z,\hat{\mathbf{w}})} A = 0.$$

Sumando un cero, escribimos (4.5) como,

$$\int_{\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})} A = \left(\int_{L(x,\hat{\mathbf{v}})} A - \int_{L(x+z,\hat{\mathbf{v}})} A\right) - \left(\int_{L(y,\hat{\mathbf{w}})} A - \int_{L(y+z,\hat{\mathbf{w}})} A\right). \tag{4.6}$$

Para toda $A \in \mathcal{A}_{\Phi,2\pi}(0)$ existe $\tilde{A} \in \mathcal{A}_{\Phi,2\pi}(0)$ de rango corto y una función derivable a valores reales λ, tal que $A = \tilde{A} + \nabla\lambda$. Entonces (4.6) funciona para toda $A \in \mathcal{A}_{\Phi,2\pi}(0)$.
Se sigue del teorema 4.6.1 que podemos reconstruir a partir del operador de dispersión $\int_{\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})} A$ para toda $A \in \mathcal{A}_{\Phi,2\pi}(0)$.

Teorema 4.9.3. *Supongamos que $B = 0$, entonces para todo flujo Φ y para todo $A \in \mathcal{A}_{\Phi,2\pi}(0)$, el límite de altas velocidades del $S(A,V)$ en las direcciones $\hat{\mathbf{v}}$ y $\hat{\mathbf{w}}$ determina los flujos*

$$\int_{\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})} A \tag{4.7}$$

módulo 2π, para toda curva $\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})$.

Nota 4.9.1. El teorema 4.9.3 implica que del límite a grandes velocidades del operador de dispersión podemos reconstruir los flujos

$$\int_\alpha A$$

para toda curva α tal que exista una superficie (o cadena) $\mathcal{S}$ en Λ tal que $\partial\mathcal{S} = \alpha - \gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})$, ya que por el teorema de Stokes,

$$\int_\alpha A = \int_{\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})} A + \int_{\mathcal{S}} B = \int_{\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})} A.$$

Recordemos que dado $A \in \mathcal{A}_{\Phi,2\pi}(0)$, podemos encontrar $A \in \mathcal{A}_{\Phi}(0)$ con el mismo operador de dispersión. Podemos tomar por ejemplo A_Φ. Entonces no perdemos generalidad si elegimos $A \in \mathcal{A}_\Phi(0)$. Además, notemos que podemos a lo más reconstruir los flujos módulo 2π, pues $S(A_\Phi, V) = S(A,V)$ y los flujos de A y A_Φ difieren por múltiplos enteros de 2π. Para un potencial magnético general $A \in \mathcal{A}_{\Phi,2\pi}(0)$ recuperamos los flujos por medio de la ecuación (4.6). Sin embargo, si A es de rango corto, podemos usar la ecuación más simple (4.5).

Nota 4.9.2. Como $\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})$ es un ciclo, la clase de homología $[\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})]_{H_1(\Lambda;\mathbb{R})}$ está bien definida.

Denotamos por

$$(4.8) \qquad H_{1,\text{rec}}(\Lambda;\mathbb{R}) := \left\langle \left\{ [\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})]_{H_1(\Lambda;\mathbb{R})} : L(x,\hat{\mathbf{v}}) \cup L(x,\hat{\mathbf{w}}) \subset \Lambda \right\} \right\rangle .$$

$H_{1,\text{rec}}(\Lambda;\mathbb{R})$ es un subespacio vectorial del grupo de homología $H_1(\Lambda;\mathbb{R})$. Denotemos por $H^1_{\text{de R, rec}}(\Lambda)$ el subespacio vectorial de $H^1_{\text{de R}}(\Lambda)$ que es dual a $H_{1,\text{rec}}(\Lambda;\mathbb{R})$ en el sentido del teorema de de Rham. Entonces para toda Φ y para toda $A \in \mathcal{A}_{\Phi,2\pi}(0)$, del límite de altas velocidades del operador de dispersión podemos reconstruir la proyección de A en $H^1_{\text{de R, rec}}(\Lambda)$ módulo 2π, como mostraremos a continuación. Sea

$$\left\{ [\sigma_j]_{H_{1,\text{rec}}(\Lambda;\mathbb{R})} \right\}_{j=1}^{m},$$

una base de $H_{1,\text{rec}}(\Lambda;\mathbb{R})$, y sea

$$\left\{ [A_j]_{H^1_{\text{de R, rec}}(\Lambda)} \right\}_{j=1}^{m},$$

la base dual en el sentido de de Rham, es decir,

$$\int_{\sigma_j} A_k = \delta_{j,k}, j,k = 1,2,\cdots,m.$$

Denotemos por P_{rec} la proyección en $H^1_{\text{de R, rec}}(\Lambda)$. Entonces, para toda $A \in \mathcal{A}_{\Phi,2\pi}(B)$

$$P_{\text{rec}}\, [A]_{H^1_{\text{de R}}(\Lambda)} = \sum_{j=1}^{m} \lambda_j [A_j]_{H^1_{\text{de R, rec}}(\Lambda)},$$

además, como

$$\lambda_j = \int_{\sigma_j} A,$$

podemos reconstruir $\lambda_j, j = 1,2,\cdots,m$ (módulo 2π) del límite de grandes energías del operador de dispersión.

Capítulo 5

Conclusiones

- Demostramos que el Ansatz de Aharonov y Bohm [2] es una buena aproximación para la función de onda exacta del electrón para todo tiempo. Nuestra predicción teórica coincide con los resultados experimentales de Tonomura et al. [63, 64]

- El Ansatz de Aharonov y Bohm es, de hecho, una buena aproximación para la función de onda del electrón si el electrón permanece (aproximadamente) en una región simplemente conexa y no choca con el magneto, como fue sugerido por Aharonov y Bohm.

- Los factores principales que producen el error son el tamaño del electrón y el ángulo de apertura.

- Para sigma intermedio ($\sigma \in [6.\,7591 \times 10^{-6} r_1, \frac{r_1}{22}]$), la evolución dada por el Ansatz de Aharonov-Bohm (3.21) difiere de la solución exacta en norma por un número menor que 10^{-99}.

- Para sigma intermedio la probabilidad de interacción del electrón con el magneto es prácticamente nula (menor que 10^{-199}) y, por lo tanto, no hay campos electromagnéticos dentro de la trayectoria del electrón. Empero, la solución de la ecuación de Schrödinger está dada por el Ansatz de Aharonov y Bohm (3.21) y es afectada por el potencial vectorial A por medio de una fase $e^{i\lambda^h_{A,0}}$. Esta fase es la que aparece en los experimentos de Tonomura et al. [63], [64].

- Aunque en los experimentos de Tonomura et al. [63], [64] no hay interacción con el campo magnético, sí la hay con el magneto impenetrable.

Tonomura et al. argumentan que no es necesario considerar la parte del electrón que choca con el magneto porque podemos ver la clara figura de la sombra del magneto.

- Nuestros resultados muestran que para valores de sigma intermedios, la física cuántica predice el patrón de interferencia observado en los experimentos de Tonomura et al. con una precisión extraordinaria. Sería muy interesante realizar experimentos utilizando electrones de tamaño intermedio (con varianza intermedia).

- Los resultados que obtenemos cuantitativamente al tomar los datos experimentales de Tonomura et al. [63, 64, 65] y un paquete de ondas incidente gaussiano no son restrictivos a este caso. Analizamos también de manera cualitativa el operador de dispersión en el límite de altas velocidades con la presencia de un obstáculo general que es una unión finita de cuerpos con asas. En este caso, el paquete de ondas incidente tiene la única restricción de que en el límite a altas velocidades, en el cual el electrón sigue la trayectoria clásica, este mismo no choque con el obstáculo.

- En el caso de un obstáculo general dado por una unión finita de cuerpos con asas, y en el límite de altas velocidades, el operador de dispersión es un operador de multiplicación por un número complejo constante unitario sobre los electrones que pasan por un mismo agujero; la fase de este número complejo está dada por el flujo del campo magnético sobre cierta sección transversal del obstáculo. Esto nos permite saber la localización de los agujeros a través de experiencias de dispersión. Lo que hace posible recuperar cierta información de la topología del obstáculo.

- Obtenemos también, en el caso de un obstáculo general, información de la clase de cohomología de de Rham del potencial magnético. De esta forma, concluimos que el potencial magnético tiene un significado físico y, además, se demuestran los efectos topológicos sobre la dispersión de los electrones.

- Damos una caracterización de las cantidades físicas asociadas al potencial magnético que son fundamentales para la física cuántica; éstas están dadas por los flujos módulo 2π del potencial magnético sobre los elementos de una base de la homología singular con coeficientes enteros del complemento del obstáculo.

Capítulo 6

Perspectivas a Futuro

En este capítulo se plantean problemas abiertos en los que el autor de esta tesis, en colaboración con el doctor Ricardo Weder, tenemos resultados parciales. Estos problemas plantean resolver cuestiones físicas inconclusas relacionadas con el efecto Aharonov-Bohm, como lo son los efectos relativistas y de spin, y las diferencias entre el caso bidimensional y tridimensional.

6.1. El Efecto Aharonov-Bohm en 2 Dimensiones

Se ha hecho una cantidad numerosa de trabajos desde el punto de vista experimental y teórico relativo al efecto Aharonov-Bohm en 2 dimensiones. En el famoso artículo de Aharonov y Bohm [2] se estudia el caso bidimensional como una simplificación del caso tridimensional. Ellos usan un solenoide recto infinito como aproximación de un solenoide recto muy largo; esto es lo que les permite reducir el problema tridimensional a uno bidimensional. En [76] Weder estudia el caso bidimensional para un campo magnético incluido en un cilindro infinito de sección transversal arbitraria, con los métodos dependientes del tiempo que se utiliza en esta tesis.

Sin embargo, es claro que las propiedades topológicas del complemento del solenoide cambian de manera radical al cambiar un solenoide finito por uno infinito, y el efecto Aharonov-Bohm es de cierta manera un efecto topológico. Se hicieron experimentos con solenoides finitos rectos, pero todos fueron criticados por la imposibilidad de confinar el campo magnético dentro de ellos.

Hay diferencias fundamentales entre el caso tridimensional y el caso bidimensional. Estas diferencias hacen físicamente incorrecto suponer que el problema tridimensional se pueda reducir al caso bidimensional. Una de ellas es que no existen potenciales magnéticos de rango corto asociados al solenoide (ver, por ejemplo, [76]). Es, en consecuencia, interesante estudiar el caso bidimensional y analizar estas diferencias fundamentales que impiden modelar el fenómeno físico en dos dimensiones.

6.2. El Efecto Aharonov-Bohm y las Ecuaciónes de Klein-Gordon y de Dirac

En [4] se obtiene el límite de grandes velocidades del operador de dispersión y se proporcionan cotas de error que tienen la forma de una constante sobre el módulo de la velocidad. La constante involucrada depende de las propiedades de la función de onda y puede ser grande. La velocidad de las partículas no puede ser más grande que la velocidad de la luz, por los postulados básicos de la teoría de la relatividad, de suerte puede ser que se deba tomar una velocidad demasiado grande para que el cociente de la constante entre la velocidad que aparece en las cotas de error sea pequeño. Como se demuestra en el artículo [5] esto no sucede en el caso de los experimentos de Tonomura et al. De todas maneras, este argumento muestra es de interés considerar efectos relativísticos. Para considerar estos efectos, es necesario aplicar modelos relativistas. La ecuación de Klein-Gordon modela partículas cuánticas relativistas con spin cero y la de Dirac partículas con espín 1/2. Por medio de estas ecuaciones podemos resolver el problema que estamos planteando, lo cual se apoya en el siguiente argumento:

Usando la ecuación de Klein-Gordon y la de Dirac esperamos obtener cotas de error de la forma $\frac{C}{v}$, pero ahora, a diferencia del caso de la ecuación de Schrödinger, v no representa la velocidad. La velocidad de las partículas (en el límite de altas energías) es $c\frac{v}{\sqrt{c^2+v^2}}$, en donde c es la velocidad de la luz. Entonces podemos hacer tender v a infinito (y, por lo tanto, la cota de error tiende a cero), manteniendo la velocidad de las partículas acotada por la velocidad de la luz.

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Capítulo 7

The Aharonov-Bohm Effect and Tonomura et al. Experiments. Rigorous Results

En este capítulo se presenta el artículo [5].

The Aharonov-Bohm Effect and Tonomura et al. Experiments. Rigorous Results *†

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Abstract

The Aharonov-Bohm effect is a fundamental issue in physics. It describes the physically important electromagnetic quantities in quantum mechanics. Its experimental verification constitutes a test of the theory of quantum mechanics itself. The remarkable experiments of Tonomura et al. are widely considered as the only experimental evidence of the physical existence of the Aharonov-Bohm effect. Here we give the first rigorous proof that the classical Ansatz of Aharonov and Bohm of 1959 , that was tested by Tonomura et al., is a good approximation to the exact solution to the Schrödinger equation. This also proves that the electron, that is represented by the exact solution, is not accelerated, in agreement with the recent experiment of Caprez et al. in 2007, that shows that the results of the Tonomura et al. experiments can not be explained by the action of a force. Under the assumption that the incoming free electron is a gaussian wave packet, we estimate the exact solution to the Schrödinger equation for all times. We provide a rigorous, quantitative error bound for the difference in norm between the exact solution and the Aharonov-Bohm Ansatz. Our bound is uniform in time. We also prove that on the gaussian asymptotic state the scattering operator is given by a constant phase shift, up to a quantitative error bound that we provide. Our results show that for intermediate size electron wave packets, smaller than the ones used in the Tonomura et al. experiments, quantum mechanics predicts the results observed by Tonomura et al. with an error bound smaller than 10^{-99}. It would be quite interesting to perform experiments with electron wave packets of intermediate size. Furthermore, we provide a physical interpretation of our error bound.

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1 Introduction

In classical electrodynamics the force produced by a magnetic field on a charged particle is given by the Lorentz force, $F = q\mathbf{v} \times B$, where q and $\mathbf{v}$ are, respectively, the charge and the velocity of the particle, and B is the magnetic field. In regions where the magnetic field is zero the Lorentz force is zero and the particle travels in a straight line. In particular, the dynamics of a classical particle is unaffected by magnetic fields enclosed in regions that are not accessible to the particle. This also means that in classical electrodynamics the relevant physical quantity is the magnetic field and that the magnetic potentials are only a convenient mathematical tool.

The situation is different in quantum mechanics, where the dynamics is described by the Schrödinger equation that can not be formulated directly in terms of the magnetic field. It is required to introduce the magnetic potential. It was pointed out by Aharonov and Bohm [2] that this implies that in quantum mechanics the magnetic potentials have a real physical significance. Aharonov and Bohm [2] proposed an experiment to confirm the theoretical prediction. They suggested to use a thin, straight solenoid, centered at the origin and with axis in the vertical direction. They supposed that the magnetic field was essentially confined to the solenoid. They advised to employ a coherent electron wave packet that splits in two parts, each one going trough one side of the solenoid. Both wave packets should be brought together behind the solenoid, to create an interference pattern due to the difference in phase in the wave function of each part of the wave packet, produced by the magnetic field enclosed inside the solenoid. Actually, the existence of this interference pattern was first predicted by Franz [9]. The Aharonov-Bohm effect plays a prominent role in fundamental physics, among other reasons, because it describes the physically important electromagnetic quantities in quantum mechanics, and since it is a quantum mechanical effect, the verification of its existence constitutes a test of the validity of the theory of quantum mechanics itself.

The case of a solenoid has been extensively studied from the theoretical and experimental points of view. The theoretical analysis is reduced to a two dimensional problem after making the assumption that the solenoid is infinite. Nevertheless, experimentally it is impossible to have an infinite solenoid and, therefore, the magnetic field can not be completely confined into the solenoid. The leakage of the magnetic field was a highly controversial point. To avoid this problem it was suggested to use a toroidal magnet, that can contain a magnetic field inside without a leak. The experiments with toroidal magnets where carried over by Tonomura et al. [17, 25, 26]. In remarkable experiments they were able to superimpose behind the magnet an electron wave packet that traveled inside the hole of the magnet with another electron wave packet that traveled outside the magnet, and they measured the phase shift produced by the magnetic flux enclosed in the magnet, giving a strong evidence of the existence of the Aharonov-Bohm effect. In fact, the Tonomura et al. experiments [17, 25, 26] are widely considered as the only experimental evidence of the existence of the Aharonov-Bohm effect.

In the case of toroidal magnets, several Ansätze have been provided for the solution to the Schrödinger equation and for the scattering matrix without giving error bound estimates for the difference, respectively, between the exact solution and the exact scattering matrix, and the Ansätze. Most of these works are qualitative, although some of them give numerical values for their Ansätze. Methods like, Fraunhöfer diffraction, first-order Born and high-energy approximations, Feynman path integrals and the Kirchhoff method in optics were used to propose the Ansätze. The amount of work related to the Aharonov-Bohm effect is very large. For a review of the literature up to 1989 see [15] and [18]. In particular, in [18] there is a detailed discussion of the large controversy -involving over three hundred papers- concerning the existence of the Aharonov-Bohm effect. For a recent update of this controversy see [23, 27].

The paper [4] presents a discussion of a version of the Aharonov-Bohm Ansatz for an infinite solenoid. For recent rigorous work in the case of an infinite solenoid see [14, 28] where, among other results, it is proven that in the high-velocity limit the scattering operator is given by a constant phase shift, as predicted by Franz [9] and Aharonov and Bohm [2]. In [16] rigorous mathematical ground is given for the presence of the magnetic potential in the Schrödinger operator describing the Aharonov-Bohm effect in the case of a solenoid. In [11], a semi-classical analysis of the Aharonov-Bohm effect in bound-states in two dimensions is given. For a rigorous mathematical analysis of the Aharonov-Bohm effect in three dimensions for toroidal magnets -actually in the general case of handle bodies- see [3], where the high-velocity limit of the scattering operator was evaluated in the case where the direction of the velocity is kept fixed as its absolute value goes to infinity. A rigorous error bound was given for the difference between the scattering operator and its high-velocity limit for incoming asymptotic states that have small interaction with the magnet in the high-velocity limit. The error bound goes to zero as the inverse of the velocity. A detailed analysis of the Aharonov-Bohm effect in the case of the Tonomura et al. experiments [17, 25, 26] was given in [3], as well as other results. The results of [3] give a rigorous qualitative proof that quantum mechanics predicts the interference patterns observed in the Tonomura et al. experiments [25, 26, 17] with toroidal magnets. The papers [3, 14, 28], as well as this paper, use the method introduced in [8] to estimate the high-velocity limit of solutions to Schrödinger equations and of the scattering operator. The papers [21], [22], [29], and [30] study the scattering matrix for potentials of Aharonov-Bohm type in the whole space.

In this paper we give the first rigorous proof that the classical Ansatz of Aharonov and Bohm is a good approximation to the exact solution of the Schrödinger equation. We provide, for the first time, a rigorous quantitative mathematical analysis of the Aharonov-Bohm effect with toroidal magnets under the conditions of the experiments of Tonomura et al. [17, 25, 26]. We assume that the incoming free electron is a gaussian wave packet, what from the physical point of view is a reasonable assumption. The technical advantage of using a gaussian wave packet for the incoming free electrons is that in this case we know very well the dynamics of the free asymptotic gaussian state, and we can carry over the estimates of [3] in a precise manner. We provide a rigorous, simple, quantitative, error bound for the difference in norm between the exact solution and the approximate solution given by the Aharonov-Bohm Ansatz. Our error bound is uniform in time. We also prove that on the gaussian asymptotic state, the scattering operator is given by multiplication by $e^{i\frac{q}{\hbar c}\tilde{\Phi}}$ -where q is the charge of the electron, c is the speed of light, $\hbar$ is Planck's constant, and $\tilde{\Phi}$ is the magnetic flux in a transversal section of the magnet- up to a quantitative error bound, that we provide.

Actually, the error bound is the same in the cases of the exact solution and the scattering operator.

Aharonov and Bohm [2] and Tonomura et al. [17, 25, 26] suggested to split the electron wave packet into the part that goes through the hole of the magnet and the part that goes outside. Tonomura et al. observed that an image was produced behind the magnet that clearly showed that shadow of the magnet and also the hole and the exterior of the magnet. They concluded [25] that this indicates that there was not interference between the part of the electron wave packet that went trough the hole and the one that either hit the magnet or traveled outside. The part of the wave packet that goes outside the magnet can be taken as the reference wave packet. Therefore, we only model the part of the electron wave packet that goes through the hole of the magnet. Using the experimental data of Tonomura et al. [17, 25, 26] we provide lower and upper bounds on the variance of the gaussian state in order that the electron wave packet actually goes through the hole. We also rigorously prove that the results of the Tonomura et al. experiments [17, 25, 26], that were predicted by Aharonov and Bohm, actually follow from quantum mechanics. Furthermore, our results show that it would be quite interesting to perform experiments for intermediate size electron wave packets (smaller than the ones used in the Tonomura et al. experiments, that where much larger than the magnet) that satisfies appropriate lower and upper bounds that we provide. One could as well take a larger magnet. In this case, the interaction of the electron wave packet with the magnet is negligible -the probability that the electron wave packet interacts with the magnet is smaller than 10^{-199} (See Remark 8.12 and Section 9.2)- and, moreover, quantum mechanics predicts the results observed by Tonomura et al. with an error bound smaller than 10^{-99}, in norm.

Our error bound has a physical interpretation. For small variances, it is due to Heisenberg's uncertainty principle. If the variance in configuration space is small, the variance in momentum space is big, and then, the component of the momentum transversal to the axis of the magnet is large. In consequence, the opening angle of the electron wave packet is large, and there is a large interaction with the magnet. If the variance is large, the opening angle is small, but as the electron wave packet is big we have again a large interaction with the magnet.

It has been claimed that the outcome of the Tonomura et al. experiments [17, 25, 26] can be explained by the action of a force acting on the electron that travels through the hole of the magnet. See, for example, [5, 10] and the references quoted there. Such a force would accelerate the electron and it would produce a time delay. In a recent crucial experiment Caprez et al. [6] found that the time delay is zero, thus experimentally excluding the explanation of the results of the Tonomura et al. experiments by the action of a force. In the Aharonov-Bohm Ansatz the electron is not accelerated, it propagates following the free evolution, with the wave function multiplied by a phase. Since, as mentioned above, we prove that the Aharonov-Bohm Ansatz approximates the exact solution with an error bound uniform in time that can be smaller that 10^{-99} in norm, we rigorously prove that quantum mechanics predicts that no force acts on the electron, in agreement with the experimental results of Caprez et al. [6].

1.1 Tonomura et al. Experiments

The remarkable experiments of Tonomura at al. [17, 25, 26] are widely considered as the only experimental evidence of the physical existence of the Aharonov-Bohm effect. Tonomura et. al. constructed small toroidal magnets such that the magnetic field is practically zero outside them. In [26], the magnets are impenetrable and, furthermore, they are covered by super conductive layers that forbid the leakage of magnetic field outside the magnets. We denote by $\tilde{K} := \{(x_1, x_2, x_3) \in \mathbb{R}^3 : 0 < \tilde{r}_1 \leq (x_1^2 + x_2^2)^{1/2} \leq \tilde{r}_2, |x_3| \leq \tilde{h}\}$ the magnet ($\tilde{r}_1$ is the inner radius, $\tilde{r}_2$ the outer radius and $2\tilde{h}$ is the height), and by $\tilde{B}(x)$ the magnetic field. We suppose that $\tilde{B}(x)$ is zero for x outside the magnet.

An electron wave packet was sent towards the magnet. It was superimposed behind it with a reference electron wave packet to produce the interference pattern. The experiments were set up in such a way that the reference electron wave packet was not influenced by the magnet, and that the electron wave packet and the reference electron wave packet only interfered behind the magnet, were the interference patterns were formed. The observed interference patterns provided a strong evidence of the physical existence of the Aharonov-Bohm effect.

The electron wave packet was much larger than the magnet. It was 3 micrometers in size in the direction of the electron propagation and 20 micrometers in size in a plane perpendicular to the propagation direction [24]. It covered the magnet completely. Recall that it was observed that an image was produced behind the magnet that clearly showed the shadow of the magnet and also the hole and the exterior of the magnet (see [25, 26]) and that it was pointed out by Tonomura et al. [25, 26], that this indicates that there was no interference between the part of the electron wave packet that went through the hole, and the one that either hit the magnet or traveled outside, because of the clear image of the shadow of the magnet [25, 26]. As mentioned before, we will concentrate our analysis on the part of the wave packet that goes through the hole, and we will take it as the electron wave packet itself. It is either the part of the electron wave packet that goes trough the hole, or a smaller electron wave packet that really goes trough the hole.

1.2 Aharonov-Bohm Ansatz for the Exact Solution

At the time of emission, i.e., as $t \to -\infty$, the electron wave packet is far away from the magnet and it does not interact with it, therefore, it can be assumed that it follows the free evolution,

$$i\hbar \frac{\partial}{\partial t}\phi(x,t) = H_0 \phi(x,t), x \in \mathbb{R}^3, t \in \mathbb{R}. \tag{1.1}$$

where H_0 is the free Hamiltonian.

$$H_0 := \frac{1}{2M}\mathbf{P}^2. \tag{1.2}$$

M is the mass of the electron and $\mathbf{P} := -i\hbar\nabla$ is the momentum operator. We represent the emitted electron wave packet by the free evolution of a gaussian wave function, $\varphi_{\mathbf{v}}$, with velocity $\mathbf{v}$,

$$\varphi_{\mathbf{v}} := e^{i\frac{M}{\hbar}\mathbf{v}\cdot x}\,\varphi, \text{ where } \quad \varphi := \frac{1}{(\sigma^2\pi)^{3/4}} e^{-\frac{x^2}{2\sigma^2}}, \tag{1.3}$$

with variance σ smaller than the inner radius of the magnet. We have chosen the variance transverse to the velocity of propagation, $\mathbf{v}$, equal to the longitudinal variance in the direction of propagation. In fact, the size of the longitudinal variance is not essential for our arguments and we have chosen it equal to the transversal variance only for simplicity. Notice that in the momentum representation, $e^{i\frac{M}{\hbar}\mathbf{v}\cdot x}$ is a translation operator by the vector $M\mathbf{v}$, what implies that the wave function (1.3) is centered at the classical momentum $M\mathbf{v}$ in the momentum representation,

$$\hat{\varphi}_{\mathbf{v}}(p) = \hat{\varphi}(p - M\mathbf{v}),$$

where for any state represented by the wave function $\phi(x)$ in the configuration representation, the momentum representation is given by the Fourier transform,

$$\hat{\phi}(p) := \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbb{R}^3} e^{-i\frac{p}{\hbar}\cdot x}\,\phi(x)\,dx.$$

By the previous analysis, the electron wave packet is represented at the time of emission by the following gaussian wave packet that is a solution to the free Schrödinger equation (1.1)

$$\psi_{\mathbf{v},0}(x,t) := e^{-i\frac{t}{\hbar}H_0}\,\varphi_{\mathbf{v}}(x). \tag{1.4}$$

The (exact) electron wave packet, $\psi_{\mathbf{v}}(x,t)$, satisfies the interacting Schrödinger equation for all times,

$$i\hbar\frac{\partial}{\partial t}\psi_{\mathbf{v}}(x,t) = H\psi_{\mathbf{v}}(x,t), x \in \Lambda := \mathbb{R}^3 \setminus \tilde{K}, t \in \mathbb{R}, \tag{1.5}$$

where

$$H := H(A) := \frac{1}{2M}(\mathbf{P} - \hbar A)^2 \tag{1.6}$$

is the Hamiltonian and $A = \frac{q}{\hbar c}\tilde{A}$, where c is the speed of light, q is the charge of the electron, $\hbar$ is Plank's constant, and $\tilde{A}$ is a magnetic potential with curl$\tilde{A} = \tilde{B}$ where $\tilde{B}$ is the magnetic field. We define the Hamiltonian (1.6) in $L^2(\Lambda)$ with Dirichlet boundary condition at $\partial\Lambda$, i.e. $\psi = 0$ for $x \in \partial\Lambda$. This is the standard boundary condition that corresponds to an impenetrable magnet. It implies that the probability that the electron is at the boundary of the magnet is zero. Note that the Dirichlet boundary condition is invariant under gauge transformations. In the case of the impenetrable magnet the existence of the Aharonov-Bohm effect is more striking, because in this situation there is zero interaction of the electron with the magnetic field inside the magnet. Note, however, that once a magnetic potential is chosen the particular self-adjoint boundary condition taken at $\partial\Lambda$ does not play an essential role in our calculations. Furthermore, our results hold also for a penetrable magnet where the interacting Schrödinger equation (1.5) is defined in all space. Actually, this later case is slightly simpler because we do not need to work with two Hilbert spaces, $L^2(\mathbb{R}^3)$ for the free evolution, and $L^2(\Lambda)$ for the interacting evolution, what simplifies the proofs. In consequence, the electron wave packet is the unique solution, $\psi_{\mathbf{v}}$, to the interacting Schrödinger equation (1.5) that is asymptotic to the free gaussian wave packet, $\psi_{\mathbf{v},0}$, as $t \to -\infty$,

$$\psi_{\mathbf{v}}(x,t) \approx \psi_{\mathbf{v},0}(x,t), \quad t \to -\infty. \tag{1.7}$$

Aharonov and Bohm [2] proposed an approximate solution to the Schrödinger equation over simply connected regions (regions with no holes) where the magnetic field is zero, by a change of gauge formula from the zero vector potential. Of course, it is not possible to have a gauge transformation from the zero potential everywhere because that would imply that the magnetic flux on a transversal section of the magnet would be zero. Hence, the gauge transformation has to be discontinuous somewhere. As mentioned in Section 1.1, in the case of Tonomura et al. [17, 25, 26] experiments the magnet is a cylindrical torus, $\tilde{K}$.

We take as the surface of discontinuity of the gauge transformation

$$\mathcal{S} := \{(x_1, x_2, x_3) \in \mathbb{R}^3 : (x_1^2 + x_2^2)^{1/2} > \tilde{r}_2, x_3 = 0\}$$

and we define the gauge transformation in the domain, $\mathcal{D}$, given by

$$\mathcal{D} := \Lambda \setminus \mathcal{S}.$$

Without loss of generality we can suppose that the support of A is contained on the convex hull of $\tilde{K}$ (see Section 7.1). For every $x \in \mathcal{D}$, and a fixed point x_0 in $\mathcal{D}$ with vertical component less than $-\tilde{h}$, we define the gauge transformation as follows,

$$\lambda_{A,0}(x) := \int_{x_0}^{x} A,$$

where the integral is over a path in $\mathcal{D}$. Note that for any $x \in \mathcal{D}$ with $x_3 > 0$ the integration contour has to go necessarily through the hole of the magnet.

For any solution to the Schrödinger equation (1.5), $\phi(x,t)$, that stays in $\mathcal{D}$, Aharonov and Bohm [2] propose that the solution is given by the following Ansatz, motivated by the change of gauge formula from the zero vector potential,

$$\phi_{AB}(x,t) := e^{i\lambda_{A,0}(x)} e^{-i\frac{t}{\hbar}H_0} e^{-i\lambda_{A,0}(x)}\, \phi(x,0). \tag{1.8}$$

Note that if the initial state at $t = 0$ is taken as $e^{-i\lambda_{A,0}(x)}\, \phi(x,0)$ the Aharonov-Bohm Ansatz is the multiplication of the free solution by the Dirac magnetic factor $e^{i\lambda_{A,0}(x)}$ [7].

The Aharonov-Bohm Ansatz is expected to be a good approximation to the exact solution if the electron wave packet stays in a connected domain, away from the surface $\mathcal{S}$ where the gauge transformation is discontinuous. This Aharonov-Bohm Ansatz is valid for solutions whose initial data is given at time equal to zero.

For the incoming electron wave packet that satisfies (1.7) the initial data is given as time tends to $-\infty$ and then, the Aharonov-Bohm Ansatz has to be modified. To formulate the appropriate Ansatz we define the wave operators,

$$W_{\pm}(A) := W_{\pm} := \text{s-}\lim_{t \to \pm\infty} e^{i\frac{t}{\hbar}H(A)}\, J\, e^{-i\frac{t}{\hbar}H_0}.$$

where J is the identification operator from $L^2(\mathbb{R}^3)$ into $L^2(\Lambda)$ given by multiplication by the characteristic function of Λ, i.e., $J\phi(x) := \chi_\Lambda(x)\,\phi(x)$ where, $\chi_\Lambda(x) = 1, x \in \Lambda, \chi_\Lambda(x) = 0, x \in \mathbb{R}^3 \setminus \Lambda$. It is proved in [3] that the strong limits exist and that we can replace the operator J by the operator of multiplication by any smooth characteristic cutoff function $\chi(x) \in C^\infty$ such that $\chi(x) = 0, x \in \tilde{K}$ and $\chi(x) = 1$ for x in the complement of a bounded set that contains $\tilde{K}$ on its interior.

The solution to the Schrödinger equation that is asymptotic to the free solution $e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}}$ as $t \to -\infty$ is given by

$$\psi_{\mathbf{v}} := e^{-i\frac{t}{\hbar}H(A)}\, W_- \varphi_{\mathbf{v}}. \tag{1.9}$$

It satisfies,

$$\lim_{t \to -\infty} \|\psi_{\mathbf{v}} - J\,\psi_{\mathbf{v},0}\| = 0. \tag{1.10}$$

Using this fact we prove in Section 7 that the Aharonov-Bohm Ansatz for the exact solution to the Schrödinger equation (1.5) with initial data as time tends to $-\infty$ is given by,

$$\psi_{AB,\mathbf{v}}(x,t) = e^{i\lambda_{A,0}(x)} e^{-i\frac{t}{\hbar}H_0} \varphi_{\mathbf{v}}, \tag{1.11}$$

what, again, is the multiplication of the free incoming solution by the Dirac magnetic factor $e^{i\lambda_{A,0}(x)}$ [7].

It is expected that if the electron wave packet stays in a connected region of space, away from the surface of discontinuity $\mathcal{S}$, the Aharonov-Bohm Ansazt should be a good approximation to the exact solution, i.e., that,

$$\psi_{\mathbf{v}} \approx \psi_{AB,\mathbf{v}}. \tag{1.12}$$

The Aharonov-Bohm Ansatz, $\psi_{AB,\mathbf{v}}$, is what is observed in the Tonomura et. al. experiments [17, 25, 26]: as the support of the vector potential A is contained in the convex hull of $\tilde{K}$, for every x whose vertical component is bigger than $\tilde{h}$, $\lambda_{A,0}(x)$ is equal to the constant $\frac{q}{\hbar c}\tilde{\Phi}$, where $\tilde{\Phi}$ is the flux of the magnetic field over a transverse section of the magnet. Then, for $x_3 > \tilde{h}$, the Aharonov-Bohm Ansatz is given by

$$\psi_{AB,\mathbf{v}}(x) = e^{i\frac{q}{\hbar c}\tilde{\Phi}} e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}}, \quad x_3 > \tilde{h}. \tag{1.13}$$

This is exactly what it was observed in the Tonomura et al. experiments [17, 25, 26].

The scattering operator is defined as

$$S := W_+^* W_-.$$

For large positive times, when the exact electron wave packet is far away from the magnet, and it is localized in the region with large positive x_3, it can be again approximated with an outgoing solution to the free Schrödinger equation,

$$\psi_{+,\mathbf{v},0} := e^{-i\frac{t}{\hbar}H_0}\varphi_{+,\mathbf{v}}, \tag{1.14}$$

such that,

$$\lim_{t\to\infty} \|\psi_{\mathbf{v}} - J\,\psi_{+,\mathbf{v},0}\| = 0. \tag{1.15}$$

The initial data of the incoming and the outgoing solutions to the free Schrödinger equation are related by the scattering operator (see Section 3.1),

$$\varphi_{+,\mathbf{v}} = S\varphi_{\mathbf{v}}. \tag{1.16}$$

By equations (1.10) and (1.12-1.16) the Aharonov-Bohm Ansatz suggests that

$$\varphi_{+,\mathbf{v}} = S\varphi_{\mathbf{v}} \approx e^{i\frac{q}{\hbar c}\tilde{\Phi}}\,\varphi_{\mathbf{v}}, \tag{1.17}$$

i.e., that on the gaussian asymptotic state, $\varphi_{\mathbf{v}}$, the scattering operator is given by multiplication by $e^{i\frac{q}{\hbar c}\tilde{\Phi}}$, to a good approximation. This also is precisely what was observed in the Tonomura et al. experiments [17, 25, 26]. Furthermore, in the Aharonov-Bohm Ansatz (1.11) the electron is not accelerated, it propagates along the free evolution, with the wave function multiplied by a phase. This implies that in the Aharonov-Bohm Ansatz no force acts on the electron, and hence, it is not accelerated. This is precisely what was observed in the Caprez et al. [6] experiments.

1.3 The Main Results

As under the free evolution the electron wave packet is concentrated along the classical trajectory, we can expect that if the velocity $\mathbf{v}$ -that is directed along the positive vertical axis- is large enough, the exact electron wave packet will keep away, for all times, from the surface, $\mathcal{S}$, where the gauge transformation is discontinuous. In consequence, the Aharonov-Bohm Ansatz should be a good approximation, and equations (1.12) and (1.17) should hold. In the following theorem (see also Theorem 8.10) we prove that this is true under the conditions of the Tonomura et al. experiments [17, 25, 26], provided that appropriate, quantitative, lower and upper bounds on the variance, σ, of the gaussian wave function are satisfied. The requirement for the variance σ to lie within the interval below assures that interaction of the electron with the magnet and the surface $\mathcal{S}$ is small.

THEOREM 1.1. *Aharonov-Bohm Ansatz, Scattering Operator and Tonomura et al. Experiments*

Suppose that the magnets and energies are the ones of the experiments of Tonomura et al.. Then, for every gaussian wave function, φ, with variance $\sigma \in [\frac{4.5}{mv}, \frac{\tilde{r}_1}{2}]$ and every $t \in \mathbb{R}$, the solution to the Schrödinger equation, $e^{-i\frac{t}{\hbar}H(A)}\, W_-\, \varphi_{\mathbf{v}}$, that behaves as $e^{-i\frac{t}{\hbar}H_0}\, \varphi_{\mathbf{v}}$ as $t \to -\infty$ is given at the time t by

$$\psi_{AB,\mathbf{v}} := e^{i\lambda_{A,0}(x)} e^{-i\frac{t}{\hbar}H_0} \varphi_{\mathbf{v}}, \tag{1.18}$$

up to the following error,

$$\begin{aligned} &\| e^{-i\frac{t}{\hbar}H} W_-(A) \varphi_{\mathbf{v}} - e^{i\lambda_{A,0}} e^{-i\frac{t}{\hbar}H_0} \varphi_{\mathbf{v}} \| \leq \\ &7 e^{-\frac{r_1^2}{2\sigma^2}} + 177 \times 10^3 e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} + 10^{-100}, \end{aligned} \tag{1.19}$$

where, $m := M/\hbar$. Furthermore, the scattering operator satisfies

$$\begin{aligned} &\| S\, \varphi_{\mathbf{v}} - e^{i\frac{q}{\hbar c}\tilde{\Phi}} \varphi_{\mathbf{v}} \| \leq \\ &7 e^{-\frac{r_1^2}{2\sigma^2}} + 177 \times 10^3 e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} + 10^{-100}. \end{aligned} \tag{1.20}$$

The main factors that produce the error bound in equation (1.19, 1.20) are the terms,

- Size of the electron wave packet factor,

$$e^{-\frac{r_1^2}{2\sigma^2}}. \tag{1.21}$$

- Opening angle of the electron wave packet factor,

$$e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}}. \tag{1.22}$$

When the variance σ is close to the inner radius of the magnet (the electron wave packet is big), (1.21) is close to 1 and (1.22) is extremely small (because in this case $\sigma m v$ is big). Then, when the electron wave packet is big compared to the inner radius, (1.21) is the important term, what justifies our name. When the variance is small (such that $\sigma m v$ is close to 1) the factor (1.22) is close to one and (1.21) is extremely small ($\frac{r_1}{\sigma}$ is big) and so, the important factor is (1.22). Note that when the variance in position, σ, is small, by Heisenberg uncertainly principle the variance in momentum is big. In particular, the transversal component of momentum is large and the electron wave packet spreads a lot as it propagates, what makes the opening angle of the electron wave packet large . This justifies the name that we give to (1.22). Note that in both cases the part of the electron wave packet that hits the obstacle is big. When σ is big, because the wave packet is big, and when σ is small, because the opening angle is big, and even if the wave packet was initially small, it spreads rapidly as it propagates inside the magnet and, in consequence, a large part of the wave packet hits the obstacle. For variances, σ, that are neither to small nor too big the part of the electron wave packet that hits the obstacle is small and the error is very small. In Section 9 we discuss in detail the physical interpretation of our error bound and we present a detailed quantitative analysis for a large range of σ.

In particular, we give a rigorous proof that if $1.1592 \times 10^{-9} \leq \sigma \leq 7.7955 \times 10^{-6}$ the error bound is smaller than 10^{-99}. As mentioned above, it would be quite interesting to perform an experiment with electron wave packets that satisfy our bounds. One could as well take a larger magnet. In this case the probability that the electron wave packet interacts with the magnet is smaller than 10^{-199} (See Remark 8.12 and Section 9.2), and quantum mechanics predicts with a very small error bound the interference fringes observed in the experiments of Tonomura et al. [17, 25, 26], and the absence of a force on the electron, as observed in the Caprez et al. experiment [6].

The paper is organized as follows. In Section 2 we introduce notations and definitions that we use along the paper. In Section 3 we study the time evolution of the electron wave packet. We define the wave and the scattering operators, and we introduce the solutions to the Schrödinger equation with initial condition as time goes to $-\infty$. We estimate the solution to the Schrödinger equation when it is incoming, interacting, and outgoing. In Section 4 we use the freedom that we have in the selection of the magnetic field, the magnetic potential and the smooth characteristic cutoff function to make a choice that is convenient for the computation of the error bounds. In Section 5 we make a choice of the free parameters under the experimental conditions of Tonomura et al. [17]. In Section 6 we continue our study of the time evolution of the electron wave packet when it is incoming, interacting, and outgoing. In Section 7 we consider the Aharonov-Bohm Ansatz for initial data at time zero and for initial data at time $-\infty$. In Section 8 we estimate the difference between the exact solution to the Schrödinger equation and the Aharonov-Bohm Ansatz as the electron is incoming, interacting, and outgoing. In particular, in Theorem 8.11 we prove our main result that is quoted as Theorem 1.1 in the Introduction. In Section 9 give a detailed analysis of the physical interpretation of our error bound with quantitative results. In Section 10 we give the conclusions of our paper. In appendix A we prove estimates for the free evolution of gaussian states that we use in our work. In Appendix B we prove upper bounds for integrals that we need to compute our error bound.

2 Notations and Definitions

In this section we collect notations and definitions that are used along the paper.

The magnet $\tilde{K}$ - see Section 1.1 - is defined by the following formula,

$$\tilde{K} := \left\{ (x_1, x_2, x_3) \in \mathbb{R}^3 : 0 < \tilde{r}_1 \leq (x_1^2 + x_2^2)^{1/2} \leq \tilde{r}_2, |x_3| \leq \tilde{h} \right\}. \tag{2.1}$$

We call $\tilde{D}$ the convex hull of $\tilde{K}$. We use the notation,

$$\Lambda := \mathbb{R}^3 \setminus \tilde{K}. \tag{2.2}$$

We employ the symbol $\chi = \chi(x) = \chi(x,\sigma)$ for a twice continuously differentiable cut-off function that depends on the variance of the wave packet, σ, - see (1.3). The support of $1-\chi$ is contained in the set

$$K := K(\sigma) := \left\{(x_1,x_2,x_3) \in \mathbb{R}^3 : 0 < r_1 \leq (x_1^2+x_2^2)^{1/2} \leq r_2, |x_3| \leq h(\sigma)\right\}, \tag{2.3}$$

where r_1 and r_2 are some positive numbers such that $r_1 < \tilde{r}_1$, $r_2 > \tilde{r}_2$, $\tilde{r}_1 - r_1 = r_2 - \tilde{r}_2$ and $h = h(\sigma) : \mathbb{R}_+ \to \mathbb{R}_+$ is an increasing function such that $h(\sigma) > \tilde{h}$ for all σ in $\mathbb{R}_+$. We will write either h or $h(\sigma)$ for the same object.
We designate by

$$\epsilon := \tilde{r}_1 - r_1 = r_2 - \tilde{r}_2, \quad \delta(\sigma) := \delta := h(\sigma) - \tilde{h}, \tag{2.4}$$

and by $D := D(\sigma)$ the convex hull of K.

For every $\zeta,\ \tilde{\omega},\ \sigma \in \mathbb{R}_+$ such that $0 < \tilde{\omega}^{-1} < \sigma m v$, we denote by $z_{\tilde{\omega},\sigma}(\zeta)$ the unique solution of the equation,

$$(z_{\tilde{\omega},\sigma}(\zeta) - \zeta)\frac{\sigma m v}{(\sigma^4 m^2 v^2 + z_{\tilde{\omega},\sigma}(\zeta)^2)^{1/2}} = \tilde{\omega}^{-1}, \tag{2.5}$$

and for every $\sigma_1, \sigma_2 \in (0, r_1)$ (see (2.3)) we define

$$z_{\tilde{\omega},\sigma_1,\sigma_2}(\zeta) := \max(z_{\tilde{\omega},\sigma_1}(\zeta), z_{\tilde{\omega},\sigma_2}(\zeta)), \quad r_{\sigma_1,\sigma_2} := \min_{i\in\{1,2\}}\{\lambda > 0 : \frac{(r_1\sigma_i m v)^2}{\sigma_i^4(mv)^2 + \lambda^2} = 1\}. \tag{2.6}$$

For every $\sigma \in \mathbb{R}_+$, we define

$$\tilde{\omega}(\sigma) := \frac{1}{\min\left(\sqrt{\frac{33}{34}}\,\sigma m v, \sqrt{2000}\right)}, \quad z(\sigma) := z_{\tilde{\omega}(\sigma),\sigma}(h(\sigma)), \quad \sigma_0 := \sqrt{\frac{34}{33}}\,\frac{\sqrt{2000}}{mv}. \tag{2.7}$$

Note that (see equation (11.23) in Appendix A)

$$z(\sigma) > h(\sigma). \tag{2.8}$$

For every $\sigma \in \mathbb{R}_+$ and every $z, \zeta, s \in \mathbb{R}$ we use the following notation,

$$\rho = \rho(z) = \rho(\sigma, z) := \frac{\sigma m v}{(\sigma^4 m^2 v^2 + z^2)^{1/2}}, \tag{2.9}$$

$$\theta_{inv}(\sigma,z,s,\zeta) := (\zeta - s)\frac{\sigma m v}{(\sigma^4 m^2 v^2 + z^2)^{1/2}},\ \ \theta_{inv}(\sigma,z) := \theta_{inv}(\sigma,z,z,h(\sigma)), \tag{2.10}$$

and

$$\Upsilon(\sigma,z,s,\zeta) := \int_{\theta_{inv}(\sigma,z,s,-\zeta)}^{\theta_{inv}(\sigma,z,z,\zeta)} e^{-\tau^2}\,d\tau, \quad \Upsilon(\sigma,z) := \Upsilon(\sigma,z,z,h(\sigma)), \tag{2.11}$$

$$\Theta(\sigma,z,s,\zeta) := \int_{\theta_{inv}(\sigma,z,s,-\zeta)}^{\theta_{inv}(\sigma,z,z,\zeta)} \tau^2\, e^{-\tau^2}\,d\tau, \quad \Theta(\sigma,z) := \Theta(\sigma,z,z,h(\sigma)). \tag{2.12}$$

We utilize the symbols $\hbar$, c, M and q for the Planck constant, the speed of light and the mass and charge of the electron, respectively. We define,

$$m := \frac{M}{\hbar}.$$

We denote by $\mathbf{v} \in \mathbb{R}^3$ the velocity - see (1.3) - and we designate by $v := |\mathbf{v}|$, and $\hat{\mathbf{v}} := \mathbf{v}/v$, respectively, the modulus and the direction of the velocity. We suppose that $\hat{\mathbf{v}} = (0,0,1)$. We designate by $\mathbf{p} := -i\nabla_x$. The momentum operator is $\mathbf{P} := \hbar\mathbf{p}$.

We use the letters $\tilde{B}$ and $\tilde{A}$ for the magnetic field and the magnetic potential, respectively. The details of the distribution of the magnetic field inside $\tilde{K}$ are not relevant for the dynamics of the electron that propagates outside $\tilde{K}$, as long as $\tilde{B}$ is contained inside $\tilde{K}$. Actually, what is relevant is the flux of $\tilde{B}$ along a transversal section of $\tilde{K}$ modulo 2π. See [3] for this issue. We use this freedom to choose $\tilde{B}$ and $\tilde{A}$ in a technically convenient way Then, unless we specify something else, we assume that the support of $\tilde{B}$ is contained in $\tilde{K}$, that the support of $\tilde{A}$ is contained in the convex hull of $\tilde{K}$ (what is always possible), and that both are continuously differentiable. In Section 4, for any given flux in the transversal section of the magnet we explicitly construct a magnetic field and a magnetic potential that satisfy our assumptions. We define $A := \frac{q}{\hbar c}\tilde{A}$, $B := \frac{q}{\hbar c}\tilde{B}$, and

$$\eta(x,\tau) := \int_0^\tau (\hat{\mathbf{v}} \times B)(x + \rho\hat{\mathbf{v}})\, d\rho. \tag{2.13}$$

We denote by $\tilde{\Phi}$ the flux of the magnetic field $\tilde{B}$ over a transversal section (TS) of the magnet,

$$\tilde{\Phi} := \int_{\mathrm{T}S} \tilde{B}. \tag{2.14}$$

Then, the flux of B over a transversal section of the magnet is given by,

$$\Phi := \int_{\mathrm{T}S} B = \frac{q}{\hbar c}\tilde{\Phi}. \tag{2.15}$$

By Stokes theorem, for every $x = (x_1, x_2, x_3) \in \mathbb{R}^3$ such that $\sqrt{x_1^2 + x_2^2} \leq \tilde{r}_1$ we have that,

$$\tilde{\Phi} = \int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot \tilde{A}(x + \tau\hat{\mathbf{v}})d\tau, \quad \Phi = \int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(x + \tau\hat{\mathbf{v}})d\tau. \tag{2.16}$$

Given a function F with domain $\mathcal{D} \subset \mathbb{R}^n, n = 1, 2, \cdots$ that takes values on a normed space $\tilde{C}$ with norm $\|\cdot\|$, we denote by $\|F\|_\infty :=$ ess sup$\{\|f(x)\| : x \in \mathcal{D}\}$.

The vector $\bar{M} = \bar{M}(\chi, A, \mathbf{v}) = (M_1(\chi, A, \mathbf{v}), \cdots, M_5(\chi, A, \mathbf{v})) := (M_1, \cdots, M_5) \in \mathbb{R}^5$ is given by ($\mathbf{v}$ and A and χ are defined above in this section),

$$
\begin{aligned}
&M_1 := \|\mathbf{p}^2\chi\|_\infty + \|\chi\mathbf{p}\cdot A\|_\infty + \|2(\mathbf{p}\chi)\cdot A\|_\infty + \|\chi A^2\|_\infty,\\
&M_2 := \|2(\mathbf{p}\chi)\|_\infty + \|2\chi A\|_\infty,\\
&M_3 = \|(\mathbf{p}\chi)\cdot\hat{v}\|_\infty + \|\chi A\cdot\hat{v}\|_\infty,\\
&M_4 := \|\chi(x)(\mathbf{p}\cdot A)(x+t\hat{v})\|_\infty + \|\chi(x)A^2(x+t\hat{v})\|_\infty + 2\|A(x+t\hat{v})\cdot(\mathbf{p}\chi)(x)\|_\infty + 2\|\chi(x)A(x+t\hat{v}))\cdot\eta(x,t)\|_\infty,\\
&M_5 := 2\|\chi(x)A(x+t\hat{v})\|_\infty.
\end{aligned}
\tag{2.17}
$$

The norms in M_4 and M_5 are taken with respect to $x\in\mathbb{R}^3$ and $t\in\mathbb{R}$.

We define the linear function $\mathcal{A}:\mathbb{R}^5\to\mathbb{R}^5$ by the following: given a vector $w := (w_1,\cdots w_5)\in\mathbb{R}^5$, we take $\mathcal{A}(w) := (\mathcal{A}(w)_1,\cdots,\mathcal{A}(w)_5)$ as,

$$
\begin{aligned}
&\mathcal{A}(w)_1 := \tfrac{1}{\sqrt{2}mv}w_1 + \sqrt{2}w_3, \quad \mathcal{A}(w)_2 := \tfrac{4}{\pi^{1/4}}[\tfrac{\sqrt{2}}{2mv}w_1 + \tfrac{2+\sqrt{2}}{2}w_2 + \sqrt{2}w_3],\\
&\mathcal{A}(w)_3 := \frac{\frac{1}{\sqrt{2}}+\frac{\sqrt{3}\pi^{1/4}}{2}}{\sqrt{mv}\pi^{1/4}}w_2, \quad \mathcal{A}(w)_4 := \tfrac{1}{\sqrt{2}mv}w_4, \quad \mathcal{A}(w)_5 := \frac{\frac{1}{\sqrt{2}}+\frac{\sqrt{3}\pi^{1/4}}{2}}{\sqrt{mv}\pi^{1/4}}w_5.
\end{aligned}
\tag{2.18}
$$

The symbols used on the formulae below where defined in this section. Given S_1, $v\in\mathbb{R}_+$, $w\in\mathbb{R}^5$ and $j\in\{-\infty,0,\infty\}$, we define the function $\widetilde{\mathbf{A}}^j_{w,v} = \widetilde{\mathbf{A}}^j_w : \mathbb{R}\times\mathbb{R}_+\to\mathbb{R}$ by

$$
\begin{aligned}
&\widetilde{\mathbf{A}}^{-\infty}_w(z,\sigma) = \widetilde{\mathbf{A}}^{-\infty}(z,\sigma) :=\\
&\max(z,S_1)\tfrac{\mathcal{A}(w)_1}{2} + \max(z,S_1)^{-1/2}(hr_2^2(\sigma mv)^3)^{1/2}\tfrac{\mathcal{A}(w)_2}{2} + \tfrac{\max(z,S_1)}{\sigma^{1/2}}\tfrac{\mathcal{A}(w)_3}{2} - z\tfrac{\mathcal{A}(w)_1}{2} - \tfrac{z}{\sigma^{1/2}}\tfrac{\mathcal{A}(w)_3}{2},\\
&\widetilde{\mathbf{A}}^0_w(z,\sigma) = \widetilde{\mathbf{A}}^0(z,\sigma) := \widetilde{\mathbf{A}}^{-\infty}_w(z,\sigma) + z\mathcal{A}(w)_4 + \tfrac{z}{\sigma^{1/2}}\mathcal{A}(w)_5,\\
&\widetilde{\mathbf{A}}^\infty_w(z,\sigma) = \widetilde{\mathbf{A}}^\infty(z,\sigma) := 3\widetilde{\mathbf{A}}^{-\infty}_w(z,\sigma) + z\mathcal{A}(w)_4 + \tfrac{z}{\sigma^{1/2}}\mathcal{A}(w)_5.
\end{aligned}
\tag{2.19}
$$

We will not make explicit the dependence on S_1 because it will be fixed in our estimates. Actually, S_1 is a free parameter that we introduce to optimize the error bound for the incoming electron wave packet in Theorem 3.1. We fix S_1 in Section 5.2. Note, furthermore, that $\widetilde{\mathbf{A}}^{-\infty}_w(z,\sigma)$ is independent of w_3 and of w_4. We define it as a function of $w\in\mathbb{R}^5$ to simplify the statement of our results.

We define the following quantities,

$$
\begin{aligned}
&C_{pp}(\sigma) = C_{pp}(\sigma,B,\chi) := \tfrac{1}{\pi^{1/4}mv}(\|\triangle\chi\|_\infty + 2\|\eta(x,t)\cdot(\mathbf{p}\chi)(x)\|) + \tfrac{2}{\pi^{1/4}}\|\mathbf{p}\chi(x)\cdot\hat{\mathbf{v}}\|_\infty,\\
&C_{ps}(\sigma) = C_{ps}(\sigma,B,\chi) := \tfrac{1}{\pi^{1/4}mv}(\|\chi\mathbf{p}\cdot\eta(x,t)\|_\infty + \|\chi(x)\eta(x,t)\|^2_\infty),\\
&C_{sp}(\sigma) = C_{sp}(\sigma,B,\chi) := \tfrac{2}{\pi^{1/4}\sigma mv}(\|\mathbf{p}\chi(x)\|_\infty),\\
&C_{ss}(\sigma) = C_{ss}(\sigma,B,\chi) := \tfrac{2}{\pi^{1/4}\sigma mv}(\|\chi\eta(x,t)\|_\infty),\\
&\mathcal{R}(\zeta) = \mathcal{R}(\zeta,Z) = \mathcal{R}(\zeta,Z,A) := \|A\|_\infty\tfrac{\pi^{1/2}(\sigma^4m^2v^2+\zeta^2)^{1/2}}{\sigma mv}e^{-\frac{1}{2}(h-Z)^2\frac{(\sigma mv)^2}{\sigma^4m^2v^2+\zeta^2}}.
\end{aligned}
\tag{2.20}
$$

3 Time Evolution of the Electron Wave Packet

3.1 Wave and Scattering Operators

The Hamiltonian operator (1.6) is self-adjoint when it is defined on the domain $D(H) := \mathcal{H}_2(\Lambda) \cap \mathcal{H}_{1,0}(\Lambda)$, where by $\mathcal{H}_s(\Lambda), s = 1, 2, \cdots$ we denote the Sobolev spaces and by $\mathcal{H}_{1,0}(\Lambda)$ we denote the closure in the norm of $\mathcal{H}_1(\Lambda)$ of the set $C_0^\infty(\Lambda)$ of all infinitely differentiable functions with compact support in Λ [1]. Note that as the functions in $\mathcal{H}_{1,0}(\Lambda)$ vanish in trace sense at $\partial\Lambda$, H is the positive self-adjoint realization in $L^2(\Lambda)$ of the formal differential operator $\frac{1}{2M}(\mathbf{P} - \hbar A)^2$ with Dirichlet boundary condition at the boundary of Λ [12, 19]. The free Hamiltonian (1.2) is self-adjoint when it is defined on the domain $D(H_0) := \mathcal{H}_2(\mathbb{R}^3)$. Let J be the identification operator from $L^2(\mathbb{R}^3)$ into $L^2(\Lambda)$ given by multiplication by the characteristic function of Λ, i.e.,

$$J\phi(x) = \chi_\Lambda(x)\, \phi(x), \tag{3.1}$$

where $\chi_\Lambda(x) = 1, x \in \Lambda, \chi_\Lambda(x) = 0, x \in \mathbb{R}^3 \setminus \Lambda$. As mentioned in the introduction, the wave operators are defined as follows [20],

$$W_\pm(A) = W_\pm := \text{s-}\lim_{t \to \pm\infty} e^{i\frac{t}{\hbar}H}\, J\, e^{-i\frac{t}{\hbar}H_0}. \tag{3.2}$$

It is proved in [3] that the strong limits (3.2) exist, that they are partially isometric, and that we can replace J by the operator of multiplication by any smooth characteristic function, $\chi(x) \in C^2$ such that $\chi(x) = 0, x \in \tilde{K}$ and $\chi(x) = 1$ for x in the complement of a bounded set that contains $\tilde{K}$ on its interior.

$$W_\pm(A) = W_\pm = \text{s-}\lim_{t \to \pm\infty} e^{i\frac{t}{\hbar}H}\, \chi\, e^{-i\frac{t}{\hbar}H_0}. \tag{3.3}$$

It is also known [13] that the wave operators are asymptotically complete, i.e., that the ranges of $W_\pm$ are the same, and that they coincide with the subspace of absolute continuity of H. Moreover, the $W_\pm$ are unitary from $L^2(\mathbb{R}^3)$ onto the subspace of absolute continuity of H, and they satisfy the intertwining relations,

$$e^{-i\frac{t}{\hbar}H}\, W_\pm = W_\pm\, e^{-i\frac{t}{\hbar}H_0}. \tag{3.4}$$

Recall that the scattering operator is defined as [20],

$$S := W_+^*\, W_-. \tag{3.5}$$

3.2 Initial Conditions at Minus Infinity

In scattering experiments we know the wave packet of the electron at the emission time. Thus, if we want to know the evolution of the emitted electron for all times, we have to solve the interacting Schrödinger equation (1.5) with initial conditions at minus infinity. As mentioned in the introduction this is accomplished with wave operator W_-. The incoming electron wave packet is described at the time of emission ($t \to -\infty$) by a solution to the free Schrödinger equation, (1.1),

$$e^{-i\frac{t}{\hbar}H_0}\,\phi_-. \tag{3.6}$$

As $e^{-i\frac{t}{\hbar}H}$ is unitary, for all $\phi_- \in L^2(\mathbb{R}^3)$

$$\lim_{t\to\pm\infty}\left\| e^{-i\frac{t}{\hbar}H}\,W_\pm\phi_- - J\,e^{-i\frac{t}{\hbar}H_0}\phi_-\right\| = 0. \tag{3.7}$$

Then, the solution to (1.5) that behaves as (3.6) as $t \to -\infty$ is given by,

$$e^{-i\frac{t}{\hbar}H}W_-\,\phi_-. \tag{3.8}$$

And, moreover,

$$\lim_{t\to\infty}\left\| e^{-i\frac{t}{\hbar}H}\,W_-\,\phi_- - J\,e^{-i\frac{t}{\hbar}H_0}\phi_+\right\| = 0, \quad \text{where}\,\phi_+ := W_+^* W_-\,\phi_-. \tag{3.9}$$

This means that -as to be expected- for large positive times, when the exact electron wave packet is far away from the magnet, it behaves as the outgoing solution to the free Schrödinger equation (1.1)

$$e^{-i\frac{t}{\hbar}H_0}\phi_+, \tag{3.10}$$

where the data at $t = 0$ of the incoming and the outgoing free wave packets (3.6, 3.10) are related by the scattering operator,

$$\phi_+ = S\phi_-.$$

3.3 The Incoming Electron Wave Packet

We first introduce concepts that will be used latter in our estimates.

We define the re-scaled boosted Hamiltonians [3, 28] as follows (see (1.2), (1.6)),

$$H_1 = H_1(\mathbf{v}) := \frac{1}{\hbar v} e^{-im\mathbf{v}\cdot x}\,H_0\,e^{im\mathbf{v}\cdot x},\;\; H_2 = H_2(A,\mathbf{v}) := \frac{1}{\hbar v} e^{-im\mathbf{v}\cdot x}\,H(A)\,e^{im\mathbf{v}\cdot x}. \tag{3.11}$$

Recall that $m = \frac{M}{\hbar}$ and $\mathbf{v}$ is the velocity (see (1.3)). Let us denote by

$$W_{\pm,\mathbf{v}} := e^{-im\mathbf{v}\cdot x}\,W_\pm\,e^{im\mathbf{v}\cdot x} \tag{3.12}$$

the boosted wave operators. We have that,

$$W_{\pm,\mathbf{v}} = \mathrm{s}\lim_{\zeta\to\pm\infty} e^{i\zeta H_2}\,\chi(x)\,e^{-i\zeta H_1}, \tag{3.13}$$

where ζ represents the classical x_3-coordinate of the electron at the time $t = \zeta/v$.

We notice that,

$$e^{-i\zeta H_2} = e^{-im\mathbf{v}\cdot x} e^{-i\frac{\zeta}{\hbar v} H(A)} e^{im\mathbf{v}\cdot x},\ e^{-i\zeta H_1} = e^{-im\mathbf{v}\cdot x} e^{-i\frac{\zeta}{\hbar v} H_0} e^{im\mathbf{v}\cdot x} = e^{-i\frac{\zeta}{2mv}(\mathbf{p}+m\mathbf{v})^2}. \tag{3.14}$$

The following theorem gives us an estimate of the exact electron wave packet $e^{-i\frac{Z}{v\hbar}H} W_-(A)\varphi_{\mathbf{v}}$ for distances $Z \leq -z(\sigma) < -h(\sigma)$, i.e., where it is incoming.

THEOREM 3.1. *Let $w = (w_1, \cdots, w_5) \in \mathbb{R}^5$ be such that $w_i \geq M_i(\chi, A, \mathbf{v})$ for $i \in \{1, 2, 3\}$. Assume that $\sigma m v \geq \sqrt{34/33}$. Then, for any $Z \in \mathbb{R}^+$ such that $Z \geqq z(\sigma) > h(\sigma)$,*

$$\| e^{\mp i \frac{Z}{v\hbar} H} W_{\pm} \varphi_{\mathbf{v}} - \chi e^{\mp i \frac{Z}{v\hbar} H_0} \varphi_{\mathbf{v}} \| \leq e^{-\frac{1}{2\tilde{w}(\sigma)^2}} \widetilde{\mathbf{A}}_w^{-\infty}(z(\sigma), \sigma). \tag{3.15}$$

Proof: First we prove (3.15) for $W_+(A)$. By Duhamel's formula and (3.14) we have that,

$$\left\| \left(W_{+,\mathbf{v}} - e^{iZH_2}\, \chi e^{-iZH_1} \right) \varphi \right\| \leq \frac{1}{2mv} \int_Z^\infty \left[\left\| m_1\, e^{-izH_1}\, \varphi \right\| + 2 \left\| m_2 \cdot \mathbf{p}\, e^{-izH_1} \varphi \right\| + 2mv \left\| m_2 \cdot \hat{\mathbf{v}} e^{-izH_1} \varphi \right\| \right] dz, \tag{3.16}$$

where,

$$m_1 := (\mathbf{p}^2 \chi) - \chi(\mathbf{p} \cdot A) - 2(\mathbf{p}\chi) \cdot A + A^2 \chi. \tag{3.17}$$

$$m_2 := (\mathbf{p}\chi) - \chi A. \tag{3.18}$$

Equation (3.15) for $W_+(A)$ follows from (3.16), Lemmata 11.3 and 11.5 in Appendix A, the facts that the function $\theta_{inv}(\sigma, Z)$ is decreasing as a function of Z, for $Z \geq 0$, that $1/\tilde{w}(\sigma) = -\theta_{inv}(\sigma, z(\sigma))$ and the following estimates:

$$\int_{\max(Z, S_1)}^\infty \left(\frac{1}{\sigma^4 m^2 v^2 + \zeta^2} \right)^{3/4} \leq 2 \max(z, S_1)^{-1/2},$$

$$|\theta_{inv}(\sigma, Z)| \leq \sigma m v.$$

The last inequality follows from the definition of $\theta_{inv}(\sigma, Z)$, since $Z \geqq z(\sigma) > h(\sigma)$ (see equation (2.8)).

We now consider the case of $W_-(A)$. Note that by the uniqueness of the solutions to the Schrödinger equation we have that,

$$\overline{e^{-iZH_2(A,\mathbf{v})}\, \psi} = e^{iZH_2(-A,-\mathbf{v})}\, \overline{\psi}. \tag{3.19}$$

This is the invariance under time reversal and charge conjugation. Hence,

$$W_{-,-\mathbf{v}}(-A)\psi = \overline{W_{+,\mathbf{v}}(A)\overline{\psi}}, \tag{3.20}$$

and then,

$$\left(W_{-,-\mathbf{v}}(-A) - e^{-iZH_2(-A,-\mathbf{v})}\, \chi e^{iZH_1(-\mathbf{v})} \right) \varphi = \overline{\left(W_{+,\mathbf{v}}(A) - e^{iZH_2(A,\mathbf{v})}\, \chi e^{-iZH_1(\mathbf{v})} \right) \varphi}. \tag{3.21}$$

It follows that (3.15) for $W_-(-A)$ and $\varphi_{-\mathbf{v}}$ follows from (3.15) for $W_+(A)$ and $\varphi_{\mathbf{v}}$, and the fact that $\bar{M}(\chi, A, \mathbf{v}) = \bar{M}(\chi, -A, -\mathbf{v})$.

Let $L : \mathbb{R}^3 \to \mathbb{R}^3$ be defined as $L(x) = -x$, for $x \in \mathbb{R}^3$. Note that,

$$(e^{-i\zeta H_2(A,\mathbf{v})}\psi) \circ L = e^{-i\zeta H_2(-A\circ L, -\mathbf{v})}\,(\psi \circ L). \tag{3.22}$$

Equation (3.22) implies that,

$$(W_{-,\mathbf{v}}(A)\varphi) \circ L = W_{-,-\mathbf{v}}(-A \circ L)\,(\varphi \circ L)\,, \tag{3.23}$$

where we used that as $\chi(x) = 1$ for x in the complement of a bounded set,

$$\mathrm{s}-\lim_{\zeta \to \pm\infty} (\chi(-x) - \chi(x)) e^{-i\zeta H_1} = 0.$$

We obtain (3.15) for $W_-(A)$ and $\varphi_{\mathbf{v}}$ from (3.15) for $W_-(-A \circ L)$, $\varphi_{-\mathbf{v}}$, $\chi \circ L$ instead of χ, and $B \circ L$ instead of B using equations (3.22, 3.23) and observing that $\bar{M}(\chi, A, \mathbf{v}) = \bar{M}(\chi \circ L, -A \circ L, -\mathbf{v})$. For this purpose we use $B \circ L$ instead of B in the definition of η in (2.13).

□

3.4 The Interacting Electron Wave Packet

We first introduce an assumption that we use often.

ASSUMPTION 3.2. *Let μ_i, $i \in \{1,2,3\}$ belong to $\mathbb{R}_+$. Suppose that the following conditions hold.*

1. *Either $\mu_i \leqq \sigma_0$, $i \in \{1,2,3\}$, or $\mu_i \geqq \sigma_0$, $i \in \{1,2,3\}$.*

2. *Either, $\mu_i \leqq \mu_3$, $i \in \{1,2\}$, or $\mu_i \geqq \mu_3$, $i \in \{1,2\}$.*

We define $\mu_{\max} := \max(\mu_1, \mu_2)$, $\mu_{\min} := \min(\mu_1, \mu_2)$, and take $\nu = \mu_{\min}$, if $\mu_i \leqq \mu_3, i \in \{1,2\}$ and $\nu = \mu_{\max}$, if $\mu_i \geqq \mu_3, i \in \{1,2\}$. We denote by $Z := z(\mu_{\max})$, if $\mu_i \leqq \sigma_0, i \in \{1,2,3\}$; and $Z := \max_{i\in\{1,2\}}\{z_{\tilde{\omega}(\mu_{\max}),\mu_i}(h(\mu_{\max}))\}$, if $\mu_i \geqq \sigma_0, i \in \{1,2,3\}$. We suppose that $Z \geqq z_{\sqrt{\frac{2}{3}},\nu,\mu_3}(h(\mu_{\max}))$ and $r_1 \rho(\mu_i, z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))) \geq 1$ for $i \in \{1,2\}$.

□

The quantities I_{ps}, I_{pp}, I_{ss}, and I_{sp} that we use below are defined, respectively, in equations (11.26), (11.32), (11.35), and (11.55) in Appendix A.

LEMMA 3.3. *Suppose that Assumption 3.2 is satisfied and that $\sigma m v \geq 1$. Then, for every gaussian wave function φ with variance $\sigma \in [\mu_{\min}, \mu_{\max}]$ and every $\zeta \in \mathbb{R}$ with $|\zeta| \leq z(\sigma)$,*

$$\left\| \left(e^{i(z(\sigma)-\zeta)H_2}\, \chi(x)\, e^{-i(z(\sigma)-\zeta)H_1} - \chi(x) e^{-i\int_0^{(z(\sigma)-\zeta)} \hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})d\tau} \right) e^{-i\zeta H_1} \varphi \right\| \leq$$

$$e^{-\frac{1}{2}\frac{1}{\tilde{\omega}(\sigma)^2}} (Z-\zeta) \left(\frac{1}{\sqrt{2}2mv} M_4 + M_5 \frac{(\frac{\sigma m v}{2})^{1/2} + \frac{\sqrt{3}\pi^{1/4}}{2}}{\pi^{1/4} 2\sigma m v} \right) + C_{pp}(\sigma) I_{pp}(\mu_1,\mu_2,\mu_3) + \tag{3.24}$$

$$\frac{C_{ps}(\sigma)}{2} I_{ps}(\mu_1,\mu_2,\mu_3,\zeta) + C_{sp}(\sigma) I_{sp}(\mu_1,\mu_2,\mu_3) + \frac{C_{ss}(\sigma)}{2} I_{ss}(\mu_1,\mu_2,\mu_3,\zeta),$$

$$\left\| \left(e^{iz(\sigma)H_2}\, \chi(x)\, e^{-iz(\sigma)H_1} - \chi(x) e^{-i\int_0^{z(\sigma)} \hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})d\tau} \right) \varphi \right\| \leq$$

$$e^{-\frac{1}{2}\frac{1}{\tilde{\omega}(\sigma)^2}} (Z) \left(\frac{1}{\sqrt{2}2mv} M_4 + M_5 \frac{(\frac{\sigma m v}{2})^{1/2} + \frac{\sqrt{3}\pi^{1/4}}{2}}{\pi^{1/4} 2\sigma m v} \right) + \frac{C_{pp}(\sigma)}{2} I_{pp}(\mu_1,\mu_2,\mu_3) + \tag{3.25}$$

$$\frac{C_{ps}(\sigma)}{2} I_{pp}(\mu_1,\mu_2,\mu_3) + \frac{C_{sp}(\sigma)}{2} I_{sp}(\mu_1,\mu_2,\mu_3) + \frac{C_{ss}(\sigma)}{2} I_{sp}(\mu_1,\mu_2,\mu_3).$$

Proof: As in the proof of Lemma 5.6 of [3] (see also [28]) we prove that,

$$\left(e^{i(z(\sigma)-\zeta)H_2}\, \chi(x)\, e^{-i(z(\sigma)-\zeta)H_1} - \chi(x) e^{-i\int_0^{z(\sigma)-\zeta} \hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})d\tau} \right) e^{-i\zeta H_1}\varphi = \int_0^{z(\sigma)-\zeta} dz\, i e^{izH_2} e^{-i\int_0^{z(\sigma)-\zeta-z} \hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})d\tau}$$

$$\left[\sum_{i=1}^{2} \left(f_i(x, z(\sigma)-\zeta-z) + g_i(x, z(\sigma)-\zeta-z)\cdot \mathbf{p} \right) e^{-izH_1} + f_3(x)\, e^{-izH_1} \right] e^{-i\zeta H_1}\varphi, \tag{3.26}$$

where,

$$f_1(x,\tau) := \frac{1}{2mv} \left[-\chi(x)(\mathbf{p}\cdot A)(x+\tau\hat{\mathbf{v}}) + \chi(x)(A(x+\tau\hat{\mathbf{v}}))^2 - 2A(x+\tau\hat{\mathbf{v}})\cdot(\mathbf{p}\chi)(x) + \right.$$
$$\left. 2\chi(x) A(x+\tau\hat{\mathbf{v}})\cdot \eta(x,\tau) \right], \tag{3.27}$$

$$f_2(x,\tau) := \frac{1}{2mv} \left[-\chi(x)(\mathbf{p}\cdot\eta)(x,\tau) + \chi(x)(\eta(x,\tau))^2 - (\Delta\chi)(x) - 2\eta(x,\tau)\cdot(\mathbf{p}\chi)(x) \right], \tag{3.28}$$

$$f_3(x) := (\mathbf{p}\chi)(x)\cdot\hat{\mathbf{v}}, \tag{3.29}$$

$$g_1(x,\tau) := -\frac{1}{mv}\chi(x)\, A(x+\tau\hat{\mathbf{v}}), \tag{3.30}$$

$$g_2(x,\tau) := \frac{1}{mv} \left[-\chi(x)\,\eta(x,\tau) + (\mathbf{p}\chi)(x) \right]. \tag{3.31}$$

It follows that,

$$\left\| \left(e^{i(z(\sigma)-\zeta)H_2}\, \chi(x)\, e^{-i(z(\sigma)-\zeta)H_1} - \chi(x) e^{-i\int_0^{z(\sigma)-\zeta} \hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})d\tau} \right) e^{-i\zeta H_1}\varphi \right\| \leq$$

$$\int_0^{z(\sigma)-\zeta} dz\, \left\| f_1(x, z(\sigma)-\zeta-z) e^{-izH_1} e^{-i\zeta H_1}\,\varphi \right\| + \int_0^{z(\sigma)-\zeta} dz\, \left\| f_2(x, z(\sigma)-\zeta-z) e^{-izH_1}\; e^{-i\zeta H_1}\,\varphi \right\| +$$
$$\int_0^{z(\sigma)-\zeta} dz\, \left\| f_3(x) e^{-izH_1} e^{-i\zeta H_1}\,\varphi \right\| + \int_0^{z(\sigma)-z} dz\, \left\| g_1(x, z(\sigma)-\zeta-z)\cdot \mathbf{p} e^{-izH_1} e^{-i\zeta H_1}\,\varphi \right\| + \tag{3.32}$$
$$\int_0^{z(\sigma)-\zeta} dz\, \left\| g_2(x, z(\sigma)-\zeta-z)\cdot \mathbf{p} e^{-izH_1} e^{-i\zeta H_1}\,\varphi \right\|.$$

We estimate the first integral in the right-hand side of (3.32) using equation (11.57), the second using (11.25) and (11.31), the third using (11.31), the fourth using (11.59), and the fifth using (11.34) and (11.54). To use (11.59) note that $\theta_{inv}(\sigma, z(\sigma)) = -1/\tilde{\omega}(\sigma)$. Then, as $\sigma m v \geq 1$, $\theta_{inv}(\sigma, z(\sigma))^2 \geq 1/2$. After reordering terms we obtain equation (3.24). Equation (3.25) is obtained in the same way but using (11.33) instead of (11.31) and (11.56) instead of (11.54).

$\square$

LEMMA 3.4. *For $Z \geq h$,*

$$\left\| \left(\chi(x) e^{-i\int_0^\infty \hat{\mathbf{v}} \cdot A(x+\tau\hat{\mathbf{v}}) d\tau} - \chi(x) e^{-i\int_0^{Z-\zeta} \hat{\mathbf{v}} \cdot A(x+\tau\hat{\mathbf{v}}) d\tau} \right) e^{-i\zeta H_1} \varphi \right\| \leq \frac{1}{2} \mathcal{R}(\zeta, Z). \tag{3.33}$$

Proof: By Duhamel's formula and (11.7),

$$\begin{aligned} &\left\| \left(\chi(x) e^{-i\int_0^\infty \hat{\mathbf{v}} \cdot A(x+\tau\hat{\mathbf{v}}) d\tau} - \chi(x) e^{-i\int_0^{Z-\zeta} \hat{\mathbf{v}} \cdot A(x+\tau\hat{\mathbf{v}}) d\tau} \right) e^{-i\zeta H_1} \varphi \right\| \leq \int_{Z-\zeta}^\infty \| \chi(x) \hat{\mathbf{v}} \cdot A(x+\tau\hat{\mathbf{v}}) \, e^{-i\zeta H_1} \varphi \| \, d\tau \\ &\leq \frac{\|A\|_\infty}{\sqrt{2}} \int_Z^\infty e^{-\frac{1}{2} \, (h-\tau)^2 \frac{(\sigma m v)^2}{\sigma^4 m^2 v^2 + \zeta^2}} \, d\tau = \frac{\|A\|_\infty}{\sqrt{2}} \, e^{-\frac{1}{2}(h-Z)^2 \frac{(\sigma m v)^2}{\sigma^4 m^2 v^2 + \zeta^2}} \int_Z^\infty \, d\tau \, e^{-\frac{1}{2}(\tau - Z)(\tau + Z - 2h) \frac{(\sigma m v)^2}{\sigma^4 m^2 v^4 + \zeta^2}}, \end{aligned} \tag{3.34}$$

where we used that $(h-\tau)^2 - (h-Z)^2 = (\tau - Z)(\tau + Z - 2h)$. Finally since, $(\tau - Z)(\tau + Z - 2h) \geq (\tau - Z)^2$,

$$\begin{aligned} &\left\| \left(\chi(x) e^{-i\int_0^\infty \hat{\mathbf{v}} \cdot A(x+\tau\hat{\mathbf{v}}) d\tau} - \chi(x) e^{-i\int_0^{Z-\zeta} \hat{\mathbf{v}} \cdot A(x+\tau\hat{\mathbf{v}}) d\tau} \right) e^{-i\zeta H_1} \varphi \right\| \leq \\ &\frac{\|A\|_\infty}{\sqrt{2}} \, e^{-\frac{1}{2}(h-Z)^2 \frac{(\sigma m v)^2}{\sigma^4 m^2 v^2 + \zeta^2}} \int_Z^\infty \, d\tau \, e^{-\frac{1}{2}(\tau - Z)^2 \frac{(\sigma m v)^2}{\sigma^4 m^2 v^4 + \zeta^2}}, \end{aligned} \tag{3.35}$$

what proves the lemma.

$\square$

In the Theorem below we estimate the exact electron wave packet $e^{-i\frac{\zeta}{v\hbar}H} W_\pm(A) \varphi_{\mathbf{v}}$ for distances ζ such that, $|\zeta| \leq z(\sigma)$. As $z(\sigma) > h(\sigma)$ -see equation (2.8)- this is the interaction region.

THEOREM 3.5. *Suppose that Assumption 3.2 is satisfied, and, furthermore that $\sigma m v \geq 1$. Let $w = (w_1, \cdots, w_5) \in \mathbb{R}^5$ be such that $w_i \geq M_i(\chi, A, \mathbf{v})$ for $i \in \{1, \cdots, 5\}$. Then, for every gaussian wave function φ with variance $\sigma \in [\mu_{\min}, \mu_{\max}]$ and every $\zeta \in \mathbb{R}$ with $|\zeta| \leq z(\sigma)$,*

$$\begin{aligned} &\| e^{-i\frac{\zeta}{v\hbar}H} W_\pm(A) \varphi_{\mathbf{v}} - \chi e^{-i\int_0^{\pm\infty} \hat{\mathbf{v}} \cdot A(x+\tau\hat{\mathbf{v}}) d\tau} e^{-i\frac{\zeta}{v\hbar}H_0} \varphi_{\mathbf{v}} \| \leq e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}} \widetilde{\mathbf{A}}_w^0(z(\sigma), \sigma) + C_{pp}(\sigma) I_{pp}(\mu_1, \mu_2, \mu_3) + \\ &\frac{C_{ps}(\sigma)}{2} I_{ps}(\mu_1, \mu_2, \mu_3, \pm\zeta) + C_{sp}(\sigma) I_{sp}(\mu_1, \mu_2, \mu_3) + \frac{C_{ss}(\sigma)}{2} I_{ss}(\mu_1, \mu_2, \mu_3, \pm\zeta) + \frac{1}{2} \mathcal{R}(\pm\zeta, z(\sigma)), \end{aligned} \tag{3.36}$$

$$\begin{aligned} &\| W_\pm(A) \varphi_{\mathbf{v}} - \chi e^{-i\int_0^{\pm\infty} \hat{\mathbf{v}} \cdot A(x+\tau\hat{\mathbf{v}}) d\tau} \varphi_{\mathbf{v}} \| \leq e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}} (\widetilde{\mathbf{A}}_w^{-\infty}(z(\sigma), \sigma) + \frac{z(\sigma)}{2} \mathcal{A}(w)_4 + \frac{z(\sigma)}{2\sigma^2} \mathcal{A}(w)_5) + \\ &\frac{C_{pp}(\sigma)}{2} I_{pp}(\mu_1, \mu_2, \mu_3) + \frac{C_{ps}(\sigma)}{2} I_{pp}(\mu_1, \mu_2, \mu_3) + \frac{C_{sp}(\sigma)}{2} I_{sp}(\mu_1, \mu_2, \mu_3) + \\ &\frac{C_{ss}(\sigma)}{2} I_{sp}(\mu_1, \mu_2, \mu_3) + \frac{1}{2} \mathcal{R}(0, z(\sigma)). \end{aligned} \tag{3.37}$$

Proof:

We prove (3.36) for $W_+(A)$, the proof for $W_-(A)$ follows as in (3.19-3.23). Note that by the intertwining relations of the wave operators (3.4) and by (3.14) we have that,

$$\left\|\left(W_{+,\mathbf{v}}(A) - e^{i(z(\sigma)-\zeta)H_2}\chi\, e^{-i(z(\sigma)-\zeta)H_1}\right) e^{-i\zeta H_1}\varphi\right\| = \left\|e^{-i\frac{(z(\sigma)-\zeta)}{v\hbar}H}W_+(A)e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}} - \chi e^{-i\frac{(z(\sigma)-\zeta)}{v\hbar}H_0}e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\right\| =$$
$$\left\|e^{-i\frac{z(\sigma)}{v\hbar}H}W_+(A)\varphi_{\mathbf{v}} - \chi e^{-i\frac{z(\sigma)}{v\hbar}H_0}\varphi_{\mathbf{v}}\right\|. \tag{3.38}$$

We use the intertwining relations and (3.14) again to obtain,

$$\left\|e^{-i\frac{\zeta}{v\hbar}H}W_+(A)\varphi_{\mathbf{v}} - \chi e^{-i\int_0^{\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})d\tau}e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\right\| =$$
$$\|W_{+,\mathbf{v}}(A)e^{-i\zeta H_1}\varphi - \chi e^{-i\int_0^{\pm\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})d\tau}e^{-i\zeta H_1}\varphi\| \leq \|(W_{+,\mathbf{v}}(A) - e^{i(z(\sigma)-\zeta)H_2}\chi e^{-i(z(\sigma)-\zeta)H_1})e^{-i\zeta H_1}\varphi\| +$$
$$\|(e^{i(z(\sigma)-\zeta)H_2}\chi\, e^{-i(z(\sigma)-\zeta)H_1} - \chi e^{-i\int_0^{z(\sigma)-\zeta}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})d\tau})e^{-i\zeta H_1}\varphi\| + \tag{3.39}$$
$$\|(\chi e^{-i\int_0^{\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})d\tau} - \chi e^{-i\int_0^{z(\sigma)-\zeta}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})d\tau})e^{-i\zeta H_1}\varphi\|.$$

Equation (3.36) is obtained by (3.38), (3.39), Theorem 3.1, equation (3.24) and Lemma 3.4. The proof of (3.37) is similar, but instead of (3.24) we use (3.25).

3.5 Estimates for the Scattering Operator

We first prove the following lemma.

LEMMA 3.6. *Suppose that the conditions of Theorem 3.5 are satisfied. Then,*

$$\left\|\left(W^*_{+,\mathbf{v}}\, e^{-i\int_0^{-\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\,d\tau} - e^{i\Phi}\right)\chi(x)\,\varphi\right\| \leq 3e^{-\frac{1}{2}\frac{r_1^2}{\sigma^2}} + e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}}(\widetilde{\mathbf{A}}_w^{-\infty}(z(\sigma),\sigma) + \frac{z(\sigma)}{2}\mathcal{A}(w)_4 + \frac{z(\sigma)}{2\sigma^2}\mathcal{A}(w)_5) +$$
$$\frac{C_{pp}(\sigma)}{2}I_{pp}(\mu_1,\mu_2,\mu_3) + \frac{C_{ps}(\sigma)}{2}I_{pp}(\mu_1,\mu_2,\mu_3) + \frac{C_{sp}(\sigma)}{2}I_{sp}(\mu_1,\mu_2,\mu_3) + \frac{C_{ss}(\sigma)}{2}I_{sp}(\mu_1,\mu_2,\mu_3) +$$
$$\frac{1}{2}\mathcal{R}(0,z(\sigma)). \tag{3.40}$$

Proof: As $W_+^*\, W_+ = I$,

$$\left\|\left(W^*_{+,\mathbf{v}}\, e^{-i\int_0^{-\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\,d\tau} - e^{i\Phi}\right)\chi(x)\,\varphi\right\| = \left\|W^*_{+,\mathbf{v}}\,\left(e^{-i(\int_0^{-\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\,d\tau+\Phi)}\chi - W_{+,\mathbf{v}}\chi\right)e^{i\Phi}\varphi\right\| \leq$$
$$\left\|\left(e^{-i\int_0^{\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\,d\tau}\chi - W_{+,\mathbf{v}}\right)\varphi\right\| + \|(1-\chi)\varphi\| + \left\|(e^{-i(\int_0^{-\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\,d\tau+\Phi)} - e^{-i\int_0^{\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\,d\tau})\chi\varphi\right\|. \tag{3.41}$$

Since $\int_{-\infty}^{\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\,d\tau = \Phi$ for x in the cylinder $\{x\in\mathbb{R}^3 : x_1^2+x_2^2\leq r_1^2\}$, (3.40) follows from Theorem 3.5 and the following estimates,

$$\|(1-\chi(x))\varphi\| \leq e^{-r_1^2/2\sigma^2}, \quad \left\|(e^{-i(\int_0^{-\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\,d\tau+\Phi)} - e^{-i\int_0^{\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\,d\tau})\chi\varphi\right\| \leq 2e^{-r_1^2/2\sigma^2}. \tag{3.42}$$

□

In the theorem below we approximate the scattering operator by its high-velocity limit (see [3]).

THEOREM 3.7. *Suppose that Assumption 3.2 is satisfied. Let $w = (w_1, \cdots, w_5) \in \mathbb{R}^5$ be such that $w_i \geq M_i(\chi, A, \mathbf{v})$ for $i \in \{1, \cdots, 5\}$. Then, for every gaussian wave function φ with variance $\sigma \in [\mu_{\min}, \mu_{\max}]$,*

$$\begin{aligned} &\left\| \left(S - e^{i\Phi}\chi\right) \varphi_{\mathbf{v}} \right\| \leq 3 e^{-\frac{1}{2}\frac{r_1^2}{2\sigma^2}} + e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}} (2 \widetilde{\mathbf{A}}_w^{-\infty}(z(\sigma), \sigma) + z(\sigma)\mathcal{A}(w)_4 + \frac{z(\sigma)}{\sigma^{1/2}}\mathcal{A}(w)_5) + C_{pp}(\sigma) I_{pp}(\mu_1, \mu_2, \mu_3) + \\ &C_{ps}(\sigma) I_{pp}(\mu_1, \mu_2, \mu_3) + C_{sp}(\sigma) I_{sp}(\mu_1, \mu_2, \mu_3) + C_{ss}(\sigma) I_{sp}(\mu_1, \mu_2, \mu_3) + \mathcal{R}(0, z(\sigma)). \end{aligned} \tag{3.43}$$

Proof: We denote,

$$S_{\mathbf{v}} := e^{-im\mathbf{v}\cdot x}\, S\, e^{im\mathbf{v}\cdot x}. \tag{3.44}$$

We have that,

$$\begin{aligned} &\left\| \left(S - e^{i\Phi}\chi\right) \varphi_{\mathbf{v}} \right\| = \left\| \left(S_{\mathbf{v}} - e^{i\Phi}\chi\right) \varphi \right\| = \left\| W_{+,\mathbf{v}}^* \left(W_{-,\mathbf{v}} - \chi(x)\, e^{-i\int_0^{-\infty} \hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}}) d\tau} \right) \varphi + \right. \\ &\left. \left(W_{+,\mathbf{v}}^*\, e^{-i\int_0^{-\infty} \hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}}) d\tau} - e^{i\Phi} \right) \chi(x)\, \varphi \right\|. \end{aligned} \tag{3.45}$$

Equation (3.43) follows from Theorem 3.5, Lemma 3.6 and (3.45).

3.6 The Outgoing Electron Wave Packet

In the following theorem we estimate the exact electron wave packet $e^{-i\frac{\zeta}{v\hbar}H} W_-(A)\varphi_{\mathbf{v}}$ for distances ζ in the outgoing region, $\zeta \geq z(\sigma) > h(\sigma)$.

THEOREM 3.8. *Suppose that Assumption 3.2 is satisfied. Let $w = (w_1, \cdots, w_5) \in \mathbb{R}^5$ be such that $w_i \geq M_i(\chi, A, \mathbf{v})$ for $i \in \{1, \cdots, 5\}$. Then, for every gaussian wave function φ with variance $\sigma \in [\mu_{\min}, \mu_{\max}]$ and every $\zeta \in \mathbb{R}$ with $\zeta \geq z(\sigma)$,*

$$\begin{aligned} &\| e^{-i\frac{\zeta}{v\hbar}H} W_-(A)\varphi_{\mathbf{v}} - \chi e^{i\Phi} e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}} \| \leq 3 e^{-\frac{1}{2}\frac{r_1^2}{2\sigma^2}} + e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}} \widetilde{\mathbf{A}}_w^{\infty}(z(\sigma), \sigma) + C_{pp}(\sigma) I_{pp}(\mu_1, \mu_2, \mu_3) + \\ &C_{ps}(\sigma) I_{pp}(\mu_1, \mu_2, \mu_3) + C_{sp}(\sigma) I_{sp}(\mu_1, \mu_2, \mu_3) + C_{ss}(\sigma) I_{sp}(\mu_1, \mu_2, \mu_3) + \mathcal{R}(0, z(\sigma)). \end{aligned} \tag{3.46}$$

Proof:

Using the definition of S (see (3.5)) and the fact that $e^{-i\frac{\zeta}{v\hbar}H}$ is unitary we get,

$$\begin{aligned} &\| e^{-i\frac{\zeta}{v\hbar}H} W_-(A)\varphi_{\mathbf{v}} - \chi e^{i\Phi} e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}} \| = \| W_-(A)\varphi_{\mathbf{v}} - e^{i\frac{\zeta}{v\hbar}H} \chi e^{i\Phi} e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}} \| \leq \\ &\| e^{i\Phi} \left(W_+(A)\varphi_{\mathbf{v}} - e^{i\frac{\zeta}{v\hbar}H} \chi e^{-i\frac{\zeta}{v\hbar}H_0} \right) \varphi_{\mathbf{v}} \| + \| W_-(A)\varphi_{\mathbf{v}} - W_+(A) e^{i\Phi}\varphi_{\mathbf{v}} \|. \end{aligned} \tag{3.47}$$

Furthermore,

$$\| W_-(A)\varphi_{\mathbf{v}} - W_+(A) e^{i\Phi}\varphi_{\mathbf{v}} \| \leq \| W_-(A)\varphi_{\mathbf{v}} - W_+(A) S\varphi_{\mathbf{v}} \| + \| W_+(A)(S - e^{i\Phi})\varphi_{\mathbf{v}} \|. \tag{3.48}$$

Since the wave operators are asymptotically complete [13], the operators $W_\pm W_\pm^*$ are the orthogonal projector onto the common range of $W_\pm$. Then, $W_+ W_+^* W_- = W_-$, and we have that,

$$W_-(A)\varphi_{\mathbf{v}} - W_+(A)S\varphi_{\mathbf{v}} = W_-(A)\varphi_{\mathbf{v}} - W_+(A)\, W_+^*(A)\, W_-(A)\varphi_{\mathbf{v}} = 0,$$

and by (3.47, 3.48)

$$\|e^{-i\frac{\varsigma}{v\hbar}H} W_-(A)\varphi_{\mathbf{v}} - \chi e^{i\Phi} e^{-i\frac{\varsigma}{v\hbar}H_0}\varphi_{\mathbf{v}}\| \leq \|W_+(A)\varphi_{\mathbf{v}} - e^{i\frac{\varsigma}{v\hbar}H}\chi e^{-i\frac{\varsigma}{v\hbar}H_0}\varphi_{\mathbf{v}}\| + \|S\varphi_{\mathbf{v}} - e^{i\Phi}\varphi_{\mathbf{v}}\|. \tag{3.49}$$

The inequality (3.46) follows from Theorems 3.1 and 3.7, and from equation (3.49).

4 The Magnetic Field, the Magnetic Potential and the Cutoff Function

We have proven in Theorem 4.1 of [3] that the Hamiltonias (1.6) with Dirichlet boundary condition on $\partial\Lambda$ that correspond to two different magnetic fields contained inside the magnet, and that have the same flux Φ modulo 2π are unitarily equivalent. We have also proven in [3] that the scattering operator only depends on the total flux Φ enclosed inside the magnet, modulo 2π. This implies that without losing generality we can assume that

$$|\Phi| < 2\pi, \tag{4.1}$$

what we do from now on. This also means that we have a large freedom to choose the magnetic field, as long as it is contained inside the magnet. As mentioned in the introduction, we also have a large freedom to choose the smooth cutoff function χ. We use this freedom to choose the magnetic field, the magnetic potential and the smooth cutoff function that is convenient for the computation of the error bounds. Below we construct a magnetic field inspired in the experimental results of Tonomura et. al. [25]. We also choose a magnetic potential and a cutoff function, and we provide bounds for them.

4.1 Mollifiers

We denote for $z \in \mathbb{R}$,

$$\psi(z) := \frac{1}{\iota}\begin{cases} e^{-1/(1-z^2)}, & |z| \leq 1, \\ 0, & |z| \geq 1, \end{cases} \tag{4.2}$$

where,

$$\iota := \int_{-1}^{1} e^{-1/(1-z^2)}\, dz. \tag{4.3}$$

For $\varepsilon > 0$ we define,

$$\psi_\varepsilon(z) := \frac{1}{\varepsilon}\psi(z/\varepsilon), \tag{4.4}$$

and for every $a, b \in \mathbb{R}$, with $a < b$ and every $\varepsilon \in \mathbb{R}_+$ with $\varepsilon < \frac{1}{2}(b-a)$, we take,

$$\psi_{a,b,\varepsilon}(z) := \int_a^b dy\, \psi_\varepsilon(z-y) = \begin{cases} 1, z \in [a+\varepsilon, b-\varepsilon], \\ \\ 0, z \notin [a-\varepsilon, b+\varepsilon]. \end{cases} \tag{4.5}$$

Then,

$$\|\psi_{a,b,\varepsilon}\|_\infty = 1, \tag{4.6}$$

$$\|\psi'_{a,b,\varepsilon}\|_\infty \leq \frac{1}{\iota e\, \varepsilon}, \tag{4.7}$$

$$\left\|\psi''_{a,b,\varepsilon}\right\|_\infty \leq \frac{2N}{\iota\, \varepsilon^2}, \text{ where } N := 2e^{-(3/2+\sqrt{3/4})}(3/2+\sqrt{3/4})^2(1-(3/2+\sqrt{3/4})^{-1})^{1/2}. \tag{4.8}$$

4.2 The Magnetic Field

Recall that the magnet is the set,

$$\tilde{K} := \left\{(x_1, x_2, x_3) \in \mathbb{R}^3 : 0 < \tilde{r}_1 \leq (x_1^2 + x_2^2)^{1/2} \leq \tilde{r}_2, |x_3| \leq \tilde{h}\right\}. \tag{4.9}$$

We use cylindrical coordinates: for $(x_1, x_2, x_3) \in \mathbb{R}^3$, we take $r := (x_1^2 + x_2^2)^{1/2}$, $0 \leq \theta < 2\pi$, x_3. For $\tilde{\varepsilon} < \frac{\tilde{r}_2 - \tilde{r}_1}{4}, \tilde{\delta} < \frac{\tilde{h}}{2}$, we define,

$$B = B(x, \tilde{\varepsilon}, \tilde{\delta}) := \frac{\Phi}{C_{\tilde{\varepsilon},\tilde{\delta}}}\, \psi_{\tilde{r}_1+\tilde{\varepsilon},\tilde{r}_2-\tilde{\varepsilon},\tilde{\varepsilon}}(r)\, \psi_{-\tilde{h}+\tilde{\delta},\tilde{h}-\tilde{\delta},\tilde{\delta}}(x_3)(-\sin\theta, \cos\theta, 0), \tag{4.10}$$

where for a transverse section of $\tilde{K}$, TS,

$$C_{\tilde{\varepsilon},\tilde{\delta}} := \int_{\mathrm{TS}} \psi_{\tilde{r}_1+\tilde{\varepsilon},\tilde{r}_2-\tilde{\varepsilon},\tilde{\varepsilon}}(r)\, \psi_{-\tilde{h}+\tilde{\delta},\tilde{h}-\tilde{\delta},\tilde{\delta}}(x_3) \geq 2(\tilde{h} - 2\tilde{\delta})\, (\tilde{r}_2 - \tilde{r}_1 - 4\tilde{\varepsilon}). \tag{4.11}$$

Then, $\nabla \cdot B = 0$ and the flux of B over any transverse section of $\tilde{K}$ is Φ.

This choice of B, that is approximately constant along any transverse section of $\tilde{K}$ and is directed along the unit vector $(-\sin(\theta), \cos(\theta), 0)$ is inspired by the experimental results of Tonomura et al. [25]: in Figure 4 (a) of [25], the fringes on the shadow of the magnet suggest that the component of the magnetic field that is orthogonal to a transverse section of the magnet is constant over this transverse section.

By (4.6, 4.7, 4.11),

$$\|B\|_\infty \leq \frac{\pi}{(\tilde{h} - 2\tilde{\delta})\, (\tilde{r}_2 - \tilde{r}_1 - 4\tilde{\varepsilon})}, \tag{4.12}$$

$$\left\|\frac{\partial}{\partial x_j} B\right\|_\infty \leq \frac{\pi}{(\tilde{h} - 2\tilde{\delta})\, (\tilde{r}_2 - \tilde{r}_1 - 4\tilde{\varepsilon})} (\frac{1}{\iota e\tilde{\varepsilon}} + \frac{1}{\tilde{r}_1}),\ j = 1, 2, \tag{4.13}$$

$$\left\| \frac{\partial}{\partial x_3} B \right\|_\infty \leq \frac{\pi}{(\tilde{h} - 2\tilde{\delta})\,(\tilde{r}_2 - \tilde{r}_1 - 4\tilde{\varepsilon})} \frac{1}{\iota e \tilde{\delta}}. \tag{4.14}$$

With this choice of B we have that (see (2.13)).

$$\|\eta(x,\tau)\|_\infty \leq 2\tilde{h} \frac{\pi}{(\tilde{h} - 2\tilde{\delta})\,(\tilde{r}_2 - \tilde{r}_1 - 4\tilde{\varepsilon})}, \tag{4.15}$$

$$\|\mathbf{p} \cdot \eta(x,\tau)\|_\infty \leq 2\tilde{h} \frac{\pi}{(\tilde{h} - 2\tilde{\delta})\,(\tilde{r}_2 - \tilde{r}_1 - 4\tilde{\varepsilon})} \left(\frac{1}{\iota e \tilde{\varepsilon}} + \frac{1}{\tilde{r}_1} \right). \tag{4.16}$$

4.3 The Magnetic Potential

The potential $A = A(x, \tilde{\varepsilon}, \tilde{\delta})$ associated to the field $B = B(x, \tilde{\varepsilon}, \tilde{\delta})$ satisfies the differential equation $\nabla \times A = B$. As B has no vertical component, we can take A parallel to the vertical axis.

$$A = A(x, \tilde{\varepsilon}, \tilde{\delta}) := \frac{-\Phi}{C_{\tilde{\varepsilon},\tilde{\delta}}}\, \psi_{-\tilde{h}+\tilde{\delta},\tilde{h}-\tilde{\delta},\tilde{\delta}}(x_3) \left(0, 0, \int_{(y_1,y_2)}^{(x_1,x_2)} \psi_{\tilde{r}_1+\tilde{\varepsilon},\tilde{r}_2-\tilde{\varepsilon},\tilde{\varepsilon}}(r)\,(\cos\theta, \sin\theta) \right), \tag{4.17}$$

where (y_1, y_2) is any point with $|(y_1, y_2)| \geq \tilde{r}_2$ and the line integral is over any curve in $\mathbb{R}^2$ that connects the point (y_1, y_2) with (x_1, x_2). The value of A is independent of the curve chosen. The potential A has support in the convex hull of $\tilde{K}$, that we denoted by $\tilde{D}$. Moreover, by (4.6, 4.7),

$$\|A\|_\infty \leq \frac{\pi}{(\tilde{h} - 2\tilde{\delta})\,(\tilde{r}_2 - \tilde{r}_1 - 4\tilde{\varepsilon})} (\tilde{r}_2 - \tilde{r}_1), \tag{4.18}$$

$$\left\| \frac{\partial}{\partial x_j} A \right\|_\infty \leq \frac{\pi}{(\tilde{h} - 2\tilde{\delta})\,(\tilde{r}_2 - \tilde{r}_1 - 4\tilde{\varepsilon})}, j = 1, 2, \tag{4.19}$$

$$\left\| \frac{\partial}{\partial x_3} A \right\|_\infty \leq \frac{\pi}{(\tilde{h} - 2\tilde{\delta})\,(\tilde{r}_2 - \tilde{r}_1 - 4\tilde{\varepsilon})} \frac{1}{\iota e \tilde{\delta}} (\tilde{r}_2 - \tilde{r}_1). \tag{4.20}$$

4.4 The Cutoff Function

We use the freedom that we have in the choice of the cutoff function $\chi(x)$ to select it in a convenient way. Take $0 < \varepsilon < \tilde{r}_1, \delta > 0$. We define (see (2.4)),

$$r_1 := \tilde{r}_1 - \varepsilon > 0,\; r_2 := \tilde{r}_2 + \varepsilon,\; h := \tilde{h} + \delta. \tag{4.21}$$

We define

$$\chi(x) := 1 - \psi_{r_1+\varepsilon/2, r_2-\varepsilon/2, \varepsilon/2}(r)\, \psi_{-h+\delta/2, h-\delta/2, \delta/2}(x_3). \tag{4.22}$$

Then (see (2.3)),

$$\chi(x)=\begin{cases}0, & x\in\tilde{K},\\ \\ 1, & x\in\mathbb{R}^3\setminus K.\end{cases} \tag{4.23}$$

Moreover, by (4.6, 4.7, 4.8),

$$\|\chi\|_\infty=1, \tag{4.24}$$

$$\left\|\frac{\partial}{\partial x_j}\chi\right\|_\infty\leq\frac{2}{\iota e\varepsilon}, j=1,2, \tag{4.25}$$

$$\left\|\frac{\partial}{\partial x_3}\chi\right\|_\infty\leq\frac{2}{\iota e\delta}, \tag{4.26}$$

$$\left\|\mathbf{p}^2\chi\right\|_\infty\leq\frac{8\,N}{\iota\varepsilon^2}+\frac{2}{er_1\iota\varepsilon}+\frac{8\,N}{\iota\delta^2}. \tag{4.27}$$

We denote by

$$\begin{aligned}&I:=\tfrac{1}{\pi}(\tilde{h}-2\tilde{\delta})(\tilde{r}_2-\tilde{r}_1-4\tilde{\varepsilon}),\\ &J:=\tfrac{\tilde{r}_2-\tilde{r}_1}{I}.\end{aligned} \tag{4.28}$$

We designate by $\bar{m}(\chi)=\bar{m}:=(m_1(\chi),\cdots,m_5(\chi))\in\mathbb{R}^5$ the vector with the following components,

$$\begin{aligned}&m_1(\chi)=m_1:=\tfrac{8N}{\iota\varepsilon^2}+\tfrac{2}{\iota\varepsilon r_1 e}+\tfrac{8N}{\iota\delta^2}+\left(2+(\tilde{r}_2-\tilde{r}_1)\frac{1}{\iota\tilde{\delta}e}\right)I^{-1}+\tfrac{4}{\iota\delta e}J+J^2,\\ &m_2(\chi)=m_2:=2\left(\tfrac{4}{\iota\varepsilon e}+\tfrac{2}{\iota\delta e}\right)+2J,\\ &m_3(\chi)=m_3:=\frac{2}{\iota\delta e}+J,\\ &m_4(\chi)=m_4:=\left(2+(\tilde{r}_2-\tilde{r}_1)\frac{1}{\iota\tilde{\delta}e}\right)I^{-1}+J^2+\tfrac{4}{\iota\delta e}J,\\ &m_5(\chi)=m_5:=2J.\end{aligned} \tag{4.29}$$

Now we define the following quantities,

$$\begin{aligned}&c_{pp}(\sigma):=\tfrac{1}{\pi^{1/4}mv}\left(\frac{8N}{\iota\varepsilon^2}+\frac{2}{\iota\varepsilon r_1 e}+\frac{8N}{\iota\delta^2}+\frac{4\tilde{h}}{I}\frac{4}{\iota\varepsilon e}\right)+\frac{4}{\pi^{1/4}\iota\delta e},\\ &c_{ps}(\sigma):=\tfrac{1}{\pi^{1/4}mv}\left(\tfrac{2\tilde{h}}{I}\left(\frac{1}{\iota\tilde{\varepsilon}e}+\frac{1}{\tilde{r}_1}\right)+\left(\tfrac{2\tilde{h}}{I}\right)^2\right),\\ &c_{sp}(\sigma):=\tfrac{1}{\pi^{1/4}\sigma mv}\left(\tfrac{8}{\iota\varepsilon e}+\frac{4}{\iota\delta e}\right),\\ &c_{ss}(\sigma):=\tfrac{1}{\pi^{1/4}\sigma mv}\tfrac{4\tilde{h}}{I},\\ &R(\zeta,Z)=R(\zeta):=\frac{m_5}{2}\frac{(\sigma^4m^2v^2+\zeta^2)^{1/2}}{\sigma mv}\pi^{1/2}e^{-\frac{1}{2}\frac{(h-Z)^2(\sigma mv)^2}{\sigma^4m^2v^2+\zeta^2}}.\end{aligned} \tag{4.30}$$

REMARK 4.1. *For the field, the potential and cutoff function constructed in this section we have that,*

$$
\begin{aligned}
&M_i \leq m_i, \;\; i \in \{1, \cdots, 5\}, \\
&C_{pp}(\sigma) \leq c_{pp}(\sigma), \; C_{ps}(\sigma) \leq c_{ps}(\sigma), \; C_{ss}(\sigma) \leq c_{ss}(\sigma), \; C_{sp}(\sigma) \leq c_{sp}(\sigma), \\
&\mathcal{R}(\zeta, Z) \leq R(\zeta, Z).
\end{aligned}
\tag{4.31}
$$

Proof: the Remark follows from explicit computation.

□

We introduce some notation that we use below. We define the vectors $\overline{\mathbf{A}}^j(v, \bar{m}) = \overline{\mathbf{A}}^j := (\mathbf{A}_1^j, \mathbf{A}_{1/2}^j, \mathbf{A}_0^j, \mathbf{A}_{-1/2}^j, \mathbf{A}_{-1}^j)$, for $j \in \{-\infty, 0, \infty\}$:

$$
\begin{aligned}
&\overline{\mathbf{A}}^{-\infty}(v, \bar{m}) = \overline{\mathbf{A}}^{-\infty} := (mvr_1 \tfrac{\mathcal{A}(\bar{m})_1}{2} + mvr_2 (\tfrac{2\tilde{h}}{r_1})^{1/2} \tfrac{1}{(1-5\times 10^{-10})^{1/2}} \tfrac{\mathcal{A}(\bar{m})_2}{2}, mvr_1 \tfrac{\mathcal{A}(\bar{m})_3}{2}, - \\
&134.99\tilde{h} \tfrac{\mathcal{A}(\bar{m})_1}{2}, -134.99\tilde{h} \tfrac{\mathcal{A}(\bar{m})_3}{2}, 0), \\
&\overline{\mathbf{A}}^{-0}(v, \bar{m}) = \overline{\mathbf{A}}^{-0} := (\mathbf{A}_1^{-\infty}, \mathbf{A}_{1/2}^{-\infty}, \mathbf{A}_0^{-\infty} + 135.91\tilde{h}\mathcal{A}(\bar{m})_4, \mathbf{A}_{-1/2}^{-\infty} + \\
&135.91\tilde{h}\mathcal{A}(\bar{m})_5, \tfrac{\sqrt{\pi}}{2} \tfrac{m_5}{2} (1 + 1.11 \times 10^{-6})^{1/2} \tfrac{136.82}{mv} \tilde{h}), \\
&\overline{\mathbf{A}}^{\infty}(v, \bar{m}) = \overline{\mathbf{A}}^{\infty} := (3\mathbf{A}_1^{-\infty}, 3\mathbf{A}_{1/2}^{-\infty}, 3\mathbf{A}_0^{-\infty} + 138\tilde{h}\mathcal{A}(\bar{m})_4, 3\mathbf{A}_{-1/2}^{-\infty} + 138\tilde{h}\mathcal{A}(\bar{m})_5, 0).
\end{aligned}
\tag{4.32}
$$

Finally, for $j \in \{-\infty, 0, \infty\}$ we denote,

$$
\mathbf{A}^j(\sigma, v, \bar{m}) = \mathbf{A}^j(\sigma) := \sum_{i \in \{1, 1/2, 0, -1/2, -1\}} \mathbf{A}_i^j \sigma^i. \tag{4.33}
$$

5 Tonomura et al. Experiments. Continued

5.1 Experimental Data

We consider the 2 different magnets with their dimensions given in table I of [17]. We denote them by $\{\tilde{K}_j\}_{j \in \{1,2\}}$,

$$
\tilde{K}_j := \{x = (x_1, x_2, x_3) \in \mathbb{R}^3 : \tilde{r}_{1,j} \leq \sqrt{x_1^2 + x_2^2} \leq \tilde{r}_{2,j}, |x_3| \leq \tilde{h}\}. \tag{5.1}
$$

We use the notation

$$
\chi_j, \, j \in \{1, 2\} \tag{5.2}
$$

for the corresponding cutoff function constructed in Section 4.4.

The height $\tilde{h}$ is $10^{-6}cm$ for both magnets and

$$
\tilde{r}_{1,1} = 1.5 \times 10^{-4} cm
$$

$$\tilde{r}_{2,1} = 2.5 \times 10^{-4} cm$$

$$\tilde{r}_{1,2} = 1.75 \times 10^{-4} cm$$

$$\tilde{r}_{2,2} = 2.75 \times 10^{-4} cm$$

In the Tonomura et al. experiments [26] the electron has an energy of $150\, keV$. In this experiments they consider impenetrable magnets as we do in this paper. In the experiments [25] they consider penetrable magnets and energies of $80\, keV$, $100\, keV$ and $125\, keV$. Since our method applies also in the case of penetrable magnets, we will consider in our estimates below the two extreme energies and an intermediate energy, although the most important one is the one of $150\, keV$ that is the one used for the case of impenetrable magnets. Thus we consider the following energies.

$$E_1 = 150\, keV,$$

$$E_2 = 100\, keV,$$

$$E_3 = 80\, keV.$$

They used an electron wave packet that might be represented at the time of emission ($t \to -\infty$) by the gaussian wave function,

$$\left(\frac{1}{\alpha_z^2 \pi}\right)^{1/4} \left(\frac{1}{\alpha_r^2 \pi}\right)^{2/4} e^{-i\frac{t}{\hbar}H_0} e^{i\frac{M}{\hbar}\mathbf{v}\cdot x} e^{-\frac{x_1^2+x_2^2}{2\alpha_r^2}}\, e^{-\frac{x_3^2}{2\alpha_z^2}}. \tag{5.3}$$

The transverse variance of the wave function α_r is several times the radius of the torus $(r_{2,j}, j = 1,2)$, so the electron wave packet covers the magnet.

The part of the wave packet that goes through the hole of the torus has a different behavior than the one that goes outside the hole. There appears to be no interference between those two parts of the wave packet, because a clear figure of the shadow of magnet is formed behind the torus. This was pointed out by Tonomura et al. [25], [26]. We can, therefore, model only the part of the electron wave packet that goes trough the hole of the magnet. Hence, we take the transverse variance α_r smaller than the inner radius of the magnet. The anisotropy of the variance $(\alpha_z \neq \alpha_r)$ does not introduce new ideas to the analysis and all the proofs that we do assuming that $\alpha_z = \alpha_r$ can be done in the same way if $\alpha_z \neq \alpha_r$. We obtain similar results in both situations. Taking $\alpha_z \neq \alpha_r$ complicates the notations and, therefore, for simplicity, we will assume that $\alpha_z = \alpha_r = \sigma$. So, when emitted, the electron that goes trough the hole is represented by,

$$\psi_{\mathbf{v},0}(x,t) := \frac{1}{(\sigma^2\pi)^{3/4}} e^{-i\frac{t}{\hbar}H_0} e^{i\frac{M}{\hbar}\mathbf{v}\cdot x} e^{-\frac{x^2}{2\sigma^2}}, \tag{5.4}$$

with the variance σ smaller than the inner radius of the magnet.

The real electron wave packet, under the experiment conditions, that behaves as (5.4) when the time goes to $-\infty$ is given by the wave function (see (1.9)),

$$\psi_{\mathbf{v}}(x,t) := e^{-i\frac{t}{\hbar}H}\, W_{-}\varphi_{\mathbf{v}} = e^{-i\frac{\zeta}{\hbar v}H}\, W_{-}\varphi_{\mathbf{v}}. \tag{5.5}$$

Remember that we take $\mathbf{v} = (0,0,v)$ and that $\zeta := vt$ is the classical position of the electron, in the vertical direction, at time t.

The energy for the free wave packet (or of the perturbed wave packet at $-\infty$) is given by

$$\langle \frac{1}{2M}\mathbf{P}^2\varphi_{\mathbf{v}}, \varphi_{\mathbf{v}}\rangle = \frac{1}{2}Mv^2 + \frac{3}{4}\frac{\hbar^2}{M\sigma^2} \approx \frac{1}{2M}v^2. \tag{5.6}$$

When σ is big ($\sigma mv >> 1$) the second factor is much smaller than the first. If we take for example $\sigma mv \geq \sqrt{15}$ the second factor is less that 1/10 times the first. Therefore, when $\sigma mv >> 1$, we can suppose that the energy is given by the classical energy, $\frac{1}{2M}v^2$. With this assumption we can calculate the velocities, and the velocities times m corresponding to the energies E_1, E_2, E_3:

$$v_1 = 2.2971 \times 10^{10} cm/s, \quad mv_1 = 1.9842 \times 10^{10} cm^{-1},$$

$$v_2 = 1.8755 \times 10^{10} cm/s, \quad mv_2 = 1.6201 \times 10^{10} cm^{-1},$$

$$v_3 = 1.6775 \times 10^{10} cm/s, \quad mv_3 = 1.4491 \times 10^{10} cm^{-1}.$$

For now on we suppose that the obstacle $\tilde{K}$ is either $\tilde{K}_1$ or $\tilde{K}_2$ and that the velocity v is either v_1, v_2 or v_3.

5.2 Selection of the Parameters

We have obtained rigorous upper bounds for the difference between the exact solution to the Schrödinger equation and the Aharonov-Bohm Ansatz, and for the difference between the scattering operator and its high-velocity limit. These bounds hold for any choice of the parameters $S_1, \tilde{\delta}, \tilde{\varepsilon}, \delta$ and ε. We use this freedom to choose these parameters in a convenient way. From now on, we choose the parameter $S_1 > 0$ such that

$$r_1\rho(S_1) = 1. \tag{5.7}$$

This choice is made to optimize the error bound in Theorem 3.1. This theorem was proven using Lemmata 11.3, 11.5. For example, for the convergence of the integral on the left-hand side of equation (11.10) we need the decay of $\rho(\sigma, z)$ for large z, but for z small this factor is very large. For this reason we split this integral in two regions (where we use different estimates) introducing the parameter S_1.

Furthermore.,

$$
\begin{aligned}
&\tilde{\varepsilon} := \tfrac{\tilde{r}_2-\tilde{r}_1}{200},\\
&\tilde{\delta} := \tfrac{\tilde{h}}{100},\\
&\delta := \max(10\,\sigma, \tilde{h}),\\
&\varepsilon := \tfrac{\tilde{r}_1}{50}.
\end{aligned}
\tag{5.8}
$$

This selection was obtained using numerical estimates to optimize the error bound for the time evolution of the electron wave packet.

6 The Time Evolution of the Electron Wave Packet. Continued

LEMMA 6.1. *For the data used in the Tonomura et al. experiments, $v \in \{v_1, v_2, v_3\}$ and $\tilde{K} \in \{\tilde{K}_1, \tilde{K}_2\}$, suppose that $\sigma \in [\frac{4.5}{mv}, \tilde{r}_1/2]$ and $\zeta \in \mathbb{R}$. Then,*

$$
\begin{aligned}
&e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}}\, \widetilde{\mathbf{A}}_{\tilde{m}}^{-\infty}(z(\sigma),\sigma) \leq e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}}\, \mathbf{A}^{-\infty}(\sigma) + 10^{-420},\\
&e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}}\, \widetilde{\mathbf{A}}_{\tilde{m}}^{0}(z(\sigma),\sigma) + \tfrac{1}{2}R(\zeta, z(\sigma)) \leq e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}}\, \mathbf{A}^{0}(\sigma) + 10^{-420},\\
&e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}}\, \widetilde{\mathbf{A}}_{\tilde{m}}^{\infty}(z(\sigma),\sigma) + R(0, z(\sigma)) \leq e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}}\, \mathbf{A}^{\infty}(\sigma) + 10^{-420}.
\end{aligned}
\tag{6.1}
$$

Proof:

- First case, $\sigma \in [\sigma_0, \frac{\tilde{r}_1}{2}]$.

  As $\tilde{\omega}(\sigma)^{-1} \leq \sqrt{\frac{33}{34}}\sigma m v$, we have that

$$
1 \leq \frac{(\sigma m v)^2}{(\sigma m v)^2 - \tilde{\omega}(\sigma)^{-2}} \leq 34. \tag{6.2}
$$

  For these values of σ, $\tilde{\omega}(\sigma)^{-1} = \sqrt{2000}$. Then, using (11.23) and the experimental values we get,

$$
2.1023 \times 10^{-6} \leq z(\sigma) \leq .0673. \tag{6.3}
$$

  We also have,

$$
.0042 \leq S_1 \leq 303.8306. \tag{6.4}
$$

  Using (6.3) and (6.4) we get,

$$
(h r_2^2 \sigma^3 m^3 v^3)^{1/2}\, \left(\max(z(\sigma), S_1)\right)^{-1/2} \leq 2.9127 \times 10^5, \tag{6.5}
$$

and

$$\frac{(\sigma^4 m^2 v^2 + \zeta^2)^{1/2}}{\sigma m v} \leq (\sigma^2 + \frac{33 z(\sigma)^2}{34 \times 2000})^{1/2} \leq 0.0015. \tag{6.6}$$

Now we note that (see the definition of $R(\zeta, z(\sigma))$ in (4.30)).

$$R(\zeta, z(\sigma)) \leq \frac{m_5}{2} \frac{(\sigma^4 m^2 v^2 + z(\sigma)^2)^{1/2}}{\sigma m v} \pi^{1/2} e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}}, \qquad R(0, z(\sigma)) \leq \frac{m_5}{2} \pi^{1/2} \sigma e^{-\frac{(h - z(\sigma))^2}{2\sigma^2}}. \tag{6.7}$$

We bound the quantities $\widetilde{\mathbf{A}}^{-j}$, $j \in \{-\infty, 0, \infty\}$ uniformly for $\sigma \in [\sigma_0, \frac{\tilde{r}_1}{2}]$ and for the experimental energies and magnets, using (6.3, 6.4, 6.5, 6.7) and the smaller experimental values of $\tilde{r_1}, (\tilde{r}_2 - \tilde{r}_1), \tilde{h}$ and mv to determine the components of $\bar{m}$. We use the fact that for the values of sigma that we consider, $e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}} \leq e^{-1000}$ to obtain,

$$\begin{aligned}
&e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}} \widetilde{\mathbf{A}}^{-\infty}(z(\sigma), \sigma) \leq 10^{-420}, \\
&e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}} \widetilde{\mathbf{A}}^{0}(z(\sigma), \sigma) + \tfrac{1}{2} R(\zeta, z(\sigma)) \leq 10^{-420}, \\
&e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}} \widetilde{\mathbf{A}}^{\infty}(z(\sigma), \sigma) + R(0, z(\sigma)) \leq 10^{-420}.
\end{aligned} \tag{6.8}$$

- Second case, $\sigma \in [\frac{4.5}{mv}, \sigma_0]$. For these values of σ, $\frac{(\sigma m v)^2}{(\sigma m v)^2 + \tilde{\omega}(\sigma)^{-2}} = 34$, then by (11.23), $34\, h + \sqrt{34}\,\sqrt{33}\, h \leq z(\sigma) \leq 34\, h + \sqrt{34}\,\sqrt{\frac{33}{34}\sigma^4 m^2 v^2 + 33\, h^2}$ and by triangle inequality $z(\sigma) \leq 34h + \sqrt{33}\,\sigma^2 m v + 34h$ and then, we have that,

$$134.99\, \tilde{h} \leq z(\sigma) \leq 136.82\, \tilde{h}. \tag{6.9}$$

It can be verified that,

$$\begin{aligned}
&\max(z(\sigma), S_1) = S_1 \leq \sigma m v r_1, \\
&\max(z(\sigma), S_1)^{-1/2} (h r_2^2 \sigma^3 m^3 v^3)^{1/2} \leq \sigma m v r_2 (\tfrac{h}{r_1})^{1/2} \tfrac{1}{(1 - 5 \times 10^{-10})^{1/2}}, \\
&\tfrac{(\sigma^4 m^2 v^2 + z(\sigma)^2)^{1/2}}{\sigma m v} \leq (1.11 \times 10^{-6} + 1)^{1/2} \tfrac{136.82 \tilde{h}}{\sigma m v},
\end{aligned} \tag{6.10}$$

where in the last inequality we used (6.9). Using (6.9) again we get

$$R(0, z(\sigma)) \leq \frac{m_5}{2} \pi^{1/2} \sigma e^{-\frac{1}{2}(\frac{133.99 \tilde{h}}{\sigma})^2} \leq 10^{-10^8}. \tag{6.11}$$

Finally we obtain (6.1) using (2.19), (4.32), (6.7), (6.9), (6.10), (6.11) and the fact that $\mathcal{A}_4(\bar{m}) \leq \mathcal{A}_1(\bar{m})$ and $\mathcal{A}_5(\bar{m}) \leq \mathcal{A}_3(\bar{m})$ (note that in this case $e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}} = e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}}$).

REMARK 6.2. *For $j \in \{-\infty, 0, \infty\}$, $e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} \mathbf{A}^j(\sigma)$ is decreasing on the interval $[\frac{4.5}{mv}, \infty)$.*

Proof: Calculating the numbers $\mathbf{A}_i^j$ we find that $\mathbf{A}_i^j \geq 0$ for $i \in \{1, 1/2, -1\}$, and also $\mathbf{A}^0_{-1/2} \geq 0$. The other components of the vectors $\mathbf{A}^j$ are negative. We suppose that $j \in \{-\infty, \infty\}$, the case $j = 0$ can be done in the same way (the term $\mathbf{A}^0_{-1/2}$ is manipulated as the term $\mathbf{A}^0_{-1}$). Since $\mathbf{A}^j(\sigma) \geq 0$ and $\sigma mv \geq 4.5$, we have that $\frac{d}{d\sigma} e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}} \mathbf{A}^j \leq e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}(-b_1(\sigma)+b_2(\sigma))$, where $b_1(\sigma) = \frac{33}{34}4.5mv(\mathbf{A}^j_1\sigma + \mathbf{A}^j_{1/2}\sigma^{1/2}) \geq 0$ and $b_2 = -\frac{33}{34}4.5mv(\mathbf{A}^j_0 + \mathbf{A}^j_{-1/2}\sigma^{-1/2}) + \sum_{i\in\{1,1/2,0,-1/2\}} i\mathbf{A}^j_i \sigma^{i-1} \geq 0$. As b_1 is increasing and b_2 decreasing, $-b_1 + b_2$ is decreasing, as $-b_1(\frac{4.5}{mv}) + b_2(\frac{4.5}{mv}) \leq 0$, we have that $\frac{d}{d\sigma} e^{-\frac{1}{2\tilde{\omega}(\sigma)^2}} \mathbf{A}^j \leq 0$ for $\sigma \in [\frac{4.5}{mv}, \sigma_0]$.

□

Below we introduce a partition of an interval that is adapted to the magnitude.

DEFINITION 6.3. For any number $a > 0$ we designate by $O_a \in \mathbb{Z}$ the order of a, (i.e. O_a is such that $10^{O_a} \leq a < 10^{O_a+1}$). For an interval $[a, b], a > 0$ and a positive number N_0 we define the partition $\mathcal{P}(a, b, N_0) := \{p_i\}_{i=1}^k$ ($p_i < p_{i+1} \forall i \in \{1, \cdots, k-1\}$) as follows:

- case 1: $b \leq 10^{O_a+1}$. If $b - a \leq N_0 10^{O_a}$ we take $k = 2$, $p_1 = a$, $p_2 = b$. If $b - a > N_0 10^{O_a}$ we take $k \geq 3$, $p_1 = a$, $p_k = b$ and $p_i, i \in \{2, \cdots k-1\}$ such that $p_i < p_{i+1}$, $p_{i+1} - p_i = N_0 10^{O_a}$ for $i \in \{1, \cdots, k-2\}$ and $p_k - p_{k-1} \leq N_0 10^{0_a}$.
- case 2: $b > 10^{O_a+1}$. For every $j \in \{0, \cdots, O_b - O_a\}$ we define a set $\mathcal{P}^j$ as follows. We take $\mathcal{P}^0$ as in the case 1 but taking 10^{O_a+1} instead of b. $\mathcal{P}^{O_b - O_a}$ is taken as in the case 1 taking 10^{O_b} instead of a. If $O_b - O_a \geq 2$, for $j \in \{1, \cdots, O_b - O_a - 1\}$ we define $\mathcal{P}^j$ as in the case 1 taking 10^{O_a+j} instead of a and 10^{O_a+j+1} instead of b. Now we define $\mathcal{P}(a, b, N_0) = \cup_{j\in\{0,\cdots,O_b-O_a\}} \mathcal{P}^j$.

DEFINITION 6.4. *We denote by* $\{\Sigma_j\}_{j=1}^{11}$ *the following sets:*
$\Sigma_1 := \mathcal{P}(\frac{r_1}{\log(10)250}, \frac{r_1}{\log(10)197}, .0003)$, $\Sigma_2 := \mathcal{P}(\frac{r_1}{\log(10)197}, \frac{r_1}{\log(10)150}, .0005)$, $\Sigma_3 := \mathcal{P}(\frac{r_1}{\log(10)150}, 10^{-5}, .0008)$, $\Sigma_4 := \mathcal{P}(10^{-5}, 1.1 \times 10^{-5}, .0001)$, $\Sigma_5 := \mathcal{P}(1.1 \times 10^{-5}, 1.3 \times 10^{-5}, .0002)$, $\Sigma_6 := \mathcal{P}(1.3 \times 10^{-5}, 1.7 \times 10^{-5}, .0004)$, $\Sigma_7 := \mathcal{P}(1.7 \times 10^{-5}, 2 \times 10^{-5}, .0008)$, $\Sigma_8 := \mathcal{P}(2 \times 10^{-5}, \frac{\tilde{r}_1}{2}, .0015)$, $\Sigma_9 := \mathcal{P}(10^{-6}, \frac{r_1}{\log(10)250}, 1000)$, $\Sigma_{10} := \mathcal{P}(\sigma_0, 10^{-6}, 1000)$, $\Sigma_{11} := \mathcal{P}(\frac{4.5}{mv}, \sigma_0, .1)$.

LEMMA 6.5. *Suppose that the energies and magnets are the ones used on Tonomura et al. experiments. Let* $\mu_i \in \mathbb{R}_+, i \in \{1, 2, 3\}$. *Suppose that* $\{\mu_i\}_{i=1}^2$ *is contained in one of the sets* Σ_j *for* $j \in \{1, \cdots, 11\}$. *We take* $\mu_3 = 10^{-6}$ *if* $\{\mu_i\}_{i=1}^2$ *is contained in* Σ_j *for* $j \in \{1, \cdots, 10\}$ *and we take* $\mu_3 = \sigma_0$ *if* $\{\mu_i\}_{i=1}^2$ *is contained in the last set. We suppose furthermore, that* μ_1 *and* μ_2 *are consecutive numbers in the set where they belong and* $\mu_1 < \mu_2$. *Then, for every* $\sigma \in [\mu_1, \mu_2]$ *and every* $\zeta \in \mathbb{R}$ *with* $|\zeta| \leq z(\sigma)$ *we have that,*

$$\begin{aligned}
&c_{pp}(\sigma)I_{pp}(\mu_1,\mu_2,\mu_3) + \frac{c_{ps}(\sigma)}{2}I_{ps}(\mu_1,\mu_2,\mu_3,\zeta) + c_{sp}(\sigma)I_{sp}(\mu_1,\mu_2,\mu_3) + \frac{c_{ss}(\sigma)}{2}I_{ss}(\mu_1,\mu_2,\mu_3,\zeta) \leq \\
&4e^{-\frac{r_1^2}{2\sigma^2}} + 10^{-3}e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}\mathbf{A}^0(\sigma) + 10^{-101}, \\
&c_{pp}(\sigma)I_{pp}(\mu_1,\mu_2,\mu_3) + c_{ps}(\sigma)I_{pp}(\mu_1,\mu_2,\mu_3) + c_{sp}(\sigma)I_{sp}(\mu_1,\mu_2,\mu_3) + c_{ss}(\sigma)I_{sp}(\mu_1,\mu_2,\mu_3) \leq \\
&4e^{-\frac{r_1^2}{2\sigma^2}} + 10^{-7}e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}\mathbf{A}^\infty(\sigma) + 10^{-101},
\end{aligned} \tag{6.12}$$

where the functions I_{pp}, I_{ps}, I_{sp}, and I_{ss} are evaluated at $Z := z(\mu_2)$ if $\mu_j \leq \sigma_0$ and at $Z := \max_{j\in\{1,2\}}\{z_{\omega(\mu_2),\mu_j}(h(\mu_2))\}$, if $\mu_j \geq \sigma_0$.

Proof: We use a computer to calculate $r_1\rho(\mu_i, Z)$ for $i \in \{1,2,3\}$ and we prove that these quantities are bigger than 1. As $z(\sigma) \leq Z$ (see 11.27), $r_1\rho(\mu_i, Z) \geq 1$ for $i \in \{1,2,3\}$ implies that $|\zeta| \leq r_{\mu_1,\mu_2}$ and that $r_{\nu,\mu_3} \geq Z$, what simplifies I_{ss} (see equation (11.35)). We estimate the integrals as it is shown in the appendix using a computer, taking $\delta_0 = 1$ if $\mu_1 mv > 10$ and $\delta_0 = \frac{1}{10}$ if $\mu_1 mv \leq 10$. We use the computer again to show that (6.12) is valid with $(4e^{-\frac{r_1^2}{2\mu_1^2}} + 10^{-3}e^{-\frac{33}{34}\frac{(\mu_2 mv)^2}{2}}\mathbf{A}^0(\mu_2))$ instead of $(4e^{-\frac{r_1^2}{2\sigma^2}} + 10^{-3}e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}\mathbf{A}^0(\sigma))$, $(4e^{-\frac{r_1^2}{2\mu_1^2}} + 10^{-7}e^{-\frac{33}{34}\frac{(\mu_2 mv)^2}{2}}\mathbf{A}^\infty(\mu_2))$ instead of $(4e^{-\frac{r_1^2}{2\sigma^2}} + 10^{-7}e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}\mathbf{A}^\infty(\sigma))$, $-Z$ instead of ζ and $c_T(\mu_1)$ instead of $c_T(\sigma)$ (for $T \in \{pp, ps, sp, ss\}$). Finally by Remark 6.2 and the fact that $c_T(\sigma) \leq c_T(\mu_1)$, $I_T(\mu_1,\mu_2,\mu_3,\zeta) \leq I_T(\mu_1,\mu_2,\mu_3,-Z)$, $T \in \{pp, ps, sp, ss\}$ (see (11.27)) , we obtain (6.12).

□

6.1 The Incoming Electron Wave Packet. Continued

THEOREM 6.6. *Suppose that the magnets and energies are the ones of the experiments of Tonomura et al.. Then for every gaussian wave function with variance $\sigma \in [\frac{4.5}{mv}, \frac{\tilde{r}_1}{2}]$ and every $\zeta \in \mathbb{R}$ with $\zeta \leq -z(\sigma)$ we have,*

$$\|e^{-i\frac{\zeta}{v\hbar}H}W_-(A)\varphi_{\mathbf{v}} - \chi e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\| \leq e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}\sum_{i\in\{1,1/2,0,-1/2,-1\}}\mathbf{A}_i^{-\infty}\sigma^i + 10^{-420}, \tag{6.13}$$

where the quantities $\mathbf{A}_i^{-\infty}$ are explicit numbers that depend only on the magnet and the energy that we take (see (4.32))

Proof: Equation (6.13) is a consequence of Theorem 3.1, Remark 4.1 and Lemma 6.1.

6.2 The Interacting Electron Wave Packet. Continued

THEOREM 6.7. *Suppose that the magnets and energies are the ones of the experiments of Tonomura et al.. Then for every gaussian wave function with variance $\sigma \in [\frac{4.5}{mv}, \frac{\tilde{r}_1}{2}]$ and every $\zeta \in \mathbb{R}$ with $|\zeta| \leq z(\sigma)$ we have,*

$$\begin{aligned}&\|e^{-i\frac{\zeta}{v\hbar}H}W_-(A)\varphi_{\mathbf{v}} - \chi e^{-i\int_0^{-\infty}\hat{\mathbf{v}}\cdot A(x+\tau\mathbf{v})d\tau}e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\| \leq \\ &4e^{-\frac{r_1^2}{2\sigma^2}} + e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}\sum_{i\in\{1,1/2,0,-1/2,-1\}}(1+10^{-3})\mathbf{A}_i^0\sigma^i + 10^{-101} + 10^{-420},\end{aligned} \tag{6.14}$$

where the quantities $\mathbf{A}_i^0$ are explicit numbers that depend only on the magnet and the energy that we take (see (4.32))

Proof: Let $\sigma \in [\frac{4.5}{mv}, \frac{\tilde{r}_1}{2}]$, then there are μ_1, μ_2 and μ_3 such that μ_1, μ_2, μ_3 and σ satisfies the hypothesis of Lemma 6.5. We prove using a computer that they satisfy also the hypothesis of the Theorem 3.5. We obtain (6.14) from Theorem 3.5, Remark 4.1 and Lemmata 6.1, 6.5.

□

6.3 Outgoing Electron Wave Packet and Scattering Operator. Continued

THEOREM 6.8. *Suppose that the magnets and energies are the ones of the experiments of Tonomura et al.. Then, for every gaussian wave function with variance* $\sigma \in [\frac{4.5}{mv}, \frac{\tilde{r}_1}{2}]$ *and every* $\zeta \in \mathbb{R}$ *with* $\zeta \geq z(\sigma)$ *we have,*

$$\begin{aligned} &\| e^{-i\frac{\zeta}{v\hbar}H} W_-(A)\varphi_{\mathbf{v}} - e^{i\Phi}\chi e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}} \| \leq \\ &7e^{-\frac{r_1^2}{2\sigma^2}} + e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} \sum_{i\in\{1,1/2,0,-1/2,-1\}} (1+10^{-7})\mathbf{A}_i^{\infty}\sigma^i + 10^{-101} + 10^{-420}, \end{aligned} \tag{6.15}$$

$$\begin{aligned} &\| S\varphi_{\mathbf{v}} - e^{i\Phi}\chi\varphi_{\mathbf{v}} \| \leq \\ &7e^{-\frac{r_1^2}{2\sigma^2}} + e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} \sum_{i\in\{1,1/2,0,-1/2,-1\}} (1+10^{-7})\mathbf{A}_i^{\infty}\sigma^i + 10^{-101} + 10^{-420}, \end{aligned} \tag{6.16}$$

where the quantities $\mathbf{A}_i^{\infty}$ *are explicit numbers that depend only on the magnet and the energy that we take (see (4.32)).*

Proof: Let $\sigma \in [\frac{4.5}{mv}, \frac{\tilde{r}_1}{2}]$. Then, there are μ_1, μ_2 and μ_3 such that μ_1, μ_2, μ_3 and σ satisfies the hypothesis of Lemma 6.5. We prove using a computer that they satisfy also the hypothesis of the Theorem 3.8. We obtain (6.14) from Theorem 3.8, Remark 4.1 and Lemmata 6.1, 6.5. To get equation (6.16) we remember that to obtain the error bound in Theorem 3.8 we used the error bound for the scattering operator of Theorem 3.7. Then, the error bound that we get for the outgoing wave function in Theorem 3.8 bounds the error bound for the scattering operator.

7 Aharonov-Bohm Ansatz. Discontinuous Change of Gauge Formula from the Zero Vector Potential

In this section we denote by A the vector potential constructed in Section 4. We take also the parameters, magnets and energies introduced in Section 5.

7.1 Statement of the Aharonov-Bohm Ansatz

Let A_1 and A_2 be two differentiable magnetic potentials defined in $\mathbb{R}^3 \setminus \tilde{K}$ with curl zero and that have the same flux Φ. Suppose, furthermore, that

$$|A_i(x)| \leq C\frac{1}{1+|x|}, \; a_i(r) := \max_{x\in\mathbb{R}^3\setminus\tilde{K}, |x|\geq r} \{|A_i(x)\cdot\hat{x}|\} \in L^1(0,\infty). \tag{7.1}$$

Choose any point $x_0 \in \mathbb{R} \setminus \tilde{K}$. We define

$$\lambda_{A_2,A_1}(x) := \int_{x_0}^{x} (A_2 - A_1), \tag{7.2}$$

where the integral is over any curve in $\mathbb{R}^3 \setminus \tilde{K}$ that connects x_0 with x. This integral does not depends on the curve because both potentials have curl zero, and both have the same flux Φ. If this last condition is not true we can not define λ_{A_2,A_1}. Then,

$$A_2 = A_1 + \nabla \lambda_{A_2,A_1}. \tag{7.3}$$

The solution to the Schrödinger equation with magnetic potential A_2 and initial condition given when the time is zero by the estate ψ, is obtained in terms of the corresponding one for the magnetic potential A_1, by the change of gauge formula,

$$e^{-i\frac{t}{\hbar}H(A_2)}\psi = e^{i\lambda_{A_2,A_1}} e^{-i\frac{t}{\hbar}H(A_1)} e^{-i\lambda_{A_2,A_1}}\psi. \tag{7.4}$$

The solution to the Schrödinger equation for the vector potential A_1 that behaves as

$$e^{-i\frac{t}{\hbar}H_0}\psi \tag{7.5}$$

when the time goes to minus infinity is given by the formula (see equation 1.9),

$$e^{-i\frac{t}{\hbar}H(A_1)} W_-(A_1)\psi. \tag{7.6}$$

In other words, (7.6) is the solution to the Schrödinger equation when the initial conditions are taken at time minus infinity by (7.5). Now we give the change of gauge formula for the Schrödinger equation with initial conditions taken at time minus infinity:

$$e^{-i\frac{t}{\hbar}H(A_2)} W_-(A_2)\psi = e^{i\lambda_{A_2,A_1}(x)} e^{-i\frac{t}{\hbar}H(A_1)} W_-(A_1) e^{-i\lambda_{A_2,A_1,\infty}(-\mathbf{p})}\psi, \tag{7.7}$$

where $\lambda_{A_2,A_1,\infty}(x) := \lim_{r\to\infty} \lambda_{A_2,A_1}(rx)$. (see equation (5.8) in [3]).

Although the magnetic potential, A, constructed in Section 4 has curl equal zero, it has non zero flux. Therefore, there is no change of gauge between the vector potential zero and A. Suppose now that for every time the electron is practically localized in a region, $\mathcal{D}$, that has no holes (that is simply connected) or, in other words, in a region where $\lambda_{A,0}$ can be defined by equation (7.2) if we take curves that connects x_0 with x lying on this region. On this region A is gauge equivalent to the vector potential zero and the change of gauge formulae (7.4) should follow approximately (although not exactly, because there is not a real change of gauge between A and the zero potential). The error will depend on how much of the electron lies in the complement of $\mathcal{D}$. This is the Ansatz of Aharonov and Bohm [2]. Let us be more specific. In our case we take,

$$\mathcal{D} := (\mathbb{R}^3 \setminus \tilde{K}) \setminus \mathcal{S}, \tag{7.8}$$

where

$$\mathcal{S} := \{(x_1, x_2, 0) \in \mathbb{R}^3 : \sqrt{x_1^2 + x_2^2} > \tilde{r}_2\}. \tag{7.9}$$

For two vector potentials A_1 and A_2 whose curl is zero (and that do not necessarily have the same flux) we define the function given in (7.2) in the simply connected region $\mathcal{D}$: given $x_0 = (x_{0,1}, x_{0,2}, x_{0,3}) \in \mathcal{D}$ with $x_{0,3} < -\tilde{h}$ and x

in $\mathcal{D}$ we define,

$$\lambda_{A_2,A_1}(x) := \int_{x_0}^{x} (A_2 - A_1), \tag{7.10}$$

where the integral is over any curve in $\mathcal{D}$ connecting x_0 with x. Note that for an electron to cross from the negative vertical axis to the positive one over $\mathcal{D}$, it has to go through the hole of the magnet.

Then, we have that,

$$A_2(x) = A_1(x) + \nabla\lambda_{A_2,A_1}(x), \quad x \in \mathcal{D}. \tag{7.11}$$

We extend λ_{A_2,A_1} to $\mathbb{R}^3 \setminus \tilde{K}$ by zero without changing notation, i.e., $\lambda_{A_2,A_1}(x) = 0$, for $x \in \mathcal{S}$. Note that λ_{A_2,A_1} is discontinuous on $\mathcal{S}$.

The Ansatz of Aharonov and Bohm can be stated in the following way.

DEFINITION 7.1. *Aharonov-Bohm Ansatz with Initial Condition at Zero*
Let A_1 be a magnetic potential defined in $\mathbb{R}^3 \setminus \tilde{K}$ such curl $A_1 = 0$, and with flux not necessarily zero. Let ψ the initial data at time zero of a solution to the Schrödinger equation that stays in $\mathcal{D}$ for all times. Then, the change of gauge formula ([2], page 487),

$$e^{-i\frac{t}{\hbar}H(A_1)}\psi \approx e^{i\lambda_{A_1,0}(x)}e^{-i\frac{t}{\hbar}H_0}e^{-i\lambda_{A_1,0}(x)}\psi \tag{7.12}$$

holds.

Note that if the initial state at $t = 0$ is taken as $e^{-i\lambda_{A_1,0}(x)}\,\psi$ the Aharonov-Bohm Ansatz is the multiplication of the free solution by the Dirac magnetic factor $e^{i\lambda_{A_1,0}(x)}$ [7].

Equation (7.12) is formulated when the initial conditions are taken at time zero. Now we reformulate it taking initial conditions when the time is minus infinity and for the high velocity state $\varphi_{\mathbf{v}}$. For the high-velocity state $\varphi_{\mathbf{v}}$ and for big v, we have that,

$$e^{-i\lambda_{A_2,A_1,\infty}(-\mathbf{p})}\varphi_{\mathbf{v}} \approx e^{-i\lambda_{A_2,A_1,\infty}(-\hat{\mathbf{v}})}\varphi_{\mathbf{v}}. \tag{7.13}$$

For this statement see the proof of Theorem 5.7 of [3]. Formula (7.7) with $W_-(0) = I$, and equation (7.13) suggest the following formulation of the Aharonov-Bohm Ansatz, with initial condition at time minus infinity and for high-velocity states.

DEFINITION 7.2. *Aharonov-Bohm Ansatz with Initial condition at $-\infty$. General Potentials*
Let A_1 be a magnetic potential defined in $\mathbb{R}^3 \setminus \tilde{K}$ such curl$A_1 = 0$, and with flux not necessarily zero. Let $\psi_{\mathbf{v}}(A_1)(x,t)$,

$$\psi_{\mathbf{v}}(A_1)(x,t) := e^{-i\frac{t}{\hbar}H(A_1)}W_-(A_1)\,\varphi_{\mathbf{v}}$$

be the solution to the Schrödinger equation that behaves as

$$e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}} \tag{7.14}$$

when the time goes to minus infinity. We suppose that $\psi_{\mathbf{v}}(A_1)(x,t)$ is approximately localized in $\mathcal{D}$ for every time. Then, the following change of gauge formula follows,

$$\psi_{\mathbf{v}}(A_1)(x,t) \approx e^{i\lambda_{A_1,0}(x)} e^{-i\frac{t}{\hbar}H_0} e^{-i\lambda_{A_1,0,\infty}(-\hat{\mathbf{v}})} \varphi_{\mathbf{v}}, \tag{7.15}$$

where $\lambda_{A_1,0,\infty}(x) = lim_{r\to\infty}\lambda_{A_1,0}(rx)$.

□

Let us show that formula (7.15) can formally be derived from (7.12). We take $\psi = e^{i\lambda_{A_1,0}(x)} e^{-i\lambda_{A_1,0,\infty}(-\hat{\mathbf{v}})} \varphi_{\mathbf{v}}$ in (7.12). Then, we have that $e^{-i\frac{t}{\hbar}H(A_1)}\psi \approx e^{i\lambda_{A_1,0}(x)} e^{-i\frac{t}{\hbar}H_0} e^{-i\lambda_{A_1,0,\infty}(-\hat{\mathbf{v}})} \varphi_{\mathbf{v}}$. For big velocities, the time evolution $e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}}$ is localized near the classical position $\mathbf{v}t$ [8] . Therefore,

$$e^{i\lambda_{A_1,0}(x)} e^{-i\frac{t}{\hbar}H_0} e^{-i\lambda_{A_1,0,\infty}(-\hat{\mathbf{v}})} \varphi_{\mathbf{v}} \approx e^{i\lambda_{A_1,0}(\mathbf{v}t)} e^{-i\frac{t}{\hbar}H_0} e^{-i\lambda_{A_1,0,\infty}(-\hat{\mathbf{v}})} \varphi_{\mathbf{v}},$$

and thus, $e^{-i\frac{t}{\hbar}H(A_1)}\psi$ behaves as (7.14) when the time goes to minus infinity. Then,

$$\psi_{\mathbf{v}}(A_1)(x,t) \approx e^{-i\frac{t}{\hbar}H(A_1)}\psi \approx e^{i\lambda_{A_1,0}(x)} e^{-i\frac{t}{\hbar}H_0} e^{-i\lambda_{A_1,0,\infty}(-\hat{\mathbf{v}})} \varphi_{\mathbf{v}}$$

and (7.15) follows.

For a general C^1 vector potential A_1 with curl equal zero and flux Φ, there is a real change of gauge (given by formula (7.2)) between this potential and the vector potential A with support in the convex hull of $\tilde{K}$ constructed in Section 4. As the vector potentials A and A_1 are gauge equivalent, they define the same physics and, therefore, we can always chose the vector potential A. For this potential, $\lambda^h_{A,0,\infty}(-\hat{\mathbf{v}}) = 0$, and then, the Aharonov-Bohm Ansatz for initial conditions at minus infinity and the potential A is as follows.

DEFINITION 7.3. *Aharonov-Bohm Ansatz*

Let A be the magnetic potential constructed in Section (4).
Let $\psi_{\mathbf{v}}(x,t) := e^{-i\frac{t}{\hbar}H(A)} W_-(A)\,\varphi_{\mathbf{v}}$ be the solution to the Schrödinger equation that behaves like

$$\psi_{\mathbf{v},0} := e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}} \tag{7.16}$$

when time goes to minus infinity. We suppose that $\psi_{\mathbf{v}}$ is approximately localized in $\mathcal{D}$ for all times. Then, the following change of gauge formula holds,

$$\psi_{\mathbf{v}} \approx e^{i\lambda_{A,0}(x)} e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}}. \tag{7.17}$$

□

Observe that the Aharonov-Bohm Ansatz is the multiplication of the free solution by the Dirac magnetic factor $e^{i\lambda_{A,0}(x)}$ [7].

Note that as we noticed before, the electron -when emitted, would follow the free evolution $e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}}$ under the assumption that we take a representation where the magnetic potential (A) vanishes at this time. If we take a representation given by a general vector potential (A_1) with flux Φ, we should change the initial conditions at minus infinity by $e^{i\lambda^h_{A_1,0,\infty}(-\hat{\mathbf{v}})}e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}}$ (notice that $\lambda^h_{A_1,0,\infty}(-\hat{\mathbf{v}}) = \lambda^h_{A_1,A,\infty}(-\hat{\mathbf{v}})$).

In the following sections we give a rigorous proof that (7.17) holds and we obtain error bounds for the difference between the exact solution and the Aharonov-Bohm Ansatz. We also provide a physical interpretation of the error bound and we relate it to the probability for the electron to be outside the region $\mathcal{D}$.

8 The Time Evolution of the electron Wave Packet. Final Estimates

In this Section we use the same symbol, $e^{-i\frac{\zeta}{v\hbar}H_0}$, for the restriction of the free evolution to Λ and, moreover, we designate by $\|\cdot\|$ the norm in $L^2(\Lambda)$.

8.1 Incoming Electron Wave Packet. Final Estimates

LEMMA 8.1. *For every gaussian wave function, φ, with variance σ and for every $\zeta \in \mathbb{R}$ with $\zeta \leq -z(\sigma)$, the following estimate holds.*

$$\|\chi e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}} - e^{i\lambda_{A,0}}e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\| \leq \sqrt{2}e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} + 10^{-420}. \tag{8.1}$$

Proof: Let $\mathcal{D}_{-h}$ be the set $\{(x_1,x_2,x_3) \in \mathbb{R}^3 : x_3 \leq -h\}$. We have that, $\lambda_{A,0}(x) = 0$ and $\chi(x) = 1$ for $x \in \mathcal{D}_{-h}$. Using polar coordinates we obtain (see (3.14), (11.3) and Remark 11.1).

$$\|\chi e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}} - e^{i\lambda_{A,0}}e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\|^2 \leq \frac{4}{\pi^{3/2}}\int_{(\mathbb{R}^3\setminus\mathcal{D}_{-h}-\hat{\mathbf{v}}\zeta)\rho(\sigma,\zeta)} e^{-x^2}dx \leq 2e^{-\theta_{inv}(\sigma,z(\sigma))^2}. \tag{8.2}$$

Finally we notice that $\sqrt{2}\,e^{-\frac{\theta_{inv}(\sigma,z(\sigma))^2}{2}} \leq 10^{-434}$ for $\sigma \geq \sigma_0$.

□

Using Theorem 6.6 and Lemma 8.1 we prove that,

THEOREM 8.2. *Aharonov-Bohm Ansatz. Incoming Wave Packet*

Suppose that the magnets and energies are the ones of the experiments of Tonomura et al.. Then for every gaussian wave function with variance $\sigma \in [\frac{4.5}{mv}, \frac{\tilde{r}_1}{2}]$ and every $\zeta \in \mathbb{R}$ with $\zeta \leq -z(\sigma)$, the solution to the Schrödinger equation that behaves as (7.16) when the time goes to minus infinity, $e^{-i\frac{\zeta}{v\hbar}H}W_-(A)\varphi_{\mathbf{v}}$, is given at the time $t = \frac{\zeta}{v}$ (ζ being the vertical coordinate) by the Aharonov-Bohm Ansatz,

$$e^{i\lambda_{A,0}(x)}e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}}, \tag{8.3}$$

up to an error bound of the form:

$$\|e^{-i\frac{\zeta}{v\hbar}H}W_-(A)\varphi_{\mathbf{v}} - e^{i\lambda_{A,0}}e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\| \leq e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}}(\sum_{i\in\{1,1/2,0,-1/2,-1\}}\mathbf{A}_i^{-\infty}\sigma^i + \sqrt{2}) + 10^{-419}, \tag{8.4}$$

where the quantities $\mathbf{A}_i^{-\infty}$ *are explicit numbers that depend only on the magnet and the energy that we take (see (4.32)).*

8.2 Interacting Electron Wave Packet. Final Estimates

LEMMA 8.3. *For every gaussian wave function,* φ*, with variance* $\sigma \in [4.5/mv, \tilde{r}_1/2]$ *and for every* $\zeta \in \mathbb{R}$ *with* $|\zeta| \leq z(\sigma)$*, the following estimate holds.*

$$\|\chi e^{-i\int_0^{-\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})d\tau}e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}} - e^{i\lambda_{A,0}}e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\| \leq 2e^{-\frac{1}{2}r_1^2\rho(\sigma,\zeta)^2} \leq 2.0031\ e^{-\frac{1}{2}\frac{r_1^2}{\sigma^2}} + 2e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} + 10^{-456}. \tag{8.5}$$

Proof: We denote by $\mathcal{H}M := \{(x_1,x_2,x_3) \in \mathbb{R}^3 : \sqrt{x_1^2+x_2^2} \leq r_1\}$. For $x \in \mathcal{H}M$, $-\int_0^{-\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})d\tau = \lambda_{A,0}^h(x)$ and $\chi(x) = 1$. Using polar coordinates we obtain (see (3.14, 11.3)),

$$\|\chi e^{-i\int_0^{-\infty}\hat{\mathbf{v}}A(x+\tau\hat{\mathbf{v}})d\tau}e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}} - e^{i\lambda_{A,0}}e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\|^2 \leq \frac{4}{\pi^{3/2}}\int_{(\mathbb{R}^3\setminus\mathcal{HM}-\hat{\mathbf{v}}\zeta)\rho(\sigma,\zeta)} e^{-x^2}dx \leq 4e^{-r_1^2\rho(\sigma,\zeta)^2}. \tag{8.6}$$

The second inequality in (8.5) is proved in three cases:

- $\sigma \in [\frac{4.5}{mv}, \sigma_0]$.

  By (6.9), see also Sections 2 and 5.2,

$$e^{-r_1^2\rho(\sigma,\zeta)^2} \leq e^{-\frac{r_1^2}{(z(\sigma)-h)^2}\frac{1}{\tilde{\omega}(\sigma)^2}} \leq e^{-\frac{r_1^2}{(134.82\tilde{h})^2}\frac{33}{34}(\sigma m v)^2} \leq e^{-\frac{33}{34}(\sigma m v)^2}. \tag{8.7}$$

- $\sigma \in [\sigma_0, 3.2\times 10^{-6}]$. For these values of σ we have that $\tilde{\omega}(\sigma) = 2000^{-1/2}$. We use (6.2), (11.23) and the triangle inequality for the square-root term to obtain,

$$\frac{z(\sigma)}{\sigma^2 m v} \leq \frac{1}{mv}\left(\frac{68h}{\sigma^2} + \frac{\sqrt{2000\times 34}}{\sigma}\right). \tag{8.8}$$

  Then,

$$e^{-\frac{1}{2}\rho(\sigma,\zeta)^2 r_1^2} \leq exp\left[-\frac{r_1^2}{2\sigma^2}\frac{1}{1+\frac{1}{(mv)^2}(\frac{68h}{\sigma^2}+\frac{\sqrt{2000\times34}}{\sigma})^2}\right] = exp\left[-\frac{r_1^2}{2}\frac{1}{\sigma^2+\frac{1}{(mv)^2}(\frac{68h}{\sigma}+\sqrt{2000\times 34})^2}\right]. \tag{8.9}$$

  The function $f(\sigma) = 1/\left(\sigma^2 + \frac{1}{(mv)^2}(\frac{68h}{\sigma}+\sqrt{2000\times 34})^2\right)$ restricted to the interval $[\sigma_0, 10^{-7}]$ has derivative equal to zero on the positive axis only at the unique point of intersection of the function σ^4 and the line $\frac{68h}{(mv)^2}(68h+\sqrt{2000\times 34}\sigma)$, see Sections 2 and 5.2. For the interval $[10^{-7}, 3.2\times 10^{-6}]$ the derivative of f is zero over the positive axis in the unique solution of the equation $\sigma^4 = \frac{68\tilde{h}}{(mv)^2}(68\tilde{h} + (\sqrt{2000 \times 34} + 680)\sigma)$, see Sections 2 and 5.2. Then, it follows that,

$$\begin{aligned} &\exp\left[-\frac{r_1^2}{2}\frac{1}{\sigma^2 + \frac{1}{(mv)^2}(\frac{68\tilde{h}}{\sigma} + \sqrt{2000\times 34})^2}\right] \leq \\ &\max_{\nu \in \{\sigma_0,\, 10^{-7},\, 3.2\times 10^{-6}\}} exp\left[-\frac{r_1^2}{2}\frac{1}{\nu^2 + \frac{1}{(mv)^2}(\frac{68\tilde{h}}{\nu} + \sqrt{2000\times 34})^2}\right]. \end{aligned} \tag{8.10}$$

Evaluating (8.10) using the experimental energies and magnets, we find that,

$$e^{-\frac{1}{2}\rho(\sigma,\zeta)^2} \leq 10^{-458}. \tag{8.11}$$

- $\sigma \in [3.2 \times 10^{-6}, \frac{\tilde{r}_1}{2}]$.

  Now we use that

$$e^{-\ r_1^2\rho(\sigma,\zeta)^2} \leq e^{-\frac{r_1^2}{\sigma^2}} e^{-\left(r_1^2\rho(\sigma,z(\sigma))^2 - \frac{r_1^2}{\sigma^2}\right)} = e^{-\frac{r_1^2}{\sigma^2}} \exp\left[\frac{r_1^2}{\sigma^2}\frac{(\frac{z(\sigma)}{\sigma^2 mv})^2}{1 + (\frac{z(\sigma)}{\sigma^2 mv})^2}\right]. \tag{8.12}$$

  By (11.23) $\frac{z(\sigma)}{\sigma^2 mv}$ is decreasing as a function of σ (see Sections 2, and 5.2 and notice that $\frac{(\sigma mv)^2}{(\sigma mv)^2 - \tilde{\omega}^2}$ is decreasing on σ) and then, we have that,

$$\sqrt{2}\, exp\left[\frac{r_1^2}{2\sigma^2}\frac{(\frac{z(\sigma)}{\sigma^2 mv})^2}{1 + (\frac{z(\sigma)}{\sigma^2 mv})^2}\right] \leq \sqrt{2}\, exp\left[\frac{r_1^2}{2(3.2\times 10^{-6})^2}\frac{(\frac{z(3.2\times 10^{-6})}{(3.2\times 10^{-6})^2 mv})^2}{1 + (\frac{z(3.2\times 10^{-6})}{(3.2\times 10^{-6})^2 mv})^2}\right] \leq 1.4171. \tag{8.13}$$

REMARK 8.4. The term appearing in the middle inequality of equation (8.5) is two times the square root of the probability for the free particle to be outside the hole of the magnet ($\mathcal{H}M$) when the electron is classically at the position $(0, 0, \zeta)$:

$$\int_{\mathbb{R}^3 \setminus \mathcal{H}M} |(e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}})(x)|^2 dx = e^{-r_1^2\rho(\sigma,\zeta)^2}. \tag{8.14}$$

Recall that $\mathcal{H}M$ is defined in the proof of Lemma 8.3. Equation (8.14) is a measure of the part of the electron that hits the magnet when the classical electron (the electron under classical mechanics rules) lies within a distance less than $z(\sigma)$ from the center of the magnet. By the second inequality in (8.5) we can see that the probability of the electron to be outside the hole of the magnet at time ζ/v splits in two terms: one, $e^{-\frac{1}{2}\frac{r_1^2}{\sigma^2}}$, is due to the probability of the free electron to be outside the hole when $\zeta = 0$ (see formula (8.14)). This factor provides us an idea of the influence of the magnet over the electron given by the size of the wave packet (i.e., how much does the electron hits the magnet -see Section 9.4), and the other, $e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}$, is related with the spreading of the electron as time increases - see Section 9.5. This factor is important when σ is small, because by Heisenberg uncertainly principle when the electron is localized in a small region, its momentum is not localized and therefore the electron spreads. Those two factors are essentially the causes of all the error bounds that we have in this paper. The error bounds are mainly produced by the probability of the electron to hit the magnet when it is classically at the position $(0,0,\zeta)$, with $|\zeta| \leq z(\sigma)$. In Section 9 we provide an analysis of these terms and we give precise definitions of the size of the electron wave packet and of the opening angle, that is due to the spreading.

Using Theorem 6.7 and Lemma 8.3 we prove,

THEOREM 8.5. *Aharonov-Bohm Ansatz. Interacting Electron Wave Packet*
Suppose that the magnets and energies are the ones of the experiments of Tonomura et al.. Then, for every gaussian wave function with variance $\sigma \in [\frac{4.5}{mv}, \frac{\tilde{r}_1}{2}]$ *and every* $\zeta \in \mathbb{R}$ *with* $|\zeta| \leq z(\sigma)$ *the solution to the Schrödinger equation,* $e^{-i\frac{\zeta}{v\hbar}H} W_-(A)\varphi_{\mathbf{v}}$*, that behaves as (7.16) when time goes to minus infinity is given at the time* $t = \frac{\zeta}{v}$ *(* ζ *being the vertical coordinate) by the Aharonov-Bohm Ansatz,*

$$e^{i\lambda_{A,0}} e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}}, \tag{8.15}$$

up to an error bound of the form:

$$\begin{aligned} &\|e^{-i\frac{\zeta}{v\hbar}H} W_-(A)\varphi_{\mathbf{v}} - e^{i\lambda_{A,0}} e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\| \leq \\ &6.0031 e^{-\frac{r_1^2}{2\sigma^2}} + e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} \left(\sum_{i\in\{1,1/2,0,-1/2,-1\}} (1+10^{-3})\mathbf{A}_i^0 \sigma^i + 2\right) + 10^{-101} + 10^{-420} + 10^{-456}, \end{aligned} \tag{8.16}$$

where the quantities $\mathbf{A}_i^0$ *are explicit numbers that depend only on the magnet and the energy that we take (see (4.32)).*

8.3 Outgoing Electron Wave Packet and Scattering Operator. Final Estimates

LEMMA 8.6. *For every gaussian wave function,* φ*, with variance* σ *and for every* $\zeta \in \mathbb{R}$ *with* $\zeta \geq z(\sigma)$*, the following estimate holds.*

$$\|\chi e^{i\Phi} e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}} - e^{i\lambda_{A,0}} e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\| \leq \sqrt{2}\, e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} + 10^{-420}. \tag{8.17}$$

Proof: Let $\mathcal{D}_h$ be the set $\{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_3 \geq h\}$, note that $\lambda_{A,0}(x) = \Phi$ and $\chi(x) = 1$ for $x \in \mathcal{D}_h$. The proof follows in the same way as the proof of Lemma 8.1.

□

Theorem 6.8 and Lemma 8.6 imply the following theorem.

THEOREM 8.7. *Aharonov-Bohm Ansatz. Outgoing Electron Wave Packet*
Suppose that the magnets and energies are the ones of the experiments of Tonomura et al.. Then for every gaussian wave function with variance $\sigma \in [\frac{4.5}{mv}, \frac{\tilde{r}_1}{2}]$ *and every* $\zeta \in \mathbb{R}$ *with* $\zeta \geq z(\sigma)$ *the solution to the Schrödinger equation,* $e^{-i\frac{\zeta}{v\hbar}H} W_-(A)\varphi_{\mathbf{v}}$*, that behaves as (7.16) when the time goes to minus infinity is given at the time* $t = \frac{\zeta}{v}$ *(*ζ *being the vertical coordinate) by the Aharonov-Bohm Ansatz,*

$$e^{i\lambda_{A,0}} e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}}, \tag{8.18}$$

up to an error bound of the form:

$$\|e^{-i\frac{\zeta}{v\hbar}H}W_-(A)\varphi_{\mathbf{v}} - e^{i\lambda_{A,0}}e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\| \leq$$
$$7e^{-\frac{r_1^2}{2\sigma^2}} + e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}(\sum_{i\in\{1,1/2,0,-1/2,-1\}}(1+10^{-7})\mathbf{A}_i^{\infty}\sigma^i + \sqrt{2}) + 10^{-101} + 2\times 10^{-420}, \tag{8.19}$$

and, furthermore, the scattering operator satisfies,

$$\|S(A)\varphi_{\mathbf{v}} - e^{i\Phi}\varphi_{\mathbf{v}}\| \leq 7e^{-\frac{r_1^2}{2\sigma^2}} + e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}(\sum_{i\in\{1,1/2,0,-1/2,-1\}}(1+10^{-7})\mathbf{A}_i^{\infty}\sigma^i + \sqrt{2}) + 10^{-101} + 2\times 10^{-420}, \tag{8.20}$$

where the quantities $\mathbf{A}_i^{\infty}$ are explicit numbers that depend only on the magnet and the energy that we take (see (4.32)).

8.4 Uniform in Time Estimates for the Electron Wave Packet

REMARK 8.8. The error bound of Theorem 8.2 is smaller that the one of Theorem 8.5 and this last one is bounded by the error bound of Theorem 8.7. This is physically reasonable, because for an electron to be an interacting electron, it has to be first incoming electron and for an electron to be outgoing electron it has to be before an interacting electron, so the error should be accumulative. Let us prove this. That the error of Theorem 8.2 is smaller than the one of the Theorem 8.5 follows directly from the definitions (4.32). To prove that the error in Theorem 8.7 bounds the one of Theorem 8.5 we use again (4.32) and that (remember that $\sigma mv \geq 4.5$),

$$(1+10^{-3})\frac{\mathbf{A}_{-1}^0}{\sigma} + (2-\sqrt{2}) = (1+10^{-3})\left[\frac{\sqrt{\pi}}{2}\frac{m_5}{2}(1+1.11\times 10^{-6})^{1/2}\frac{136.82}{\sigma mv}\tilde{h}\right] + (2-\sqrt{2}) \leq$$
$$(2-10^{-3})(150(1-\tfrac{1}{50})\sigma mv - 134.99)\frac{\tilde{h}}{2}\frac{\frac{1}{\sqrt{2}}+\frac{\sqrt{3}\pi^{1/4}}{2}}{\sqrt{\sigma mv}\pi^{1/4}}m_5 \leq (2-10^{-3})(\sigma^{1/2}mvr_1 - \sigma^{-1/2}134.99\tilde{h})\frac{\mathcal{A}_3(\bar{m})}{2} \leq \tag{8.21}$$
$$(2-10^{-3})(\sigma^{1/2}\mathbf{A}_{1/2}^{-\infty} + \sigma^{-1/2}\mathbf{A}_{-1/2}^{-\infty}).$$

□

This gives us the following theorem.

THEOREM 8.9. *Aharonov-Bohm Ansatz. Time-Uniform Estimates*
Suppose that the magnets and energies are the ones of the experiments of Tonomura et al.. Then, for every gaussian wave function with variance $\sigma \in [\frac{4.5}{mv}, \frac{\tilde{r}_1}{2}]$ and every $\zeta \in \mathbb{R}$ the solution to the Schrödinger equation, $e^{-i\frac{\zeta}{v\hbar}H}W_-(A)\varphi_{\mathbf{v}}$, that behaves as (7.16) when the time goes to minus infinity is given at the time $t = \frac{\zeta}{v}$ (ζ being the vertical coordinate) by the Aharonov-Bohm Ansatz,

$$e^{i\lambda_{A,0}(x)}e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}}, \tag{8.22}$$

up to an error bound of the form:

$$\|e^{-i\frac{\zeta}{v\hbar}H}W_-(A)\varphi_{\mathbf{v}} - e^{i\lambda_{A,0}}e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\| \leq$$
$$7e^{-\frac{r_1^2}{2\sigma^2}} + e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}(\sum_{i\in\{1,1/2,0,-1/2,-1\}}(1+10^{-7})\mathbf{A}_i^{\infty}\sigma^i + \sqrt{2}) + 10^{-101} + 2\times 10^{-420}. \tag{8.23}$$

Moreover, the scattering operator satisfies,

$$\|S\varphi_{\mathbf{v}} - e^{i\Phi}\varphi_{\mathbf{v}}\| \leq 7e^{-\frac{r_1^2}{2\sigma^2}} + e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}\left(\sum_{i\in\{1,1/2,0,-1/2,-1\}}(1+10^{-7})\mathbf{A}_i^{\infty}\sigma^i + \sqrt{2}\right) + 10^{-101} + 2\times 10^{-420}. \tag{8.24}$$

The quantities $\mathbf{A}_i^{\infty}$ are explicit numbers that depend only on the magnet and the energy that we take (see (4.32)).

□

By (4.29) and (5.2) $m_i(\chi_1) \geq m_i(\chi_2)$, $i \in \{1, \cdots, 5\}$, and as $\sigma^{1/2} mvr_1 \geq \frac{134.99\,\tilde{h}}{\sigma^{1/2}}$ ($\sigma mvr_1 \geq 134.99\,\tilde{h}$, remember that $\sigma mv \geq 4.5$), we have that $\mathbf{A}^j(\sigma, v, \bar{m}(\chi_1)) \geq \mathbf{A}^j(\sigma, v, \bar{m}(\chi_2))$ (see (4.33)). We have also (see (4.32) and (4.33)) that $\mathbf{A}^{\infty}(\sigma, v_i, \bar{m}(\chi_1)) \leq \mathbf{A}^{\infty}(\sigma, v_1, \bar{m}(\chi_1))$ for $i \in \{1, 2, 3\}$ and $j \in \{1, 2\}$ (notice that $\mathcal{A}(\bar{m})_1 \geq \mathcal{A}(\bar{m})_4$ and $\mathcal{A}(\bar{m})_3 \geq \mathcal{A}(\bar{m})_5$). So if we write $\mathbf{A}_i^{\infty}(v_1, \bar{m}(\chi_1))$ in (8.23, 8.24) instead of $\mathbf{A}_i^{\infty}$ we obtain also error bounds, but now the coefficients $\mathbf{A}_i^{\infty}$ are fixed for all the magnets and velocities. Taking this into consideration we calculate the values of $\overline{\mathbf{A}}^{\infty}(v_1, \bar{m}(\chi_1))$ and we obtain the following theorem.

THEOREM 8.10. *Aharonov-Bohm Ansatz and Tonomura et al. Experiments*

Suppose that the magnets and energies are the ones of the experiments of Tonomura et al.. Then, for every gaussian wave function with variance $\sigma \in [\frac{4.5}{mv}, \frac{\tilde{r}_1}{2}]$ and every $\zeta \in \mathbb{R}$, the solution to the Schrödinger equation, $e^{-i\frac{\zeta}{v\hbar}H}W_-(A)\varphi_{\mathbf{v}}$, that behaves as (7.16) when the time goes to minus infinity is given at the time $t = \frac{\zeta}{v}$ (ζ being the vertical coordinate) by the Aharonov-Bohm Ansatz,

$$e^{i\lambda_{A,0}(x)}e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}}, \tag{8.25}$$

up to an error bound of the form:

$$\begin{aligned}&\|e^{-i\frac{\zeta}{v\hbar}H}W_-(A)\varphi_{\mathbf{v}} - e^{i\lambda_{A,0}}e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\| \leq \\ &7e^{-\frac{r_1^2}{2\sigma^2}} + e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}(1.04\times 10^{14}\sigma + 3.91\times 10^8\sigma^{1/2} - 1.41\times 10^3 - 1.14\times 10^{-2}\frac{1}{\sigma^{1/2}}) + 10^{-101} + 2\times 10^{-420}.\end{aligned} \tag{8.26}$$

Furthermore, the scattering operator satisfies,

$$\begin{aligned}&\|S\varphi_{\mathbf{v}} - e^{i\Phi}\varphi_{\mathbf{v}}\| \leq 7e^{-\frac{r_1^2}{2\sigma^2}} + e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}(1.04\times 10^{14}\sigma + 3.91\times 10^8\sigma^{1/2} - 1.41\times 10^3 - 1.14\times 10^{-2}\frac{1}{\sigma^{1/2}}) + \\ &10^{-101} + 2\times 10^{-420}.\end{aligned} \tag{8.27}$$

□

We now bound the right hand side of (8.26) by $7e^{-\frac{r_1^2}{2\sigma^2}} + \mathcal{F}(\sigma, mv)$, where $\mathcal{F}(\sigma, mv) := e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}(1.04\times 10^{14}\sigma + 3.91\times 10^8\sigma^{1/2}) + 10^{-101} + 2\times 10^{-420}$. We notice that $\mathcal{F}$ is decreasing for mv fixed and $\sigma mv \geq 4.5$. We compute $\mathcal{F}(15.5\times 10^{-10}, mv_3)$ and show that this quantity is less than 10^{-100}, it follows that $\mathcal{F}(\sigma, mv) \leq 10^{-100}$ for $\sigma \geq 15.5\times 10^{-10}$ and the experimental velocities. Then $\mathcal{F}(\sigma, mv) \leq e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}}(1.04\times 10^{14}(15.5\times 10^{-10}) + 3.91\times 10^8(15.5\times 10^{-10})^{1/2}) + 10^{-100}$ $= 177\times 10^3 e^{-\frac{33}{34}\frac{(\sigma mv)^2}{2}} + 10^{-100}$. We obtain the following theorem, that is our main result, and that is quoted as Theorem 1.1 in the introduction.

THEOREM 8.11. *Aharonov-Bohm Ansatz and Tonomura et al. Experiments. Final Estimates*

Suppose that the magnets and energies are the ones of the experiments of Tonomura et al.. Then, for every gaussian wave function with variance $\sigma \in [\frac{4.5}{mv}, \frac{\tilde{r}_1}{2}]$ *and every* $\zeta \in \mathbb{R}$*, the solution to the Schrödinger equation,* $e^{-i\frac{\zeta}{v\hbar}H} W_-(A)\varphi_{\mathbf{v}}$*, that behaves as (7.16) when the time goes to minus infinity is given at the time* $t = \frac{\zeta}{v}$ *(*ζ *being the vertical coordinate) by the Aharonov-Bohm Ansatz,*

$$e^{i\lambda_{A,0}(x)} e^{-i\frac{t}{\hbar}H_0}\varphi_{\mathbf{v}}, \tag{8.28}$$

up to an error bound of the form:

$$\begin{gathered} \|e^{-i\frac{\zeta}{v\hbar}H} W_-(A)\varphi_{\mathbf{v}} - e^{i\lambda_{A,0}} e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\| \leq \\ 7e^{-\frac{r_1^2}{2\sigma^2}} + 177 \times 10^3 e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} + 10^{-100}. \end{gathered} \tag{8.29}$$

Furthermore, the scattering operator satisfies,

$$\|S\varphi_{\mathbf{v}} - e^{i\Phi}\varphi_{\mathbf{v}}\| \leq 7e^{-\frac{r_1^2}{2\sigma^2}} + 177 \times 10^3 e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} + 10^{-100}. \tag{8.30}$$

REMARK 8.12. In the experiments of Tonomura et al. [26], they send an electron wave packet that partially hits the magnet. The part of the electron wave packet that hits the magnet does not go behind the magnet because we can see the black shadow of the magnet behind it. In other words, this part of the electron wave packet will be in the region $\{(x_1, x_2, x_3) \in \Lambda : x_3 \leq h\}$. We can bound, therefore, the probability of interaction of the electron with the magnet by the probability for the electron to not be behind the magnet for large time. We denote, as in the proof of Lemma 8.6, by $\mathcal{D}_h$ the set $\{(x_1, x_2, x_3) \in \mathbb{R}^3 : x_3 \geq h\}$. Actually $\mathcal{D}_h$ is the region behind the magnet. Then the probability of interaction of the electron with the magnet is bounded by,

$$\|\chi_{\Lambda \setminus \mathcal{D}_h} e^{-i\frac{t}{\hbar}H} W_-(A)\varphi_{\mathbf{v}}\|^2 \tag{8.31}$$

when the time goes to ∞, where $\chi_{\Lambda \setminus \mathcal{D}_h}$ is the characteristic function of the set $\Lambda \setminus \mathcal{D}_h$. We take as before $\zeta = vt$, then we have,

$$\|\chi_{\Lambda \setminus \mathcal{D}_h} e^{-i\frac{t}{\hbar}H} W_-(A)\varphi_{\mathbf{v}}\|^2 \leq (\|e^{-i\frac{\zeta}{v\hbar}H} W_-(A)\varphi_{\mathbf{v}} - e^{i\lambda_{A,0}} e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\| + \|\chi_{\Lambda \setminus \mathcal{D}_h} e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\|)^2. \tag{8.32}$$

We take $\hat{\omega}(\sigma) := \frac{1}{\sqrt{\frac{33}{34}}\sigma m v}$ and $\hat{z}(\sigma) := z_{\hat{\omega}(\sigma),\sigma}(h(\sigma))$, see Section 2. Using polar coordinates we obtain for $\zeta \geq \hat{z}(\sigma)$ (see Section 2, (3.14), (11.3) and Remark 11.1),

$$\|\chi_{\Lambda \setminus \mathcal{D}_h} e^{-i\frac{\zeta}{v\hbar}H_0}\varphi_{\mathbf{v}}\|^2 \leq \frac{1}{\pi^{3/2}} \int_{(\mathbb{R}^3 \setminus \mathcal{D}_h - \hat{\mathbf{v}}\zeta)\rho(\sigma,\zeta)} e^{-x^2} dx \leq \frac{1}{2} e^{-\theta_{inv}(\sigma, \hat{z}(\sigma))^2} = \frac{1}{2} e^{-\frac{33}{34}(\sigma m v)^2}. \tag{8.33}$$

Letting the time go to ∞ in (8.31) and using Theorem 8.11, (8.32) and (8.33) we obtain that the probability of interaction of the electron with the magnet is bounded by,

$$(7e^{-\frac{r_1^2}{2\sigma^2}} + 177001 e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} + 10^{-100})^2. \tag{8.34}$$

9 Physical Interpretation of the Error Bounds

We analyze the error bounds given in equation (8.29, 8.30). The error bounds appearing in the whole paper are produced by the same factors. Equations (8.29, 8.30) provide uniform in time error bounds that apply to all experimental magnets and energies. The behaviour of the error bound is the same for the three energies and the two magnets, so there is no loss of generality if we select a magnet and an energy in our analysis. We will use the biggest energy (E_1) and the second magnet (K_2) to provide numbers and graphics. So, for now on we take the magnet K_2 and the energy E_1.

The main factors that produce the error bound in equation (8.29, 8.30) are the terms,

1. Size of electron wave packet factor.
$$e^{-\frac{r_1^2}{2\sigma^2}}. \tag{9.1}$$

2. Opening angle of the electron wave packet factor.
$$e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}}. \tag{9.2}$$

When the variance σ is close to the radius of the magnet, (9.1) is close to 1 and (9.2) is extremely small, because in this case σmv is big. Then, when the electron is big compared to the inner radius, (9.1) is the important term, which justifies our name. When the variance is very small -such that σmv is close to 1- the factor (9.2) is close to one and (9.1) is extremely small ($\frac{r_1}{\sigma}$ is big), and then, the important factor is (9.2). But when the variance in position (σ) is small, by Heisenberg uncertainly principle the variance in momentum is big, and then, the component of the momentum transversal to the axis of the magnet is large. In consequence, the opening angle of the electron wave packet is large, and the electron spreads fast as it propagates. This justifies the name of (9.2).

By the previous discussion, we divide the analysis of the error bounds in (8.29, 8.30) in three sections: big sigma (σ close to the inner radius of the magnet), small sigma (σmv close to 1) and intermediate sigma (sigma neither big, nor small).

9.1 Big Sigma, $\sigma \in [\frac{r_1}{22}, \frac{\tilde{r}_1}{2}]$

Remember that $r_1 = \tilde{r}_1 - \varepsilon$ and that ε is defined in Section 5.2. Here $\tilde{r}_1 = 1.75 \times 10^{-4} cm$ (see Section 5.1). Then, in terms of absolute values, big sigma ranges over the interval $[7.7955 \times 10^{-6}, 8.7500 \times 10^{-5}]$. In Figure 1 we show the graphic of the error bound in (8.29) as a function of $\frac{\sigma}{r_1}$, for big sigma, and in the table below we give some representative values.

Error Bound as a Function of Sigma Over r_1 for Big Sigma.	
Sigma Over r_1	***Error Bound***
.34305	10^{-1}
.27626	10^{-2}
.23764	10^{-3}
.21170	10^{-4}
.19274	10^{-5}
.17811	10^{-6}
.16637	10^{-7}
.15668	10^{-8}
.14851	10^{-9}
.14150	10^{-10}

9.2 Intermediate Sigma, $\sigma \in [6.7591 \times 10^{-6} r_1, \frac{r_1}{22}]$, or $\sigma \in [\frac{23}{mv}, \frac{154678}{mv}]$

Remember that $mv = 1.9842 \times 10^{10}$ (see Section 5.1). Therefore, in terms of absolute values, intermediate sigma ranges over the interval $[1.1592 \times 10^{-9}, 7.7955 \times 10^{-6}]$. For these values of sigma, $\frac{r_1}{\sigma} \geq 22$ and $\sigma mv \geq 23$, and therefore, the error bound in (8.29) is less than 10^{-99}.

For intermediate sigma the probability of interaction of the electron with the magnet is less than 10^{-199} (see Remark 8.12).

9.3 Small Sigma, $\sigma \in [1.3224 \times 10^{-6} r_1, 6.7591 \times 10^{-6} r_1]$, or $\sigma \in [\frac{4.5}{mv}, \frac{23}{mv}]$

In terms of absolute values we have that $\sigma \in [2.2679 \times 10^{-10}, 1.1592 \times 10^{-9}]$. In Figure 2 we show the graphic of the error bound in (8.29) as a function of $\frac{\sigma}{r_1}$, for small sigma, and in the table below we give some representative values.

Error Bound as a Function of Sigma Over r_1 for Small Sigma.	
Sigma Over r_1	***Error Bound***
1.6001 $\times 10^{-6}$	10^{-1}
1.7234 $\times 10^{-6}$	10^{-2}
1.8384 $\times 10^{-6}$	10^{-3}
1.9467 $\times 10^{-6}$	10^{-4}
2.0492 $\times 10^{-6}$	10^{-5}
2.1469 $\times 10^{-6}$	10^{-6}
2.2403 $\times 10^{-6}$	10^{-7}
2.3299e $\times 10^{-6}$	10^{-8}
2.4162 $\times 10^{-6}$	10^{-9}
2.4996 $\times 10^{-6}$	10^{-10}

9.4 The Radius of the Electron Wave Packet

As before, we denote by $\mathcal{H}M$ the cylinder $\{(x, y, z) \in \mathbb{R}^3 : \sqrt{x^2 + y^2} \leq r_1\}$. $\mathcal{H}M$ is basically the hole of the magnet. The factor $e^{-\frac{r_1^2}{2\sigma^2}}$ is practically the square root of the probability for the free particle at time zero to be outside the hole of the magnet:

$$e^{-\frac{r_1^2}{2\sigma^2}} = \left\| \chi_{\mathbb{R}\setminus\mathcal{H}M} (\frac{1}{\sigma^2\pi})^{3/4} e^{-\frac{x^2}{2\sigma^2}} \right\|. \tag{9.3}$$

This factor represents the part of the electron wave packet that hits the magnet or goes outside (the square root appears because our estimations are in norm and not in probability). It is natural to have this factor in the error bound because we are only modeling the particles that go trough the hole. This factor is significant only when the variance is close to the inner radius of the magnet. As the proximity of the electron to the magnet increases the error in equations (8.29, 8.30), it is important to define intuitively what is the meaning of this closeness or, in other words, what is the size of the electron wave packet. We agree that the free electron is actually localized in configuration space in a ball centered in the classical position $\mathbf{v}t$ and with radius chosen in such a way that the probability of finding the electron on this ball is 99%. We measure the radius of the wave packet at the time $t = 0$ - when the free particle is in the center of the magnet - and denote it by $R(\sigma)$. Then, we have:

$$R := R(\sigma) = 2.382\ \sigma.$$

The error due to the part of the electron that hits the magnet (9.3) is practically zero (smaller than 10^{-99}) when $R \leq .1082 r_1 (R \leq 1.8556 \times 10^{-5})$. In Figure 3 we show the error bound of equation (8.29) as a function of the radius of the wave packet over r_1 for big sigma, $\sigma \in [\frac{r_1}{22}, \frac{\tilde{r}_1}{2}]$ $(.1082\, r_1 \leq R \leq .5102\, r_1)$.

Even when the size of the wave packet is comparable to the inner radius of the magnet we have error bounds extremely small. We give some data to show this behavior:

Error Bound as a Function of the Radius of the Wave Packet Over r_1 for Big Sigma.	
Radius of the Wave Packet over r_1	***Error Bound***
.81716	10^{-1}
.65806	10^{-2}
.56606	10^{-3}
.50427	10^{-4}
.45911	10^{-5}
.42425	10^{-6}
.39629	10^{-7}
.37322	10^{-8}
.35376	10^{-9}
.33703	10^{-10}

9.5 The Opening Angle of the Electron Wave Packet

Although it is impossible to define an opening angle of the electron, because it is everywhere, we agree to say that the free electron (in momentum representation) is actually in a ball, $B_P(M\mathbf{v})$ with center the classical momentum $(M\mathbf{v})$ and radius P such that there is a 99% probability for the electron to have its momentum within this ball. We define the opening angle, $\omega(\sigma)$, in the obvious way (see Figure 4),

$$\sin(\frac{\omega(\sigma)}{2}) := \frac{P}{Mv} = \frac{2.382}{\sigma m v}.$$

When sigma is big, the opening angle is very small and when sigma is small, the opening angle is big, this is nothing more than Heisenberg uncertainty principle.

The factor $e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}}$ of the error bound (8.29, 8.30) has the following interpretation in terms of the opening angle:

$$e^{-\frac{33}{34}\frac{(\sigma m v)^2}{2}} = e^{-2.7535(\frac{1}{\sin(\omega(\sigma)/2)})^2}.$$

This factor is practically zero (smaller than 10^{-100}) when $\omega \leq 11.8$ degrees ($\sigma \geq 1.1592 \times 10^{-9}$ or $\sigma m v \geq 23$), and then, it begins to increase as ω increases (σ decreases). In Figure 5 we show the error bound in equation (8.29) as a function of the opening angle for small sigma, $\sigma \in [1.3224 \times 10^{-6} r_1, 6.7591 \times 10^{-6} r_1]$, and in the table below we give some representative values.

Error Bound as a Function of the Opening Angle for Small Sigma.	
Opening Angle (degrees)	***Error Bound***
51.8407	10^{-1}
47.8885	10^{-2}
44.7231	10^{-3}
42.1135	10^{-4}
39.9137	10^{-5}
38.0265	10^{-6}
36.3842	10^{-7}
34.9380	10^{-8}
33.6517	10^{-9}
32.4979	10^{-10}

10 Conclusions

In Theorems 8.2, 8.5, 8.7, 8.9, 8.10 and 8.11 we found the time evolution of the electron up to an error bound that we provide explicitly. The approximate wave function of the electron that we give is the one given by the Aharonov-Bohm Ansatz. It coincides also with the part of the electron wave packet that goes through the hole of the magnet in Tonomura et al. experiments [26]. As we noticed before (see Section 7.1) the Aharonov-Bohm Ansatz is valid if the evolution of the exact wave packet is localized at every time in a simply connected region, with no holes, (for example in (7.8)). The main factors that produce the error bounds are the size of the wave packet (see (9.1)) and the opening angle (see (9.2)). These factors can be understood also in terms of the part of the wave packet that hits the magnet when the electron crosses the hole of the magnet (see Remark 8.4) and, therefore, they are related with the part of the electron not localized in a simple connected region (see (7.8)) at every time. In Section 9 we analyzed the error bounds and we have shown that our estimates for the time evolution are valid for a rather big interval that starts when the opening angle is close to 55 degrees ($\sigma \approx 1.3224 \times 10^{-6} r_1$) and ends when the size of the wave packet is close to the inner radius of the magnet (close to r_1). We have shown also that the error bounds decrease very fast -exponentially- as the variance gets away from the extremes of the interval. For intermediate sigma ($\sigma \in [6.7591 \times 10^{-6} r_1, \frac{r_1}{22}]$), the time evolution given by Aharonov-Bohm Ansatz (8.28) differs from the exact one only by a number less than 10^{-99} in norm. As it is shown in Remark 8.12 and Section 9.2, for intermediate sigma, the probability that the electron wave packet interacts with the magnet is smaller than 10^{-199} and so, there are no fields in the trajectory of the electron. Nevertheless, the solution is the one given by the Aharonov-Bohm Ansatz (8.28) and it is affected by the vector potential A by a phase factor $e^{i\lambda_{A,0}}$. This phase factor is the one that appears in Tonomura et al. experiments [26]. Although in the experiments of Tonomura et al. [25] there is no interaction with the magnetic field, there is an interaction with the impenetrable magnet. Tonomura et al. [26] argued that it is not necessary to consider the part of the electron wave packet that hits the magnet -they used a rather big one- because the shadow of the magnet was clearly seen in the hologram. Our results show that it would be quite interesting to perform an experiment with a medium size electron wave packet with an intermediate sigma. One could use, as well, a bigger magnet. Our results show that quantum mechanics predicts in this case the interference patterns observed by Tonomura et al. [26] with extraordinary precision.

In the Aharonov-Bohm Ansatz the electron is not accelerated, it propagates following the free evolution, with the wave function multiplied by a phase. As we prove that the Aharonov-Bohm Ansatz approximates the exact solution with an error bound uniform in time that can be smaller that 10^{-99} in norm, we rigorously prove that quantum mechanics predicts that no force acts on the electron, in agreement with the experimental results of Caprez et al. [6].

Summing up, the experiments of Tonomura et al. [17, 25, 26] give a strong evidence of the existence of the interference fringes predicted by Franz [9] and by Aharonov and Bohm [2]. The experiment of Caprez et al. [6] verifies that the interference fringes are not due to a force acting on the electron, and the results of this paper rigorously prove that quantum mechanics theoretically predicts the observations of these experiments in a extremely precise way. This gives a firm experimental and theoretical basis to the existence of the Aharonov-Bohm effect [2], namely, that magnetic fields act at a distance on charged particles, even if they are identically zero in the space accessible to the particles, and that this action at a distance is carried by the circulation of the magnetic potential, what gives magnetic potentials a real physical significance.

11 Appendix A. Estimates for the Free Evolution of gaussian States

In this appendix we prove estimates for the solutions to the boosted free Schrödinger equation,

$$i\frac{\partial}{\partial z}\varphi(x,z) = H_1\varphi(x,z), \;\; \varphi(x,0) = \varphi(x), \tag{11.1}$$

where the boosted free Hamiltonian H_1 is defined in (3.11).

Recall that under the change of variable $t := z/v$, the solutions of (11.1) are solutions of the boosted free Schrödinger equation with Hamiltonian $e^{-im\mathbf{v}\cdot x}H_0\, e^{im\mathbf{v}\cdot x}$. Classically, a particle that starts at the origin with velocity $\mathbf{v}=(0,0,v)$, will be located at time t at the position $(0,0,z)$. At the high-velocity limit, the quantum evolution follows the classical one and the parameter z can be taken as the position in the $z-$direction of the particle. We consider the case where the initial state is gaussian,

$$\varphi(x) := \frac{1}{(\sigma^2\pi)^{3/4}}\, e^{-x^2/2\sigma^2}, \tag{11.2}$$

with variance σ. The solution to (11.1) is given by,

$$e^{-izH_1}\varphi = e^{-izmv/2}\,\frac{\sigma^{3/2}}{\pi^{3/4}}\,\frac{1}{(\sigma^2+iz/mv)^{3/2}}\, e^{-(x-z\hat{\mathbf{v}})^2/2(\sigma^2+iz/mv)}. \tag{11.3}$$

we will often use the following simple result.

REMARK 11.1. *Suppose that $C_3 \leq C_2 \leq C_1 \leq 0$. Then,*

1.

$$\int_{C_3}^{C_2} e^{-z^2}dz \leq e^{-C_1^2}\int_{C_3-C_1}^{C_2-C_1} e^{-z^2}dz \leq e^{-C_1^2}\int_0^{\infty} e^{-z^2}dz. \tag{11.4}$$

2.

$$\int_{C_3}^{C_2} z^2 e^{-z^2}dz \leq -\frac{C_2}{2}e^{-C_2^2}+\frac{C_3}{2}e^{-C_3^2}+\frac{1}{2}e^{-C_1^2}\int_{C_3-C_1}^{C_2-C_1} e^{-z^2}dz \leq e^{-C_1^2}(-\frac{C_2}{2}+\frac{1}{2}\int_0^{\infty} e^{-z^2}dz). \tag{11.5}$$

Proof:

$$\int_{C_3}^{C_2} e^{-z^2}dz \leq e^{-C_1^2}\int_{C_3}^{C_2} e^{-(z^2-C_1^2)} \leq e^{-C_1^2}\int_{C_3}^{C_2} e^{(z-C_1)^2}dz,$$

where we used that, $z^2-C_1^2 \geq (z-C_1)^2$. This proves 1. Furthermore, 2 follows from 1 and the following equation.

$$\int_{C_3}^{C_2} \frac{z}{2}\, 2z\, e^{-z^2}dz = -\frac{z}{2}e^{-z^2}|_{C_3}^{C_2} + \int_{C_3}^{C_2}\frac{1}{2}e^{-z^2}dz.$$

.

LEMMA 11.2. *Let f be a bounded complex valued function with support contained in D. Then, for $z \geq h$ and $d \geq h-z$,*

1.

$$\left\|f(x)e^{-izH_1}\varphi\right\| \leq \frac{\|f\|_\infty}{\sqrt{2}}\, e^{-\theta_{inv}(\sigma,z)^2/2}, \tag{11.6}$$

2.

$$\left\|f(x+d\hat{\mathbf{v}})e^{-izH_1}\varphi\right\| \leq \frac{\|f\|_\infty}{\sqrt{2}}\, e^{-\theta_{inv}(\sigma,z,z+d,h(\sigma))^2/2}, \tag{11.7}$$

3.

$$\left\|f(x)e^{-izH_1}\varphi\right\| \leq \frac{\|f\|_\infty}{\pi^{1/4}}\, e^{-\theta_{inv}(\sigma,z)^2/2}\sqrt{2h}\, r_2\, \rho(z)^{3/2}. \tag{11.8}$$

Proof: We use the function $\rho(z)$ defined in (2.9),

$$\left\|f(x)e^{-izH_1}\varphi\right\|^2 \leq \frac{\|f\|_\infty^2}{\pi^{3/2}} \int_{(D-\hat{\mathbf{v}}z)\rho(z)} e^{-x^2}\,dx \leq \frac{\|f\|_\infty^2}{\pi^{1/2}} \int_{(-h-z)\rho(z)}^{(h-z)\rho(z)} d\mu\, e^{-\mu^2}\left(1-e^{-r_2^2\rho(z)^2}\right) \leq$$

$$\frac{\|f\|_\infty^2}{\pi^{1/2}} e^{-\theta_{inv}(\sigma,z)^2} \int_{-2h\rho(z)}^{0} dz\, e^{-z^2}\left(1-e^{-r_2^2\rho(z)^2}\right), \tag{11.9}$$

where in the last inequality we used (11.4). Equation (11.6) follows from (11.9). Equation (11.7) is obtained similarly. Equation (11.8) follows from (11.9) and the estimate,

$$\int_{-2h\rho(z)}^{0} dz e^{-z^2}\left(1-e^{-r_2^2\rho(z)^2}\right) \leq 2hr_2^2\rho(z)^3.$$

LEMMA 11.3. *Let f be a bounded complex valued function with support contained in D. Then, for $Z \geq h, s \geq 0$,*

$$\begin{aligned}&\textstyle\int_Z^\infty \left\|f(x)e^{-izH_1}\varphi\right\| \leq \frac{\|f\|_\infty}{\sqrt{2}} e^{-\theta_{inv}(\sigma,Z)^2/2}(\max(Z,s)-Z)+\\ &\textstyle\frac{\|f\|_\infty}{\pi^{1/4}} e^{-\theta_{inv}(\sigma,\max(Z,s))^2/2}\sqrt{2h}r_2(\sigma m v)^{3/2}\int_{\max(Z,s)}^\infty \frac{1}{(\sigma^4 m^2 v^2+\zeta^2)^{3/4}}d\zeta.\end{aligned} \tag{11.10}$$

Proof: We prove the lemma writing the integral in the left hand side of (11.10) as follows

$$\int_Z^\infty \left\|f(x)e^{-izH_1}\varphi\right\| = \int_Z^{\max(Z,s)} \left\|f(x)e^{-izH_1}\varphi\right\| + \int_{\max(Z,s)}^\infty \left\|f(x)e^{-izH_1}\varphi\right\|$$

and using (11.6) in the first integral, (11.8) in the second, and the fact that $\theta_{inv}(\sigma,z)^2$ is increasing in z for $z \geq h$.

□

LEMMA 11.4. *Let $g : \mathbb{R}^3 \to \mathbb{C}^3$ be bounded and with support contained in D and let $z \geq h$. Then,*

1.

$$\left\|g(x)\cdot\mathbf{p}\, e^{-izH_1}\varphi\right\| \leq \frac{\|g\|_\infty}{\pi^{1/4}\sigma} e^{-\theta_{inv}(\sigma,z)^2/2}\left[\frac{-\theta_{inv}(\sigma,z)}{2}+\frac{3\sqrt{\pi}}{4}\right]^{1/2}. \tag{11.11}$$

2.

$$\left\|g(x)\cdot\mathbf{p}\, e^{-izH_1}\varphi\right\| \leq \frac{\|g\|_\infty}{\pi^{1/4}\sigma} e^{-\theta_{inv}(\sigma,z)^2/2}\left[4(\sigma m v)^2+2\right]^{1/2}\sqrt{h}\, r_2\, \rho(z)^{3/2}. \tag{11.12}$$

Proof:

$$\left\|g(x)\cdot\mathbf{p}\, e^{-izH_1}\varphi\right\|^2 \leq \frac{\|g\|_\infty^2}{\pi^{3/2}\sigma^2}\int_{(D-\hat{\mathbf{v}}z)\rho(z)} x^2\, e^{-x^2}\,dx \leq \frac{\|g\|_\infty^2}{\pi^{1/2}\sigma^2}[\Upsilon(\sigma,z)+\Theta(\sigma,z)]\left(1-e^{-r_2^2\rho(z)^2}\right), \tag{11.13}$$

where Θ and Υ are defined in Section 2. Equation (11.11) follows from (11.13) applying the last inequality in (11.4) to $\Upsilon(\sigma,z)$ and the last inequality in (11.5) to $\Theta(\sigma,z)$. Furthermore, using the middle inequality in (11.5) we obtain that,

$$\Theta(\sigma,z) \leq \frac{\rho(z)}{2}[(z-h)e^{-(z-h)^2\rho^2(z)}-(z+h)e^{-(z+h)^2\rho^2(z)}] + \frac{1}{2}e^{-\theta_{inv}(\sigma,z)^2}\int_{-2h\rho(z)}^{0} e^{-z^2}\,dz. \tag{11.14}$$

Note that,

$$e^{-(z-h)^2\rho(z)^2} - e^{-(z+h)^2\rho(z)^2} \leq e^{-\theta_{inv}(\sigma,z)^2} 4zh\rho(z)^2, \tag{11.15}$$

$$\int_{-2h\rho(z)}^{0} e^{-z^2}\, dz \leq 2h\rho(z). \tag{11.16}$$

Writing $z-h = z+h-2h$ in (11.14) we obtain that,

$$\Theta(\sigma,z) \leq \frac{\rho(z)}{2}(z+h)e^{-\theta_{inv}(\sigma,z)^2} 4zh\rho(z)^2 \leq e^{-\theta_{inv}(\sigma,z)^2} 4h\rho(z)(\sigma m v)^2. \tag{11.17}$$

Moreover, applying the middle inequality in (11.4) to $\Upsilon(\sigma,z)$ we prove that,

$$\Upsilon(\sigma,z) \leq e^{-\theta_{inv}(\sigma,z)^2}\, 2h\,\rho(z). \tag{11.18}$$

Equation (11.12) follows from (11.13, 11.17, 11.18).

LEMMA 11.5. *Let $g: \mathbb{R}^3 \to \mathbb{C}^3$ be bounded and with support contained in D. Then, for any $Z \geq h$ with $\theta_{inv}(\sigma,Z) \geq 1$, $s \geq 0$,*

$$\begin{aligned} \textstyle\int_Z^\infty \left\|g(x)\cdot \mathbf{p}\, e^{-izH_1}\varphi\right\| &\leq \tfrac{\|g\|_\infty}{\pi^{1/4}\sigma} e^{-\theta_{inv}(\sigma,Z)^2/2}\left(\tfrac{|\theta_{inv}(\sigma,Z)|^{1/2}}{\sqrt{2}} + \tfrac{\sqrt{3}\,\pi^{1/4}}{2}\right)(\max(Z,s)-Z) + \\ & \tfrac{\|g\|_\infty}{\pi^{1/4}\sigma} e^{-\theta_{inv}(\sigma,\max(Z,s))^2/2}\left(2\sigma m v + \sqrt{2}\right)\sqrt{h}\ r_2(\sigma m v)^{3/2} \textstyle\int_{\max(Z,s)}^\infty (\sigma^4 m^2 v^2 + \zeta^2)^{-3/4}. \end{aligned} \tag{11.19}$$

Proof: We split the integral in the left hand side of (11.19) as follows

$$\int_Z^\infty \left\|g(x)\cdot \mathbf{p}\, e^{-izH_1}\varphi\right\| = \int_Z^{\max(Z,s)} \left\|g(x)\cdot \mathbf{p}\, e^{-izH_1}\varphi\right\| + \int_{\max(Z,s)}^\infty \left\|g(x)\cdot \mathbf{p}\, e^{-izH_1}\varphi\right\|$$

and using (11.11) in the first integral, (11.12) in the second, and the fact that the functions $e^{-x/2}\sqrt{x}, e^{-x/2}\,x^{1/4}$ are decreasing for $x \geq 1$ (notice also that $\theta_{inv}(\sigma,z)^2$ is increasing in z for $z \geq h$).

REMARK 11.6. *Suppose that z, $\zeta \in \mathbb{R}^+$, s and b are real numbers such that $z \geq \zeta$, $s \geq z - 2\zeta$, $b > 0$. Then,*

1. *In any interval $I := [\sigma_1,\sigma_2]$ such that $\forall \sigma \in I, -\theta_{inv}(\sigma,z,s,\zeta) \geq \sqrt{1/2}$,*

$$\Upsilon(\sigma,z,s,\zeta)e^{-b\rho(\sigma,z)^2} \leq \max[\Upsilon(\sigma_1,z,s,\zeta)e^{-b\rho(\sigma_1,z)^2}, \Upsilon(\sigma_2,z,s,\zeta)e^{-b\rho(\sigma_2,z)^2}]. \tag{11.20}$$

2. *In any interval $I := [\sigma_1,\sigma_2]$ such that $\forall \sigma \in I, -\theta_{inv}(\sigma,z,s,\zeta) \geq \sqrt{3/2}$,*

$$\Theta(\sigma,z,s,\zeta)e^{-b\rho(\sigma,z)^2} \leq \max[\Theta(\sigma_1,z,s,\zeta)e^{-b\rho(\sigma_1,z)^2}, \Theta(\sigma_2,z,s,\zeta)e^{-b\rho(\sigma_2,z)^2}]. \tag{11.21}$$

Proof: We give the proof of 1. The proof of 2 is similar. We have that

$$\frac{\partial}{\partial \sigma}\Upsilon(\sigma,z,s,\zeta)\, e^{-b\rho(\sigma,z)^2} = \frac{1}{\sigma}\frac{m^2v^2}{(\sigma^4 m^2 v^2+z^2)}\left(\left(\frac{z}{mv}\right)^2-\sigma^4\right) e^{-b\rho(\sigma,z)^2}\Big[e^{-(\zeta+s)^2\rho(\sigma,z)^2}(\zeta+s)\rho(\sigma,z)- \tag{11.22}$$
$$e^{-(z-\zeta)^2\rho(\sigma,z)^2}(z-\zeta)\rho(\sigma,z)\ -2b\,\rho(\sigma,z)^2\,\Upsilon(\sigma,z,s,\zeta)\Big].$$

As the function $e^{-x^2}x$ is decreasing for $x \geq 1/\sqrt{2}$, the term in the square brackets is (11.22) is negative. Then, the left-hand side of (11.22) is different from zero for $\sigma \in I$ if $\sqrt{z/mv} \notin I$ and otherwise, it is negative for $\sigma < \sqrt{z/mv}$ and it is positive for $\sigma > \sqrt{z/mv}$. This proves 1.

□

Remember that $z_{\tilde{\omega},\sigma}(h)$ is defined in Section 2. It is given by,

$$z_{\tilde{\omega},\sigma}(h) = \frac{h(\sigma mv)^2}{(\sigma mv)^2-\tilde{\omega}^{-2}} + \frac{\sigma mv}{((\sigma mv)^2-\tilde{\omega}^{-2})^{1/2}}\left(\tilde{\omega}^{-2}\sigma^2+h^2\left(\frac{(\sigma mv)^2}{(\sigma mv)^2-\tilde{\omega}^{-2}}-1\right)\right)^{1/2}. \tag{11.23}$$

REMARK 11.7. *Suppose that $\sigma_2 \leq \sigma \leq \sigma_1$. Then,*

$$z_{\tilde{\omega},\sigma}(\zeta) \leq \max(z_{\tilde{\omega},\sigma_1}(\zeta), z_{\tilde{\omega},\sigma_2}(\zeta)). \tag{11.24}$$

Proof: Note that as a function of σ, $\rho(\sigma,z)$ is increasing for $\sigma \leq \sqrt{z/mv}$ and that it is decreasing for $\sigma > \sqrt{z/mv}$. Suppose that $z_{\tilde{\omega},\sigma_1}(\zeta) \leq z_{\tilde{\omega},\sigma}(\zeta)$. Then, $\sigma \leq \sqrt{z/mv}$, because if $\sigma > \sqrt{z/mv}$,

$$\tilde{\omega}^{-1} = -\theta_{inv}(\sigma_1, z_{\tilde{\omega},\sigma_1}(\zeta), z_{\tilde{\omega},\sigma_1}(\zeta),\zeta) < -\theta_{inv}(\sigma, z_{\tilde{\omega},\sigma_1}(\zeta), z_{\tilde{\omega},\sigma_1}(\zeta),\zeta),$$

since, $-\theta_{inv}(\sigma,z,z,\zeta) = (z-\zeta)\rho(\sigma,z)$ and as $-\theta_{inv}$ is increasing in $z \geq 0$, this implies that $z_{\tilde{\omega},\sigma}(\zeta) < z_{\tilde{\omega},\sigma_1}(\zeta)$. Then, $\sigma_2 < \sigma \leq \sqrt{z/mv}$, and it follows that,

$$\tilde{\omega}^{-1} = -\theta_{inv}(\sigma, z_{\tilde{\omega},\sigma}(\zeta), z_{\tilde{\omega},\sigma}(\zeta),\zeta) \geq -\theta_{inv}(\sigma_2, z_{\tilde{\omega},\sigma}(\zeta), z_{\tilde{\omega},\sigma}(\zeta),\zeta).$$

But as also,

$$\tilde{\omega}^{-1} = -\theta_{inv}(\sigma_2, z_{\tilde{\omega},\sigma_2}(\zeta), z_{\tilde{\omega},\sigma_2}(\zeta),\zeta),$$

and $-\theta_{inv}$ is increasing in $z \geq 0$, we have that $z_{\tilde{\omega},\sigma}(\zeta) \leq z_{\tilde{\omega},\sigma_2}(\zeta)$.

LEMMA 11.8. *Let μ_i, $i \in \{1,2,3\}$ belong to $\mathbb{R}_+$. Suppose that the following conditions are satisfied,*

1. *Either $\mu_i \leq \sigma_0$, $i \in \{1,2,3\}$, or $\mu_i \geq \sigma_0$, $i \in \{1,2,3\}$.*

2. *$\mu_i \leq \mu_3$, $i \in \{1,2\}$, or $\mu_i \geq \mu_3$, $i \in \{1,2\}$.*

We define $\mu_{\max} := \max(\mu_1, \mu_2)$*,* $\mu_{\min} := \min(\mu_1, \mu_2)$ *and take* $\nu = \mu_{\max}$*, if* $\mu_i \geq \mu_3, i \in \{1,2\}$ *and* $\nu = \mu_{\min}$*, if* $\mu_i \leq \mu_3, i \in \{1,2\}$*. We denote by* $Z := z(\mu_{\max})$*, if* $\mu_i \leq \sigma_0$*; and* $Z := \max_{i\in\{1,2\}}\{z_{\tilde{\omega}(\mu_{\max}),\mu_i}(h(\mu_{\max}))\}$*, if* $\mu_i \geq \sigma_0$*. We suppose that* $Z \geq z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))$*. Let* $f : \mathbb{R}^3 \times \mathbb{R}_+ \times \mathbb{R} \to \mathbb{C}$ *be a complex valued function and we take* $f_{\sigma,z}(x) := f(x, \sigma, z)$*. Suppose the support of* $f_{\sigma,z}$ *is contained in* $K - [0, (z(\sigma) - \zeta - z)]\hat{\mathbf{v}}$ *for some* $\zeta \in \mathbb{R}$*, every* $\sigma \in \mathbb{R}_+$ *and every* $z \in \mathbb{R}$ *with* $z + \zeta \leq z(\sigma)$*. Then, for every gaussian wave function* φ *with variance* $\sigma \in [\mu_{\min}, \mu_{\max}]$*,*

$$\int_0^{z(\sigma)-\zeta} \left\| f_{\sigma,z}(x) e^{-izH_1} e^{-i\zeta H_1} \varphi \right\| \leq \frac{\|f\|_\infty}{\pi^{1/4}} I_{ps}(\mu_1, \mu_2, \mu_3, \zeta), \tag{11.25}$$

where,

$$\begin{aligned} I_{ps}(\mu_1, \mu_2, \mu_3, \zeta) &:= \pi^{1/4}\, z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max})) \max_{\mu_i\in\{\mu_1,\mu_2\}} e^{-\frac{r_1^2}{2}\rho(\mu_i, z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max})))^2} + \pi^{1/4} \max\{-\zeta, 0\} \\ &\max_{\mu_i\in\{\mu_1,\mu_2\}} e^{-\frac{r_1^2}{2}\rho(\mu_i,\zeta)^2} + \sum_{\mu_i\in\{\nu,\mu_3\}} \int_{z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))}^{Z} \Upsilon(\mu_i, \tau, Z, h(\mu_{\max}))^{1/2} e^{-\frac{r_1^2}{2}\rho(\mu_i,\tau)^2} d\tau. \end{aligned} \tag{11.26}$$

Proof: It follows from equation (11.23) that $z(\sigma) \leq z_{\tilde{\omega}(\sigma),\sigma}(h(\mu_{\max}))$. If $\mu_i \geq \sigma_0$ then $\tilde{\omega}(\sigma) = \tilde{\omega}(\mu_{\max})$ for $\sigma \in [\mu_{\min}, \mu_{\max}]$. It follows from Remark 11.7 that $z(\sigma) \leq \max_{i\in\{1,2\}}\{z_{\tilde{\omega}(\mu_{\max}),\mu_i}(h(\mu_{\max}))\} = Z$. If $\mu_i \leq \sigma_0$ then from formula (11.23) and the definition of $\tilde{\omega}(\sigma)$ we have that $z_{\tilde{\omega}(\sigma),\sigma}(h(\mu_{\max})) \leq z_{\tilde{\omega}(\mu_{\max}),\mu_{\max}}(h(\mu_{\max})) = z(\mu_{\max})$. We conclude that

$$z(\sigma) \leq Z, \tag{11.27}$$

and then,

$$\int_0^{z(\sigma)-\zeta} dz\, \left\| f_{\sigma,z}(x) e^{-izH_1} e^{-i\zeta H_1} \varphi \right\| \leq \int_0^{Z-\zeta} dz\, \left\| f_{\sigma,z}(x) e^{-izH_1} e^{-i\zeta H_1} \varphi \right\|. \tag{11.28}$$

As in (11.9) we prove that

$$\left\| f_{\sigma,z}(x) e^{-izH_1} e^{-i\zeta H_1} \varphi \right\|^2 \leq \frac{\|f\|_\infty^2}{\pi^{1/2}} \Upsilon(\sigma, z+\zeta, Z, h(\mu_{\max}))\, e^{-r_1^2 \rho(\sigma, z+\zeta)^2}. \tag{11.29}$$

Then,

$$\begin{aligned} &\int_0^{Z-\zeta} \left\| f_{\sigma,z}(x) e^{-izH_1} e^{-i\zeta H_1} \varphi \right\| dz \leq \tfrac{\|f\|_\infty}{\pi^{1/4}} \Big[\max(\textstyle\int_\zeta^0 \Upsilon(\sigma, z, Z, h(\mu_{\max}))^{1/2} e^{-\frac{r_1^2}{2}\rho(\sigma,z)^2}, 0) + \\ &\textstyle\int_0^{z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))} \Upsilon(\sigma, z, Z, h(\mu_{\max}))^{1/2}\, e^{-\frac{r_1^2}{2}\rho(\sigma,z)^2} + \int_{z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))}^{Z} \Upsilon(\sigma, z, Z, h(\mu_{\max}))^{1/2}\, e^{-\frac{r_1^2}{2}\rho(\sigma,z)^2} \Big] \leq \\ &\tfrac{\|f\|_\infty}{\pi^{1/4}} \Big[\pi^{1/4} \max(-\zeta, 0) e^{-\frac{r_1^2}{2}\rho(\sigma,\zeta)^2} + \pi^{1/4}\, z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max})) e^{-\frac{r_1^2}{2}\rho(\sigma, z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max})))^2} + \\ &\textstyle\int_{z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))}^{Z} \Upsilon(\sigma, z, Z, h(\mu_{\max}))^{1/2}\, e^{-\frac{r_1^2}{2}\rho(\sigma,z)^2} \Big], \end{aligned} \tag{11.30}$$

where we used that, $\Upsilon \leq \sqrt{\pi}$. If $z \geq z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))$, it follows from Remark 11.7 that $z \geq z_{\sqrt{2},\sigma}(h(\mu_{\max}))$ for every σ belonging to the interval limited by ν and μ_3. We complete the proof of the lemma using (11.20) in the integral in the right-hand side of (11.30), and for the other two terms we argue as in the proof of (11.20).

□

Using the proof of the preceding lemma, we prove the following,

LEMMA 11.9. *Suppose that the hypothesis of the Lemma 11.8 are fulfilled and furthermore, assume that the support of $f_{\sigma,z}$ is contained in K for every $\sigma \in \mathbb{R}_+$ and every $z \in \mathbb{R}$. Then, for every $\zeta \in \mathbb{R}$ with $|\zeta| \leq z(\sigma)$,*

$$\int_0^{z(\sigma)-\zeta} \left\| f_{\sigma,z}(x) e^{-izH_1} e^{-i\zeta H_1} \varphi \right\| \leq \frac{\|f\|_\infty}{\pi^{1/4}} 2 I_{pp}(\mu_1, \mu_2, \mu_3), \tag{11.31}$$

where,

$$I_{pp}(\mu_1, \mu_2, \mu_3) := I_{ps}(\mu_1, \mu_2, \mu_3, 0). \tag{11.32}$$

and

$$\int_0^{z(\sigma)} \left\| f_{\sigma,z}(x) e^{-izH_1} \varphi \right\| \leq \frac{\|f\|_\infty}{\pi^{1/4}} I_{pp}(\mu_1, \mu_2, \mu_3). \tag{11.33}$$

LEMMA 11.10. *Let $\mu_i, \mu_{max}, \mu_{min}, \nu$ and Z be as in Lemma 11.8. We suppose furthermore that $Z \geqq z_{\sqrt{\frac{2}{3}},\nu,\mu_3}(h(\mu_{max}))$ and $r_1 \rho(\mu_i, z_{\sqrt{2},\nu,\mu_3}(h(\mu_{max}))) \geq 1$ for $i \in \{1,2\}$. Let $g : \mathbb{R}^3 \times \mathbb{R}_+ \times \mathbb{R} \to \mathbb{C}^3$ be a complex vector valued function and we take $g_{\sigma,z}(x) := g(x,\sigma,z)$. Suppose that the support of $g_{\sigma,z}$ is contained in $K - [0, z(\sigma) - \zeta - z]\hat{\mathbf{v}}$ for some $\zeta \in \mathbb{R}$, all $\sigma \in \mathbb{R}_+$ and for all z with $z + \zeta \leq z(\sigma)$. Then, for every gaussian wave function φ with variance $\sigma \in [\mu_{min}, \mu_{max}]$,*

$$\int_0^{z(\sigma)-\zeta} \left\| g_{\sigma,z}(x) \cdot \mathbf{p}\, e^{-izH_1} e^{-i\zeta H_1} \varphi \right\| dz \leq \frac{\|g\|_\infty}{\pi^{1/4}\, \sigma} I_{ss}(\mu_1, \mu_2, \mu_3, \zeta) \tag{11.34}$$

where,

$$I_{ss}(\mu_1,\mu_2,\mu_3,\zeta) := \frac{\pi^{1/4}}{\sqrt{2}}\, z_{\sqrt{\frac{2}{3}},\nu,\mu_3}(h(\mu_{\max}))\max_{\mu_i\in\{\mu_1,\mu_2\}}(e^{-\frac{r_1^2}{2}\rho(\mu_i,z_{\sqrt{\frac{2}{3}},\nu,\mu_3}(h(\mu_{\max})))^2})+$$

$$\frac{\pi^{1/4}}{\sqrt{2}}\,\max\{-\zeta,0\}\max_{\mu_i\in\{\mu_1,\mu_2\}}(e^{-\frac{r_1^2}{2}\rho(\mu_i,\zeta)^2})+$$

$$\pi^{1/4}\, z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))\max_{\mu_i\in\{\mu_1,\mu_2\}}(r_1\rho(\mu_i,z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max})))e^{-\frac{r_1^2}{2}\rho(\mu_i,z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max})))^2})+$$

$$\pi^{1/4}\,\max(-\zeta,0)\left\{\begin{array}{c}\max_{\mu_i\in\{\mu_1,\mu_2\}}(r_1\rho(\mu_i,\zeta)e^{-\frac{r_1^2}{2}\rho(\mu_i,\zeta)^2}),\ if\ |\zeta|\leq r_{\mu_1,\mu_2}\\ e^{-1/2},\ if\ |\zeta|>r_{\mu_1,\mu_2}\end{array}\right\}+$$

$$\pi^{1/4}\, z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))\max_{\mu_i\in\{\mu_1,\mu_2\}}(e^{-\frac{r_1^2}{2}\rho(\mu_i,z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max})))^2})+ \tag{11.35}$$

$$\pi^{1/4}\,\max(-\zeta,0)\max_{\mu_i\in\{\mu_1,\mu_2\}}(e^{-\frac{r_1^2}{2}\rho(\mu_i,\zeta)^2})+$$

$$\sum_{\mu_i\in\{\nu,\mu_3\}}\int_{z_{\sqrt{\frac{2}{3}},\nu,\mu_3}(h(\mu_{\max}))}^{Z}\Theta(\mu_i,\tau,Z,h(\mu_{\max}))^{1/2}e^{-\frac{r_1^2}{2}\rho(\mu_i,\tau)^2}d\tau+$$

$$\sum_{\mu_i\in\{\nu,\mu_3\}}\max(\int_{z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))}^{\min(r_{\nu,\mu_3},Z)}\Upsilon(\mu_i,\tau,Z,h(\mu_{\max}))^{1/2}r_1\rho(\mu_i,\tau)e^{-\frac{r_1^2}{2}\rho(\mu_i,\tau)^2}d\tau,0)+$$

$$\sum_{\mu_i\in\{\nu,\mu_3\}}\int_{\min(r_{\nu,\mu_3},Z)}^{Z}\Upsilon(\mu_i,\tau,Z,h(\mu_{\max}))^{1/2}e^{-1/2}d\tau+$$

$$\sum_{\mu_i\in\{\nu,\mu_3\}}\int_{z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))}^{Z}\Upsilon(\mu_i,\tau,Z,h(\mu_{\max}))^{1/2}e^{-\frac{r_1^2}{2}\rho(\mu_i,\tau)^2}]d\tau.$$

Proof: By (11.27),

$$\int_0^{z(\sigma)-\zeta}\left\|g_{\sigma,z}(x)\cdot\mathbf{p}e^{-izH_1}e^{-i\zeta H_1}\varphi\right\|\leq\int_0^{Z-\zeta}\left\|g_{\sigma,z}(x)\cdot\mathbf{p}e^{-izH_1}e^{-i\zeta H_1}\varphi\right\|. \tag{11.36}$$

Estimating as in the proof of (11.13) we prove that,

$$\left\|g_{\sigma,z}(x)\cdot\mathbf{p}e^{-izH_1}e^{-i\zeta H_1}\varphi\right\|^2\leq\frac{\|g\|_\infty^2}{\pi^{1/2}\sigma^2}\left[\Theta(\sigma,z+\zeta,Z,h(\mu_{max}))+\right.$$
$$\left.\Upsilon(\sigma,z+\zeta,Z,h(\mu_{\max}))(1+r_1^2\rho(\sigma,z+\zeta)^2)\right]e^{-r_1^2\rho(\sigma,z+\zeta)^2}. \tag{11.37}$$

We have that,

$$\int_0^{Z-\zeta}\left\|g_{\sigma,z}(x)\cdot\mathbf{p}\,e^{-izH_1}e^{-i\zeta H_1}\varphi\right\|\,d\tau\leq\frac{\|g\|_\infty}{\pi^{1/4}\,\sigma}\sum_{j=1}^{7}I_j, \tag{11.38}$$

where,

$$I_1 := max(\int_\zeta^0\left(\Theta(\sigma,\tau,Z,h(\mu_{\max}))\,e^{-r_1^2\rho(\sigma,\tau)^2}\right)^{1/2}d\tau,0)+$$
$$\int_0^{z_{\sqrt{\frac{2}{3}},\nu,\mu_3}(h(\mu_{\max}))}\left(\Theta(\sigma,\tau,Z,h(\mu_{\max}))\,e^{-r_1^2\rho(\sigma,\tau)^2}\right)^{1/2}d\tau, \tag{11.39}$$

$$I_2 := \int_{z_{\sqrt{\frac{2}{3}},\nu,\mu_3}(h(\mu_{\max}))}^{Z}\left(\Theta(\sigma,\tau,Z,h(\mu_{\max}))\,e^{-r_1^2\rho(\sigma,\tau)^2}\right)^{1/2}d\tau, \tag{11.40}$$

$$I_3 := max(\int_{\zeta}^{0} \left(\Upsilon(\sigma,\tau,Z,h(\mu_{\max}))\, r_1^2 \rho(\sigma,\tau)^2 e^{-r_1^2\rho(\sigma,\tau)^2}\right)^{1/2}\, d\tau, 0)$$
$$+\int_{0}^{z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))} \left(\Upsilon(\sigma,\tau,Z,h(\mu_{\max}))\, r_1^2 \rho(\sigma,\tau)^2 e^{-r_1^2\rho(\sigma,\tau)^2}\right)^{1/2}\, d\tau, \tag{11.41}$$

$$I_4 := \int_{z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))}^{\max(z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max})),\min(r_{\nu,\mu_3},Z))} \left(\Upsilon(\sigma,\tau,Z,h(\mu_{\max}))\, r_1^2 \rho(\sigma,\tau)^2 e^{-r_1^2\rho(\sigma,\tau)^2}\right)^{1/2}\, d\tau, \tag{11.42}$$

$$I_5 := \int_{\max(z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max})),\min(r_{\nu,\mu_3},Z))}^{Z} \left(\Upsilon(\sigma,\tau,Z,h(\mu_{\max}))\, r_1^2 \rho(\sigma,\tau)^2 e^{-r_1^2\rho(\sigma,\tau)^2}\right)^{1/2}\, d\tau, \tag{11.43}$$

$$I_6 := \max(\int_{\zeta}^{0} \left(\Upsilon(\sigma,\tau,Z,h(\mu_{\max}))\, e^{-r_1^2\rho(\sigma,\tau)^2}\right)^{1/2}\, d\tau, 0)+$$
$$\int_{0}^{z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))} \left(\Upsilon(\sigma,\tau,Z,h(\mu_{\max}))\, e^{-r_1^2\rho(\sigma,\tau)^2}\right)^{1/2}\, d\tau, \tag{11.44}$$

$$I_7 := \int_{z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))}^{Z} \left(\Upsilon(\sigma,\tau,Z,h(\mu_{\max}))\, e^{-r_1^2\rho(\sigma,\tau)^2}\right)^{1/2}\, d\tau. \tag{11.45}$$

Since $\Upsilon \leq \sqrt{\pi}$ and $\Theta \leq \sqrt{\pi}/2$ we have that,

$$I_1 + I_6 \leq \pi^{1/4} \left(\tfrac{1}{\sqrt{2}}\, \max(-\zeta,0)\, e^{-\frac{r_1^2}{2}\rho(\sigma,\zeta)^2} + \tfrac{1}{\sqrt{2}}\, z_{\sqrt{\frac{2}{3}},\nu,\mu_3}(h(\mu_{\max}))\, e^{-\frac{r_1^2}{2}\rho(\sigma,z_{\sqrt{\frac{2}{3}},\nu,\mu_3}(h(\mu_{\max})))^2} \right)$$
$$+\pi^{1/4} \left(\max(-\zeta,0)\, e^{-\frac{r_1^2}{2}\rho(\sigma,\zeta)^2} + z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))\, e^{-\frac{r_1^2}{2}\rho(\sigma,z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max})))^2} \right). \tag{11.46}$$

By Remark 11.6

$$I_2 \leq \sum_{\mu_i \in \{\nu,\mu_3\}} \int_{z_{\sqrt{\frac{2}{3}},\nu,\mu_3}(h(\mu_{\max}))}^{Z} \left(\Theta(\mu_i,\tau,Z,h(\mu_{\max}))\, e^{-r_1^2\rho(\mu_i,\tau)^2}\right)^{1/2}\, d\tau, \tag{11.47}$$

$$I_7 \leq \sum_{\mu_i \in \{\nu,\mu_3\}} \int_{z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))}^{Z} \left(\Upsilon(\mu_i,\tau,Z,h(\mu_{\max}))\, e^{-r_1^2\rho(\mu_i,\tau)^2}\right)^{1/2}\, d\tau. \tag{11.48}$$

Moreover, since $xe^{-x^2/2}$ is increasing for $0 \leq x < 1$ and decreasing for $x \geq 1$,

$$I_3 \leq \pi^{1/4}\, \max(-\zeta,0) \left\{ \begin{array}{c} r_1\rho(\sigma,\zeta)e^{-\frac{r_1^2}{2}\rho(\sigma,\zeta)^2},\ if\ |\zeta| \leq r_{\mu_1,\mu_2} \\ e^{-1/2},\ if\ |\zeta| > r_{\mu_1,\mu_2} \end{array} \right\}$$
$$+\pi^{1/4}\, z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))\, r_1\, \rho(\sigma, z_{\sqrt{2},\nu,\mu_3})\, e^{-\frac{r_1^2}{2}\rho(\sigma,z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max})))^2}. \tag{11.49}$$

By Remark 11.6, if $\tau \geq z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))$,

$$\Upsilon(\sigma,\tau,Z,h(\mu_{\max})) \leq \max_{\mu_i \in \{\nu,\mu_3\}} \Upsilon(\mu_i,\tau,Z,h(\mu_{\max})). \tag{11.50}$$

By (11.50) and as $x\,e^{-x}$ takes its maximum at $x = 1$,

$$I_5 \leq \sum_{\mu_i \in \{\nu, \mu_3\}} \int_{\max(z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max})),\min(r_{\nu,\mu_3},Z))}^{Z} \left(\Upsilon(\mu_i, \tau, Z, h(\mu_{\max}))\, e^{-1}\right)^{1/2} d\tau. \tag{11.51}$$

Note that if $r_1^2 \rho(\mu_i, \tau)^2 \geq 1, \mu_i \in \{\nu, \mu_3\}$ then, $r_1^2 \rho(\sigma, \tau)^2 \geq 1, \forall \sigma$ between ν and μ_3 . Hence, as in the proof of Remark 11.6 we prove that,

$$\begin{aligned} & r_1^2 \rho(\sigma, \tau)^2 \Upsilon(\sigma, \tau, Z, h(\mu_{\max}))\, e^{-r_1^2 \rho(\sigma,\tau)^2} \chi_{\cap_{\mu_i \in \{\nu,\mu_3\}} \{r_1^2 \rho(\mu_i,\tau)^2 \geq 1\}}(\tau) \\ & \leq \max_{\mu_i \in \{\nu, \mu_3\}} r_1^2 \rho(\mu_i, \tau)^2 \Upsilon(\mu_i, \tau, Z, h(\mu_{\max}))\, e^{-r_1^2 \rho(\mu_i,\tau)^2} \chi_{\cap_{\mu_i \in \{\nu,\mu_3\}} \{r_1^2 \rho^2(\mu_i,\tau) \geq 1\}}(\tau), \end{aligned} \tag{11.52}$$

and then,

$$I_4 \leq \sum_{\mu_i \in \{\nu, \mu_3\}} \int_{z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max}))}^{\max(z_{\sqrt{2},\nu,\mu_3}(h(\mu_{\max})),\min(r_{\nu,\mu_3},Z))} \left(r_1^2 \rho(\mu_i, \tau)^2\, \Upsilon(\mu_i, \tau, Z, h(\mu_{\max}))\, e^{-r_1^2 \rho(\mu_i,\tau)^2}\right)^{1/2} d\tau. \tag{11.53}$$

To obtain equation (11.34), we use (11.38, 11.46–11.49, 11.51, 11.53) and we argue as in the proofs of Remark 11.6 to estimate equations (11.46) and (11.49).

□

Using the proof of the preceding lemma we prove the following,

LEMMA 11.11. *Suppose that the hypothesis of the Lemma 11.10 are fulfilled, assume furthermore, that the support of $g_{\sigma,z}$ is contained in K, for all $\sigma \in \mathbb{R}_+$ and for all z. Then, for every $\zeta \in \mathbb{R}$ with $|\zeta| \leq z(\sigma)$ and every gaussian wave function φ with variance $\sigma \in [\mu_{min}, \mu_{max}]$,*

$$\int_0^{z(\sigma)-\zeta} \left\| g_{\sigma,z}(x) \cdot \mathbf{p}\, e^{-izH_1} e^{-i\zeta H_1} \varphi \right\| dz \leq \frac{\|g\|_\infty}{\pi^{1/4}\,\sigma} 2 I_{sp}(\mu_1, \mu_2, \mu_3), \tag{11.54}$$

where,

$$I_{sp}(\mu_1, \mu_2, \mu_3) := I_{ss}(\mu_1, \mu_2, \mu_3, 0). \tag{11.55}$$

And

$$\int_0^{z(\sigma)} \left\| g_{\sigma,z}(x) \cdot \mathbf{p}\, e^{-izH_1} \varphi \right\| dz \leq \frac{\|g\|_\infty}{\pi^{1/4}\,\sigma} I_{sp}(\mu_1, \mu_2, \mu_3). \tag{11.56}$$

LEMMA 11.12. *Let $f : \mathbb{R}^3 \to \mathbb{C}$ be bounded and with support contained in D. Then, for $Z \geq h$, and ζ such that $\zeta \leqq Z$,*

$$\int_0^{Z-\zeta} \left\| f(x + (Z - (z + \zeta))\hat{\mathbf{v}}) e^{-izH_1} e^{-i\zeta H_1} \varphi \right\| dz \leq (Z - \zeta) \frac{\|f\|_\infty}{\sqrt{2}}\, e^{-\frac{1}{2}\theta_{inv}(\sigma,Z)^2}. \tag{11.57}$$

Proof: Estimating as in the proof of(11.9) we prove that,

$$\left\| f(x + (Z-(z+\zeta))\hat{\mathbf{v}})e^{-izH_1}\varphi \right\|^2 \leq \frac{\|f\|_\infty^2}{\pi^{3/2}} \int_{(-Z-h)\rho(\sigma,z+\zeta)}^{(-Z+h)\rho(\sigma,z+\zeta)} e^{-z^2}\, dz\, \pi \int_0^{r_2\rho(\sigma,z+\zeta)} e^{-r^2} 2r\, dr$$
$$\leq \frac{\|f\|_\infty^2}{2} e^{-\theta_{inv}(\sigma,Z)^2}, \tag{11.58}$$

where we used (11.4).

LEMMA 11.13. *Let $g : \mathbb{R}^3 \to C^3$ be bounded and with support contained in D, suppose that $\theta_{inv}(\sigma, Z)^2 \geq \frac{1}{2}$. Then, for $Z \geq h$, and ζ such that $\zeta \leq Z$, we have that,*

$$\int_0^{Z-\zeta} \left\| g(x + (Z-(z+\zeta))\hat{\mathbf{v}}) \cdot \mathbf{p}\, e^{-izH_1} e^{-i\zeta H_1}\varphi \right\| dz \leq (Z-\zeta)\frac{\|g\|_\infty}{\pi^{1/4}\sigma} e^{-\frac{1}{2}\theta_{inv}(\sigma,Z)^2} \left[\frac{-\theta_{inv}(\sigma,Z)}{2} + \frac{3\sqrt{\pi}}{4}\right]^{1/2}. \tag{11.59}$$

Proof: The lemma is proven estimating as in the proof of (11.11) using Remark 11.1.

12 Appendix B. Upper Bounds for the Integrals

In this appendix we prove upper bounds for the integrals appearing in the terms I_{ps}, I_{pp}, I_{ss} and I_{sp} (see (11.26), (11.32), (11.35), (11.55)).

Suppose that $Z \geq s \geq \zeta, \delta_0 > 0$. Designate $\sqrt{\mathbb{N}} := \{0, 1, \sqrt{2}, \sqrt{3}, \cdots\}$. We denote,

$$\{Z_1, Z_2, \cdots, Z_K\} := \sqrt{\delta_0}\sqrt{\mathbb{N}} \cap [-\theta_{inv}(\sigma, s, s, \zeta), -\theta_{inv}(\sigma, Z, Z, \zeta)], \tag{12.1}$$

where $Z_1 < Z_2 < \cdots < Z_K$. As $-\theta_{inv}(\sigma, \tau, \tau, \zeta)$ is increasing as a fuction of τ we have that,

$$s \leq z_{Z_1^{-1},\sigma}(\zeta) < z_{Z_2^{-1},\sigma}(\zeta) < z_{Z_3^{-1},\sigma}(\zeta) < \cdots < z_{Z_K^{-1},\sigma}(\zeta) \leq Z, \tag{12.2}$$

LEMMA 12.1. *Suppose that $Z \geq s \geq \zeta, r > 0$, and let $f : \mathbb{R} \to \mathbb{R}$ satisfy $f(\tau) \geq \tau - 2\zeta$. Then,*

$$\int_s^Z d\tau \Upsilon(\sigma,\tau,f(\tau),\zeta)^{1/2} \leq$$
$$\frac{\pi^{1/4}}{\sqrt{2}} \left[e^{-\frac{1}{2}\theta_{inv}(\sigma,s,s,\zeta)^2}(z_{Z_1^{-1},\sigma}(\zeta) - s) + \sum_{j=1}^{K-1} e^{-\frac{1}{2}Z_j^2} (z_{Z_{j+1}^{-1},\sigma}(\zeta) - z_{Z_j^{-1},\sigma}(\zeta)) + e^{-\frac{1}{2}Z_K^2}(Z - z_{Z_k^{-1},\sigma}(\zeta))\right], \tag{12.3}$$

$$\int_s^Z d\tau \Upsilon(\sigma,\tau,f(\tau),\zeta)^{1/2} e^{-\frac{r_1^2}{2}\rho(\tau)^2} \leq \frac{\pi^{1/4}}{\sqrt{2}}[e^{-\frac{r_1^2}{2}\rho(z_{Z_1^{-1},\sigma}(\zeta))^2} e^{-\frac{1}{2}\theta_{inv}(\sigma,s,s,\zeta)^2}(z_{Z_1^{-1},\sigma}(\zeta) - s) +$$
$$\sum_{j=1}^{K-1} e^{-\frac{r_1^2}{2}\rho(z_{Z_{j+1}^{-1},\sigma}(\zeta))^2} e^{-\frac{1}{2}Z_j^2} (z_{Z_{j+1}^{-1},\sigma}(\zeta) - z_{Z_j^{-1},\sigma}(\zeta)) + e^{-\frac{r_1^2}{2}\rho(Z)^2} e^{-\frac{1}{2}Z_k^2} (Z - z_{Z_k^{-1},\sigma}(\zeta))], \tag{12.4}$$

$$\int_s^Z d\tau \Theta(\sigma,\tau,f(\tau),\zeta)^{1/2} e^{-\frac{r_1^2}{2}\rho(\tau)^2} \leq \frac{1}{\sqrt{2}}[e^{-\frac{r_1^2}{2}\rho(z_{Z_1^{-1},\sigma}(\zeta))^2} e^{-\frac{1}{2}\theta_{inv}(\sigma,s,s,\zeta)^2}(Z_1 + \sqrt{\pi}/2)^{1/2}(z_{Z_1^{-1},\sigma}(\zeta) - s) +$$
$$\sum_{j=1}^{K-1} e^{-\frac{r_1^2}{2}\rho(z_{Z_{j+1}^{-1},\sigma}(\zeta))^2} e^{-\frac{1}{2}Z_j^2} (Z_{j+1} + \sqrt{\pi}/2)^{1/2} (z_{Z_{j+1}^{-1},\sigma}(\zeta) - z_{Z_j^{-1},\sigma}(\zeta)) +$$
$$e^{-\frac{r_1^2}{2}\rho(Z)^2} e^{-\frac{1}{2}Z_k^2} (\theta_{inv}(\sigma,Z,Z,\zeta) + \sqrt{\pi}/2)^{1/2} (Z - z_{Z_k^{-1},\sigma}(\zeta))]. \tag{12.5}$$

If moreover, $r_1\rho(Z) \geq 1$,

$$\int_s^Z d\tau \Upsilon(\sigma,\tau,f(\tau),\zeta)^{1/2}\, r_1\rho(\tau) e^{-\frac{r_1^2}{2}\rho(\tau)^2} \leq \frac{\pi^{1/4}}{\sqrt{2}}[r_1\rho(z_{Z_1^{-1},\sigma}(\zeta))$$

$$e^{-\frac{r_1^2}{2}\rho(z_{Z_1^{-1},\sigma}(\zeta))^2}\, e^{-\frac{1}{2}\theta_{inv}(\sigma,s,s,\zeta)^2}(z_{Z_1^{-1},\sigma}(\zeta)-s) + \sum_{j=1}^{K-1} r_1\rho(z_{Z_{j+1}^{-1},\sigma}(\zeta)) e^{-\frac{r_1^2}{2}\rho(z_{Z_{j+1}^{-1},\sigma}(\zeta))^2}\, e^{-\frac{1}{2}Z_j^2}\,(z_{Z_{j+1}^{-1},\sigma}(\zeta) - z_{Z_j^{-1},\sigma}(\zeta)) +$$

$$r_1\rho(Z)e^{-\frac{r_1^2}{2}\rho(Z)^2}\, e^{-\frac{1}{2}Z_k^2}\,(Z - z_{Z_k^{-1},\sigma}(\zeta))\,]. \tag{12.6}$$

Proof: We split the integral in the left-hand side of (12.3) as follows,

$$\int_s^Z d\tau \Upsilon(\sigma,\tau,f(\tau),\zeta)^{1/2} = \int_s^{z_{Z_1^{-1},\sigma}(\zeta)} d\tau \Upsilon(\sigma,\tau,f(\tau),\zeta)^{1/2} + \sum_{j=1}^{K-1}\int_{z_{Z_j^{-1},\sigma}(\zeta)}^{z_{Z_{j+1}^{-1},\sigma}(\zeta)} d\tau \Upsilon(\sigma,\tau,f(\tau),\zeta)^{1/2} + \int_{z_{Z_K^{-1},\sigma}(\zeta)}^{Z} d\tau \Upsilon(\sigma,\tau,f(\tau),\zeta)^{1/2}, \tag{12.7}$$

and we apply (11.4). This proves (12.3). (12.4) is proved in a similar way. Equation (12.5) is proven in the same way, but using (11.5). Finally, we prove (12.6) as above, using (11.4) and observing that the function $x\, e^{-x^2/2}$ is decreasing for $x \geq 1$.

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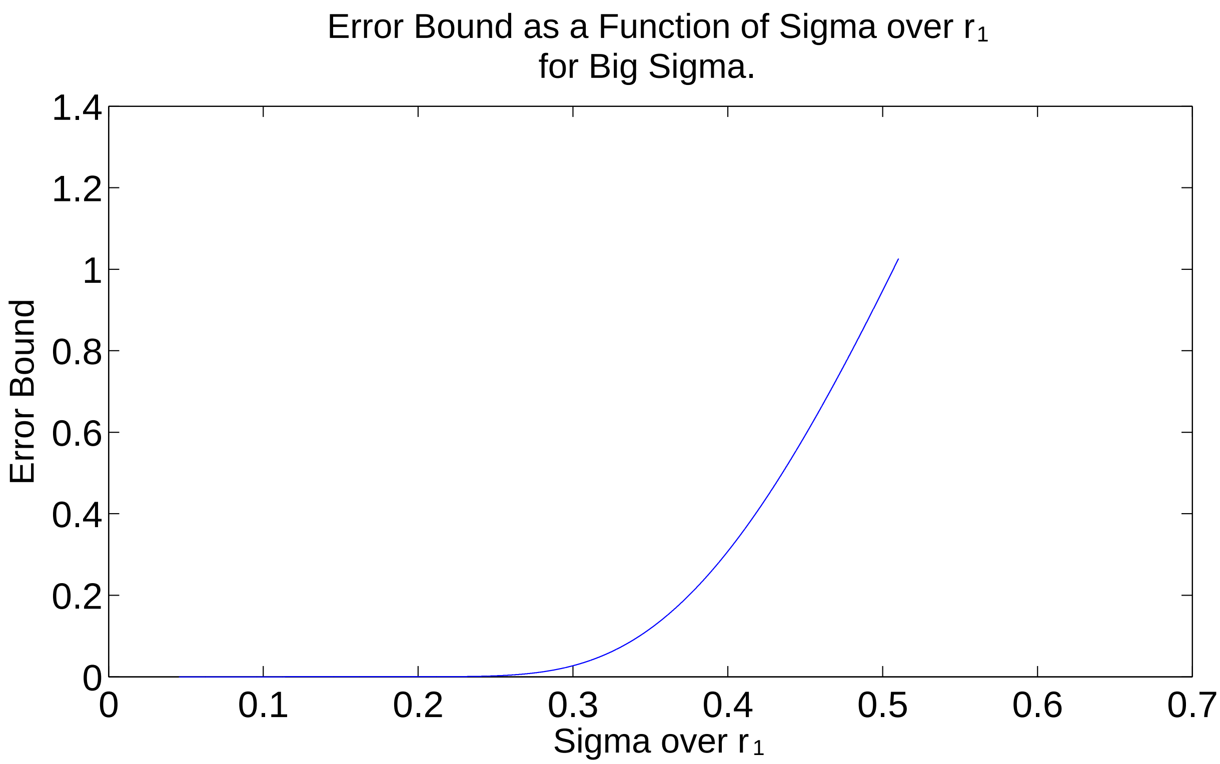

Figure 1: Error bound as a function of σ over r_1 for big sigma

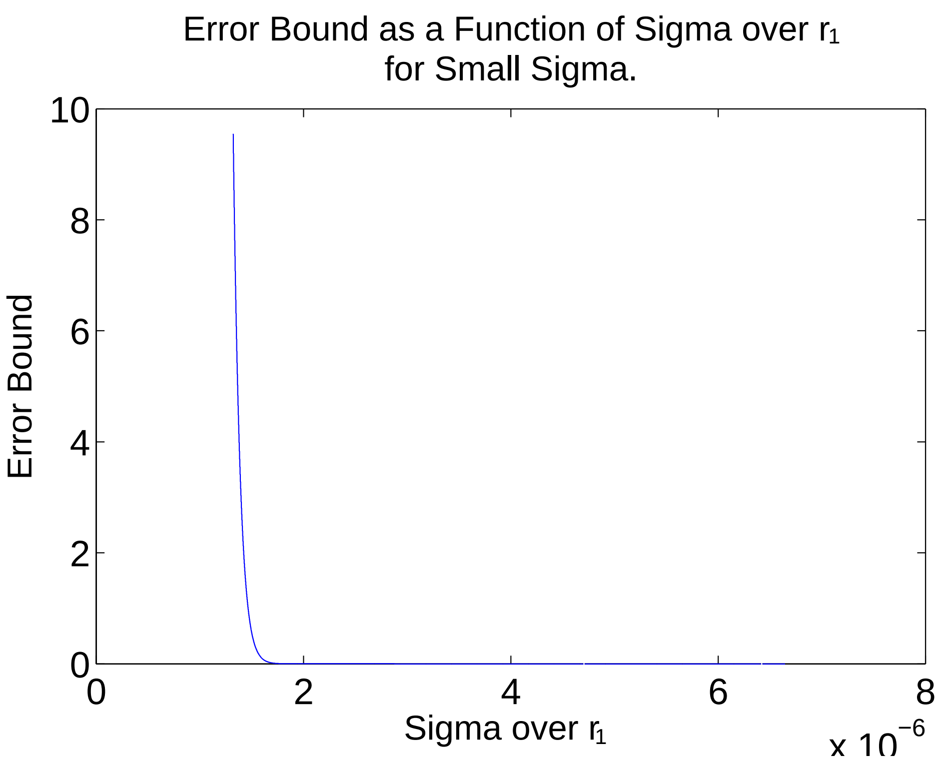

Figure 2: Error bound as a function of $\frac{\sigma}{r_1} \times 10^{-6}$ for small sigma

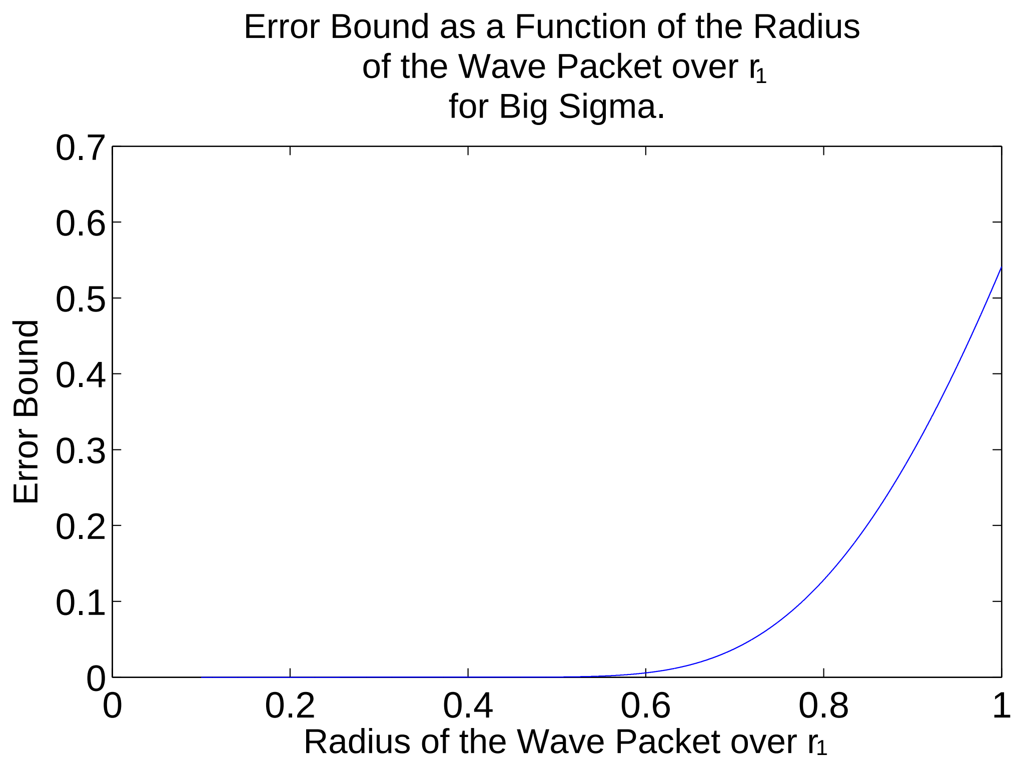

Figure 3: Error bound as a function of the radius of the wave packet over r_1 for big sigma

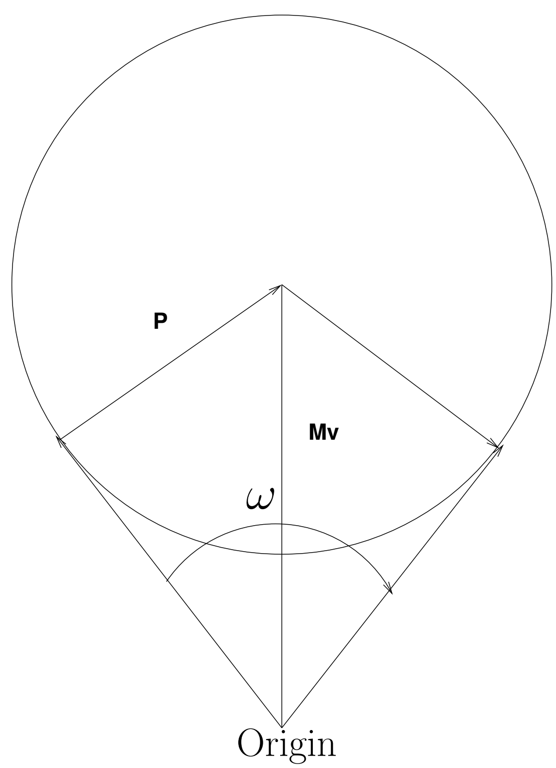

Figure 4: Opening angle

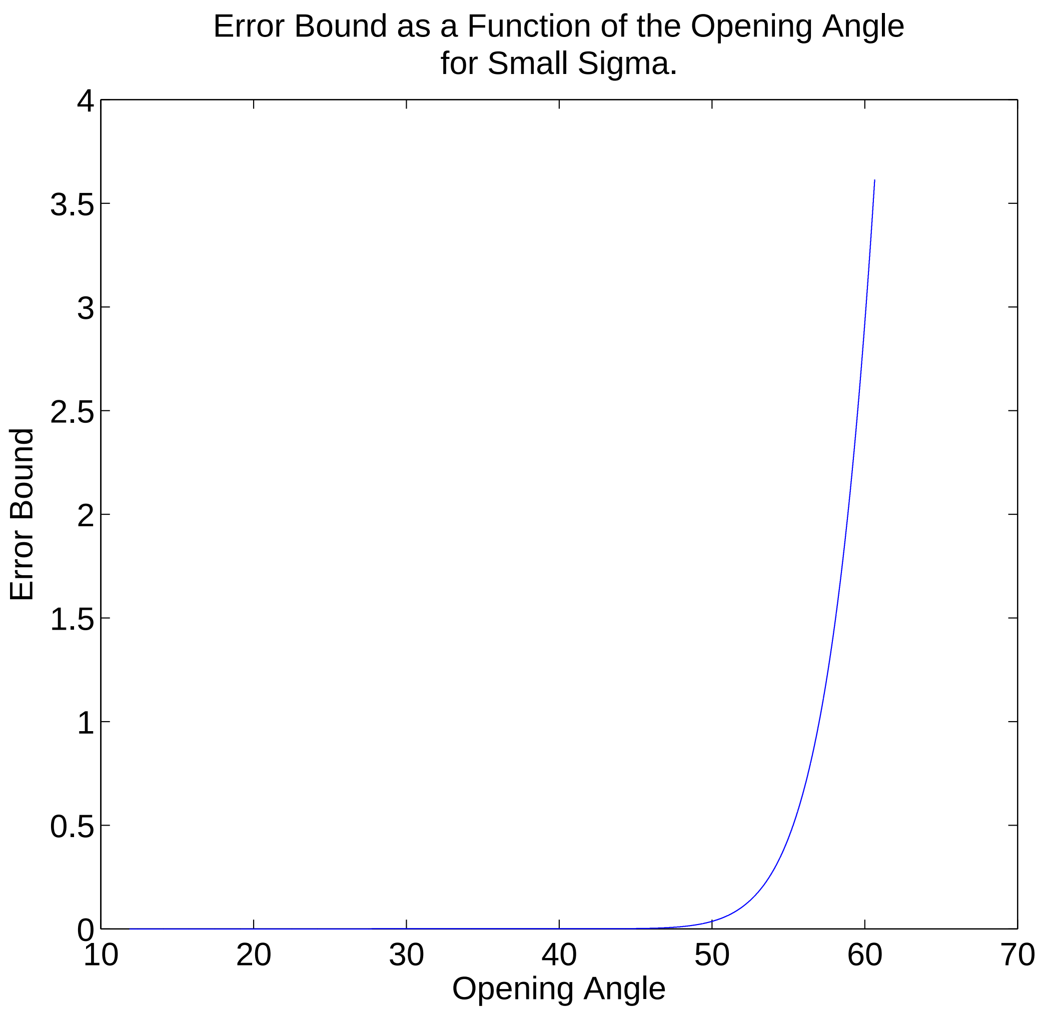

Figure 5: Error bound as a function of the opening angle for small sigma

Capítulo 8

High-Velocity Estimates for the Scattering Operator and Aharonov-Bohm Effect in Three Dimensions

En este capítulo se presenta el artículo [4]

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High-Velocity Estimates for the Scattering Operator and Aharonov-Bohm Effect in Three Dimensions*

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Abstract: We obtain high-velocity estimates with error bounds for the scattering operator of the Schrödinger equation in three dimensions with electromagnetic potentials in the exterior of bounded obstacles that are handlebodies. A particular case is a finite number of tori. We prove our results with time-dependent methods. We consider high-velocity estimates where the direction of the velocity of the incoming electrons is kept fixed as its absolute value goes to infinity. In the case of one torus our results give a rigorous proof that quantum mechanics predicts the interference patterns observed in the fundamental experiments of Tonomura et al. that gave conclusive evidence of the existence of the Aharonov-Bohm effect using a toroidal magnet. We give a method for the reconstruction of the flux of the magnetic field over a cross-section of the torus modulo 2π. Equivalently, we determine modulo 2π the difference in phase for two electrons that travel to infinity, when one goes inside the hole and the other outside it. For this purpose we only need the high-velocity limit of the scattering operator for one direction of the velocity of the incoming electrons. When there are several tori-or more generally handlebodies-the information that we obtain in the fluxes, and on the difference of phases, depends on the relative position of the tori and on the direction of the velocities when we take the high-velocity limit of the incoming electrons. For some locations of the tori we can determine all the fluxes modulo 2π by taking the high-velocity limit in only one direction. We also give a method for the unique reconstruction of the electric potential and the magnetic field outside the handlebodies from the high-velocity limit of the scattering operator.

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1. Introduction

The Aharonov-Bohm effect is a fundamental quantum mechanical phenomenon wherein charged particles, like electrons, are physically influenced, in the form of a phase shift, by the existence of magnetic fields in regions that are inaccessible to the particles. This genuinely quantum mechanical phenomenon was predicted by Aharonov and Bohm [3]. See also Ehrenberg and Siday [9]. This phenomenon has been extensively studied both from the theoretical and the experimental points of view. For a review of the literature see [29] and [30]. There has been a large controversy, involving over three hundred papers, concerning the existence of the Aharonov-Bohm effect. For a detailed discussion of this controversy see [30]. The issue was finally settled by the fundamental experiments of Tononura et al. [37,38], who used toroidal magnets to enclose a magnetic flux inside them. In remarkable experiments they were able to superimpose behind the magnet an electron beam that traveled inside the hole of the magnet with another electron beam that traveled outside the magnet, and they measured the phase shift produced by the magnetic flux enclosed in the magnet, giving conclusive evidence of the existence of the Aharonov-Bohm effect.

In this paper we give a rigorous mathematical analysis of this scattering problem with time-dependent methods. In particular, we give a rigorous mathematical proof that quantum mechanics predicts the phase shifts observed in the Tonomura et al. experiments [37,38].

We consider bounded obstacles, K, whose connected components are handlebodies. In particular, they can be the union of a finite number of bodies diffeomorphic to tori or to balls. Some of them can be patched through the boundary.

We study the high-velocity limit of the scattering operator in the complement, Λ, of the obstacle, K, for the Schrödinger equation with magnetic field and electric potential in Λ and with magnetic fluxes enclosed in the obstacle K. We obtain high-velocity estimates with error bounds for the scattering operator using the time-dependent method of [14]. We consider high-velocity limits where the direction of the velocity of the incoming electrons is kept fixed as its absolute value goes to infinity.

The leading term of our estimate gives us a reconstruction formula that allows us to reconstruct the circulation of the magnetic potential modulo 2π along lines in the direction of the velocity (the X-ray transform). From these line integrals we uniquely reconstruct the magnetic field in some region of Λ. The error term for the leading order goes to zero as a constant divided by the absolute value of the velocity.

The next term in our high-velocity estimate allows us to reconstruct the integral of the electric potential along lines in the direction of the velocity (the X-ray transform). We uniquely reconstruct the electric potential in a region of Λ from these lines' integrals. The error term for this high-velocity estimate goes to zero as a constant divided by a power of the absolute value of the velocity, that depends on the decay rate at infinity of the magnetic field and of the electric potential. If we have enough decay this power is one, as for the leading order.

The leading-order high-velocity estimate is given in Theorem 5.7 and the next term in our high-velocity estimate is given in Theorem 5.9. The unique reconstruction of the magnetic field and the electric potential in a region of Λ is given in Theorem 6.3. The reconstruction method is summarized in Remark 6.4.

Then, we consider the Aharonov-Bohm effect. We assume that the magnetic field in Λ is identically zero. On the contrary, the electric potential is not assumed to be zero. In other words, we analyze the Aharonov-Bohm effect in the presence of an electric potential. We use for reconstruction only the leading-order high-velocity estimate. As for high-velocities, the electric potential gives a lower-order contribution; it plays no role in the Aharonov-Bohm effect. However, to allow for a non-trivial electric potential could be of interest from the experimental point of view.

In Theorem 7.1 we reconstruct the circulation of the magnetic potential, modulo 2π, over a set of closed paths in Λ and in Remark 7.3 we reconstruct the projection of the de Rham cohomology class of the magnetic potential onto a subspace of $H^1_{\text{de R}}(\Lambda)$ in the sense that we reconstruct, modulo 2π, the expansion coefficients of the projection into the subspace of the de Rham cohomology class of the magnetic potential in any basis of the subspace. The set of circulations and the projection of the de Rham cohomology class of the magnetic potential that we can reconstruct depend on the relative position of the handlebodies and on the direction of the velocity of the incoming electrons. In Theorem 7.11, Corollary 7.12 and Remark 7.13 we give our method for the reconstruction of the fluxes inside the obstacle K, modulo 2π. Since the scattering operator is invariant under short-range gauge transformations that change the fluxes by multiples of 2π, the fluxes can only be reconstructed modulo 2π. Again, the fluxes that we reconstruct depend on the relative position of the handlebodies and on the direction of the velocity of the incoming electrons. In Example 7.14 we give obstacles that consist of a finite number of tori and manifolds diffeomorphic to balls, where from the high-velocity limit of the scattering operator in only one direction we reconstruct modulo 2π all the circulations in Λ of the magnetic potential, its de Rham cohomology class modulo 2π, and the flux modulo 2π of the magnetic field over the cross section of all the tori.

Finally, we discuss the fundamental experiments of Tonomura et al. [37,38] in Sect. 8. We show that our results give a rigorous proof that quantum mechanics predicts the interference patterns between electron beams that go inside and outside the torus, that were observed in these remarkable experiments.

The paper is organized as follows. In Sect. 2 we give a precise definition of the obstacle, K, and we study in a detailed way the homology and the cohomology of K and Λ. This allows us to construct a homology and cohomlogy basis that have clear physical significance. Using these results we construct in Sect. 3 classes of magnetic potentials characterized by the magnetic field in Λ and by the fluxes of the magnetic field in the cross sections of the components of K that have holes. We construct classes of magnetic potentials where the fluxes are fixed, and classes where the fluxes are only fixed modulo 2π. We study the gauge transformations between these magnetic potentials. In Sect. 4 we define the Hamiltonian of our system. In Sect. 5 we study our direct scattering problem. We prove the existence of the wave operators and we define the scattering operator. We analyze how the wave and scattering operators change under the change of the magnetic potential when the fluxes are only fixed modulo 2π. We also prove our high-velocity estimates. In Sect. 6 we give our method for the reconstruction of the magnetic field and the electric potential in a region of Λ. In Sect. 7 we obtain our results in the Aharonov-Bohm effect and in Sects. 8 we discuss the Tonomura et al. experiments [37,38]. In Appendixes A and B we prove results in homology that we need.

For the Aharonov-Bohm effect in scattering in two dimensions see [28] and [40]. For inverse scattering by magnetic fields in all space see [4–6,20–22]. For properties of the scattering matrix for scattering by Aharonov-Bohm potentials in all space see [33,34] and [42,43]. For the Ahanov-Bohm effect in inverse boundary-value problems see [10–13], [24] and [25].

Finally, some words about our notations and definitions. We use notions of homology and cohomology as defined, for example, in [7,16,17,8] and [41]. In particular, we consider homology and cohomology groups on open sets of $\mathbb{R}^n$, $n = 2, 3$ with coefficients in

$\mathbb{Z}$ and in $\mathbb{R}$. As these singular homology and cohomology groups are isomorphic to the C^∞ homology and cohomology groups, [7], p. 291, we will identify them. We also use differential forms, or just forms, in open sets of $\mathbb{R}^3$ with regular boundary—or in their closure- with the Euclidean metric, as defined, for example, in [8,35,41]. For such a set, O, we denote by $\Omega^k(O)$ the set of all $k-$forms in O.

We use the standard identification between concepts of vector calculus and differential forms in three dimensions in the interior of O, that we denote by $\overset{o}{O}$, [35]. Let $\{x^i\}_{i=1}^3$ be the Euclidean coordinates of $\mathbb{R}^3$.

We identify vectors and $1-$differential forms as

$$(A_1, A_2, A_3) \Longleftrightarrow \sum_{i=1}^{3} A_j dx^j.$$

We identify vectors and $2-$differential forms as

$$(B_1, B_2, B_3) \Longleftrightarrow B_3 dx^1 \wedge dx^2 - B_2 dx^1 \wedge dx^3 + B_1 dx^2 \wedge dx^3.$$

We identify scalars and $3-$differential forms as

$$f \Longleftrightarrow f dx^1 \wedge dx^2 \wedge dx^3.$$

The exterior derivative, d, in $1-$forms is equivalent to the curl of the associated vector, and in $2-$forms is equivalent to the divergence of the associated vector. In particular, a $1-$form, A, is closed if $dA = 0$, or equivalently, if the associated vector has curl zero, and a $2-$form, B, is closed if $dB = 0$, or equivalently, if the associated vector has divergence zero. For $0-$forms the exterior derivative coincides with the gradient ∇.

We will always assume that the coefficients of our forms are at least locally integrable in any coordinate chart. Hence, they define distributions or currents [8]. We say that a form belongs to some space if its coefficients in any coordinate chart belong to that space. For example, we say that a form is continuous if it has continuous coefficients or that is L^p if its coefficients are in L^p. In the case of a $2-$form, B, we will say that $B \in L^p\Omega^2(O)$, or, equivalently, that the associated vector $B \in L^p(\overset{o}{O})$. For forms defined in O that are not differentiable in the classical sense, the derivatives are taken in the distribution sense in O, if O is open, or in $\overset{o}{O}$ if it is closed.

For any $x \in \mathbb{R}^3$, $x \neq 0$, we denote $\hat{x} := x/|x|$. By $B_r^{\mathbb{R}^n}(x_0)$, $n = 2, 3$, we denote the open ball of center x_0 and radius r. By $\mathbb{S}^2$ we denote the unit sphere in $\mathbb{R}^3$. For any set O we denote by $F(x \in O)$ the operator of multiplication by the characteristic function of O. The symbol $\cong$ means isomorphism, the symbol $\simeq$ means homotopic equivalence and the symbol $\approx$ means homeomorphism.

We define the Fourier transform as a unitary operator on $L^2(\mathbb{R}^3)$ as follows:

$$\hat{\phi}(p) := F\phi(p) := \frac{1}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} e^{-ip\cdot x} \phi(x)\, dx.$$

We define functions of the operator $\mathbf{p} := -i\nabla$ by Fourier transform,

$$f(\mathbf{p})\phi := F^* f(p) F\phi,\ D(f(\mathbf{p})) := \{\phi \in L^2(\mathbb{R}^3) : f(p)\,\hat{\phi}(p) \in L^2(\mathbb{R}^3)\},$$

for every measurable function f.

2. The Obstacle

2.1. Handlebodies. Let us designate by $\mathbb{S}^1$ the unit circle. We denote by $T := \mathbb{S}^1 \times \overline{B_1^{\mathbb{R}^2}(0)}$ the solid torus of dimension 3. We orient T assuming that the inverse of the following function is a chart that belongs to the orientation of T,

$$\mathcal{U} : (0,1) \times B_1^{\mathbb{R}^2}(0) \to T, \ \mathcal{U}(t,x,y) = (e^{2\pi i t}, x, y). \tag{2.1}$$

The boundary sum of T with itself is defined as follows. See [15], p. 19. Let $D_1 \subseteq \partial T$ be a disc contained in a chart, (U_1, ϕ_1), belonging to the orientation of T and let $D_2 \subseteq \partial T$ be a disc contained in a chart, (U_2, ϕ_2), belonging to the opposite orientation. We define the boundary sum $T \natural T$ as the disjoint union of T with itself, identifying D_1 in the first torus with D_2 in the second torus by means of the charts, in such a way that $T\natural T$ is an oriented differentiable manifold, the inclusion $l_1 : T \hookrightarrow T\natural T$ in the first torus is an homeomorphism onto its image whose restriction to $\overset{o}{T}$ is a diffeomorphism that preserves orientation and the inclusion $l_2 : T \hookrightarrow T\natural T$ in the second torus is an homeomorphism onto its image whose restriction to $\overset{o}{T}$ is a diffeomorphism that inverts orientation. We define the boundary sum of k tori by induction. Suppose that we already defined the boundary sum $\natural(k-1)\,T := T\natural T \cdots \natural T,\ k-1$ times of $k-1$ tori. Let $l_j, j = 1, 2, \ldots, k-1$ be the inclusion of T on the j^{th} torus. As before, Let $D_1 \subseteq \partial T$ be a disc contained in a chart (U_1, ϕ_1) belonging to the orientation of T if $k-1$ is odd, or belonging to the opposite orientation if $k-1$ is even. Moreover, we assume that $l_{k-1}(U_1)$ does not intersect any of the union charts in $\natural\,(k-1)T$. This is always possible choosing the union charts small enough. Let $D_2 \subseteq \partial T$ be a disc contained in a chart (U_2, ϕ_2) belonging to the opposite orientation of T. Then, the boundary sum $\natural k\, T := T\natural T \cdots \natural T,\ k$ times is obtained from $\natural T \cdots \natural T,\ k-1$ times identifying $l_{k-1}(D_1)$ with D_2 by means of the charts $(l_{k-1}(U_1), \phi_1 \circ l_{k-1}^{-1})$ and (U_2, ϕ_2) in such a way that $\natural\, kT$ is an oriented differentiable manifold, the inclusion $\natural\,(k-1)T \hookrightarrow \natural\, kT$ in the first $k-1$ tori is an homeomorphism onto its image whose restriction to the interior is a diffeomorphism that preserves orientation and the inclusion $l_k : T \hookrightarrow \natural\, kT$ in the last torus is an homeomorphism onto its image whose restriction to $\overset{0}{T}$ is a diffeomorphism that inverts orientation. The structure of $\natural\, kT$ as an oriented differentiable manifold does not depend on the discs used to join the tori [15], p. 19. We will say that any oriented differentiable manifold diffeomorphic to $\natural kT$ is a handlebody with k handles, where the diffeomorphism is oriented. We will denote by $\natural 0T$ any oriented manifold that is diffeomorphic to the closed ball in $\mathbb{R}^3$ of center zero and radius one. Note that the inclusions $l_j : T \hookrightarrow \natural kT$ onto the j^{th} torus are homeomorphisms onto their images whose restriction to the interior are diffeomorphisms that preserve orientation if j is odd and change orientation if j is even.

2.2. Homology of handlebodies. We define the functions $\gamma_\pm : [0,1] \to T : \gamma_\pm(t) = (e^{\pm 2\pi i t}, 0, 0)$ and

$$Z_j(t) := \begin{cases} l_j \circ \gamma_+(t) & \text{if } j \text{ is odd,} \\ l_j \circ \gamma_-(t) & \text{if } j \text{ is even.} \end{cases} \tag{2.2}$$

For any $\xi \in \mathbb{S}^1$ we define

$$B_\xi := \left(\{\xi\} \times \overline{B_1(0)}\right) \subseteq T. \tag{2.3}$$

We orient B_ξ by requiring that the inverse of the inclusion $B_1(0) \hookrightarrow B_\xi$ belongs to the orientation of B_ξ, i.e., the inverse of the inclusion is a chart.

The image of Z_j in $\natural kT$ is a submanifold that we orient by means of the curve Z_j. We assume that $l_j(B_\xi)$ does not intersect any of the union charts, which is always possible if the union charts are small enough. We orient the submanifold $l_j(B_\xi)$ by the orientation of B_ξ. Let $v_1 \in T_{l_j(\xi,0,0)}(Z_j([0,1])) \subseteq T_{l_j(\xi,0,0)}(\natural kT)$ be a tangent vector in the orientation of $Z_j([0,1])$, and let $v_2, v_3 \in T_{l_j(\xi,0,0)}(l_j(B_\xi)) \subseteq T_{l_j(\xi,0,0)}(\natural kT)$ with (v_2, v_3) in the positive orientation of $l_j(B_\xi)$. Then, (v_1, v_2, v_3) is positively oriented in the tangent space $T_{l_j(\xi,0,0)}(\natural kT)$. This means that $Z_j([0,1])$ and $l_j(B_\xi)$ intersect in a positive way.

Let us denote by $H_1(\natural kT;\mathbb{R})$ the first group of singular homology of $\natural kT$ with coefficients in $\mathbb{R}$. See [16], p. 47. In Appendix A we give a proof, for the reader's convenience, that $\left\{[Z_j]_{H_1(\natural kT;\mathbb{R})}\right\}_{j=1}^k$ is a basis of $H_1(\natural kT;\mathbb{R})$.

2.3. Definition of the obstacle.

Assumption 2.1. *We assume that the obstacle K is a compact submanifold of $\mathbb{R}^3$ of dimension three oriented with the orientation of $\mathbb{R}^3$. Moreover, $K = \cup_{j=1}^L K_j$, where $K_j, 1 \le j \le L$ are the connected components of K. We assume that the K_j are handlebodies.*

By our assumption there exist numbers $m_j \in \mathbb{N} \cup 0$ and oriented diffeomorphisms $F_j : \natural m_j T \to K_j, 1 \le j \le L$. We denote by $\mathcal{J}_j$ the inclusion $K_j \hookrightarrow K$. The diffeomorphisms F_j induce a diffeomorphism

$$G : \bigvee_{j=1}^{L} \natural m_j T \to K,$$

where the symbol $\bigvee$ means disjoint union. We denote,

$$J := \{j \in \{1,2,\ldots,L\} : m_j > 0\}, \quad m := \sum_{j=1}^{L} m_j,$$

$$\{\gamma_k\}_{k=1}^m := \left\{\mathcal{J}_j \circ F_j \circ Z_i | j \in J, i \in \{1,2,\ldots m_j\}\right\}. \tag{2.4}$$

Choose a $\xi \in \mathbb{S}^1$ such that $l_i(B_\xi)$ does not intersect any chart of union in $\natural m_j T$, $\forall j \in J, \forall i \in \{1,2,\ldots,m_j\}$. This is always possible by choosing the charts of union in a proper way. If $\gamma_k = \mathcal{J}_j \circ F_j \circ Z_i$ we define $B_k := \mathcal{J}_j \circ F_j \left(l_i(B_\xi)\right)$. B_k is a manifold that we orient by means of the orientation of B_ξ. As F_j is a oriented diffeomorphism and Z_i intersects $l_i(B_\xi)$ in a positive way, it follows that γ_k intersects B_k in a positive way.

We define, $\mathcal{W}_\xi : [0,1] \to T : \mathcal{W}_\xi(t) := (\xi, \cos t, \sin t)$ and

$$\tilde{\gamma}_k := \mathcal{J}_j \circ F_j \circ l_i \circ \mathcal{W}_\xi. \tag{2.5}$$

Take $\varepsilon > 0$ such that $\{x| \text{distance}(x, \partial K) < \varepsilon\}$ is diffeomorphic to $\partial K \times (-\varepsilon, \varepsilon)$. This is possible by the tubular neighborhood theorem. See Theorem 11.4, p. 93 of [7]. We define,

$$\hat{\gamma}_k(t) := \tilde{\gamma}_k(t) + \frac{\varepsilon}{2} N(\tilde{\gamma}_k(t)), \tag{2.6}$$

where $N(\tilde{\gamma}_k(t))$ is the exterior normal to K at the point $\tilde{\gamma}_k(t)$. Note that $\partial B_k = \tilde{\gamma}_k([0, 1])$, the orientation on $\tilde{\gamma}_k([0, 1])$ induced by B_k is the orientation induced by the curve $\tilde{\gamma}_k$.

2.4. The homology of the obstacle.

Proposition 2.2. *$\{[\gamma_k]_{H_1(K;\mathbb{R})}\}_{k=1}^m$ is a basis of $H_1(K; \mathbb{R})$.*

Proof. As $G : \bigvee_{j=1}^L \natural m_j T \to K$ is a diffeomorphism and since

$$H_1 \left(\bigvee_{j=1}^L \natural m_j T; \mathbb{R} \right) \cong \oplus_{j=1}^L H_1 \left(\natural m_j T; \mathbb{R} \right),$$

by Proposition 9.5, p. 47 of [16], it follows from Proposition 9.3 of Appendix A that $\{[\gamma_k]_{H_1(K;\mathbb{R})}\}_{k=1}^m$ is a basis of $H_1(K; \mathbb{R})$. □

2.5. The cohomology of the obstacle. As K is an ANR (absolute neighborhood retract, p. 225 and Theorem 26.17.4 of [16]) we have that

$$\check{H}^1(K; \mathbb{R}) \cong H^1(K; \mathbb{R}), \tag{2.7}$$

by Proposition 27.1, p. 230 of [16] (see also p. 347, Theorem 7.15 of [7]).

By Alexander's duality theorem (see Theorem 27.5, p. 233 of [16])

$$\check{H}^1(K; \mathbb{R}) \cong H_2(\mathbb{R}^3, \mathbb{R}^3 \setminus K; \mathbb{R}). \tag{2.8}$$

By Theorem 14.1, p. 75 of [16] we have the following exact sequence:

$$H_2(\mathbb{R}^3; \mathbb{R}) \to H_2(\mathbb{R}^3, \mathbb{R}^3 \setminus K; \mathbb{R}) \to H_1(\mathbb{R}^3 \setminus K; \mathbb{R}) \to H_1(\mathbb{R}^3; K).$$

As $\mathbb{R}^3$ is homotopically equivalent to a point, it follows from Theorem 11.3, p. 59 and Example 9.4, p. 47 of [16] that $H_2(\mathbb{R}^3; \mathbb{R}) = 0$ and $H_1(\mathbb{R}^3; \mathbb{R}) = 0$. Then, we have the exact sequence

$$0 \to H_2(\mathbb{R}^3, \mathbb{R}^3 \setminus K; \mathbb{R}) \to H_1(\mathbb{R}^3 \setminus K; \mathbb{R}) \to 0,$$

and then,

$$H_2(\mathbb{R}^3, \mathbb{R}^3 \setminus K; \mathbb{R}) \cong H_1(\mathbb{R}^3 \setminus K; \mathbb{R}). \tag{2.9}$$

By (2.7,2.8, 2.9),

$$H^1(K; \mathbb{R}) \cong H_1(\mathbb{R}^3 \setminus K; \mathbb{R}). \tag{2.10}$$

By the theorem of universal coefficients, p. 198 of [17], $H^1(K; \mathbb{R}) \cong \text{Hom}_{\mathbb{R}} (H_1(K; \mathbb{R}), \mathbb{R})$. Then, it follows that,

$$\dim H_1(K; \mathbb{R}) = \dim H_1(\mathbb{R}^3 \setminus K; \mathbb{R}) = m. \tag{2.11}$$

We denote,

$$\Lambda := \mathbb{R}^3 \setminus K.$$

We will prove in Corollary 2.4 that $\{[\hat{\gamma}_k]_{H_1(\Lambda;\mathbb{R})}\}_{k=1}^m$ is a basis of $H_1(\Lambda; \mathbb{R})$.

2.6. de Rham cohomology of Λ. Let us define

$$G^{(j)}(x) := \operatorname{curl} \frac{1}{4\pi} \int_{\gamma_j} \frac{1}{|x-y|} d\vec{\gamma}_j(y) := \operatorname{curl} \frac{1}{4\pi} \int \frac{1}{|x-\gamma_j(t)|} \dot{\gamma}_j(t)\, dt. \tag{2.12}$$

Then, $\operatorname{curl} G^{(j)}(x) = 0,\ x \in \mathbb{R}^3 \setminus \gamma_j$ and

$$\int_{\hat{\gamma}_k} G^{(j)} = \delta_{k,j},\ j,k = 1,2,\ldots,m. \tag{2.13}$$

Equation (2.12) is the law of Biot-Savart that gives the magnetic field created by a current in γ_j and (2.13) is Ampere's law. For a proof see Satz 1.4, p. 33, of [26].

Proposition 2.3. $\left\{ \left[G^{(j)}\right]_{H^1_{\text{de R}}}(\Lambda) \right\}_{j=1}^m$ *is a basis of* $H^1_{\text{de R}}(\Lambda)$.

Proof. We first prove that they are linearly independent. Suppose that $\sum \alpha_j G^{(j)} = 0$, then $\sum \alpha_j G^{(j)} = d\lambda$ for some $0-$form λ. Hence,

$$\int_{\hat{\gamma}_k} \sum \alpha_j G^{(j)} = \alpha_k = 0.$$

By de Rham's Theorem (Theorem 4.17, p. 154 of [41]) the dual space to $H_1(\Lambda;\mathbb{R})$ is isomorphic to $H^1_{\text{de R}}(\Lambda)$. The isomorphisms are given by

$$\langle [\alpha]_{H_1(\Lambda;\mathbb{R})}, [A]_{H^1_{deR}(\Lambda)} \rangle := \int_\alpha A.$$

Then, by (2.11),

$$\dim H^1_{\text{de R}}(\Lambda) = \dim H_1(\Lambda;\mathbb{R}) = m,$$

and this proves the proposition. □

Corollary 2.4. $\left\{ \left[\hat{\gamma}_r\right]_{H_1(\Lambda;\mathbb{R})} \right\}_{r=1}^m$ *is a basis of* $H_1(\Lambda;\mathbb{R})$.

Proof. By (2.13) $\left\{ \left[\hat{\gamma}_r\right]_{H_1(\Lambda;\mathbb{R})} \right\}_{r=1}^m$ is the dual basis—in the sense of de Rham's Theorem—to the basis $\left\{ \left[G^{(r)}\right]_{H^1_{\text{de R}}}(\Lambda) \right\}_{r=1}^m$ of $H^1_{\text{de R}}(\Lambda)$. □

Proposition 2.5. *Let A be a closed $1-$form with continuous coefficients defined in Λ and such that*

$$\int_{\hat{\gamma}_r} A = 0, r = 1,2,\ldots,m.$$

Then, there is a continuously differentiable 0–form, λ, such that $A = d\lambda$. Moreover, we can take $\lambda(x) := \int_{C(x_0,x)} A$, where x_0 is any fixed point in Λ and $C(x_0,x)$ is any curve from x_0 to x.

Proof. By Theorem 12, p. 68, of [8] there is a regularization $R(\epsilon)$ and an operator $\Gamma(\epsilon)$ such that if α is a continuous $k-$ form on Λ, $R\alpha$ is a C^∞ $k-$ form on Λ and $\Gamma\alpha$ is a continuous $(k-1)-$ form on Λ. Moreover, $\lim_{\epsilon\to 0} R\alpha = \alpha$ uniformly on compact sets in Λ. Furthermore,

$$R\alpha - \alpha = b\Gamma\alpha + \Gamma b\alpha, \tag{2.14}$$

where $b\alpha := (-1)^{\text{grade}\,(\alpha)-1}\, d$. Multiplying (2.14) on the left by b and applying it to $b\alpha$ we prove that $Rb = bR$. As A is closed, it follows from (2.14) that $RA - A = b\Gamma A$. In particular, this implies that $b\Gamma A$ is continuous. Let C be a closed curve. Then, by Stokes theorem,

$$\int_C b\Gamma A = \lim_{\epsilon\to 0}\int_C Rb\Gamma A = \lim_{\epsilon\to 0}\int_C bR\Gamma A = 0,$$

and then,

$$\int_C RA = \int_C A,$$

and in particular,

$$\int_{\hat{\gamma}_r} RA = \int_{\hat{\gamma}_r} A = 0, r = 1, 2, \ldots, m.$$

As RA is C^∞ and closed, and since $\left\{[\hat{\gamma}_r]_{H_1(\Lambda;\mathbb{R})}\right\}_{r=1}^m$ is a basis of $H_1(\Lambda;\mathbb{R})$ it follows from de Rham's Theorem (Theorem 4.17, p. 154, [41]) that there is an infinitely differentiable $0-$form α such that $RA = b\alpha$. But then, using Stokes theorem again,

$$\int_C RA = \int_C b\alpha = 0,$$

and we obtain that,

$$\int_C A = 0,$$

for any closed curve C and we can define $\lambda := \int_{C(x_0,x)} A$. Clearly, $A = d\lambda$. □

Recall that $\{K_j\}_{j=1}^L$ is the set of connected components of K. For each $j \in \{1, 2, \cdots, L\}$ we choose a x_j in the interior of K_j. We define the vector,

$$D_j := -\text{grad}\frac{1}{4\pi}\frac{1}{|x-x_j|},\ x \in \mathbb{R}^3 \setminus \{x_j\}, \tag{2.15}$$

and according to our convention, we denote by the same symbol the associated 2–form. Note that div $D_j(x) = dD_j = -\Delta\frac{1}{4\pi}\frac{1}{|x-x_j|} = 0, x \neq x_j, j = 1, 2, \ldots, L$ and that,

$$\left|D_j(x)\right| \leq C(1+|x|)^{-2},\ x \in \Lambda. \tag{2.16}$$

For any $r > 0$ such that $K \subset B_r^{\mathbb{R}^3}(0)$ we denote,

$$\Lambda_r := \Lambda \cap B_r^{\mathbb{R}^3}(0), \text{ and } \Lambda_\infty := \Lambda.$$

Proposition 2.6. $\left\{[D_j]_{H^2_{\text{de R}}(\Lambda_r)}\right\}_{j=1}^{L}$ *is a basis of* $H^2_{\text{de R}}(\Lambda_r)$ *for* $r \leq \infty$.

Proof. Let us first consider the case $r = \infty$. As in the proof of (2.11) we prove that

$$\dim H_0(K;\mathbb{R}) = \dim H_2(\Lambda;\mathbb{R}).$$

But by Proposition 9.6, p. 48 of [16],

$$H_0(K;\mathbb{R}) \cong \oplus_{j=1}^{L}\mathbb{R}.$$

Moreover, by de Rham's Theorem (Theorem 4.17, p. 154 of [41])

$$H^2_{\text{de R}}(\Lambda) \cong (H_2(\Lambda;\mathbb{R}))^*. \tag{2.17}$$

Then,

$$\dim H^2_{\text{de R}}(\Lambda) = \dim H_2(\Lambda;\mathbb{R}) = L. \tag{2.18}$$

Let us now consider $r < \infty$. We define, $f : \Lambda \to \Lambda_r$,

$$f(x) := \begin{cases} r_1 \frac{x}{|x|}, \text{ if } |x| \geq r_1, \\ \\ x, \text{ if } |x| \leq r_1, \end{cases}$$

and $H(x,t) : (\Lambda \times [0,1]) \to \Lambda$

$$H(x,t) := \begin{cases} x + t(r_1 \frac{x}{|x|} - x), \text{ if } |x| \geq r_1, \\ \\ x, \text{ if } |x| \leq r_1, \end{cases}$$

where $r_1 < r$ and $K \subset B_{r_1}^{\mathbb{R}^3}(0)$. Let l be the inclusion $l : \Lambda_r \hookrightarrow \Lambda$. Then as $l \circ f(x) = l \circ H(x,1) = H(x,1)$ and $H(x,0) = I(x)$, we have that $l \circ f$ is homotopic to the identity. Let us denote by $\tilde{H}(x,t)$ the restriction of $H(x,t)$ to Λ_r. Then, $f \circ l(x) = \tilde{H}(l(x),1) = \tilde{H}(x,1)$, and as $\tilde{H}(x,0) = I(x)$ we also have that $f \circ l$ is homotopic to the identity. Hence, by Theorem 11.3, p. 59 [16] the inclusion l induces an isomorphism in homology. In particular, $H_2(\Lambda_r;\mathbb{R}) \cong H_2(\Lambda;\mathbb{R})$ and then,

$$\dim H_2(\Lambda_r;\mathbb{R}) = \dim H_2(\Lambda;\mathbb{R}) = L. \tag{2.19}$$

It follows from Stoke's theorem and as $-\Delta \frac{1}{4\pi}\frac{1}{|x-x_j|} = \operatorname{div} D_j(x) = \delta(x - x_j)$ that

$$\int_{\partial K_i} D_j = \int_{\partial B_\rho^{\mathbb{R}^3}(x_i)} D_j = \delta_{i,j}, \tag{2.20}$$

for ρ small enough and $i, j = 1, 2, \ldots, L$. This easily implies that the set $\left\{[D_j]_{H^2_{\text{de R}}(\Lambda_r)}\right\}_{j=1}^{L}$ is linearly independent. $\square$

Lemma 2.7. *Suppose that* $\{[S_j]_{H_2(\Lambda_r;\mathbb{R})}\}_{j=1}^L$, *is a basis of* $H_2(\Lambda_r;\mathbb{R})$ *for* $r \leq \infty$. *Let* D *be a closed* $2-$*form with continuous coefficients in* $\overline{\Lambda_r}$. *Then,*

$$\int_{\partial K_j} D = 0, \forall j \in \{1, 2, \ldots, L\} \Longleftrightarrow \int_{S_j} D = 0, \forall j \in \{1, 2, \cdots, L\}. \quad (2.21)$$

Proof. Denote $K_{j,\varepsilon} := \{x \in \mathbb{R}^3 : \operatorname{dist}(x, K_j) < \varepsilon\}$, where ε is so small that the tubular neighborhood theorem applies and let R be the regularization operator. Suppose that the left side of (2.21) holds. Then, as D is closed we prove using the Stokes theorem that

$$\int_{\partial K_{j,\varepsilon}} RD = 0, \ \forall j \in \{1, 2, \ldots, L\}.$$

As RD is C^∞ and closed, since $bR = Rb$, there are coefficients λ_j, $j = 1, 2, \ldots, L$ and a 1–form α such that,

$$RD = \sum_{j=1}^{L} \lambda_j D_j + d\alpha.$$

Then, it follows from (2.20) (with $K_{j,\varepsilon}$ instead of K_j) and Stoke's theorem that

$$0 = \int_{\partial K_{j,\varepsilon}} RD = \lambda_j,$$

and we obtain that

$$RD = d\alpha.$$

Furthermore, using the regularization operator and Stoke's theorem we prove that

$$\int_{S_j} D = \int_{S_j} RD = \int_{S_j} d\alpha = 0, \ j \in \{1, 2, \ldots, L\}.$$

Assume now that $\int_{S_j} D = 0$, $j \in \{1, 2, \ldots, L\}$. We prove as above that $\int_{S_j} RD = 0$, $j \in \{1, 2, \ldots, L\}$, and by de Rham's Theorem (Theorem 4.17, p. 154 of [41]) there is a 1–form α such that

$$RD = d\alpha.$$

Hence,

$$\int_{\partial K_{j,\varepsilon}} D = \int_{\partial K_{j,\varepsilon}} RD = \int_{\partial K_{j,\varepsilon}} d\alpha = 0,$$

and then,

$$\int_{\partial K_j} D = \lim_{\varepsilon \to 0} \int_{\partial K_{j,\varepsilon}} D = 0, \ j \in \{1, 2, \cdots, L\}. \quad \square$$

3. Magnetic Field and Magnetic Potentials

In this section we introduce the class of magnetic fields that we consider and we construct a class of associated magnetic potentials with nice behavior at infinity that will allow us to solve our scattering problems.

Definition 3.1. *We say that a form B in $\overline{\Lambda}$ is continuous in a neighborhood of ∂K if there is a $\varepsilon > 0$ such that the coefficients of B are continuous in $\overline{\Lambda} \cap K_\varepsilon$, where $K_\varepsilon := \{x \in \mathbb{R}^3 : \operatorname{dist}(x, K) < \varepsilon\}$.*

Below we assume that the magnetic field, B, is a 2–form that is continuous in a neighborhood of ∂K and satisfies

$$\int_{\partial K_j} B = 0,\ j \in \{1, 2, \dots, L\}. \tag{3.22}$$

This condition means that the total contribution of magnetic monopoles inside each component K_j of the obstacle is 0. In a formal way we can use Stokes theorem to conclude that

$$\int_{\partial K_j} B = 0 \Longleftrightarrow \int_{K_j} \operatorname{div} B = 0,\ j \in \{1, 2, \dots, L\}.$$

As $\operatorname{div} B$ is the density of magnetic charge, $\int_{\partial K_j} B$ is the total magnetic charge inside K_j, and our condition (3.22) means that the total magnetic charge inside K_j is zero, this condition is fulfilled if there is no magnetic monopole inside K_j, $j \in \{1, 2, \dots, L\}$.

Theorem 3.2. *Let B be a 2–form in $L^p_{\text{loc}}\Omega^2(\overline{\Lambda})$, $p \geq 2$ that is continuous in a neighborhood of ∂K and satisfies (3.22). Suppose that the restriction of B to Λ is closed ($dB|_\Lambda = 0$) as a distribution (or current [8]) . Then, B has an extension to a closed 2–form $\overline{B} \in L^p_{\text{loc}}\Omega^2(\mathbb{R}^n)$ such that, $\overline{B}|_{\overline{\Lambda}} = B$.*

Proof. Let us denote $M := \overline{\Lambda_r}$, $r < \infty$. M is a compact manifold. We denote by B_M the restriction of B to M. As $dB|_\Lambda = 0$, it follows from Green's formula (Prop. 2.12, p. 60, [35]) that

$$\langle\langle B_M, \delta\eta \rangle\rangle = 0,\ \forall \eta \in C_0^\infty \Omega^3(\mathring{M}). \tag{3.23}$$

We denote (Definition 2.4.1, p. 80 [35])

$$C^k(M) := \left\{ \delta\eta | \eta \in H^1\Omega_N^{k+1}(M) \right\},$$

and (Definition 2.2.1, p. 67 [35])

$$H^1\Omega_N^k(M) := \left\{ \eta \in H^1\Omega^k(M) | \mathbf{n}\eta = 0 \right\}.$$

Let us recall (p. 27 [35]) that given $\eta \in \Omega^3(M)$ and tangent vectors $v_i \in T_x(M)$, $x \in \partial M$, $i \in \{1, 2, 3\}$,

$$\mathbf{t}\eta(v_1, v_2, v_3) = \eta \left(v_1^{\parallel}, v_2^{\parallel}, v_3^{\parallel} \right),$$

where $v_i^{\|}$ is the projection of v_i into $T_x(\partial M)$. As η is a multi-linear function and $\left\{v_1^{\|}, v_2^{\|}, v_3^{\|}\right\}$ are linearly dependent,

$$\mathbf{t}\eta = 0.$$

By the definition in p. 27 [35],

$$\mathbf{n}\eta := \eta - \mathbf{t}\eta = \eta.$$

It follows that

$$\mathbf{n}\eta = \eta,\ \eta \in H^1\Omega^3(M).$$

Let $\eta \in H^1\Omega^3_N(M)$, then there exists $f \in W^{1,2}(M)$ such that

$$\eta|_{\overset{o}{M}} = f|_{\overset{o}{M}} dx^1 \wedge dx^2 \wedge dx^3.$$

As $\mathbf{n}\eta = \eta = 0$, it follows that $f|_{\partial M} = 0$ in trace sense. Hence (Theorem 4.7.1, p. 330, [36]), f can be approximated in the $W^{1,2}(M)$ norm by functions in $C_0^\infty\left(\overset{\circ}{M}\right)$, and then η can be approximated in the $H^1\Omega^3(M)$ norm by forms in $\Omega^3(\overset{0}{M})$ with compact support. Whence, it follows from (3.23) that

$$\langle\langle B_M, \delta\eta\rangle\rangle = 0, \forall\eta \in C^2(M). \tag{3.24}$$

By Corollary 2.4.9, p. 87 [35]

$$B_M = d\alpha + \delta\beta + d\epsilon + \gamma \in \mathcal{E}^2(M) \oplus C^2(M) \oplus L^2\mathcal{H}^2_{\text{ext}}(M) \oplus \mathcal{H}^2_N(M), \tag{3.25}$$

where (Definition 2.4.1, p. 80 [35])

$$\mathcal{E}^k(M) := \left\{d\alpha | \alpha \in H^1\Omega_D^{k-1}(M)\right\}$$

and (Definition 2.2.1, p. 67 [35])

$$H^1\Omega^k_D(M) := \left\{\eta \in H^1\Omega^k(M) | \mathbf{t}\eta = 0\right\}.$$

Furthermore (p. 86 [35]),

$$\mathcal{H}^k_{\text{ext}}(M) := \left\{\eta \in \mathcal{H}^k(M) | \eta = d\epsilon\right\},$$

and (Definition 2.2.1, p. 67 [35])

$$\mathcal{H}^k(M) := \left\{\eta \in H^1\Omega^k(M) | d\eta = 0,\ \delta\eta = 0\right\}$$

are the harmonic fields, and

$$\mathcal{H}^k_N(M) := \mathcal{H}^k(M) \cap H^1\Omega^k_N(M).$$

Note that Theorem 2.2.7, p. 72 [35] implies that $\mathcal{H}^2_N(M)$ consists of C^∞ forms. Furthermore by Lemma 2.4.11, p. 90 [35] we can choose $\alpha \in W^{1,p}\Omega^1_D(M)$, and by

Theorem 2.4.8, p. 86 and Theorems 2.2.6 and 2.2.7, p. 72 [35] $\epsilon \in W^{1,p}\Omega^1_N(M)$. Moreover, the decomposition (3.25) is orthogonal in $L^2(M)$, and then by (3.24) $\delta\beta = 0$.

Let R be the regularization operator in $\Lambda_r = \overset{\circ}{M}$. Then, as in the proof of Lemma 2.7 we prove that

$$\int_{\partial K_{j,\varepsilon}} RB = 0.$$

Hence,

$$0 = \int_{\partial K_{j,\varepsilon}} RB = \int_{\partial K_{j,\varepsilon}} d(R\alpha + R\epsilon) + \int_{\partial K_{j,\varepsilon}} R\gamma = \int_{\partial K_{j,\varepsilon}} R\gamma.$$

Then, $\int_{\partial K_{j,\varepsilon}} R\gamma = 0,\ j \in \{1, 2, \dots, L\}$ and when the parameter of the regularization tends to zero we obtain $\int_{\partial K_{j,\varepsilon}} \gamma = 0,\ j \in \{1, 2, \dots, L\}$.

As γ is harmonic it is closed and it follows from Stokes theorem that

$$\int_{\partial K_j} \gamma = 0, j \in \{1, 2, \dots, L\}.$$

Then, by Lemma 2.7 $\int_{S_j} \gamma = 0, j \in \{1, 2, \dots, L\}$. By de Rham's Theorem $\gamma|_{\overset{\circ}{M}} = d\lambda, \lambda \in \Omega^1(\overset{\circ}{M})$. Denote $M_\varepsilon := \{x \in M : \operatorname{dist}(x, \partial M) \geq \varepsilon\}$. Let γ_ε be the restriction of γ to M_ε. Then γ_ε is exact and by Lemma 3.2.1, p. 119 [35], and its proof, $\gamma_\varepsilon = d\omega_\varepsilon$ with $\omega_\varepsilon \in H^1\Omega^1(M_\varepsilon)$ and

$$\|\omega_\varepsilon\|_{H^1\Omega^1(M_\varepsilon)} \leq C\|\gamma_\varepsilon\|_{L^2\Omega^2(M_\varepsilon)} \leq C\|\gamma\|_{L^2\Omega^2(M)},$$

where the constant C can be taken independent of ε for $0 < \varepsilon < \varepsilon_0$ for ε_0 small enough. Let us denote by $\Lambda^k(M)$, $\Lambda^k(M_\varepsilon)$, respectively, the exterior k–form bundle of M, M_ε (see Definition 1.3.8 in p. 39 of [35]). For any vector bundle, $\mathbb{F}$, over a manifold N we denote by $\Gamma(\mathbb{F})$ the space of all smooth sections of $\mathbb{F}$ (see Definition 1.1.9, p. 17 of [35]) . Note that the norm, C_1, of the trace operator (Theorem 1.3.7, p. 38 [35]) from $H^1(\Omega^k(M_\varepsilon))$ into $L^2\Gamma\left(\Lambda^k(M_\varepsilon)|_{\partial M_\varepsilon}\right)$ can be taken independent of ε for $0 < \varepsilon < \varepsilon_0$. By Green's formula and as $\delta\gamma_\varepsilon = 0$,

$$\langle\langle \gamma_\varepsilon, \gamma_\varepsilon \rangle\rangle = \langle\langle d\omega_\varepsilon, \gamma_\varepsilon \rangle\rangle = \int_{\partial M_\varepsilon} \mathbf{t}\omega_\varepsilon \wedge *\mathbf{n}\gamma_\varepsilon. \tag{3.26}$$

But as

$$\|\mathbf{t}\omega_\varepsilon\|_{L^2\Gamma\left(\Lambda^1(M_\varepsilon)|_{\partial M_\varepsilon}\right)} \leq C_1\|\omega_\varepsilon\|_{H^1\Omega^1(M_\varepsilon)} \leq C_1 C\|\gamma_\varepsilon\|_{L^2\Omega^2(M_\varepsilon)} \leq C_1 C\|\gamma\|_{L^2\Omega^2(M)},$$

and

$$\lim_{\epsilon\to 0} \|\mathbf{n}\gamma_\varepsilon\|_{L^2\Gamma\left(\Lambda^2(M_\varepsilon)|_{\partial M_\varepsilon}\right)} = 0,$$

it follows from (3.26) and the Schwarz inequality that

$$\|\gamma\|^2_{L^2\Omega^2(M)} = \lim_{\varepsilon\to 0} \|\gamma_\varepsilon\|^2_{L^2\Omega^2(M)} = 0.$$

Then $\gamma = 0$ and we have that

$$B_M = dA_M, \tag{3.27}$$

where $A_M := \alpha + \epsilon \in W^{1,p}\Omega^1(\overset{o}{M})$. It follows from Theorem 4.2.2, p. 311 [36] that there is $\overline{A_M} \in W^{1,p}\Omega^1(\overline{B_r^{\mathbb{R}^3}(0)})$ such that $\overline{A_M}|_M = A_M$. We define

$$\overline{B}(x) = \begin{cases} d\overline{A}_M(x), \text{ if } x \in B_r^{\mathbb{R}^3}(0), \\ \\ B(x), \text{ if } x \in \mathbb{R}^3 \setminus B_r^{\mathbb{R}^3}(0). \end{cases} \tag{3.28}$$

Hence, $\overline{B}$ is the required extension. □

Recall that the functions $\{\hat{\gamma}_j\}_{j=1}^m$ were defined in (2.6). We introduce now a function that gives the magnetic flux across surfaces that have $\{\hat{\gamma}_j\}_{j=1}^m$ as their boundaries.

Definition 3.3. *The flux, Φ is a function $\Phi : \{\hat{\gamma}_j\}_{j=1}^m \to \mathbb{R}$.*

We now define a class of magnetic potentials with a given flux.

Definition 3.4. *Let $B \in L^p\Omega^2(\overline{\Lambda})$, $p > 3$, be a closed 2–form that is continuous in a neighborhood of ∂K, where K is as in Assumption 2.1. Assume, furthermore, that (3.22) holds. We denote by $\mathcal{A}_\Phi(B)$ the set of all continuous 1−forms in $\overline{\Lambda}$ that satisfy.*

1.

$$|A(x)| \le C\frac{1}{1+|x|}, \ a(r) := \max_{x\in\Lambda,|x|\ge r}\{|A(x)\cdot\hat{x}|\} \in L^1(0,\infty). \tag{3.29}$$

2.

$$\int_{\hat{\gamma}_j} A = \Phi(\hat{\gamma}_j), \ j \in \{1, 2, \dots, m\}. \tag{3.30}$$

3.

$$dA|_\Lambda = B|_\Lambda. \tag{3.31}$$

The definition of the flux Φ depends on the particular choice of the curves $\{\hat{\gamma}_j\}_{j=1}^m$. However, the class $\mathcal{A}_\Phi(B)$ is independent of this particular choice as we prove below.

Recall that by Corollary 2.4 $\beta := \{[\hat{\gamma}_j]_{H_1(\Lambda;\mathbb{R})}\}_{j=1}^m$ is a basis of $H_1(\Lambda;\mathbb{R})$. Let $\beta' := \{[C_j]_{H_1(\Lambda;\mathbb{R})}\}_{j=1}^m$ be another basis of $H_1(\Lambda;\mathbb{R})$. We define $\Phi_{\beta'} : \{C_j\}_{j=1}^m \to \mathbb{R}$ as follows. As β is a basis of $H_1(\Lambda;\mathbb{R})$ there are real numbers b_j^i and chains σ_j such that

$$C_j = \sum_{i=1}^m b_j^i \hat{\gamma}_i + \partial\sigma_j. \tag{3.32}$$

We define

$$\Phi_{\beta'}(C_j) := \sum_{i=1}^m b_j^i \Phi(\hat{\gamma}_i) + \int_{\sigma_j} B. \tag{3.33}$$

We denote by $\mathcal{A}_{\Phi_{\beta'}}(B)$ the set of continuous 1–forms A in $\overline{\Lambda}$ that satisfy 1 and 3 of Definition 3.4 and moreover,

$$\int_{C_j} A = \Phi_{\beta'}(C_j), \; j = 1, 2, \ldots, m.$$

Proposition 3.5. $\mathcal{A}_{\Phi_{\beta'}}(B) = \mathcal{A}_{\Phi}(B)$.

Proof. Let $A \in \mathcal{A}_{\Phi}(B)$. Then, by (3.32)

$$\int_{C_j} A = \sum_{i=1}^{m} b^i_j \int_{\hat{\gamma}_i} A + \int_{\sigma_j} dA = \Phi_{\beta'}(C_j), \, j = 1, 2, \ldots, m,$$

and it follows that $A \in \mathcal{A}_{\Phi_{\beta'}}(B)$.

Suppose now that $A \in \mathcal{A}_{\Phi_{\beta'}}(B)$. As β and β' are basis, the numbers $b^i_j, i, j = 1, 2, \ldots, m$ determine an invertible matrix. We denote by $\tilde{b}^j_i$ the entries of the inverse matrix. Hence,

$$\hat{\gamma}_i = \sum_{j,s=1}^{m} \tilde{b}^j_i \, b^s_j \hat{\gamma}_s = \sum_{j=1}^{m} \tilde{b}^j_i (C_j - \partial\sigma_j),$$

and then by (3.33),

$$\int_{\hat{\gamma}_i} A = \sum_{j=1}^{m} \tilde{b}^j_i \left(\Phi_{\beta'}(C_j) - \int_{\sigma_j} B \right) = \Phi(\hat{\gamma}_i).$$

This implies that $A \in \mathcal{A}_{\Phi}(B)$. □

By Stoke's theorem the circulation $\int_{\hat{\gamma}_j} A$ of a potential $A \in \mathcal{A}_{\Phi}(B)$ represents the flux of the magnetic field B in any surface whose boundary is $\hat{\gamma}_j$, $j = 1, 2, \ldots, m$. As the magnetic field is *a priori* known outside the obstacle, it is natural to specify the magnetic potentials fixing fluxes of the magnetic field in surfaces inside the obstacle. This is accomplished fixing the circulations $\int_{\tilde{\gamma}_j} A$ instead of the circulations $\int_{\hat{\gamma}_j} A$, as we prove below. Recall that $\tilde{\gamma}_j$ is defined in (2.5). With ε as in (2.6) we define,

$$S_j := \left\{ \tilde{\gamma}_j(t) + s\frac{\varepsilon}{2} N(\tilde{\gamma}_j(t)) | t, s \in [0, 1] \right\}.$$

We give S_j the structure of an oriented surface with boundary $\hat{\gamma}_j - \tilde{\gamma}_j$. By Stoke's theorem and regularizing we prove that

$$\int_{\tilde{\gamma}_j} A = \int_{\hat{\gamma}_j} A - \int_{S_j} B.$$

We define the fluxes $\tilde{\Phi} : \{\tilde{\gamma}_j\}_{j=1}^{m} \to \mathbb{R}$ accordingly,

$$\tilde{\Phi}(\tilde{\gamma}_j) = \Phi(\hat{\gamma}_j) - \int_{S_j} B.$$

We denote by $\tilde{\mathcal{A}}_{\tilde{\Phi}}(B)$ the set of continuous $1-$forms, A, in $\overline{\Lambda}$ that satisfy 1 and 3 of Definition 3.4 and moreover,

$$\int_{\tilde{\gamma}_j} A = \tilde{\Phi}(\tilde{\gamma}_j),\ j = 1, 2, \ldots, m.$$

Proposition 3.6. $\mathcal{A}_{\tilde{\Phi}}(B) = \mathcal{A}_{\Phi}(B)$.

Proof. Let $A \in \mathcal{A}_{\Phi}(B)$. By Stoke's theorem and regularizing,

$$\int_{\tilde{\gamma}_j} A = \int_{\hat{\gamma}_j} A - \int_{S_j} B = \tilde{\Phi}_j.$$

Then, $A \in \mathcal{A}_{\tilde{\Phi}}(B)$. We prove in the same way that $A \in \mathcal{A}_{\tilde{\Phi}}(B) \Rightarrow A \in \mathcal{A}_{\Phi}(B)$. $\square$

Note that for $1-$forms $A = \sum_{i=1}^{3} A_i dx^i$, $\delta A = -\sum_{i=1}^{3} \frac{\partial}{\partial x_i} A_i = -\text{div}\, A$ [35]. We use the definition of divergence of a vector field, A, as it is usual in vector calculus. The definition given in [35] differs from ours in a $-$ sign.

Theorem 3.7. (Coulomb Potential). *Let $B \in L^p\Omega^2(\overline{\Lambda})$, $p > 3$, be a closed 2–form that is continuous in a neighborhood of ∂K, where K is as in Assumption 2.1. Assume, furthermore, that (3.22) holds and that for some r with $K \subset B_r^{\mathbb{R}^3}(0)$,*

$$|B(x)| \leq C(1 + |x|)^{-\mu},\ |x| \geq r,\ \mu > 2. \tag{3.34}$$

Then, for any flux, Φ, there is a potential $A_C \in \mathcal{A}_{\Phi}(B)$ such that $A_C = A_{(C,1)} + A_{(C,2)}$, where $A_{(C,1)}$ is continuous on $\overline{\Lambda}$, $A_{(C,2)}$ is C^∞ on $\overline{\Lambda}$, and $\delta A_{(C,j)} = -\text{div}\, A_{(C,j)} = 0$, $j = 1, 2$. Furthermore,

$$|A_{(C,1)}(x)| \leq C(1 + |x|)^{-\min(2-\varepsilon, \mu-1)},\ \forall \varepsilon > 0, \tag{3.35}$$

$$|A_{(C,2)}(x)| \leq C(1 + |x|)^{-2}. \tag{3.36}$$

Proof. Let $\overline{B}$ be the extension to $\mathbb{R}^3$ of B given by Theorem 3.2. by Proposition 2.6 of [22], and its proof we can take as $A_{(C,1)}$ the Coulomb gauge of $\overline{B}$,

$$A_{(C,1)} := -\frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{x - y}{|x - y|^3} \times \overline{B}(y)\, dy, \tag{3.37}$$

where we use the notation of vector calculus. We define $A_{(C,2)}$ as follows:

$$A_{(C,2)} := \sum_{j=1}^{m} \left(\Phi(\hat{\gamma}_j) - \int_{\hat{\gamma}_j} A_{(C,1)} \right) G^{(j)}, \tag{3.38}$$

where $G^{(j)}$, $j = 1, 2, \cdots, m$ are defined in (2.12) and we used (2.13). Clearly, $G^{(j)} \in C^\infty(\overline{\Lambda})$ and $|G^{(j)}(x)| \leq C(1 + |x|)^{-2}$. $\square$

Note that in $\mathbb{R}^3$ A_C is the Coulomb potential that corresponds to the magnetic field

$$\overline{B} + \sum_{j=1}^{m} \left(\Phi(\gamma_j) - \int_{\hat{\gamma}_j} A_{(C,1)} \right) \delta(x - \gamma_j) d\vec{\gamma}_j,$$

with

$$\left\langle \delta(x - \gamma_j) d\vec{\gamma}_j,\, \phi \right\rangle := \int_{\gamma_j} \phi\, d\vec{\gamma}_j.$$

The div-curl problem in exterior domains in the case of C^1 vector fields with Hölder continuous first derivatives was considered in [39].

Lemma 3.8. (Gauge Transformations). *Suppose that* $A, \tilde{A} \in \mathcal{A}_{\Phi}(B)$. *Then, there is a* C^1 $0-$*form* λ *in* $\overline{\Lambda}$ *such that* $\tilde{A} - A = d\lambda$. *Moreover, we can take* $\lambda(x) := \int_{C(x_0,x)} (\tilde{A} - A)$, *where* x_0 *is any fixed point in* Λ *and* $C(x_0, x)$ *is any curve from* x_0 *to* x. *Furthermore,* $\lambda_\infty(x) := \lim_{r\to\infty} \lambda(rx)$ *exists and it is continuous in* $\mathbb{R}^3 \setminus \{0\}$ *and homogeneous of order zero, i.e.* $\lambda_\infty(rx) = \lambda_\infty(x), r > 0, x \in \mathbb{R}^3 \setminus \{0\}$. *Moreover,*

$$\begin{gathered} |\lambda_\infty(x) - \lambda(x)| \le \int_{|x|}^{\infty} b(|x|), \quad \text{for some } b(r) \in L^1(0, \infty), \\ \text{and } |\lambda_\infty(x + y) - \lambda_\infty(x)| \le C|y|, \forall x : |x| = 1, \text{ and } \forall y : |y| < 1/2. \end{gathered} \tag{3.39}$$

Proof. The existence of λ follows from Proposition 2.5. The existence of λ_∞ and the first equation in (3.39) follow from Condition 1 in Definition 3.4. The homogeneity follows from the definition. Denote $G := \tilde{A} - A$. Take $m > 1$ such that $K \subset B^{\mathbb{R}^3}_{m/2}(0)$. Suppose that $|x| = 1$ and that $|y| < 1/2$.

Denote, $x' := mx, y' := m\frac{x+y}{|x+y|} - x'$. Then, $\lambda_\infty(x) = \lambda_\infty(x'), \lambda_\infty(x + y) = \lambda_\infty(x' + y')$. Hence,

$$\begin{aligned} \lambda_\infty(x + y) - \lambda_\infty(x) &= \lambda_\infty(x' + y') - \lambda_\infty(x') \\ &= \int_{x'}^{x'+y'} G + \int_{x'+y'}^{\infty} G - \int_{x'}^{\infty} G = \lim_{r\to\infty} \int_{rmx}^{rm(x+y)/|x+y|} G, \end{aligned}$$

where we used Stoke's theorem and $dG = 0$. Then,

$$|\lambda_\infty(x' + y') - \lambda_\infty(x')| \le \lim_{r\to\infty} \int_{rmx}^{rm(x+y)/|x+y|} |G| \le C|y|.$$

This proves (3.39).

We now consider potentials that satisfy the flux condition modulo 2π. □

Definition 3.9. *Let* B *be as in Definition* 3.4. *We denote by* $\mathcal{A}_{\Phi,2\pi}(B)$ *the set of all continuous* $1-$*forms in* $\overline{\Lambda}$ *that satisfy* 1 *and* 3 *of Definition* 3.4 *and moreover,*

$$\int_{\hat{\gamma}_j} A = \Phi(\hat{\gamma}_j) + 2\pi n_j(A),\ n_j(A) \in \mathbb{Z},\ j \in \{1, 2, \ldots, m\}.$$

Given $A \in \mathcal{A}_{\Phi,2\pi}(B)$ we define,

$$A_\Phi := A - \sum_{j=1}^{m} 2\pi n_j(A)\, G^{(j)}. \tag{3.40}$$

By (2.13) $A_\Phi \in \mathcal{A}_\Phi(B)$.

Suppose that $A, \tilde{A} \in \mathcal{A}_{\Phi,2\pi}(B)$. Then, A_Φ, $\tilde{A}_\Phi \in \mathcal{A}_\Phi(B)$, and by Lemma 3.8,

$$\tilde{A}_\phi - A_\Phi = d\lambda, \tag{3.41}$$

and it follows that

$$\tilde{A} - A = d\lambda + A_{\mathbb{Z}}, \tag{3.42}$$

where

$$A_{\mathbb{Z}} := \sum_{j=1}^{m} 2\pi (n_j(\tilde{A}) - n_j(A))\, G^{(j)}. \tag{3.43}$$

Let C be any closed curve in Λ. Then, by Proposition 10.1 in Appendix B,

$$C := \sum_{j=1}^{m} n_j(C)\hat{\gamma}_j + \partial\sigma, n_j(C) \in \mathbb{Z}.$$

Hence,

$$\int_C (\tilde{A} - A) = 2\pi N, \text{ for some } N \in \mathbb{Z}. \tag{3.44}$$

Whence, we can define the non-integrable factors [44],

$$U_{\tilde{A},A}(x) := e^{i \int_{C(x_0,x)} (\tilde{A}-A)} = e^{i(\lambda(x) + \int_{C(x_0,x)} A_{\mathbb{Z}})}, \tag{3.45}$$

where x_0 is any fixed point in Λ and $C(x_0, x)$ is any curve in Λ from x_0 to x. Clearly, $U_{\tilde{A},A} \in C^1(\Lambda)$ and can be extended to a continuous function defined in $\overline{\Lambda}$ that we denote with the same symbol. Moreover, if $\tilde{A}$, $A \in \mathcal{A}_\Phi(B)$ we have that $A_{\mathbb{Z}} = 0$, and then

$$U_{\tilde{A},A}(x) = e^{i\lambda(x)}, \tilde{A}, A \in \mathcal{A}_\Phi(B). \tag{3.46}$$

Lemma 3.10. *Suppose that $\tilde{A}$, $A \in \mathcal{A}_{\Phi,2\pi}(B)$. Then, for $x \neq 0$,*

$$\lim_{r\to\infty} U_{\tilde{A},A}(rx) = e^{i(\lambda_\infty(x) + C_{\tilde{A},A})}, \tag{3.47}$$

with $\lambda_\infty(x) := \lim_{r\to\infty} \lambda(rx)$ given by Lemma 3.8 with λ as in (3.41), and where $C_{\tilde{A},A}$ is a real number that is independent of x. Furthermore,

$$\left| U_{\tilde{A},A}(x) - e^{i(\lambda_\infty(x) + C_{\tilde{A},A})} \right| \leq \int_{|x|}^{\infty} c(|x|), \text{ for some } c(r) \in L^1(0,\infty). \tag{3.48}$$

Moreover, if $\tilde{A}$, $A \in \mathcal{A}_\Phi(B)$ we have that $C_{\tilde{A},A} = 0$.

Proof. Let r_0 be such that $K \subset B_{r_0}^{\mathbb{R}^3}(0)$. Take in (3.45) any curve from x_0 to $r_0\hat{x}$ and then the straight line from $r_0\hat{x}$ to $r\hat{x}$ with $r_0 \leq r < \infty$. By (2.12, 3.29, 3.39, 3.42)

$$\lim_{r\to\infty} U_{\tilde{A},A}(rx) = e^{i\lambda_\infty(x)} \lim_{r\to\infty} e^{i\int_{C(x_0,r\hat{x})} A_{\mathbb{Z}}}$$

and

$$\left| U_{\tilde{A},A}(x) - e^{i\lambda_\infty(x)} \lim_{r\to\infty} e^{i\int_{C(x_0,r\hat{x})} A_{\mathbb{Z}}} \right| \leq \int_{|x|}^{\infty} c(|x|), \text{ for some } c(r) \in L^1(0,\infty).$$

For any $y \neq 0$, $y \neq \pm x$ let $C(r\hat{x}, r\hat{y})$ be the straight line from $r\hat{x}$ to $r\hat{y}$. Then,

$$\lim_{r\to\infty} e^{i(\int_{C(x_0,r\hat{x})} A_{\mathbb{Z}} - \int_{C(x_0,r\hat{y})} A_{\mathbb{Z}})} = \lim_{r\to\infty} e^{-i\int_{C(r\hat{x},r\hat{y})} A_{\mathbb{Z}}} = 1,$$

and it follows that,

$$\lim_{r\to\infty} e^{i\int_{C(x_0,r\hat{x})} A_{\mathbb{Z}}} = \lim_{r\to\infty} e^{i\int_{C(x_0,r\hat{y})} A_{\mathbb{Z}}} = e^{iC_{\tilde{A},A}}$$

for some $C_{\tilde{A},A} \in \mathbb{R}$ that is independent of x. If $\tilde{A}, A \in \mathcal{A}_\Phi(B)$, $n_j(\tilde{A}) = n_j(A) = 0$, $j =, 1, 2, \cdots, m$ and hence, $A_{\mathbb{Z}} = 0$, which implies that $C_{\tilde{A},A} = 0$. $\square$

4. The Hamiltonian

Let us denote $\mathbf{p} := -i\nabla$. The Schrödinger equation for an electron in Λ with electric potential $\mathbf{V}$ and magnetic field $\mathbf{B}$ is given by

$$i\hbar\frac{\partial}{\partial t}\phi = \frac{1}{2M}(\mathbf{P} - \frac{q}{c}\mathbf{A})^2\phi + q\,\mathbf{V}\phi, \tag{4.1}$$

where $\hbar$ is Planck's constant, $\mathbf{P} := \hbar\mathbf{p}$ is the momentum operator, c is the speed of light, M and q are, respectively, the mass and the charge of the electron and $\mathbf{A}$ is a magnetic potential with curl$\mathbf{A} = \mathbf{B}$. To simplify the notation we multiply both sides of (4.1) by $\frac{1}{\hbar}$ and we write Schrödinger's equation as follows:

$$i\frac{\partial}{\partial t}\phi = \frac{1}{2m}(\mathbf{p} - A)^2\phi + V\phi, \tag{4.2}$$

with $m := M/\hbar$, $A = \frac{q}{\hbar c}\mathbf{A}$ and $V := \frac{q}{\hbar}\mathbf{V}$. Note that since we write Schrödinger's equation in this form our Hamiltonians below are the physical Hamiltonians divided by $\hbar$. We fix the flux modulo 2π by taking $A \in \mathcal{A}_{\Phi,2\pi}$, where $B := \frac{q}{\hbar c}\mathbf{B}$. Note that this corresponds to fix the circulations of $\mathbf{A}$ modulo $\frac{\hbar c}{q}2\pi$, or equivalently, to fix the fluxes of the magnetic field $\mathbf{B}$ modulo $\frac{\hbar c}{q}2\pi$.

For any open set, O, we denote by $\mathcal{H}_s(O)$, $s = 1, 2, \ldots$ the Sobolev spaces [1] and by $\mathcal{H}_{s,0}(O)$ the closure of $C_0^\infty(O)$ in the norm of $\mathcal{H}_s(O)$. We define the quadratic form,

$$h_0(\phi, \psi) := \frac{1}{2m}(\mathbf{p}\phi, \mathbf{p}\psi),\ D(h_0) := \mathcal{H}_{1,0}(\Lambda). \tag{4.3}$$

The associated positive operator in $L^2(\Lambda)$ [23,31] is $\frac{-1}{2m}\Delta_D$, where Δ_D is the Laplacian with Dirichlet boundary condition on $\partial\Lambda$. We define $H(0,0) := \frac{-1}{2m}\Delta_D$. By elliptic regularity [2], $D(H(0,0)) = \mathcal{H}_2(\Lambda) \cap \mathcal{H}_{1,0}(\Lambda)$.

For any $A \in \mathcal{A}_{\Phi,2\pi}(B)$ we define,

$$h_A(\phi,\psi) := \frac{1}{2m}((\mathbf{p}-A)\phi,(\mathbf{p}-A)\psi) = h_0(\phi,\psi) + \frac{1}{2m}(-(\mathbf{p}\phi, A\psi) - (A\phi,\mathbf{p}\psi)) + \frac{1}{2m}(A\phi, A\psi),\ D(h_A) = \mathcal{H}_{1,0}(\Lambda). \tag{4.4}$$

As the quadratic form $-\frac{1}{2m}((\mathbf{p}\phi, A\psi)+(A\phi,\mathbf{p}\psi)) + \frac{1}{2m}(A\phi, A\psi)$ is h_0-bounded with relative bound zero, h_A is closed and positive. We denote by $H(A,0)$ the associated positive self-adjoint operator [23,31]. $H(A,0)$ is the Hamiltonian with magnetic potential A. Note that as the operator $\frac{1}{2m}(-2A_C\cdot\mathbf{p}+A_C^2)$ is $H(0,0)$ compact we have that $H(0,0) - \frac{1}{m}A_C\cdot\mathbf{p} + \frac{1}{2m}A_C^2$ is self-adjoint on the domain of $H(0,0)$, and then

$$H(A_C,0) = H(0,0) - \frac{1}{m}A_C\cdot\mathbf{p} + \frac{1}{2m}A_C^2,\ D(H(A_C,0)) = \mathcal{H}_2(\Lambda)\cap\mathcal{H}_{1,0}(\Lambda). \tag{4.5}$$

The electric potential V is a measurable real-valued function defined on Λ. We assume that $|V|$ is h_0-bounded with relative bound zero. Under this condition [23,31] the quadratic form,

$$h_{A,V}(\phi,\psi) := h_A(\phi,\psi) + (V\phi,\psi),\ D(h_{A,V}) = \mathcal{H}_{1,0}(\Lambda), \tag{4.6}$$

is closed and bounded from below. The associated operator, $H(A,V)$, is self-adjoint and bounded from below. $H(A,V)$ is the Hamiltonian with magnetic potential A and electric potential V. If furthermore, V is $-\Delta_D$ compact, the operator $H(0,0) - \frac{1}{m}A_C\cdot\mathbf{p} + \frac{1}{2m}A_C^2 + V$ is self-adjoint on the domain of $H(0,0)$ and then,

$$H(A_C,V) = H(0,0) - \frac{1}{m}A_C\cdot\mathbf{p} + \frac{1}{2m}A_C^2 + V,\ D(H(A_C,V)) = \mathcal{H}_2(\Lambda)\cap\mathcal{H}_{1,0}(\Lambda). \tag{4.7}$$

We will denote by $U_{\tilde{A},A}$ the operator of multiplication by $U_{\tilde{A},A}(x)$. See (3.45). Note that $U_{\tilde{A},A}$ is unitary in $L^2(\Lambda)$ and that $U^*_{\tilde{A},A}$ is the operator of multiplication by $U_{A,\tilde{A}}(x)$.

Theorem 4.1. *Suppose that $\tilde{A}, A \in \mathcal{A}_{\Phi,2\pi}(B)$. Then $H(\tilde{A},V)$ and $H(A,V)$ are unitarily equivalent,*

$$H(\tilde{A},V) = U_{\tilde{A},A}\,H(A,V)\,U^*_{\tilde{A},A},\quad D(H(\tilde{A},V)) = U_{\tilde{A},A}\,D(H(A,V)). \tag{4.8}$$

Proof. As $U_{\tilde{A},A}$ and $U^*_{\tilde{A},A}$ are bijections on $\mathcal{H}_{1,0}(\Lambda)$ we have that

$$h_{\tilde{A},V}(\phi,\psi) = h_{A,V}\left(U^*_{\tilde{A},A}\phi, U^*_{\tilde{A},A}\psi\right),\ \phi,\psi\in\mathcal{H}_{1,0}(\Lambda).$$

Suppose that $\phi\in D(H(\tilde{A},V))$. Then, for every $\chi\in\mathcal{H}_{1,0}(\Lambda)$,

$$(U^*_{\tilde{A},A}\,H(\tilde{A},V)\phi,\chi) = h_{A,V}(U^*_{\tilde{A},A}\phi,\chi).$$

This implies that $U^*_{\tilde{A},A}\,\phi\in D(H(A,V))$ and that

$$H(A,V)U^*_{\tilde{A},A}\,\phi = U^*_{\tilde{A},A}H(\tilde{A},V)\phi,$$

which proves the theorem. □

5. Scattering

In the following assumptions we summarize the conditions on the magnetic field and the electric potential that we use. We denote by Δ the self-adjoint realization of the Laplacian in $L^2(\mathbb{R}^3)$ with domain $\mathcal{H}_2(\mathbb{R}^3)$. Below we assume that V is Δ-bounded with relative bound zero. By this we mean that the extension of V to $\mathbb{R}^3$ by zero is $\Delta-$bounded with relative bound zero. Using a extension operator from $\mathcal{H}_2(\Lambda)$ to $H_2(\mathbb{R}^3)$ [36] we prove that this is equivalent to require that V is bounded from $\mathcal{H}_2(\Lambda)$ into $L^2(\Lambda)$ with relative bound zero. We denote by $\|\cdot\|$ the operator norm in $L^2(\mathbb{R}^3)$.

Assumption 5.1. *We assume that the magnetic field, B, is a real-valued, bounded 2–form in $\overline{\Lambda}$, that is continuous in a neighborhood of ∂K, where K satisfies Assumption 2.1, and furthermore,*

1. B is closed : $dB|_\Lambda \equiv \operatorname{div} B = 0$.
2. *There are no magnetic monopoles in K:*

$$\int_{\partial K_j} B = 0, \; j \in \{1, 2, \ldots, L\}. \tag{5.1}$$

3.

$$|B(x)| \leq C(1 + |x|)^{-\mu}, \text{ for some } \mu > 2. \tag{5.2}$$

4. $d * B|_\Lambda \equiv \operatorname{curl} B$ *is bounded and,*

$$|\operatorname{curl} B| \leq C(1 + |x|)^{-\mu}. \tag{5.3}$$

5. *The electric potential, V, is a real-valued function, it is Δ–bounded, and*

$$\left\| F(|x| \geq r) V(-\Delta + I)^{-1} \right\| \leq C(1 + |x|)^{-\alpha}, \text{ for some } \alpha > 1. \tag{5.4}$$

Note that (5.4) implies that V is h_0-bounded with relative bound zero. Furthermore, condition (5.4) is equivalent to the following assumption [32]:

$$\left\| V(-\Delta + I)^{-1} F(|x| \geq r) \right\| \leq C(1 + |x|)^{-\alpha}, \text{ for some } \alpha > 1. \tag{5.5}$$

Condition (5.4) has a clear intuitive meaning, it is a condition on the decay of V at infinity. However, in the proofs below we use the equivalent statement (5.5).

Let us define,

$$H_0 := -\frac{1}{2m}\Delta, \; D(H_0) = \mathcal{H}_2(\mathbb{R}^3).$$

Let J be the identification operator from $L^2(\mathbb{R}^3)$ onto $L^2(\Lambda)$ given by multiplication by the characteristic function of Λ. The wave operators are defined as follows:

$$W_\pm(A, V) := \text{s-}\lim_{t \to \pm\infty} e^{itH(A,V)} \, J \, e^{-itH_0}, \tag{5.6}$$

provided that the strong limits exist. We first prove that they exist in the Coulomb gauge.

Proposition 5.2. *Suppose that B and V satisfy Assumption 5.1. Then, the wave operators $W_\pm(A_C, V)$ exist and are isometric.*

Proof. Let $\chi \in C^\infty(\mathbb{R}^3)$ satisfy $\chi(x) = 0$ in a neighborhood of K and $\chi(x) = 1$ for $|x| \geq r_0$ with r_0 large enough. Then, since $(1 - \chi(x))(H_0 + I)^{-1}$ is compact,

$$W_\pm(A_C, V) = \text{s-}\lim_{t\to\pm\infty} e^{itH(A_C,V)}\, \chi(x)\, e^{-itH_0}.$$

By Duhamel's formula, for $\phi \in D(H_0)$,

$$W_\pm(A_C, V)\phi = \chi(x)\phi(x) + \int_0^{\pm\infty} i\, e^{itH(A_C,V)}\, [H(A_C, V)\chi(x) - \chi(x)H_0]\, \phi(x)\, dt. \tag{5.7}$$

By Theorem 3.7 the proof that the integral in the right-hand side of (5.7) is absolutely convergent is standard. For example, it follows from Lemma 2.2 of [14] taking $\phi = e^{im\mathbf{v}\cdot x}\varphi$, with $\mathbf{v} \in \mathbb{R}^3$, $|\mathbf{v}| \geq 4\eta > 0$, and $\hat{\varphi} \in C_0^\infty(B_{m\eta}^{\mathbb{R}^3}(0))$, which is a dense set in $L^2(\mathbb{R}^3)$. $\square$

Lemma 5.3. (Gauge Transformations). *Suppose that Assumption 5.1 is true. Then, for every $A \in \mathcal{A}_{\Phi,2\pi}(B)$ the wave operators $W_\pm(A, V)$ exist and are isometric. Moreover, if $\tilde{A} \in \mathcal{A}_{\Phi,2\pi}(B)$, then,*

$$W_\pm(\tilde{A}, V) = e^{-iC_{\tilde{A},A}}\, U_{\tilde{A},A}\, W_\pm(A, V)\, e^{-i\lambda_\infty(\pm\mathbf{p})}. \tag{5.8}$$

Proof. Since we already know that $W_\pm(A_C, V)$ exist and are isometric it is enough to prove the gauge transformation formula (5.8). We argue as in the proof of Lemma 2.3 of [40]. By (4.8),

$$\begin{aligned} W_\pm(\tilde{A}, V) &= U_{\tilde{A},A}\, \text{s-}\lim_{t\to\pm\infty} e^{itH(A,V)} U_{A,\tilde{A}} J e^{-itH_0} \\ &= U_{\tilde{A},A}\, \text{s-}\lim_{t\to\pm\infty} e^{itH(A,V)}\, J\, e^{-i(\lambda_\infty(x)+C_{\tilde{A},A})} e^{-itH_0}, \end{aligned}$$

where we used that by Lemma 3.10 and the Rellich selection theorem $U_{A,\tilde{A}} - e^{-i(\lambda_\infty(x)+C_{\tilde{A},A})}$ is a compact operator from $D(H_0)$ into $L^2(\mathbb{R}^3)$. We finish the proof of the lemma as in the proof of Eq. (2.29) of [40], using the second equation in (3.39).

The scattering operator is defined as

$$S(A, V) := W_+^*(A, V)\, W_-(A, V).$$

By (5.8)

$$S(\tilde{A}, V) = e^{i\lambda_\infty(\mathbf{p})}\, S(A, V)\, e^{-i\lambda_\infty(-\mathbf{p})},\ \tilde{A}, A \in \mathcal{A}_{\Phi,2\pi}(B). \quad \square \tag{5.9}$$

Definition 5.4. *We say that $A \in \mathcal{A}_{\Phi,2\pi}(B)$ is short-range if*

$$|A(x)| \leq C(1 + |x|)^{-1-\varepsilon},\ \text{for some}\ \varepsilon > 0. \tag{5.10}$$

We denote the set of all short-range potentials in $\mathcal{A}_{\Phi,2\pi}(B)$ by $\mathcal{A}_{\Phi,2\pi,\mathrm{SR}}(B)$.

Note that if $\tilde{A}, A \in \mathcal{A}_{\Phi,2\pi}(B)$ and $\tilde{A} - A$ satisfies (5.10), λ_∞ is constant, and then,

$$S(\tilde{A}, V) = S(A, V), \; \tilde{A}, A \in \mathcal{A}_{\Phi,2\pi}(B) \text{ and } \tilde{A} - A \text{ satisfies (5.10)}. \tag{5.11}$$

This implies that,

$$S(A_\Phi, V) = S(A, V), \text{ for any } A \in \mathcal{A}_{\Phi,2\pi}(B), \tag{5.12}$$

where A_Φ is defined in (3.40). Remark that (5.11) holds if $\tilde{A}, A \in \mathcal{A}_{\Phi,2\pi,\mathrm{SR}}(B)$.

We quote below the following result of [40] that we will often use.

Lemma 5.5. *For any* $f \in C_0^\infty(B_{m\eta}^{\mathbb{R}^3}(0))$, $0 \le \rho < 1$, *and for any* $j = 1, 2, \dots$ *there is a constant* C_j *such that*

$$\left\| F\left(|x - \mathbf{v}t| > \frac{|\mathbf{v}t|}{4}\right) e^{-itH_0} f\left(\frac{\mathbf{p} - m\mathbf{v}}{v^\rho}\right) F\left(|x| \le |\mathbf{v}t|/8\right) \right\| \le C_j (1 + |\mathbf{v}t|)^{-j}, \tag{5.13}$$

for $v := |\mathbf{v}| > (8\eta)^{1/(1-\rho)}$.

Proof. Corollary 2.2 of [40]. □

5.1. High-velocity estimates I. The magnetic potential. We denote,

$$\Lambda_{\hat{\mathbf{v}}} := \{x \in \Lambda : x + \tau\hat{\mathbf{v}} \in \Lambda, \; \forall \tau \in \mathbb{R}\}, \text{ for } \mathbf{v} \ne 0, \tag{5.14}$$

$$L_{A,\hat{\mathbf{v}}}(t) := \int_0^t \hat{\mathbf{v}} \cdot A(x + \tau\hat{\mathbf{v}}) d\tau, -\infty \le t \le \infty. \tag{5.15}$$

Remark that under translation in configuration or momentum space generated, respectively, by $\mathbf{p}$ and x we obtain

$$e^{i\mathbf{p}\cdot\mathbf{v}t} f(x) e^{-i\mathbf{p}\cdot\mathbf{v}t} = f(x + \mathbf{v}t), \tag{5.16}$$

$$e^{-im\mathbf{v}\cdot x} f(\mathbf{p}) e^{im\mathbf{v}\cdot x} = f(\mathbf{p} + m\mathbf{v}), \tag{5.17}$$

and, in particular,

$$e^{-im\mathbf{v}\cdot x} e^{-itH_0} e^{im\mathbf{v}\cdot x} = e^{-imv^2t/2} e^{-i\mathbf{p}\cdot\mathbf{v}t} e^{-itH_0}. \tag{5.18}$$

The purpose of the obstacle K is to shield the incoming electrons from the magnetic field inside the obstacle. In order to separate the scattering effect of the magnetic potential from that of the magnetic field inside the obstacle K, we consider asymptotic configurations that have negligible interaction with K for all times in the high-velocity limit. For any non-zero $\mathbf{v} \in \mathbb{R}^3$ we take asymptotic configurations ϕ with compact support in $\Lambda_{\hat{\mathbf{v}}}$. The free evolution boosted by $\hat{\mathbf{v}}$ is given by (5.18) and-to a good approximation-in the limit when $v \to \infty$ with $\hat{\mathbf{v}}$ fixed this can be replaced (modulo an unimportant phase factor) by the classical translation $e^{-i\mathbf{p}\cdot\mathbf{v}t}$. Then, in the high-velocity limit it is a good approximation to assume that the free evolution of our asymptotic configuration is given by $e^{-i\mathbf{p}\cdot\mathbf{v}t}\phi_0 = \phi_0(x - \mathbf{v}t)$, and as ϕ_0 has support in $\Lambda_{\hat{\mathbf{v}}}$, it has negligible interaction with K for all times. Note that instead of boosting the observables we can boost the asymptotic configurations and consider the high-velocity asymptotic configurations

$$\phi_{\mathbf{v}} := e^{im\mathbf{v}\cdot x}\phi_0.$$

Lemma 5.6. *Suppose that B, V satisfy Assumption 5.1. Let Λ_0 be a compact subset of $\Lambda_{\hat{\mathbf{v}}}$, with $\mathbf{v} \in \mathbb{R} \setminus \{0\}$. Then, for all Φ and all $A \in \mathcal{A}_{\Phi,2\pi}(B)$ there is a constant C such that*

$$\left\| \left(e^{-im\mathbf{v}\cdot x}\, W_{\pm}(A, V)\, e^{im\mathbf{v}\cdot x} - e^{-iL_{A,\hat{\mathbf{v}}}(\pm\infty)} \right) \phi \right\|_{L^2(\mathbb{R}^3)} \leq C \frac{1}{v} \|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)}, \quad (5.19)$$

and if moreover, $\operatorname{div} A \in L^2_{\text{loc}}\left(\overline{\Lambda}\right)$,

$$\left\| \left(e^{-im\mathbf{v}\cdot x}\, W^*_{\pm}(A, V)\, e^{im\mathbf{v}\cdot x} - e^{iL_{A,\hat{\mathbf{v}}}(\pm\infty)} \right) \phi \right\|_{L^2(\mathbb{R}^3)} \leq C \frac{1}{v} \|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)}, \quad (5.20)$$

for all $\phi \in \mathcal{H}_2(\mathbb{R}^3)$ with $\operatorname{support} \phi \subset \Lambda_0$.

Proof. We follow the proof of Lemma 2.4 of [40]. We first give the proof in the case of the Coulomb potential A_C. We give the proof for $W_+(A_C, V)$. The proof for $W_-(A_C, V)$ follows in the same way.

By Theorem 3.7, $A_C = A_{(C,1)} + A_{(C,2)}$, where $A_{(C,1)}$ is the Coulomb potential for the extension $\overline{B}$ of the magnetic field. Then, $A_{(C,1)}$ is actually defined in $\mathbb{R}^3$. We can extend $A_{(C,2)}|_{\Omega}$ as an $n-$times, $n = 1, 2, \ldots$, continuously differentiable vector valued function defined in $\mathbb{R}^3$ (Theorem 4.2.2, p. 311 [36]). Consequently, we can extend A_C to a continuous vector valued function defined in $\mathbb{R}^3$ such that div A_C is infinitely differentiable with support contained in the obstacle K. We denote also by A_C this extension.

Let $g \in C_0^{\infty}(\mathbb{R}^3)$ satisfy $g(p) = 1$, $|p| \leq 1$, $g(p) = 0$, $|p| \geq 2$. Denote

$$\tilde{\phi} := g(\mathbf{p}/v^{\rho})\, \phi, \ \frac{1}{2} \leq \rho < 1. \quad (5.21)$$

Then,

$$\left\| \tilde{\phi} - \phi \right\|_{L^2(\mathbb{R}^3)} \leq \frac{1}{v^{2\rho}} \|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)}. \quad (5.22)$$

Hence, it is enough to prove (5.19) for $\tilde{\phi}$.

By our assumption there is a function $\chi \in C^{\infty}(\mathbb{R}^3)$ such that $\chi \equiv 0$ in a neighborhood of K and $\chi(x) = 1$, $x \in \{x : x = y + \tau\hat{\mathbf{v}},\, y \in \operatorname{support}\phi,\, \tau \in \mathbb{R}\} \cup \{x : |x| \geq M\}$ for some M large enough. We use the following notation:

$$H_1 := \frac{1}{v} e^{-im\mathbf{v}\cdot x} H_0\, e^{im\mathbf{v}\cdot x}, \ \ H_2 := \frac{1}{v} e^{-im\mathbf{v}\cdot x} H(A_C, V)\, e^{im\mathbf{v}\cdot x}. \quad (5.23)$$

Note that

$$\begin{aligned} &\left(e^{-im\mathbf{v}\cdot x}\, W_+(A_C, V)\, e^{im\mathbf{v}\cdot x} - \chi(x) e^{-iL_{A_C,\hat{\mathbf{v}}}(\infty)} \right) \tilde{\phi} \\ &\quad = \text{s-}\lim_{t\to\infty} \left[e^{itH_2} \chi(x) e^{-itH_1} - \chi(x) e^{-iL_{A_C,\hat{\mathbf{v}}}(t)} \right] \tilde{\phi}. \end{aligned} \quad (5.24)$$

Denote

$$\begin{aligned} P(t, \tau) := {}& e^{i\tau H_2} i \left[H_2 e^{-iL_{A_C,\hat{\mathbf{v}}}(t-\tau)} \chi(x) - e^{-iL_{A_C,\hat{\mathbf{v}}}(t-\tau)} \chi(x) \right. \\ &\times \left. \left(H_1 - \hat{\mathbf{v}} \cdot A_C(x + (t-\tau)\hat{\mathbf{v}}) \right) \right] e^{-i\tau H_1} \tilde{\phi}. \end{aligned} \quad (5.25)$$

Then, by Duhamel's formula,

$$\left[e^{itH_2}\chi(x)e^{-itH_1} - \chi(x)e^{-iL_{A_C,\hat{\mathbf{v}}(t)}}\right]\tilde{\phi} = \int_0^t d\tau\, P(t,\tau). \tag{5.26}$$

We designate

$$b(x,t) := A_C(x + t\hat{\mathbf{v}}) + \int_0^t (\hat{\mathbf{v}} \times B)(x + \tau\hat{\mathbf{v}})d\tau. \tag{5.27}$$

For $\mathbf{f} : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}^3$ with $\mathbf{f}_t(x) := \mathbf{f}(x,t) \in L^1_{\text{loc}}(\mathbb{R}^3, \mathbb{R}^3)$ we define

$$\Xi_{\mathbf{f}}(x,t) := \frac{1}{2m}\chi(x)\left[-\mathbf{p}\cdot\mathbf{f}(x,t) - \mathbf{f}(x,t)\cdot\mathbf{p} + (\mathbf{f}(x,t))^2\right]. \tag{5.28}$$

We have that [40]

$$P(t,\tau) = T_1 + T_2 + T_3, \tag{5.29}$$

with

$$T_1 := \frac{1}{v}e^{i\tau H_2} i e^{-iL_{A_C,\hat{\mathbf{v}}}(x,t-\tau)} \left(\Xi_b(x,t-\tau) + \chi V(x)\right) e^{-i\tau H_1}\tilde{\phi}, \tag{5.30}$$

$$T_2 := \tfrac{1}{2mv} e^{i\tau H_2} i e^{-iL_{A_C,\hat{\mathbf{v}}}(x,t-\tau)} \{-(\Delta\chi) + 2(\mathbf{p}\chi)\cdot\mathbf{p} - 2b(x,t-\tau)\cdot(\mathbf{p}\chi)\} e^{-i\tau H_1}\tilde{\phi}, \tag{5.31}$$

$$T_3 := e^{i\tau H_2} i e^{-iL_{A_C,\hat{\mathbf{v}}}(x,t-\tau)} \left[(\mathbf{p}\chi)\cdot\hat{\mathbf{v}}\right] e^{-i\tau H_1}\tilde{\phi}. \tag{5.32}$$

Note that ([4], Eq. (2.18))

$$\left\| \int_0^{t-\tau} d\nu (\hat{\mathbf{v}} \times B)(x + \nu\hat{\mathbf{v}})\, F(|x - \tau\hat{\mathbf{v}}| \le |\tau|/4) \right\|_{L^\infty(\mathbb{R}^3)} \le C\frac{1}{(1+|\tau|)^{\mu-1}}, \tag{5.33}$$

$$\begin{aligned} &\left\| \textstyle\int_0^{t-\tau} d\nu (\nabla\cdot(\hat{\mathbf{v}} \times B))(x + \nu\hat{\mathbf{v}})\, F(|x - \tau\hat{\mathbf{v}}| \le |\tau|/4) \right\|_{L^\infty(\mathbb{R}^3)} \\ &= \left\| \textstyle\int_0^{t-\tau} d\nu (\hat{\mathbf{v}}\cdot \ \text{curl}\, B)(x + \nu\hat{\mathbf{v}}) \right., \\ &F(|x - \tau\hat{\mathbf{v}}| \le |\tau|/4) \Big\|_{L^\infty(\mathbb{R}^3)} \le C\frac{1}{(1+|\tau|)^{\mu-1}}. \end{aligned} \tag{5.34}$$

Using Theorem 3.7, Lemma 5.5, (5.2, 5.3, 5.5, 5.33, 5.34) we prove as in the proof of Lemma 2.4 of [40] that

$$\|T_1(\tau)\|_{L^2(\mathbb{R}^3)} \le \frac{C}{v}\frac{1}{(1+|\tau|)^{\min(2-\varepsilon,\mu-1,\alpha)}}\|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)}, \tag{5.35}$$

$$\|T_2(\tau)\|_{L^2(\mathbb{R}^3)} \le \frac{C_j}{v}\frac{1}{(1+|\tau|)^j}\|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)},\ j = 1, 2, \ldots, \tag{5.36}$$

$$\int_{-\infty}^{\infty} d\tau \ \|T_3(\tau)\|_{L^2(\mathbb{R}^3)} \leq \frac{C}{v}\|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)}. \tag{5.37}$$

For the reader's convenience we estimate one of the terms. Denote by

$$\eta(x,t) := \int_0^t (\hat{\mathbf{v}} \times B)(x+\tau\hat{\mathbf{v}})d\tau. \tag{5.38}$$

Then, by Lemma 5.5 and (5.33),

$$\begin{aligned}
&\left\| \frac{1}{mv} e^{-iL_{A_C,\hat{\mathbf{v}}}(x,t-\tau)} \eta(x,t-\tau) e^{-i\tau H_1} \cdot \mathbf{p}\tilde{\phi} \right\|_{L^2(\mathbb{R}^3)} \\
&\quad \leq \frac{C}{v}\Big[\|\eta(x,t-\tau)|F(|x-\tau\mathbf{v}| > |\tau|/4) e^{-iH_0\tau/v} \\
&g\left(\frac{\mathbf{p}-m\mathbf{v}}{v^\rho}\right) F(|x| \leq |\tau|/8)\| \|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)} + \|\eta(x,t-\tau)F(|x-\tau\mathbf{v}| \\
&\quad \leq |\tau|/4)\|_{L^\infty(\mathbb{R}^3)} \|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)} \\
&\quad + \|F(|x| \geq |\tau|/8)\mathbf{p}\cdot\tilde{\phi}\|_{L^2(\mathbb{R}^3)}\Big] \leq \frac{C}{(1+|\tau|)^{\mu-1}} \|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)}.
\end{aligned}$$

By (5.26, 5.29, 5.35, 5.36, 5.37)

$$\left\| \left[e^{itH_2}\chi(x)e^{-itH_1} - \chi(x)e^{-iL_{A_C,\hat{\mathbf{v}}}(t)} \right] \tilde{\phi} \right\|_{L^2(\mathbb{R}^3)} \leq \frac{C}{v}\|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)}. \tag{5.39}$$

By (5.24) this proves (5.19) for A_C. Given $A \in \mathcal{A}_{\Phi,2\pi}(B)$ we define A_Φ as in (3.40). As $A_\Phi \in \mathcal{A}_\Phi(B)$, we prove that (5.19) holds for A_Φ as in the proof of Lemma 2.4 of [40] using the formulae for change of gauge (5.8). Then, we prove that it is true for A using the gauge transformation formulae between A and A_Φ, note that in this case $\lambda \equiv \lambda_\infty \equiv 0$, observing that

$$e^{-iC_{A,A_\Phi}} = e^{-i(\int_{C(x_0,x)} A_{\mathbb{Z}} + \int_0^{\pm\infty} \hat{\mathbf{v}}\cdot A_{\mathbb{Z}}(x+\tau\hat{\mathbf{v}})d\tau)} = (U_{A,A_\Phi})^* e^{-i\int_0^{\pm\infty} \hat{\mathbf{v}}\cdot A_{\mathbb{Z}}(x+\tau\hat{\mathbf{v}})d\tau}, \tag{5.40}$$

and using (3.42) with $\lambda \equiv 0$.

We now prove (5.20). Note that ([4], Eq. 2.12)

$$(\mathbf{p}-A(x))e^{-iL_{A,\hat{\mathbf{v}}}(t)} = e^{-iL_{A,\hat{\mathbf{v}}}(t)} \left(\mathbf{p} - A(x+t\hat{\mathbf{v}}) - \int_0^t (\hat{\mathbf{v}}\times B)(x+\tau\hat{\mathbf{v}})d\tau \right). \tag{5.41}$$

Then, since $\mathrm{div}A \in L^2_{\mathrm{loc}}\left(\overline{\Lambda}\right)$ it follows from Sobolev's imbedding theorem [1] that

$$\|e^{iL_{A,\hat{\mathbf{v}}}(\pm\infty)}\phi\|_{\mathcal{H}_2(\mathbb{R}^3)} \leq C\|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)}. \tag{5.42}$$

For simplicity we denote below $W_\pm(A,V)$ by $W_\pm$ and we define

$$W_{\pm,\mathbf{v}} := e^{-im\mathbf{v}\cdot x}\, W_\pm\, e^{im\mathbf{v}\cdot x}. \tag{5.43}$$

As the wave operators are isometric, $W^*_{\pm,\mathbf{v}} W_{\pm,\mathbf{v}} = I$, and then

$$\left\| \left(W^*_{\pm,\mathbf{v}} - e^{i L_{A,\hat{\mathbf{v}}}(\pm\infty)} \right) \phi \right\|_{L^2(\mathbb{R}^3)} = \left\| W^*_{\pm,\mathbf{v}} \phi - W^*_{\pm,\mathbf{v}} W_{\pm,\mathbf{v}} e^{i L_{A,\hat{\mathbf{v}}}(\pm\infty)} \phi \right\|_{L^2(\mathbb{R}^3)}$$

$$\leq \left\| \left(W_{\pm,\mathbf{v}} - e^{-i L_{A,\hat{\mathbf{v}}}(\pm\infty)} \right) e^{i L_{A,\hat{\mathbf{v}}}(\pm\infty)} \phi \right\|_{L^2(\mathbb{R}^3)} \leq C \frac{1}{v} \|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)}.$$

□

We now state the main result of this subsection.

Theorem 5.7. (Reconstruction Formula I). *Suppose that B, V satisfy Assumption 5.1. Let Λ_0 be a compact subset of $\Lambda_{\hat{\mathbf{v}}}$, with $\mathbf{v} \in \mathbb{R}\backslash\{0\}$. Then, for all Φ and all $A \in \mathcal{A}_{\Phi,2\pi}(B)$ there is a constant C such that*

$$\left\| \left(e^{-im\mathbf{v}\cdot x}\, S(A, V)\, e^{im\mathbf{v}\cdot x} - e^{i \int_{-\infty}^{\infty} \hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\, d\tau} \right) \phi \right\|_{L^2(\mathbb{R}^3)} \leq C \frac{1}{v} \|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)}, \tag{5.44}$$

$$\left\| \left(e^{-im\mathbf{v}\cdot x}\, S(A, V)^*\, e^{im\mathbf{v}\cdot x} - e^{-i \int_{-\infty}^{\infty} \hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\, d\tau} \right) \phi \right\|_{L^2(\mathbb{R}^3)} \leq C \frac{1}{v} \|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)}, \tag{5.45}$$

for all $\phi \in \mathcal{H}_2(\mathbb{R}^3)$ with support $\phi \subset \Lambda_0$.

Proof. We use the same notation as in the end of the proof of Lemma 5.6.

First we prove (5.44) and (5.45) for A_C,

$$\begin{aligned}
&\left\| \left(e^{-im\mathbf{v}\cdot x}\, S(A_C, V)\, e^{im\mathbf{v}\cdot x} - e^{i \int_{-\infty}^{\infty} \hat{\mathbf{v}}\cdot A_C(x+\tau\hat{\mathbf{v}})\, d\tau} \right) \phi \right\|_{L^2(\mathbb{R}^3)} \\
&= \Big\| W^*_{+,\mathbf{v}} W_{-,\mathbf{v}} \phi - W^*_{+,\mathbf{v}} W_{+,\mathbf{v}} e^{i(L_{A_C,\hat{\mathbf{v}}}(\infty) - L_{A_C,\hat{\mathbf{v}}}(-\infty))} \\
&\phi \Big\|_{L^2(\mathbb{R}^3)} \leq \Big\| \left[W_{-,\mathbf{v}} - e^{-i L_{A_C,\hat{\mathbf{v}}}(-\infty)} \right] \phi \\
&\quad - \left[W_{+,\mathbf{v}} - e^{-i L_{A_C,\hat{\mathbf{v}}}(\infty)} \right] e^{i(L_{A_C,\hat{\mathbf{v}}}(\infty) - L_{A_C,\hat{\mathbf{v}}}(-\infty))} \phi \Big\|_{L^2(\mathbb{R}^3)} \leq \frac{C}{v} \|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)}.
\end{aligned}$$

The proof for $S(A_C, V)^*$ follows in the same way.

Now we prove (5.44) for $A \in \mathcal{A}_{\Phi,2\pi}(B)$, the proof of (5.45) follows in the same way. By (5.12), $S(A, V) = S(A_\Phi, V)$. From (5.40) it follows that

$$e^{i \int_{-\infty}^{\infty} \hat{\mathbf{v}}\cdot A_{\mathbb{Z}}(x+\tau\hat{\mathbf{v}}) d\tau} = e^{-i C_{A,A_\Phi}} e^{i C_{A,A_\Phi}} = 1,$$

and thus

$$e^{i \int_{-\infty}^{\infty} \hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}}) d\tau} = e^{i \int_{-\infty}^{\infty} \hat{\mathbf{v}}\cdot A_\Phi(x+\tau\hat{\mathbf{v}}) d\tau}. \tag{5.46}$$

Then it is enough to prove (5.44) for $A = A_C + \nabla\lambda$.
By (5.9), (5.17) and as λ is homogenous of order zero,

$$\begin{aligned}
&\|(e^{-im\mathbf{v}\cdot x} S(A, V) e^{im\mathbf{v}\cdot x} - e^{i \int_{-\infty}^{\infty} \hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}}) d\tau}) \phi\|_{L^2(\mathbb{R}^3)} \\
&= \|(e^{i\lambda_\infty(\frac{\mathbf{p}}{mv}+\hat{\mathbf{v}})} e^{-im\mathbf{v}\cdot x} S(A_C, V) e^{im\mathbf{v}\cdot x} e^{-i\lambda_\infty(-\frac{\mathbf{p}}{mv}-\hat{\mathbf{v}})} - e^{i \int_{-\infty}^{\infty} \hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}}) d\tau}) \phi\|_{L^2(\mathbb{R}^3)} \\
&\leq \|(e^{i\lambda_\infty(\frac{\mathbf{p}}{mv}+\hat{\mathbf{v}})} e^{-im\mathbf{v}\cdot x} S(A_C, V) e^{im\mathbf{v}\cdot x} (e^{-i\lambda_\infty(-\frac{\mathbf{p}}{mv}-\hat{\mathbf{v}})} - e^{-i\lambda_\infty(-\hat{\mathbf{v}})}) \phi\|_{L^2(\mathbb{R}^3)} \\
&\quad + \|(e^{i\lambda_\infty(\frac{\mathbf{p}}{mv}+\hat{\mathbf{v}})} (e^{-im\mathbf{v}\cdot x} S(A_C, V) e^{im\mathbf{v}\cdot x} - e^{i \int_{-\infty}^{\infty} \hat{\mathbf{v}}\cdot A_C(x+\tau\hat{\mathbf{v}}) d\tau}) e^{-i\lambda_\infty(-\hat{\mathbf{v}})}) \phi\|_{L^2(\mathbb{R}^3)} \\
&\quad + \|(e^{i\lambda_\infty(\frac{\mathbf{p}}{mv}+\hat{\mathbf{v}})} - e^{i\lambda_\infty(\hat{\mathbf{v}})}) e^{i \int_{-\infty}^{\infty} \hat{\mathbf{v}}\cdot A_C(x+\tau\hat{\mathbf{v}}) d\tau} e^{-i\lambda_\infty(-\hat{\mathbf{v}})} \phi\|_{L^2(\mathbb{R}^3)} \leq C \frac{1}{v} \|\phi\|_{\mathcal{H}_2(\mathbb{R}^3)}.
\end{aligned}$$

The last inequality follows from (3.39), (5.42) and (5.44) for A_C. □

5.2. High-velocity estimates II. The electric potential. Recall that $\tilde{\phi}$ is defined in (5.21) and that H_1 is given by (5.23).

Lemma 5.8. *Let $h : \mathbb{R}^3 \to \mathbb{R}$ be a bounded function with compact support contained in $\mathbb{R}^3 \setminus \Lambda_{\hat{\mathbf{v}}}$, and let ϕ be a function in $\mathcal{H}_6(\mathbb{R}^3)$ with compact support contained in $\Lambda_{\hat{\mathbf{v}}}$. Then, for any $l \in \mathbb{N}$ there exists a constant C_l such that the following inequalities hold:*

i) $\|he^{-i\tau H_1}\tilde{\phi}\|_{L^2(\mathbb{R}^3)} \leq C_l \frac{1}{(1+|\tau|)^l} \frac{1}{v^{3-\epsilon}} \|\phi\|_{\mathcal{H}_6(\mathbb{R}^3)} \; \forall \epsilon > 0,$
ii) $\|h\mathbf{p}e^{-i\tau H_1}\tilde{\phi}\|_{L^2(\mathbb{R}^3)} \leq C_l \frac{1}{(1+|\tau|)^l} \frac{1}{v^{2-\epsilon}} \|\phi\|_{\mathcal{H}_5(\mathbb{R}^3)} \; \forall \epsilon > 0.$

Proof. We prove i), ii) follows in a similar way. Clearly,

$$\|\tilde{\phi} - \phi\|_{L^2(\mathbb{R}^3)} \leq \frac{1}{v^{6\rho}} \|\phi\|_{\mathcal{H}_6(\mathbb{R}^3)}, \text{ where } \rho \geq 1/2. \tag{5.47}$$

It follows from (5.18) and the properties of the support of h and ϕ that

$$\|he^{-i\tau H_1}\phi\|_{L^2(\mathbb{R}^3)} = \left\| he^{-i\tau \mathbf{p}\cdot\hat{\mathbf{v}}} \left(e^{-i\tau \frac{\mathbf{p}^2}{2mv}} - I - \left(-i\tau \frac{\mathbf{p}^2}{2mv}\right) - \frac{1}{2}\left(-i\tau \frac{\mathbf{p}^2}{2mv}\right)^2 \right)\phi \right\|.$$

Observing that

$$\left|\left(e^{-i\tau \frac{\mathbf{p}^2}{2mv}} - I - \left(-i\tau \frac{\mathbf{p}^2}{2mv}\right) - \frac{1}{2}\left(-i\tau \frac{\mathbf{p}^2}{2mv}\right)^2 \right)\right| \leq C|\tau|^3 \frac{\mathbf{p}^6}{(2mv)^3},$$

we obtain

$$\|he^{-i\tau H_1}\phi\|_{L^2(\mathbb{R}^3)} \leq C \frac{(1+|\tau|)^3}{(2mv)^3} \|\phi\|_{\mathcal{H}_6(\mathbb{R}^3)}. \tag{5.48}$$

We prove as in (5.36) that there exists a constant C_l such that

$$\|he^{-i\tau H_1}\tilde{\phi}\|_{L^2(\mathbb{R}^3)} \leq C_l \frac{1}{(1+|\tau|)^l} \|\phi\|_{L^2(\mathbb{R}^3)}. \tag{5.49}$$

Finally we obtain i) from (5.47) and interpolating (5.48, 5.49). $\square$

We denote

$$a(\hat{\mathbf{v}}, x) := \int_{-\infty}^{\infty} A(x + \tau\hat{\mathbf{v}}) \cdot \hat{\mathbf{v}} \, d\tau, \tag{5.50}$$

and for $\phi_0 \in \mathcal{H}_6(\mathbb{R}^3)$ with compact support in $\Lambda_{\hat{\mathbf{v}}}$,

$$\phi_{\mathbf{v}} := e^{im\mathbf{v}\cdot x}\phi_0.$$

Recall that $\Lambda_{\hat{\mathbf{v}}}$ is defined in (5.14), that $\Xi_{\mathbf{f}}(x, t)$ is defined in 5.28, that η is defined in (5.38), and that $\mathcal{A}_{\Phi,2\pi}(B)$ is defined in Definition 5.4.

Theorem 5.9. (Reconstruction Formula II). *Suppose that B, V satisfy Assumption 5.1. Let Λ_0 be a compact subset of $\Lambda_{\hat{\mathbf{v}}}$, with $\mathbf{v} \in \mathbb{R} \setminus \{0\}$. Then, for all Φ and all $A \in \mathcal{A}_{\Phi,2\pi,\mathrm{SR}}(B)$,*

$$
\begin{aligned}
v\left(\left[S(A,V) - e^{ia(\hat{\mathbf{v}},x)}\right]\phi_{\mathbf{v}}, \psi_{\mathbf{v}}\right) &= \left(-ie^{ia(\hat{\mathbf{v}},x)} \int_{-\infty}^{\infty} V(x+\tau\hat{\mathbf{v}})\, d\tau\, \phi_0,\ \psi_0\right) \\
&+ \left(-ie^{ia(\hat{\mathbf{v}},x)} \int_{-\infty}^{0} \Xi_\eta(x+\tau\hat{\mathbf{v}}, -\infty)\, d\tau\, \phi_0, \psi_0\right) \\
&+ \left(-i \int_0^{\infty} \Xi_\eta(x+\tau\hat{\mathbf{v}}, \infty)\, d\tau\, e^{ia(\hat{\mathbf{v}},x)}\phi_0, \psi_0\right) + R(\mathbf{v}, \phi_0, \psi_0),
\end{aligned}
\tag{5.51}
$$

where,

$$
|R(\mathbf{v},\phi_0,\psi_0)| \le C\|\phi_0\|_{\mathcal{H}_6(\mathbb{R}^3)}\,\|\psi_0\|_{\mathcal{H}_6(\mathbb{R}^3)} \begin{cases} \frac{1}{v^{\min(\mu-2,\alpha-1)}}, & \text{if } \min(\mu-3,\alpha-2) < 0, \\ \frac{|\ln v|}{v}, & \text{if } \min(\mu-3,\alpha-2) = 0, \\ \frac{1}{v}, & \text{if } \min(\mu-3,\alpha-2) > 0, \end{cases}
\tag{5.52}
$$

for some constant C and all $\phi_0, \psi_0 \in \mathcal{H}_6(\mathbb{R}^3)$ with compact support in Λ_0.

Proof. We first prove the theorem in the Coulomb gauge A_C. Note that

$$
\begin{aligned}
v\left(\left[S(A,V) - e^{ia}\right]\phi_{\mathbf{v}}, \psi_{\mathbf{v}}\right) &= v\left(e^{-iL_{A_C,\hat{\mathbf{v}}}(-\infty)}\phi_0, \mathcal{R}_+\psi_0\right) \\
&+ v\left(\mathcal{R}_-\phi_0, e^{-iL_{A_C,\hat{\mathbf{v}}}(\infty)}\psi_0\right) + v\left(\mathcal{R}_-\phi_0, \mathcal{R}_+\psi_0\right),
\end{aligned}
\tag{5.53}
$$

where

$$
\mathcal{R}_\pm := e^{-im\mathbf{v}\cdot x} W_\pm(A_C, V) e^{im\mathbf{v}\cdot x} - e^{-iL_{A_C,\hat{\mathbf{v}}}(\pm\infty)}.
$$

By Lemma 5.6,

$$
v\,|(\mathcal{R}_-\phi_0, \mathcal{R}_+\psi_0)| \le C\frac{1}{v}\|\phi_0\|_{\mathcal{H}_6(\mathbb{R}^3)}\,\|\psi_0\|_{\mathcal{H}_6(\mathbb{R}^3)}.
\tag{5.54}
$$

We prove below that

$$
\begin{aligned}
&v\left(e^{-iL_{A_C,\hat{\mathbf{v}}}(-\infty)}\phi_0, R_+\psi_0\right) \\
&= \left(-i\int_0^{\infty} (\Xi_\eta(x+\tau\hat{\mathbf{v}}, \infty) + \chi V(x+\tau\hat{\mathbf{v}}))\, d\tau\, e^{ia}\phi_0, \psi_0\right) + R_+(\mathbf{v}, \phi_0, \psi_0),
\end{aligned}
\tag{5.55}
$$

$$
\begin{aligned}
&v\left(\mathcal{R}_-\phi_0, e^{-iL_{A_C,\hat{\mathbf{v}}}(\infty)}\psi_0\right) \\
&= \left(-ie^{ia}\int_{-\infty}^{0} (\Xi_\eta(x+\tau\hat{\mathbf{v}}, -\infty) + \chi V(x+\tau\hat{\mathbf{v}}))\, d\tau\, \phi_0, \psi_0\right) + R_-(\mathbf{v}, \phi_0, \psi_0),
\end{aligned}
\tag{5.56}
$$

where $R_\pm$ satisfy (5.52). Note that (5.56) follows from (5.55) by time inversion and charge conjugation in the magnetic potential, i.e., by taking complex conjugates and changing A_C to $-A_C$. It can also be proved as in the proof of (5.55) that we give below in seven steps.

We use the notation of the proof of Lemma 5.6. For simplicity we denote by $O(r)$ a term that satisfies

$$|O(r)| \leq C\|\phi_0\|_{\mathcal{H}_6(\mathbb{R}^3)}\,\|\psi_0\|_{\mathcal{H}_6(\mathbb{R}^3)}\,r.$$

Step 1.

$$\begin{gathered} v\left(e^{-iL_{A_C,\hat{\mathrm{v}}}(-\infty)}\phi_0,\, R_+\psi_0\right) = \Big(e^{-iL_{A_C,\hat{\mathrm{v}}}(-\infty)}\phi_0, \\ \lim_{t\to\infty}\int_0^t d\tau e^{i\tau H_2} i e^{-iL_{A_C,\hat{\mathrm{v}}}(t-\tau)}\left[\Xi_b(x,t-\tau)+\chi V(x)\right]e^{-i\tau H_1}\tilde{\psi}_0\Big) + O(1/v). \end{gathered} \tag{5.57}$$

Equation (5.57) follows from (5.24), (5.26), (5.29) (with ϕ_0 instead of ϕ) and the following formula that is easily obtained from Lemma 5.8:

$$\|T_2+T_3\|_{L^2(\mathbb{R}^3)} \leq C_l \frac{\|\phi_0\|_{\mathcal{H}_6(\mathbb{R}^3)}}{v^{3-\epsilon}(1+|\tau|)^l},\ \forall\epsilon>0, l=1,2,\ldots, \tag{5.58}$$

that improves (5.36, 5.37).
Step 2.

$$\begin{aligned} &\lim_{t\to\infty}\int_0^t d\tau e^{i\tau H_2} i e^{-iL_{A_C,\hat{\mathrm{v}}}(t-\tau)}\left[\Xi_b(x,t-\tau)+\chi V(x)\right]e^{-i\tau H_1}\tilde{\psi}_0 \\ &\quad= \lim_{t\to\infty}\int_0^t d\tau e^{i\tau H_2} i e^{-iL_{A_C,\hat{\mathrm{v}}}(t-\tau)}\left[\Xi_\eta(x,t-\tau)+\chi V(x)\right]e^{-i\tau H_1}\tilde{\psi}_0. \end{aligned} \tag{5.59}$$

This follows from Lebesgue's dominated convergence theorem and as

$$\lim_{t\to\infty}\left\|\left(\Xi_b(x,t-\tau)-\Xi_\eta(x,t-\tau)\right)e^{-i\tau H_1}\tilde{\psi}_0\right\|_{L^2(\mathbb{R}^3)} = 0,$$

and, moreover,

$$\left\|\left(\Xi_b(x,t-\tau)-\Xi_\eta(x,t-\tau)\right)e^{-itH_1}\tilde{\psi}_0\right\|_{L^2(\mathbb{R}^3)} \leq h(\tau),\ \text{for some}\, h(\tau)\in L^1(0,\infty).$$

This estimate is proven as in the proof of Lemma 5.6, using Lemma 5.5.
Step 3.

$$\begin{aligned} &v\left(e^{-iL_{A_C,\hat{\mathrm{v}}}(-\infty)}\phi_0,\, R_+\psi_0\right) = \int_0^t d\tau\,\Big(e^{-iL_{A_C,\hat{\mathrm{v}}}(-\infty)}\phi_0, \\ &e^{i\tau H_2} i e^{-iL_{A_C,\hat{\mathrm{v}}}(\infty)}\left[\Xi_\eta(x,\infty)+\chi V(x)\right]e^{-i\tau H_1}\tilde{\psi}_0\Big) \\ &\quad+O(1/v)+0\left(1/(1+|t|)^{\min(\mu-2,\alpha-1)}\right). \end{aligned} \tag{5.60}$$

This follows from Steps 1 and 2, and from the following argument. As in the proof of Lemma 5.6 we prove that

$$\left\|\left[\Xi_\eta(x,t-\tau)+\chi V(x)\right]e^{-i\tau H_1}\tilde{\psi}_0\right\|_{L^2(\mathbb{R}^3)} \leq C\left(1/(1+|\tau|)^{\min(\mu-1,\alpha)}\right)\|\psi_0\|_{\mathcal{H}_2(\mathbb{R}^3)}. \tag{5.61}$$

Then by Fatou's lemma

$$\left\| [\Xi_\eta(x,\infty) + \chi V(x)] e^{-i\tau H_1} \tilde{\psi}_0 \right\|_{L^2(\mathbb{R}^3)} \leq C \left(1/(1+|\tau|)^{\min(\mu-1,\alpha)} \right) \|\psi_0\|_{\mathcal{H}_2(\mathbb{R}^3)}. \tag{5.62}$$

Hence, by Lebesque's dominated convergence theorem,

$$\lim_{t\to\infty} \int_0^t d\tau e^{i\tau H_2} i e^{-iL_{A_C,\hat{\mathbf{v}}(t-\tau)}} [\Xi_\eta(x, t-\tau) + \chi V(x)] e^{-i\tau H_1} \tilde{\psi}_0$$
$$= \int_0^\infty d\tau e^{i\tau H_2} i e^{-iL_{A_C,\hat{\mathbf{v}}(\infty)}} [\Xi_\eta(x,\infty) + \chi V(x)] e^{-i\tau H_1} \tilde{\psi}_0,$$

where the limit is on the strong topology of $L^2(\mathbb{R}^3)$. We complete the proof of (5.60) using (5.62).

We now estimate the integrand in (5.60).

Step 4.

$$\left(e^{-iL_{A_C,\hat{\mathbf{v}}(-\infty)}} \phi_0, e^{i\tau H_2} e^{-iL_{A_C,\hat{\mathbf{v}}(\infty)}} i [\Xi_\eta(x,\infty) + \chi V(x)] e^{-i\tau H_1} \tilde{\psi}_0 \right)$$
$$= \left(e^{i(L_{A_C,\hat{\mathbf{v}}(\tau)} - L_{A_C,\hat{\mathbf{v}}(-\infty)})} \phi_0, e^{i\tau H_1} e^{-iL_{A_C,\hat{\mathbf{v}}(\infty)}} i [\Xi_\eta(x,\infty) + \chi V(x)] e^{-i\tau H_1} \tilde{\psi}_0 \right)$$
$$+ \frac{1}{v} O\left(\frac{1}{(1+|\tau|)^{\min(\mu-2,\alpha-1)}} \right). \tag{5.63}$$

Denote by χ_Λ the characteristic function of Λ. Then

$$\left(e^{-iL_{A_C,\hat{\mathbf{v}}(-\infty)}} \phi_0, e^{i\tau H_2} e^{-iL_{A_C,\hat{\mathbf{v}}(\infty)}} i [\Xi_\eta(x,\infty) + \chi V(x)] e^{-i\tau H_1} \tilde{\psi}_0 \right)$$
$$= \left(e^{i\tau H_1} \chi_\Lambda e^{-i\tau H_2} e^{-iL_{A_C,\hat{\mathbf{v}}(-\infty)}} \phi_0, e^{i\tau H_1} e^{-iL_{A_C,\hat{\mathbf{v}}(\infty)}} i [\Xi_\eta(x,\infty) + \chi V(x)] e^{-i\tau H_1} \tilde{\psi}_0 \right).$$

Hence, (5.63) will be proved if we can replace $e^{i\tau H_1} \chi_\Lambda e^{-i\tau H_2}$ by $\chi e^{iL_{A_C,\hat{\mathbf{v}}(\tau)}}$ adding the error term. But, this follows from (5.62) and the estimate,

$$\left\| \left(e^{i\tau H_1} \chi_\Lambda e^{-i\tau H_2} - \chi e^{iL_{A_C,\hat{\mathbf{v}}(\tau)}} \right) e^{-iL_{A_C,\hat{\mathbf{v}}(-\infty)}} \phi_0 \right\| \leq C \frac{1+|\tau|}{v} \|\phi_0\|_{\mathcal{H}_2(\mathbb{R}^3)}, \tag{5.64}$$

that we prove below.

We designate

$$\varphi_\tau := e^{i(L_{A_C,\hat{\mathbf{v}}(\tau)} - L_{A_C,\hat{\mathbf{v}}(-\infty)})} \phi_0.$$

We have that

$$\left(e^{i\tau H_1} \chi_\Lambda e^{-i\tau H_2} - \chi e^{iL_{A_C,\hat{\mathbf{v}}(\tau)}} \right) e^{-iL_{A_C,\hat{\mathbf{v}}(-\infty)}} \phi_0$$
$$= e^{i\tau H_1} \chi_\Lambda e^{-i\tau H_2} \left(e^{-iL_{A_C,\hat{\mathbf{v}}(\tau)}} - e^{i\tau H_2} \chi e^{-i\tau H_1} \right) \varphi_\tau + \left(e^{i\tau H_1} \chi e^{-i\tau H_1} - \chi \right) \varphi_\tau. \tag{5.65}$$

By (5.41),

$$\|\varphi_\tau\|_{\mathcal{H}_2(\mathbb{R}^3)} \leq C \|\phi_0\|_{\mathcal{H}_2(\mathbb{R}^3)}. \tag{5.66}$$

Hence, using

$$\left| e^{-i\tau(p+m\mathbf{v})^2/2mv} - e^{-i\tau(p\cdot\hat{\mathbf{v}}+v^2/2mv)} \right| \leq C\frac{|\tau|p^2}{2mv},$$

we prove that

$$\left\| \left(e^{-i\tau H_1} - e^{-i\tau(\mathbf{p}\cdot\hat{\mathbf{v}}+v^2/2mv)} \right) \varphi_\tau \right\|_{L^2(\mathbb{R}^3)} \leq C\frac{|\tau|}{v}\|\phi_0\|_{\mathcal{H}_2(\mathbb{R}^3)}, \tag{5.67}$$

and since $\chi - 1 \equiv 0$ on the support of $e^{-i\tau(\mathbf{p}\cdot\hat{\mathbf{v}}+v^2/2mv)}\varphi_\tau$,

$$\begin{aligned} &\left\| \left(e^{i\tau H_1}\chi e^{-i\tau H_1} - \chi \right) \varphi_\tau \right\|_{L^2(\mathbb{R}^3)} \\ &= \left\| e^{i\tau H_1}(\chi - 1)(e^{-i\tau H_1} - e^{-i\tau(\mathbf{p}\cdot\hat{\mathbf{v}}+v^2/2mv)})\varphi_\tau \right\|_{L^2(\mathbb{R}^3)} \\ &\leq C\tfrac{|\tau|}{v}\|\phi_0\|_{\mathcal{H}_2(\mathbb{R}^3)}. \end{aligned} \tag{5.68}$$

Then (5.64) follows from (5.39,5.65, 5.66, 5.68).
Step 5. We now replace $e^{\pm i\tau H_1}$ by $e^{\pm i(\tau\mathbf{p}\cdot\hat{\mathbf{v}}+v^2/2mv)}$. We will prove that

$$\begin{aligned} &\left(e^{i(L_{A_C,\hat{\mathbf{v}}}(\tau)-L_{A_C,\hat{\mathbf{v}}}(-\infty))}\phi_0, e^{i\tau H_1}e^{-iL_{A_C,\hat{\mathbf{v}}}(\infty)}\, i[\Xi_\eta(x,\infty) + \chi V(x)]e^{-i\tau H_1}\tilde{\psi}_0 \right) \\ &= \Big(e^{i(L_{A_C,\hat{\mathbf{v}}}(\tau)-L_{A_C,\hat{\mathbf{v}}}(-\infty))}\phi_0, \\ &e^{i\tau\mathbf{p}\cdot\hat{\mathbf{v}}}e^{-iL_{A_C,\hat{\mathbf{v}}}(\infty)}\, i[\Xi_\eta(x,\infty) + \chi V(x)]e^{-i\tau\mathbf{p}\cdot\hat{\mathbf{v}}}\tilde{\psi}_0 \Big) + \tfrac{1}{v}O\left(\tfrac{1}{(1+|\tau|)^{\min(\mu-2,\alpha-1)}} \right) \\ &= \left(\phi_0, e^{-ia(\hat{\mathbf{v}},x)}\, i[\Xi_\eta(x+\tau\hat{\mathbf{v}},\infty) + \chi V(x+\tau\hat{\mathbf{v}})]\tilde{\psi}_0 \right) + \tfrac{1}{v}O\left(\tfrac{1}{(1+|\tau|)^{\min(\mu-2,\alpha-1)}} \right), \tau \geq 0. \end{aligned} \tag{5.69}$$

Recall that φ_τ is defined below (5.64). By (5.62) and (5.67),

$$\begin{aligned} &\left(e^{-i\tau H_1}\varphi_\tau, e^{-iL_{A_C,\hat{\mathbf{v}}}(\infty)}\, i[\Xi_\eta(x,\infty) + \chi V(x)]e^{-i\tau H_1}\tilde{\psi}_0 \right) = \Big(e^{-(i\tau\mathbf{p}\cdot\hat{\mathbf{v}}+v^2/2mv)}\varphi_\tau, \\ &\qquad e^{-iL_{A_C,\hat{\mathbf{v}}}(\infty)}\, i[\Xi_\eta(x,\infty) + \chi V(x)]e^{-i\tau H_1}\tilde{\psi}_0 \Big) + \tfrac{1}{v}O\left(\tfrac{1}{(1+|\tau|)^{\min(\mu-2,\alpha-1)}} \right). \end{aligned} \tag{5.70}$$

The first equality in (5.69) follows from (5.67) and as

$$\begin{aligned} &\|[\Xi_\eta(x,\infty) + \chi V(x)]e^{iL_{A_C,\hat{\mathbf{v}}}(\infty)}e^{-i(\tau\mathbf{p}\cdot\hat{\mathbf{v}}+v^2/2mv)}\varphi_\tau\|_{L^2(\mathbb{R}^3)} \\ &\leq C\tfrac{1}{(1+|\tau|)^{\min(\mu-1,\alpha)}}\|\phi_0\|_{\mathcal{H}_2(\mathbb{R}^3)}, \tau > 0, \end{aligned} \tag{5.71}$$

because ϕ_0 has compact support, $e^{-i\tau\mathbf{p}\cdot\hat{\mathbf{v}}}$ is just a translation and the decay properties of $V(x)$ and $\Xi_\eta(x,\infty)$ (in the direction $\hat{\mathbf{v}}$). The second equality is immediate.

By (5.60, 5.63, 5.69)

$$\begin{aligned} v\left(e^{-iL_{A_C,\hat{\mathbf{v}}}(-\infty)}\phi_0, R_+\psi_0 \right) = &\int_0^t d\tau \left(\phi_0, e^{-ia(\hat{\mathbf{v}},x)}\, i[\Xi_\eta(x+\tau\hat{\mathbf{v}},\infty) + \chi V(x+\tau\hat{\mathbf{v}})]\tilde{\psi}_0 \right) \\ &+O(1/v) + O\left(1/(1+|t|)^{\min(\mu-2,\alpha-1)} \right) \\ &+ \begin{cases} \frac{1}{v}O\left(\ln(1+|t|)\right), & \text{if } \min(\mu-2,\alpha-1) = 1, \\ \frac{1}{v}O\left(\frac{1}{(1+|t|)^{\min(\mu-3,\alpha-2,0)}} \right), & \text{otherwise.} \end{cases} \end{aligned} \tag{5.72}$$

Step 6. We now prove that

$$\begin{aligned}&\int_0^t d\tau\left(\phi_0, e^{-ia(\hat{\mathbf{v}},x)}\, i[\Xi_\eta(x+\tau\hat{\mathbf{v}},\infty)+\chi V(x+\tau\hat{\mathbf{v}})]\tilde{\psi}_0\right)\\ &\quad-\int_0^\infty d\tau\left(\phi_0, e^{-ia(\hat{\mathbf{v}},x)}\, i[\Xi_\eta(x+\tau\hat{\mathbf{v}},\infty)+\chi V(x+\tau\hat{\mathbf{v}})]\psi_0\right)\\ &\quad= O(1/v)+O\left(\frac{1}{(1+|t|)^{\min(\mu-2,\alpha-1)}}\right), t>0.\end{aligned} \tag{5.73}$$

As ϕ_0 has compact support,

$$\begin{aligned}&\left\|[\Xi_\eta(x+\tau\hat{\mathbf{v}},\infty)+\chi V(x+\tau\hat{\mathbf{v}})]e^{ia(\hat{\mathbf{v}},x)}\phi_0\right\|_{L^2(\mathbb{R}^3)}\\ &\quad\le C\frac{1}{(1+|\tau|)^{\min(\mu-1,\alpha)}}\|\phi_0\|_{\mathcal{H}_2(\mathbb{R}^3)}, \tau>0.\end{aligned} \tag{5.74}$$

Equations (5.22) and (5.74) prove (5.73).

By (5.72, 5.73)

$$\begin{aligned}v\left(e^{-iL_{A_C,\hat{\mathbf{v}}}(-\infty)}\phi_0, R_+\psi_0\right)&=\int_0^\infty d\tau\left(\phi_0, e^{-ia(\hat{\mathbf{v}},x)}\, i[\Xi_\eta(x+\tau\hat{\mathbf{v}},\infty)+\chi V(x+\tau\hat{\mathbf{v}})]\psi_0\right)\\ &\quad+O\left(1/v\right)+O\left(1/(1+|t|)^{\min(\mu-2,\alpha-1)}\right)\\ &\quad+\begin{cases}\frac{1}{v}O\left(\ln(1+|t|)\right), & \text{if } \min(\mu-2,\alpha-1)=1,\\ \frac{1}{v}O\left(\frac{1}{(1+|t|)^{\min(\mu-3,\alpha-2,0)}}\right), & \text{otherwise.}\end{cases}\end{aligned} \tag{5.75}$$

Finally, taking $t=v$ we obtain (5.55) in the Coulomb gauge, and then, (5.51) is proven for A_C.

Suppose that $A\in\mathcal{A}_{\Phi,2\pi,\mathrm{SR}}(B)$. By (5.11) $S(A,V)=S(A_C,V)$. As λ_∞ is constant, $e^{i\int_{-\infty}^{\infty}A(x+\tau\hat{\mathbf{v}})\cdot\hat{\mathbf{v}}d\tau}=e^{i\int_{-\infty}^{\infty}A_C(x+\tau\hat{\mathbf{v}})\cdot\hat{\mathbf{v}}d\tau}$, and it follows that (5.51) holds for $A\in\mathcal{A}_{\Phi,2\pi}(B)$.
□

6. Reconstruction of the Magnetic Field and the Electric Potential Outside the Obstacle

In this section we obtain a method for the unique reconstruction of the magnetic field and the electric potential outside the obstacle, K, from the high-velocity limit of the scattering operator. The method is given in the proof of Theorem 6.3 and is summarized in Remark 6.4.

Definition 6.1. *We denote by Λ_{rec} the set of points $x\in\Lambda$ such that for some two-dimensional plane P_x we have that $x+P_x\subset\Lambda$.*

Note that if K is convex $\Lambda_{\mathrm{rec}}=\Lambda$.

Lemma 6.2. *For every $A\in\mathcal{A}_{\Phi,2\pi}(B)$ and every unit vector, $\hat{\mathbf{v}}$, in $\mathbb{R}^3$, we have that*

$$\nabla\int_{-\infty}^{\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\,d\tau=\int_{-\infty}^{\infty}\hat{\mathbf{v}}\times B(x+\tau\hat{\mathbf{v}})\,d\tau, \tag{6.1}$$

in distribution sense in $\Lambda_{\hat{\mathbf{v}}}$.

Proof. The following identity holds in distribution sense in $\Lambda_{\hat{\mathbf{v}}}$ (this is just the triple vector product formula):

$$\hat{\mathbf{v}} \times (\nabla \times A) = \nabla(\hat{\mathbf{v}} \cdot A) - (\hat{\mathbf{v}} \cdot \nabla)A. \tag{6.2}$$

Then, for every $\phi \in C_0^\infty(\Lambda_{\hat{\mathbf{v}}})$,

$$\begin{aligned}
&\int_{-\infty}^{\infty} \hat{\mathbf{v}} \times B(x+\tau\hat{\mathbf{v}})\, d\tau\, [\phi] = \int_{\mathbb{R}^3} dx \int_{-\infty}^{\infty} \hat{\mathbf{v}} \times B(x+\tau\hat{\mathbf{v}})\, d\tau\, \phi(x) \\
&\quad = \int_{\mathbb{R}^3} dx \lim_{r\to\infty} \int_{-r}^{r} d\tau\, \hat{\mathbf{v}} \times B(x)\, \phi(x-\tau\hat{\mathbf{v}}) \\
&\quad = \int_{\mathbb{R}^3} dx \lim_{r\to\infty} \int_{-r}^{r} \left(-\hat{\mathbf{v}} \cdot A(x)(\nabla\phi)(x-\tau\hat{\mathbf{v}}) + A(x)\left(\hat{\mathbf{v}} \cdot \nabla\phi\right)(x-\tau\hat{\mathbf{v}})\right) \\
&\quad = \left(\nabla \int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(x+\tau\hat{\mathbf{v}})\, d\tau\right)[\phi] + \lim_{r\to\infty} \int_{\mathbb{R}^3} A(x)(\phi(x-r\hat{\mathbf{v}}) - \phi(x+r\hat{\mathbf{v}})) \\
&\quad = \left(\nabla \int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(x+\tau\hat{\mathbf{v}})\, d\tau\right)[\phi],
\end{aligned}$$

where in the last equality we used the decay of A and the fact that ϕ has compact support.

Theorem 6.3. (*Reconstruction of the Magnetic Field and the Electric Potential*). *Suppose that B, V satisfy Assumption 5.1. Then, for any flux, Φ, and all $A \in \mathcal{A}_{\Phi,2\pi}(B)$, the high-velocity limits of $S(A,V)$ in (5.44) known for all Λ_0, all unit vectors $\hat{\mathbf{v}}$ and all $\phi_0 \in \mathcal{H}_2(\mathbb{R}^3)$ with support $\phi_0 \subset \Lambda_0$, uniquely determine $B(x)$ for almost every $x \in \Lambda_{\text{rec}}$. Furthermore, for any flux, Φ, and all $A \in \mathcal{A}_{\Phi,2\pi,\text{SR}}(B)$, the high-velocity limits of $S(A,V)$ in (5.51) known for all Λ_0, all unit vectors $\hat{\mathbf{v}}$ and all $\phi_0, \psi_0 \in \mathcal{H}_6(\mathbb{R}^3)$ with support ϕ_0, support $\psi_0 \subset \Lambda_0$, uniquely determine $V(x)$ for almost every $x \in \Lambda_{\text{rec}}$.*

Proof. We proceed as in the proof of Theorem 1.1 of [14] (see also the proof of Theorem 1.4 [40]) with the modifications that are necessary to take the obstacle into account and to reconstruct the magnetic field.

Let us fix a $x_0 \in \Lambda_{\text{rec}}$. For each $j = 1, 2, 3$ we take, unit vectors $\hat{\mathbf{u}}_j, \hat{\mathbf{v}}_j$, and $\varepsilon > 0$ such that the following conditions are satisfied:

1. $$\hat{\mathbf{u}}_j \cdot \hat{\mathbf{v}}_i = 0,\ i, j \in \{1, 2, 3\}.$$
2. The unit vectors
$$\hat{\mathbf{n}}_j := \hat{\mathbf{u}}_j \times \hat{\mathbf{v}}_j,\ j = 1, 2, 3,$$
are linearly independent.
3. $$B_\varepsilon^{\mathbb{R}^3}(x_0) + p(\hat{\mathbf{u}}_j, \hat{\mathbf{v}}_j) \subset \Lambda,\ j = 1, 2, 3,$$
where $p(\hat{\mathbf{u}}_j, \hat{\mathbf{v}}_j)$ is the two-dimensional plane generated by $\hat{\mathbf{u}}_j, \hat{\mathbf{v}}_j$.

For any $z = (z_1, z_2) \in \mathbb{R}^2$ we define

$$\begin{aligned}
&\phi_j(z) := e^{-i(z_1\hat{\mathbf{u}}_j + z_2\hat{\mathbf{v}}_j)\cdot\mathbf{p}}\phi_0,\ \psi_j(z) := e^{-i(z_1\hat{\mathbf{u}}_j + z_2\hat{\mathbf{v}}_j)\cdot\mathbf{p}}\psi_0, \\
&\qquad j = 1, 2, 3, \phi_0, \psi_0 \in C_0^\infty\left(B_\varepsilon^{\mathbb{R}^3}(x_0)\right).
\end{aligned} \tag{6.3}$$

From the limit (5.44) we uniquely reconstruct

$$e^{i\int_{-\infty}^{\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\,d\tau}$$

for all $x \in \Lambda_{\hat{\mathbf{v}}}$, and then we reconstruct $\int_{-\infty}^{\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\,d\tau + 2\pi n(x,\hat{\mathbf{v}})$ with $n(x,\hat{\mathbf{v}})$ an integer that is locally constant. By Lemma 6.2 we also reconstruct uniquely

$$\int_{-\infty}^{\infty}\hat{\mathbf{v}}\times B(x+\tau\hat{\mathbf{v}})\,d\tau \tag{6.4}$$

for a.e. $x \in \Lambda_{\hat{\mathbf{v}}}$.

Take now $\hat{\mathbf{v}} \in p(\hat{\mathbf{u}}_j, \hat{\mathbf{v}}_j)$. Hence, we uniquely reconstruct

$$\int_{-\infty}^{\infty}\hat{\mathbf{n}}_j\cdot B(x+\tau\hat{\mathbf{v}})\,d\tau = -\hat{\mathbf{n}}_j\cdot\left(\hat{\mathbf{v}}\times\int_{-\infty}^{\infty}\hat{\mathbf{v}}\times B(x+\tau\hat{\mathbf{v}})\,d\tau\right), \tag{6.5}$$

for a.e. $x \in \Lambda_{\hat{\mathbf{v}}}$. We used the triple vector product formula, $a\times(b\times c) = (a\cdot c)b-(a\cdot b)c$. We now define $F_j : \mathbb{R}^2 \to \mathbb{C}$,

$$F_j(z) := \left(\hat{\mathbf{n}}_j\cdot B(x)\phi_j(z), \psi_j(z)\right).$$

F_j is continuous and

$$\left|F_j(z)\right| \le C(1+|z|)^{-\mu},\ j = 1, 2, 3.$$

Moreover, we uniquely reconstruct from (5.44) the Radon transforms,

$$\tilde{F}_j(\hat{\mathbf{w}}; z) := \int_{-\infty}^{\infty}F_j(z+\tau\hat{\mathbf{w}})d\tau = \left(\int_{-\infty}^{\infty}\hat{\mathbf{n}}_j\cdot B(x+\tau(\hat{\mathbf{w}}_1\hat{\mathbf{u}}_j+\hat{\mathbf{w}}_2\hat{\mathbf{v}}_j))\,d\tau\phi_j(z), \psi_j(z)\right),$$

where $z \in \mathbb{R}^2$ and $\hat{\mathbf{w}} := (\hat{\mathbf{w}}_1, \hat{\mathbf{w}}_2) \in \mathbb{R}^2$ has modulus one.

Inverting this Radon transform (see Theorem 2.17 of [18,19,27]) we uniquely reconstruct $F_j(z)$ and in particular $F_j(0) = \left(\hat{\mathbf{n}}_j\cdot B\phi_0, \psi_0\right)$ and hence, we uniquely reconstruct $\hat{\mathbf{n}}_j\cdot B(x),\ j = 1, 2, 3$ for a.e. $x \in B_\varepsilon^{\mathbb{R}^3}(x_0)$ and as the $\hat{\mathbf{n}}_j$ are linearly independent we uniquely reconstruct $B(x)$ for a.e. $x \in B_\varepsilon^{\mathbb{R}^3}(x_0)$. Since $x_0 \in \Lambda_{\text{rec}}$ is arbitrary we uniquely reconstruct $B(x)$ for a.e. $x \in \Lambda_{\text{rec}}$.

We now uniquely reconstruct V. Take any $x_0 \in \Lambda_{\text{rec}}$. Let $\hat{\mathbf{u}}, \hat{\mathbf{w}}$ be orthonormal vectors such that $B_\varepsilon^{\mathbb{R}^3}(x_0) + p(\hat{\mathbf{u}}, \hat{\mathbf{w}}) \subset \Lambda_{\hat{\mathbf{v}}}$. We define,

$$\phi(z) := e^{-i(z_1\hat{\mathbf{u}}+z_2\hat{\mathbf{w}})\cdot\mathbf{p}}\phi_0,\ \psi(z) := e^{-i(z_1\hat{\mathbf{u}}+z_2\hat{\mathbf{w}})\cdot\mathbf{p}}\psi_0,\ \ \phi_0, \psi_0 \in C_0^\infty\left(B_\varepsilon^{\mathbb{R}^3}(x_0)\right),$$

and the function $F : \mathbb{R}^2 \to \mathbb{C}$,

$$F(z) := (V(x)\phi(z), \psi(z)).$$

F is continuous and

$$|F(z)| \le C(1+|z|)^{-\alpha}.$$

Moreover, since B is already known in Λ_{rec}, we uniquely reconstruct from (5.51) the Radon transforms,

$$\tilde{F}(\hat{\mathbf{y}}; z) := \int_{-\infty}^{\infty} F(z + \tau\hat{\mathbf{y}})d\tau = \left(\int_{-\infty}^{\infty} V(x + \tau(\hat{\mathbf{y}}_1\hat{\mathbf{u}} + \hat{\mathbf{y}}_2\hat{\mathbf{w}}))\, d\tau\phi(z), \psi(z)\right),$$

where $z \in \mathbb{R}^2$ and $\hat{\mathbf{y}} := (\hat{\mathbf{y}}_1, \hat{\mathbf{y}}_2) \in \mathbb{R}^2$ has modulus one.

As above inverting these Radon transforms we uniquely reconstruct $F(z)$, and in particular $F(0) = (V\phi_0, \psi_0)$ which uniquely determines $V(x)$ for a.e. $x \in B_{\varepsilon}^{\mathbb{R}^3}(x_0)$. Since $x_0 \in \Lambda_{\text{rec}}$ is arbitrary, $V(x)$ is uniquely reconstructed for a.e. $x \in \Lambda_{\text{rec}}$. $\square$

Remark 6.4. Let us summarize the reconstruction method given by Theorem 6.3. From the high-velocity limit (5.44) we uniquely reconstruct

$$e^{i\int_{-\infty}^{\infty} \hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\, d\tau}, \tag{6.6}$$

and from this we uniquely reconstruct

$$\int_{-\infty}^{\infty} \hat{\mathbf{v}} \times B(x + \tau\hat{\mathbf{v}})\, d\tau, \quad x \in \Lambda_{\hat{\mathbf{v}}}, \tag{6.7}$$

which gives us the Radon transform

$$\begin{aligned} \tilde{F}_j(\hat{\mathbf{w}}; z) &:= \int_{-\infty}^{\infty} F_j(z + \tau\hat{\mathbf{w}})d\tau \\ &= \left(\int_{-\infty}^{\infty} \hat{\mathbf{n}}_j \cdot B(x + \tau(\hat{\mathbf{w}}_1\hat{\mathbf{u}}_j + \hat{\mathbf{w}}_2\hat{\mathbf{v}}_j))\, d\tau\phi_j(z), \psi_j(z)\right), \end{aligned} \tag{6.8}$$

where $z \in \mathbb{R}^2$ and $\hat{\mathbf{w}} := (\hat{\mathbf{w}}_1, \hat{\mathbf{w}}_2) \in \mathbb{R}^2$ has modulus one.

Inverting this Radon transform we uniquely reconstruct $F_j(z)$ and in particular $F_j(0) = \left(\hat{\mathbf{n}}_j \cdot B\phi_0, \psi_0\right)$ and hence, we uniquely reconstruct $\hat{\mathbf{n}}_j \cdot B(x)$, $j{=}1, 2, 3$ for a.e. $x \in B_{\varepsilon}^{\mathbb{R}^3}(x_0)$ and as the $\hat{\mathbf{n}}_j$ are linearly independent we uniquely reconstruct $B(x)$ for a.e. $x \in B_{\varepsilon}^{\mathbb{R}^3}(x_0)$. Since $x_0 \in \Lambda_{\text{rec}}$ is arbitrary we uniquely reconstruct $B(x)$ for a.e. $x \in \Lambda_{\text{rec}}$. Note that to reconstruct B almost everywhere in a neighborhood of a point x_0 we only need the high-velocity limit of the scattering operator applied to wave functions with support in a neighborhood of three two-dimensional planes. For the inversion of the Radon transform see Theorem 2.17 of [18] and [19,27].

Remember that given any $A \in \mathcal{A}_{\Phi,2\pi}(B)$ we can always find an $A \in \mathcal{A}_{\Phi}(B)$ with the same scattering operator. We can take, for example, A_{Φ}. See Eq. (5.12). Then there is no loss of generality taking $A \in \mathcal{A}_{\Phi}(B)$. Note that (6.6) is not a gauge invariant quantity. If $\tilde{A}, A \in \mathcal{A}_{\Phi}(B)$ and $\tilde{A} = A + d\lambda$, then,

$$\int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot \tilde{A}(x + \tau\hat{\mathbf{v}})d\tau = \int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(x + \tau\hat{\mathbf{v}})d\tau + \lambda_{\infty}(\hat{\mathbf{v}}) - \lambda_{\infty}(-\hat{\mathbf{v}}).$$

We can, however, reconstruct (6.7) from the gauge invariant quantity,

$$\mathcal{R}(x, y) := e^{i\int_{-\infty}^{\infty} \hat{\mathbf{v}}\cdot[A(x+\tau\hat{\mathbf{v}})-A(y+\tau\hat{\mathbf{v}})]\, d\tau}, \; x, y \in \Lambda_{\hat{\mathbf{v}}}.$$

We have that

$$\frac{1}{i}\,\overline{\mathcal{R}(x,y)}\,\nabla_x\mathcal{R}(x,y)=\nabla_x\int_{-\infty}^{\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\,d\tau=\int_{-\infty}^{\infty}\hat{\mathbf{v}}\times B(x+\tau\hat{\mathbf{v}})\,d\tau,\,x\in\Lambda_{\hat{\mathbf{v}}}.$$

We now uniquely reconstruct V. Since B is already known in Λ_{rec}, for any $\hat{\mathbf{v}}\in p(\hat{\mathbf{u}},\hat{\mathbf{w}})$ we uniquely reconstruct from (5.51) the Radon transforms,

$$\tilde{F}(\hat{\mathbf{y}};z):=\int_{-\infty}^{\infty}F(z+\tau\hat{\mathbf{y}})d\tau=\left(\int_{-\infty}^{\infty}V(x+\tau(\hat{\mathbf{y}}_1\hat{\mathbf{u}}+\hat{\mathbf{y}}_2\hat{\mathbf{w}}))\,d\tau\phi(z),\psi(z)\right),$$

where $z\in\mathbb{R}^2$ and $\hat{\mathbf{y}}:=(\hat{\mathbf{y}}_1,\hat{\mathbf{y}}_2)\in\mathbb{R}^2$ has modulus one.

As above inverting these Radon transforms we uniquely reconstruct $F(z)$, and in particular $F(0)=(V\phi_0,\psi_0)$ which uniquely determines $V(x)$ for a.e. $x\in B_\varepsilon^{\mathbb{R}^3}(x_0)$. Since $x_0\in\Lambda_{\mathrm{rec}}$ is arbitrary, $V(x)$ is uniquely reconstructed for a.e. $x\in\Lambda_{\mathrm{rec}}$.

7. The Aharonov-Bohm Effect

In this section we assume that $B\equiv 0$, i.e., that there is no magnetic field in Λ. On the contrary, the electric potential, V, is not assumed to be zero. In other words, we will analyze the Aharonov-Bohm effect in the presence of an electric potential. As we will show, for high-velocities the electric potential gives a lower-order contribution that plays no role in the Aharonov-Bohm effect. However, it could be of interest to allow for a non-trivial electric potential from the experimental point of view.

For any $x\in\mathbb{R}^3$ and any unit vector $\hat{\mathbf{v}}\in\mathbb{S}^2$ we denote

$$L(x,\hat{\mathbf{v}}):=x+\mathbb{R}\hat{\mathbf{v}},$$

and we give to $L(x,\hat{\mathbf{v}})$ the orientation of $\hat{\mathbf{v}}$. Suppose that $x,y\in\mathbb{R}^3$, $\hat{\mathbf{v}},\hat{\mathbf{w}}\in\mathbb{S}^2$ satisfy $\hat{\mathbf{v}}\cdot\hat{\mathbf{w}}\geq 0$ and that

$$L(x,\hat{\mathbf{v}})\cup L(y,\hat{\mathbf{w}})\subset\Lambda.$$

Take $\rho>0$ so large that

$$\begin{aligned}&\text{convex}\,\big((x+(-\infty,-\rho]\hat{\mathbf{v}})\cup(y+(-\infty,-\rho]\hat{\mathbf{w}})\big)\cup\\&\text{convex}\,\big((x+[\rho,\infty)\hat{\mathbf{v}})\cup(y+[\rho,\infty,)\hat{\mathbf{w}})\big)\subset B_r^{\mathbb{R}^3}(0)^c,\end{aligned}$$

where $K\subset B_r^{\mathbb{R}^3}(0)$, $B_r^{\mathbb{R}^3}(0)^c$ is the complement of $B_r^{\mathbb{R}^3}(0)$ and the symbol convex$(\cdot)$ denotes the convex hull of the indicated set.

We denote by $\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})$ the continuous, simple, oriented and closed curve with sides, $x+[-\rho,\rho]\hat{\mathbf{v}}$, oriented in the direction of $\hat{\mathbf{v}}$, $y+[-\rho,\rho]\hat{\mathbf{w}}$, oriented in the direction of $-\hat{\mathbf{w}}$ and the oriented straight lines that join the points $x+\rho\hat{\mathbf{v}}$ with $y+\rho\hat{\mathbf{w}}$ and $y-\rho\hat{\mathbf{w}}$ and $x-\rho\hat{\mathbf{v}}$.

Suppose that A is short-range (see Definition 5.4). For example, we can take $A=A_C$. We denote $x_{\perp,\hat{\mathbf{v}}}:=x-(x,\hat{\mathbf{v}})\hat{\mathbf{v}}$. It follows from Stoke's theorem that if $|x_{\perp,\hat{\mathbf{v}}}|\geq r$,

$$\int_{-\infty}^{\infty}\hat{\mathbf{v}}\cdot A(x+\tau\hat{\mathbf{v}})\,d\tau=\int_{-\infty}^{\infty}\hat{\mathbf{v}}\cdot A(x_\perp+\tau\hat{\mathbf{v}})\,d\tau=\lim_{s\to\infty}\int_{-\infty}^{\infty}\hat{\mathbf{v}}\cdot A(sx_\perp+\tau\hat{\mathbf{v}})\,d\tau=0. \tag{7.1}$$

By Stoke's theorem and arguing as in the proof of (7.1) we prove that for short-range A,

$$\int_{\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})} A = \int_{L(x,\hat{\mathbf{v}})} A - \int_{L(y,\hat{\mathbf{w}})} A. \tag{7.2}$$

Take any $z \in \mathbb{R}^3$ such that $|(x+z)_{\perp,\hat{\mathbf{v}}}| \geq r$, $|(y+z)_{\perp,\hat{\mathbf{w}}}| \geq r$. By Stoke's theorem and (7.1),

$$\int_{L(x+z,\hat{\mathbf{v}})} A = \int_{L(y+z,\hat{\mathbf{w}})} A = 0.$$

Then, adding zero we write (7.2) as

$$\int_{\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})} A = \left(\int_{L(x,\hat{\mathbf{v}})} A - \int_{L(x+z,\hat{\mathbf{v}})} A\right) - \left(\int_{L(y,\hat{\mathbf{w}})} A - \int_{L(y+z,\hat{\mathbf{w}})} A\right). \tag{7.3}$$

The point is that for any $A \in \mathcal{A}_{\Phi,2\pi}(0)$ there is $\tilde{A} \in \mathcal{A}_{\Phi,2\pi}(0)$ with $A = \tilde{A} + \nabla\lambda$ and $\tilde{A}$ short-range, consequently (7.3) holds for any $A \in \mathcal{A}_{\Phi,2\pi}(0)$.

It follows that from the high-velocity limit (5.44) we can reconstruct $\int_{\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})} A$, modulo 2π. We have proven the following theorem.

Theorem 7.1. *Suppose that $B \equiv 0$ and that V satisfies Assumption 5.1. Then, for any flux, Φ, and all $A \in \mathcal{A}_{\Phi,2\pi}(0)$, the high-velocity limits of $S(A,V)$ in (5.44) known for $\hat{\mathbf{v}}$ and $\hat{\mathbf{w}}$ determines the fluxes*

$$\int_{\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})} A \tag{7.4}$$

modulo 2π, for all curves $\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})$.

Remark 7.2. Theorem 7.1 implies that from the high-velocity limit (5.44) for $\hat{\mathbf{v}}$ and $\hat{\mathbf{w}}$ we can reconstruct the fluxes

$$\int_\alpha A$$

for any closed curve α such that there is a surface (or chain) $\mathcal{S}$ in Λ with $\partial\mathcal{S} = \alpha - \gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})$, because by Stoke's theorem,

$$\int_\alpha A = \int_{\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})} A + \int_{\mathcal{S}} B = \int_{\gamma(x,y,\hat{\mathbf{v}},\hat{\mathbf{w}})} A.$$

Remember also that given any $A \in \mathcal{A}_{\Phi,2\pi}(B)$ we can always find an $A \in \mathcal{A}_\Phi(B)$ with the same scattering operator. We can take, for example, A_Φ. See Eq. (5.12). Then, there is no loss of generality taking $A \in \mathcal{A}_\Phi(0)$. Furthermore, notice that we can at most reconstruct the fluxes modulo 2π because by (5.12) $S(A_\Phi, V) = S(A,V)$ and the fluxes of A_Φ and A differ by integer multiples of 2π. For general $A \in \mathcal{A}_{\Phi,2\pi}(0)$ we recuperate the fluxes from Eq. (7.3). However if A is short-range we can use the simpler formula (7.2).

Remark 7.3. As $\gamma(x, y, \hat{\mathbf{v}}, \hat{\mathbf{w}})$ is a cycle, the homology class $[\gamma(x, y, \hat{\mathbf{v}}, \hat{\mathbf{w}})]_{H_1(\Lambda;\mathbb{R})}$ is well defined.

We denote

$$H_{1,\text{rec}}(\Lambda;\mathbb{R}) := \left\langle \left\{ [\gamma(x, y, \hat{\mathbf{v}}, \hat{\mathbf{w}})]_{H_1(\Lambda;\mathbb{R})} : L(x, \hat{\mathbf{v}}) \cup L(x, \hat{\mathbf{w}}) \subset \Lambda \right\} \right\rangle. \tag{7.5}$$

$H_{1,\text{rec}}(\Lambda;\mathbb{R})$ is a vector subspace of $H_1(\Lambda;\mathbb{R})$. Let us denote by $H^1_{\text{de R, rec}}(\Lambda)$ the vector subspace of $H^1_{\text{de R}}(\Lambda)$ that is the dual to $H_{1,\text{rec}}(\Lambda;\mathbb{R})$, given by de Rham's Theorem. Then, for all Φ and all $A \in \mathcal{A}_{\Phi,2\pi}(0)$, from the high-velocity limit (5.44) known for all $\hat{\mathbf{v}}, \hat{\mathbf{w}}$ we reconstruct the projection of A into $H^1_{\text{de R, rec}}(\Lambda)$ modulo 2π, as we now show. Let

$$\left\{ [\sigma_j]_{H_{1,\text{rec}}(\Lambda;\mathbb{R})} \right\}_{j=1}^{m},$$

be a basis of $H_{1,\text{rec}}(\Lambda;\mathbb{R})$, and let

$$\left\{ [A_j]_{H^1_{\text{de R, rec}}(\Lambda)} \right\}_{j=1}^{m},$$

be the dual basis, i.e.,

$$\int_{\sigma_j} A_k = \delta_{j,k},\ j, k = 1, 2, \ldots, m.$$

Let us denote by P_{rec} the projector onto $H^1_{\text{de R, rec}}(\Lambda)$. Hence, for any $A \in \mathcal{A}_{\Phi,2\pi}(B)$,

$$P_{\text{rec}}\, [A]_{H^1_{\text{de R}}(\Lambda)} = \sum_{j=1}^{m} \lambda_j [A_j]_{H^1_{\text{de R, rec}}(\Lambda)},$$

and, furthermore, as

$$\lambda_j = \int_{\sigma_j} A,$$

we reconstruct λ_j, $j = 1, 2, \ldots, m$ (modulo 2π) from the high-velocity limit (5.44) known for all $\hat{\mathbf{v}}, \hat{\mathbf{w}}$.

We now give a precise definition of when a line $L(x, \hat{\mathbf{v}})$ goes through a hole of K. Take $r > 0$ such that $K \subset B_r^{\mathbb{R}^3}(0)$. Suppose that $L(x, \hat{\mathbf{v}}) \subset \Lambda$, and $L(x, \hat{\mathbf{v}}) \cap \overline{B_r^{\mathbb{R}^3}}(0) \neq \emptyset$. We denote by $c(x, \hat{\mathbf{v}})$ the curve consisting of the segment $L(x, \hat{\mathbf{v}}) \cap \overline{B_r^{\mathbb{R}^3}}(0)$ and an arc on $\partial \overline{B_r^{\mathbb{R}^3}}(0)$ that connects the points $L(x, \hat{\mathbf{v}}) \cap \partial \overline{B_r^{\mathbb{R}^3}}(0)$. We orient $c(x, \hat{\mathbf{v}})$ in such a way that the segment of straight line has the orientation of $\hat{\mathbf{v}}$.

Definition 7.4. *A line $L(x, \hat{\mathbf{v}}) \subset \Lambda$ goes through a hole of K if $L(x, \hat{\mathbf{v}}) \cap B_r^{\mathbb{R}^3}(0) \neq \emptyset$ and $[c(x, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} \neq 0$. Otherwise we say that $L(x, \hat{\mathbf{v}})$ does not go through a hole of K.*

Note that this characterization of lines that go or do not go through a hole of K is independent of the r that was used in the definition. This follows from the homotopic invariance of homology. See Theorem 11.2, p. 59 of [16].

In an intuitive sense $[c(x, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} = 0$ means that $c(x, \hat{\mathbf{v}})$ is the boundary of a surface (actually of a chain) that is contained in Λ and then it can not go through a hole of K. Obviously, as $K \subset B_r^{\mathbb{R}^3}(0)$, if $L(x, \hat{\mathbf{v}}) \cap B_r^{\mathbb{R}^3}(0) = \emptyset$ the line $L(x, \hat{\mathbf{v}})$ can not go through a hole of K.

Definition 7.5. *Two lines $L(x, \hat{\mathbf{v}}), L(y, \hat{\mathbf{w}}) \subset \Lambda$ that go through a hole of K go through the same hole if $[c(x, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} = \pm[c(y, \hat{\mathbf{w}})]_{H_1(\Lambda;\mathbb{R})}$. Furthermore, we say that the lines go through the hole in the same direction if $[c(x, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} = [c(y, \hat{\mathbf{w}})]_{H_1(\Lambda;\mathbb{R})}$.*

Lemma 7.6. *Let $A, A_0 \in \mathcal{A}_\Phi(0)$ with A_0 short-range and let λ be such that $A_0 = A + d\lambda$. Assume that $L(x, \hat{\mathbf{v}})$ and $L(y, \hat{\mathbf{w}})$ go through the same hole of K. Then,*

$$\int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(x + \tau\hat{\mathbf{v}})\, d\tau + \lambda_\infty(\hat{\mathbf{v}}) - \lambda_\infty(-\hat{\mathbf{v}})$$
$$= \pm\left(\int_{-\infty}^{\infty} \hat{\mathbf{w}} \cdot A(y + \tau\hat{\mathbf{w}})\, d\tau + \lambda_\infty(\hat{\mathbf{w}}) - \lambda_\infty(-\hat{\mathbf{w}})\right), \tag{7.6}$$

if $[c(x, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} = \pm[c(y, \hat{\mathbf{w}})]_{H_1(\Lambda;\mathbb{R})}$.

Moreover,

$$\int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(x + \tau\hat{\mathbf{v}})\, d\tau + \lambda_\infty(\hat{\mathbf{v}}) - \lambda_\infty(-\hat{\mathbf{v}})$$
$$= \int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A_0(x + \tau\hat{\mathbf{v}})\, d\tau = \int_{c(x,\hat{\mathbf{v}})} A_0 = \int_{c(x,\hat{\mathbf{v}})} A. \tag{7.7}$$

Proof. By (7.1) and Stoke's theorem,

$$\int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(x + \tau\hat{\mathbf{v}})\, d\tau + \lambda_\infty(\hat{\mathbf{v}}) - \lambda_\infty(-\hat{\mathbf{v}}) = \int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A_0(x + \tau\hat{\mathbf{v}})\, d\tau = \int_{c(x,\hat{\mathbf{v}})} A_0$$
$$= \pm\int_{c(y,\hat{\mathbf{w}})} A_0 = \pm\left(\int_{-\infty}^{\infty} \hat{\mathbf{w}} \cdot A(y + \tau\hat{\mathbf{w}})\, d\tau + \lambda_\infty(\hat{\mathbf{w}}) - \lambda_\infty(-\hat{\mathbf{w}})\right).$$

□

Lemma 7.7. *Let $A, A_0 \in \mathcal{A}_\Phi(0)$ with A_0 short-range and let λ be such that $A_0 = A + d\lambda$. Assume that $L(x, \hat{\mathbf{v}})$ does not go through a hole of K. Then,*

$$\int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(x + \tau\hat{\mathbf{v}})\, d\tau + \lambda_\infty(\hat{\mathbf{v}}) - \lambda_\infty(-\hat{\mathbf{v}}) = 0. \tag{7.8}$$

Proof. If $L(x, \hat{\mathbf{v}}) \cap B_r^{\mathbb{R}^3}(0) = \emptyset$ it follows from (7.1) and Stoke's theorem that (7.8) holds. Otherwise, $[c(x, \hat{\mathbf{v}})]_{H_1(\Lambda,\mathbb{R})} = 0$, and then, by Stoke's theorem,

$$\int_{c(x,\hat{\mathbf{v}})} A = 0.$$

Take $z \in \partial \overline{B_r^{\mathbb{R}^3}(0)} \cap c(x, \hat{\mathbf{v}})$ such that $L(z, \hat{\mathbf{v}})$ is tangent to $\partial \overline{B_r^{\mathbb{R}^3}(0)}$. By the argument above,

$$\int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(z + \tau \hat{\mathbf{v}})\, d\tau + \lambda_\infty(\hat{\mathbf{v}}) - \lambda_\infty(-\hat{\mathbf{v}}) = 0.$$

Finally, using once more Stoke's theorem we obtain that

$$0 = \int_{c(x,\hat{\mathbf{v}})} A = \int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(x + \tau \hat{\mathbf{v}})\, d\tau - \int_{-\infty}^{\infty} \hat{\mathbf{v}} \cdot A(z + \tau \hat{\mathbf{v}})\, d\tau,$$

and then, (7.8) is proven. □

Remark 7.8. If $(x, \hat{\mathbf{v}}) \in \Lambda \times \mathbb{S}^2$, there are neighborhoods $B_x \subset \mathbb{R}^3$, $B_{\hat{\mathbf{v}}} \subset \mathbb{S}^2$ such that $(x, \hat{\mathbf{v}}) \in B_x \times B_{\hat{\mathbf{v}}}$ and if $(y, \hat{\mathbf{w}}) \in B_x \times B_{\hat{\mathbf{v}}}$ then, the following is true: if $L(x, \hat{\mathbf{v}})$ does not go through a hole of K, then, also $L(y, \hat{\mathbf{w}})$ does not go through a hole of K. If $L(x, \hat{\mathbf{v}})$ goes through a hole of K, then, $L(y, \hat{\mathbf{w}})$ goes through the same hole and in the same direction. This follows from the homotopic invariance of homology, Theorem 11.2, p. 59 of [16].

Definition 7.9. *For any $\hat{\mathbf{v}} \in \mathbb{S}^2$ we denote by $\Lambda_{\hat{\mathbf{v}},\mathrm{out}}$ the set of points $x \in \Lambda_{\hat{\mathbf{v}}}$ such that $L(x, \hat{\mathbf{v}})$ does not go through a hole of K. We call this set the region without holes of $\Lambda_{\hat{\mathbf{v}}}$. The holes of $\Lambda_{\hat{\mathbf{v}}}$ is the set $\Lambda_{\hat{\mathbf{v}},\mathrm{in}} := \Lambda_{\hat{\mathbf{v}}} \setminus \Lambda_{\hat{\mathbf{v}},\mathrm{out}}$.*

We define the following equivalence relation on $\Lambda_{\hat{\mathbf{v}},\mathrm{in}}$. We say that $x R_{\hat{\mathbf{v}}} y$ if and only if $L(x, \hat{\mathbf{v}})$ and $L(y, \hat{\mathbf{v}})$ go through the same hole and in the same direction. By $[x]$ we designate the classes of equivalence under $R_{\hat{\mathbf{v}}}$.

We denote by $\left\{\Lambda_{\hat{\mathbf{v}},h}\right\}_{h \in \mathcal{I}}$ the partition of $\Lambda_{\hat{\mathbf{v}},\mathrm{in}}$ given by this equivalence relation. It is defined as follows:

$$\mathcal{I} := \{[x]\}_{x \in \Lambda_{\hat{\mathbf{v}},\mathrm{in}}}.$$

Given $h \in \mathcal{I}$ there is $x \in \Lambda_{\hat{\mathbf{v}},\mathrm{in}}$ such that $h = [x]$. We denote

$$\Lambda_{\hat{\mathbf{v}},h} := \{y \in \Lambda_{\hat{\mathbf{v}},\mathrm{in}} : y R_{\hat{\mathbf{v}}} x\}.$$

Then

$$\Lambda_{\hat{\mathbf{v}},\mathrm{in}} = \cup_{h \in \mathcal{I}} \Lambda_{\hat{\mathbf{v}},h}, \quad \Lambda_{\hat{\mathbf{v}},h_1} \cap \Lambda_{\hat{\mathbf{v}},h_2} = \emptyset,\ h_1 \neq h_2.$$

We call $\Lambda_{\hat{\mathbf{v}},h}$ the hole h of K in the direction of $\hat{\mathbf{v}}$. Note that

$$\{\Lambda_{\hat{\mathbf{v}},h}\}_{h \in \mathcal{I}} \cup \{\Lambda_{\mathbf{v},\mathrm{out}}\} \tag{7.9}$$

is an open disjoint cover of $\Lambda_{\hat{\mathbf{v}}}$.

Definition 7.10. *For any Φ, $A \in \mathcal{A}_\Phi(0)$, $\hat{\mathbf{v}} \in \mathbb{S}^2$, and $h \in \mathcal{I}$ we define,*

$$F_h := \int_{c(x,\hat{\mathbf{v}})} A,$$

where x is any point in $\Lambda_{\hat{\mathbf{v}},h}$. Note that F_h is independent of the $x \in \Lambda_{\hat{\mathbf{v}},h}$ that we choose. F_h is the flux of the magnetic field over any surface (or chain) in $\mathbb{R}^3$ whose boundary is $c(x, \hat{\mathbf{v}})$. We call F_h the magnetic flux on the hole h of K.

Let us take $\phi_0 \in \mathcal{H}_2(\mathbb{R}^3)$ with compact support in $\Lambda_{\hat{\mathbf{v}}}$. Then, since (7.9) is a disjoint open cover of $\Lambda_{\hat{\mathbf{v}}}$,

$$\phi_0 = \sum_{h \in \mathcal{I}} \varphi_h + \varphi_{\text{out}}, \tag{7.10}$$

with $\varphi_h, \varphi_{\text{out}} \in \mathcal{H}_2(\mathbb{R}^3)$, φ_h has compact support in $\Lambda_{\hat{\mathbf{v}},h}$, $h \in \mathcal{H}$, and φ_{out} has compact support in $\Lambda_{\hat{\mathbf{v}},\text{out}}$. The sum is finite because ϕ has compact support. We denote

$$\phi_{\mathbf{v}} := e^{im\mathbf{v}\cdot x}\phi_0,\ \varphi_{h,\mathbf{v}} := e^{im\mathbf{v}\cdot x}\varphi_h,\ \varphi_{\text{out},\mathbf{v}} := e^{im\mathbf{v}\cdot x}\varphi_{\text{out}}.$$

Theorem 7.11. *Suppose that $B \equiv 0$ and that V satisfies Assumption 5.1. Then, for any Φ and any $A \in \mathcal{A}_\Phi(0)$,*

$$S(A,V)\,\phi_{\mathbf{v}} = e^{-i(\lambda_\infty(\hat{\mathbf{v}})-\lambda_\infty(-\hat{\mathbf{v}}))}\left(\sum_{h\in\mathcal{I}} e^{iF_h}\varphi_{\mathbf{v},h} + \varphi_{\text{out},\mathbf{v}}\right) + O\left(\frac{1}{v}\right). \tag{7.11}$$

Proof. The theorem follows from Theorem 5.7 and Lemmas 7.6, 7.7. □

Corollary 7.12. *Under the conditions of Theorem 7.11,*

$$\left(S(A,V)\,\phi_{\mathbf{v}}, \varphi_{\mathbf{v},h}\right) = e^{-i(\lambda_\infty(\hat{\mathbf{v}})-\lambda_\infty(-\hat{\mathbf{v}}))}e^{iF_h} + O\left(\frac{1}{v}\right),\ h \in \mathcal{I}, \tag{7.12}$$

$$\left(S(A,V)\,\phi_{\mathbf{v}}, \varphi_{\mathbf{v},out}\right) = e^{-i(\lambda_\infty(\hat{\mathbf{v}})-\lambda_\infty(-\hat{\mathbf{v}}))} + O\left(\frac{1}{v}\right). \tag{7.13}$$

Moreover, the high-velocity limit of $S(A,V)$ in the direction $\hat{\mathbf{v}}$ determines $\lambda_\infty(\hat{\mathbf{v}}) - \lambda_\infty(-\hat{\mathbf{v}})$ and the fluxes F_h, $h \in \mathcal{I}$, modulo 2π.

Proof. The corollary follows immediately from Theorem 7.11. □

Remark 7.13. Equations (7.12, 7.13) are reconstruction formulae that allow us to reconstruct $\lambda_\infty(\hat{\mathbf{v}}) - \lambda_\infty(-\hat{\mathbf{v}})$ and the fluxes F_h, $h \in \mathcal{I}$, modulo 2π, from the high-velocity limit of the scattering operator in the direction $\hat{\mathbf{v}}$. Recall that $\lambda_\infty(\hat{\mathbf{v}}) - \lambda_\infty(-\hat{\mathbf{v}})$ is independent of the particular short-range potential that we use to define λ. Remember also that given any $A \in \mathcal{A}_{\Phi,2\pi}(B)$ we can always find an $A \in \mathcal{A}_\Phi(B)$ with the same scattering operator. We can take, for example, A_Φ. See Eq. (5.12). Then, there is no loss of generality taking $A \in \mathcal{A}_\Phi(0)$.

Note that it is quite remarkable that we can determine $\lambda_\infty(\hat{\mathbf{v}}) - \lambda_\infty(-\hat{\mathbf{v}})$ since it is not a gauge invariant quantity. According to the standard interpretation of quantum mechanics only gauge invariant quantities are physically relevant. Note that if A is short-range λ_∞ is constant. In this case $\lambda_\infty(\hat{\mathbf{v}}) - \lambda_\infty(-\hat{\mathbf{v}}) \equiv 0$ and it drops out from all our formulae. We see that one possibility is to consider that only short-range potentials are physically admissible. This is consistent with the usual interpretation of quantum mechanics in three dimensions. However, we can also go beyond the standard interpretation of quantum mechanics and consider the class of long-range potentials $\mathcal{A}_\Phi(B)$ as physically admissible. This raises the interesting question of what is the physical significance of the $\lambda_\infty(\hat{\mathbf{v}}) - \lambda_\infty(-\hat{\mathbf{v}})$.

Example 7.14. Here we consider a simple example where we give an explicit description of the holes. Furthermore, the fluxes of the holes are the fluxes of the magnetic field over cross sections of the tori. We reconstruct all the fluxes modulo 2π and also we determine the cohomology class of the magnetic potential modulo 2π, from the high-velocity limit of the scattering operator in only one direction.

Given a vector $z \in \mathbb{R}^3$ and $a > b > 0$ we denote by $T(z, a, b)$ the following set:

$$T(z,a,b) := \{z + a(\cos\theta, \sin\theta, 0) + b\,(x(\cos\theta, \sin\theta, 0) \\ +y(0,0,1)) : \theta \in [0, 2\pi], (x, y) \in \overline{B_1^{\mathbb{R}^2}(0)}\Big\}.$$

The map $F_{z,a,b} : T \to T(z, a, b)$ given by

$$F_{z,a,b}((\cos\theta, \sin\theta), (x, y)) \to z + a(\cos\theta, \sin\theta, 0) + b\,(x(\cos\theta, \sin\theta, 0) + y(0, 0, 1))$$

is a diffeomorphism.

The obstacle. We now define the obstacle K. We assume that $\mathbf{v} = (0, 0, 1)$.

As before the connected components of K are K_j, $j = 1, 2, \dots, L$. Let us denote $J = \{1, 2, \dots, m\}$ and $I = \{m + 1, \dots, L\}$. If $m = L$, then, $I = \emptyset$. We assume that K satisfies the following assumptions:

1. There are vectors $z_j \in \mathbb{R}^3$ and numbers $a_j > b_j$, $j = 1, 2, \dots, m$ such that,

$$K_j = T(z_j, a_j, b_j), \forall j \in J, \quad K_j \cong \overline{B_1^{\mathbb{R}^3}(0)}, \; j \in I.$$

2.

$$\big(\text{convex}\,(K_j) + \mathbb{R}\mathbf{v}\big) \cap (\text{convex}\,(K_l) + \mathbb{R}\mathbf{v}) = \emptyset, \; j, l \in J,$$
$$\big(\text{convex}\,(K_j) + \mathbb{R}\mathbf{v}\big) \cap (K_l + \mathbb{R}\mathbf{v}) = \emptyset, \; j \in J, l \in I.$$

We denote as before by convex $(\cdot)$ the convex hull of the indicated set.

The Curves $\gamma_j, \tilde{\gamma}_j, \hat{\gamma}_j$. Let θ_j be such that $z_j = r_j(\cos(\theta_j), \sin(\theta_j), 0) + (0, 0, (z_j)_3)$.

The curves γ_j, $j \in J$ are given by

$$\gamma_j(t) := z_j + a_j(\cos t, \sin t, 0),$$

and the curves $\tilde{\gamma}_j$, $j \in J$, are

$$\tilde{\gamma}_j := z_j + a_j(\cos\theta_j, \sin\theta_j, 0) + b_j\,\big(\cos t(\cos\theta_j, \sin\theta_j, 0) + \sin t(0, 0, 1)\big).$$

Furthermore, the curves $\hat{\gamma}_j$, $j \in J$, are

$$\hat{\gamma}_j := z_j + a_j(\cos\theta_j, \sin\theta_j, 0) + (b_j + \delta/2)\,\big(\cos t(\cos\theta_j, \sin\theta_j, 0) + \sin t(0, 0, 1)\big),$$

where $\delta > 0$ so small that, $\delta < a_j - b_j$, and

$$\big(\text{convex}\,(K_{j,\delta}) + \mathbb{R}\mathbf{v}\big) \cap \big(\text{convex}\,(K_{l,\delta}) + \mathbb{R}\mathbf{v}\big) \\ = \emptyset, \; j, l \in J, \;\; \big((\text{convex}\,K_{j,\delta}) + \mathbb{R}\mathbf{v}\big) \cap \big(K_{l,\delta} + \mathbb{R}\mathbf{v}\big) = \emptyset, \; j \in J, l \in I.$$

The subindex δ denotes the set of points that are at distance up to δ of the indicated set.

The flux Φ. We define the following sets:

$$h_j := \big\{z_j + t(\cos\theta, \sin\theta) : \theta \in [0, 2\pi], t \in [0, a_j - b_j)\big\} + \mathbb{R}\hat{\mathbf{v}}, \; j \in J.$$

We have that

$$[c(x, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} = [c(y, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})}, \forall x, y \in h_j, j \in J. \tag{7.14}$$

Since $c(x, \hat{\mathbf{v}})$ and $c(y, \hat{\mathbf{v}})$ are homotopic in Λ, this follows from the homotopic invariance of homology, see Theorem 11.2, p. 59 of [16] (the curves $c(x, \hat{\mathbf{v}})$ and $c(y, \hat{\mathbf{v}})$ are defined previously in this section). Then, we can associate a flux Φ_j to each h_j, $j \in J$ as follows:

$$\Phi_j = \int_{c(x,\hat{\mathbf{v}})} A, \text{ for some } x \in h_j, j \in J.$$

We have that

$$[c(y, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} = 0, \forall y \in \left(\Lambda_{\hat{\mathbf{v}}} \setminus \left(\cup_{j\in J} h_j\right)\right) \cap \left(B_r^{\mathbb{R}^3}(0) + \mathbb{R}\hat{\mathbf{v}}\right), \tag{7.15}$$

where the radius r is the one taken to define the curves $c(y, \hat{\mathbf{v}})$. Let us prove this. As the segment of straight line in $c(y, \hat{\mathbf{v}})$ does not belong to any of the sets convex $(K_j) + \mathbb{R}\hat{\mathbf{v}}$, $j \in J$, we have that for any $j \in J$ there is a surface (or a chain) σ_j contained in the complement of K_j such that $\partial\sigma_j = c(y, \hat{\mathbf{v}})$. Let $\left\{\left[G^{(j)}\right]_{H^1_{\text{de R}}}(\Lambda)\right\}_{j=1}^m$ be the basis of $H^1_{\text{de R}}$ constructed in Proposition 2.3. Then, as $dG^{(j)} = 0$ it follows from Stoke's theorem that

$$\int_{c(y,\hat{\mathbf{v}})} G^{(j)} = 0, \forall j \in J.$$

Hence, (7.15) follows from de Rham's Theorem, Theorem 4.17, p. 154 of [41].

Let us prove now that

$$\Phi_j = \Phi(\hat{\gamma}_j), j \in J. \tag{7.16}$$

For any $j \in J$ we define,

$$x_j := z_j + a_j(\cos\theta_j, \sin\theta_j, 0) - (b_j + \delta/2)(\cos\theta_j, \sin\theta_j, 0),$$

$$y_j := z_j + a_j(\cos\theta_j, \sin\theta_j, 0) + (b_j + \delta/2)(\cos\theta_j, \sin\theta_j, 0).$$

We choose the curves $c(x_j, \hat{\mathbf{v}})$, $c(y_j, \hat{\mathbf{v}})$ in such a way that the arc in $c(y_j, \hat{\mathbf{v}})$ is contained in the arc in $c(x_j, \hat{\mathbf{v}})$. Let c_j be the curve obtained by taking the segments of straight line in $c(x_j, \hat{\mathbf{v}})$ and in $c(y_j, \hat{\mathbf{v}})$ and the two arcs that are obtained by cutting from the arc in $c(x_j, \hat{\mathbf{v}})$ the arc in $c(y_j, \hat{\mathbf{v}})$. We orient c_j in such a way that the segment of straight line in $c(x_j, \hat{\mathbf{v}})$ has the orientation of $\hat{\mathbf{v}}$. Then, in homology,

$$[c_j]_{H_1(\Lambda;\mathbb{R})} = [c(x_j, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} - [c(y_j, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})}. \tag{7.17}$$

This follows from de Rham's Theorem -Theorem 4.17, p. 154 of [41]- since for any closed 1-form D,

$$\int_{c_j} D = \int_{c(x_j,\hat{\mathbf{v}})} D - \int_{c(y_j,\hat{\mathbf{v}})} D.$$

The curves $\hat{\gamma}_j$ and c_j are homotopically equivalent in Λ. Hence, by the homotopical invariance of homology, Theorem 11.2, p. 59 of [16],

$$[c_j]_{H_1(\Lambda;\mathbb{R})} = [\hat{\gamma}_j]_{H_1(\Lambda;\mathbb{R})}. \tag{7.18}$$

Then, by (7.15, 7.17),

$$[\hat{\gamma}_j]_{H_1(\Lambda;\mathbb{R})} = [c(x_j, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})}, \tag{7.19}$$

and hence,

$$\int_{c(x_j,\hat{\mathbf{v}})} A = \int_{\hat{\gamma}_j} A,\ j \in J,$$

what proves (7.16).

The holes of K. Recall that $\Lambda_{\hat{\mathbf{v}},\mathrm{out}}$ and $\Lambda_{\hat{\mathbf{v}},\mathrm{in}}$ were defined in Definition 7.9, that the holes of K are the sets $\Lambda_{\mathbf{v},h}$, $h \in \mathcal{I}$, that F_h is the flux over the hole $\Lambda_{\mathbf{v},h}$, $h \in \mathcal{I}$, that $\Lambda_{\hat{\mathbf{v}},\mathrm{in}} = \cup_{h\in\mathcal{I}}\Lambda_{\hat{\mathbf{v}},h}$.

Then, we have that

1. The index set $\mathcal{I}$ can be taken as $\mathcal{I} = \{h_j\}_{j\in J} \sim J$. Moreover, denoting $\Lambda_{\hat{\mathbf{v}},j} = \Lambda_{\hat{\mathbf{v}},h_j}$, we have that $\Lambda_{\hat{\mathbf{v}},j} = h_j$ and $\Lambda_{\hat{\mathbf{v}},\mathrm{in}} = \cup_{j\in J} h_j$.
2. We designate, $F_j := F_{h_j}$. Then
$$F_j = \Phi(\hat{\gamma}_j),\ j \in J.$$
3. $$\Lambda_{\hat{\mathbf{v}},\mathrm{out}} = \mathbb{R}^3 \setminus \left(\Lambda_{\hat{\mathbf{v}},\mathrm{in}} \cup_{j=1}^{L} (K_j + \hat{\mathbf{v}}\mathbb{R})\right).$$

Let us prove this. By (7.15) $[c(y, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} = 0, \forall y \in \left(\Lambda_{\hat{\mathbf{v}}} \setminus \cup_{j\in J} h_j\right)$ such that $B_r^{\mathbb{R}^3}(0) \cap L(y, \hat{\mathbf{v}}) \neq \emptyset$. Then

$$\left(\Lambda_{\hat{\mathbf{v}}} \setminus \cup_{j\in J} h_j\right) \cap \left(B_r^{\mathbb{R}^3}(0) + \mathbb{R}\hat{\mathbf{v}}\right) \subset \Lambda_{\hat{\mathbf{v}},\mathrm{out}}.$$

But by our definition the complement in $\Lambda_{\hat{\mathbf{v}}}$ of $B_r^{\mathbb{R}^3}(0) + \mathbb{R}\hat{\mathbf{v}}$ is contained in $\Lambda_{\hat{\mathbf{v}},\mathrm{out}}$. It follows that

$$\left(\Lambda_{\hat{\mathbf{v}}} \setminus \cup_{j\in J} h_j\right) \subset \Lambda_{\hat{\mathbf{v}},\mathrm{out}}.$$

Moreover, if $x \in h_j$ for some $j \in J$, since $[\hat{\gamma}_j]_{H_1(\Lambda;\mathbb{R})} \neq 0$, it follows from (7.14) and (7.19) that $[c(x_j, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} = [c(x, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} \neq 0$, and then, $x \notin \Lambda_{\hat{\mathbf{v}},\mathrm{out}}$. Then, we have proven that

$$\left(\Lambda_{\hat{\mathbf{v}}} \setminus \cup_{j\in J} h_j\right) = \Lambda_{\hat{\mathbf{v}},\mathrm{out}}, \tag{7.20}$$

and hence,

$$\Lambda_{\hat{\mathbf{v}},\mathrm{in}} = \cup_{j\in J} h_j.$$

Item 3 is now obvious. By (7.14) if $x, y \in h_j$, then, $[c(x, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} = [c(y, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})}$. Hence, $x R_{\hat{\mathbf{v}}} y$ which implies that h_j is contained in some hole of K. But by (7.14) and (7.19) if $x \in h_j$, $y \in h_l$, $j \neq l$, then, $[c(x, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})} \neq [c(y, \hat{\mathbf{v}})]_{H_1(\Lambda;\mathbb{R})}$ because as the $[\hat{\gamma}_j]_{H_1(\Lambda;\mathbb{R})}$, $j \in J$ are a basis of $H_1(\Lambda;\mathbb{R})$ they are different. In consequence, x and y belong to different holes of K. Then, since (7.20) holds, we have proven Item 1. Item 2 follows from (7.16).

By Corollary 7.12 and Remark 7.13, this proves that from the high-velocity limit of $S(A, V)$ in the direction of $\hat{\mathbf{v}}$ we reconstruct all the fluxes $\Phi(\hat{\gamma}_j)$, $j \in J$, modulo 2π.

Let us now prove that from the high-velocity limit of $S(A, V)$ in the direction of $\hat{\mathbf{v}}$ we also reconstruct the cohomology class $[A]_{H^1_{\text{de R}}(\Lambda)}$ modulo 2π, in the sense that we reconstruct modulo 2π the coefficients of $[A]_{H^1_{\text{de R}}(\Lambda)}$ in any basis of $H^1_{\text{de R}}(\Lambda)$.

Let $\left\{[M_j]_{H^1_{\text{de R}}(\Lambda)}\right\}_{j=1}^m$ be any basis of $H^1_{\text{de R}}(\Lambda)$ and let $\left\{[\Gamma_j]_{H_1(\Lambda;\mathbb{R})}\right\}_{j=1}^m$ be the dual basis of $H_1(\Lambda;\mathbb{R})$ given by de Rham's Theorem,

$$\int_{\Gamma_j} M_l = \delta_{j,l},\ j, l \in J.$$

Let $\{\alpha_j\}_{j\in J}$ be the expansion coefficients of A,

$$[A]_{H^1_{\text{de R}}(\Lambda)} = \sum_{j\in J} \alpha_j [M_j]_{H^1_{\text{de R}}(\Lambda)},$$

$$\alpha_j = \int_{\Gamma_j} A.$$

By Proposition 10.1 $\left\{[\hat{\gamma}_j]_{H_1(\Lambda;\mathbb{Z})}\right\}_{j=1}^m$ is a basis of $H_1(\Lambda;\mathbb{Z})$. Then,

$$[\Gamma_j]_{H_1(\Lambda;\mathbb{Z})} = \sum_{l\in J} n(j,l)[\hat{\gamma}_l]_{H_1(\Lambda;\mathbb{Z})},$$

where the coefficients $n(j,l)$ are integers. Finally,

$$\alpha_j = \int_{\Gamma_j} A = \sum_{l\in L} n(j,l) \int_{\hat{\gamma}_l} A = \sum_{l\in L} n(j,l)\Phi(\hat{\gamma}_l),\ j \in J,$$

and since we have already determined the $\Phi(\hat{\gamma}_l)$ modulo 2π, the coefficients α_j, $j \in J$ are determined modulo 2π.

8. The Tonomura et al. Experiments

The fundamental experiments of Tonomura et al. [37,38], gave a conclusive evidence of the existence of the Aharonov-Bohm effect. For a detailed account see [30].

Tonomura et al. [37,38] did their experiments in the case of toroidal magnets. This corresponds to our Example 7.14 with only one torus, i.e., $L = 1$, $J = \{1\}$. In very careful and precise experiments they managed to superimpose behind the toroidal magnet two electron beams. One of them traveled inside the hole of the toroidal magnet and the other-the reference beam-outside it. They measured the interference fringes between the two beams produced by the magnetic flux inside the torus.

We show now that our results give a rigorous mathematical proof that quantum mechanics predicts the interference fringes observed by Tonomura et al. [37,38] in their remarkable experiments.

An equivalent description of these experiments is to consider that both electron beams traveled inside the hole of the torus, one of them with a nonzero magnetic flux inside the torus, and the other-the reference beam-with the magnetic flux inside the torus set to zero. Note that it follows from Theorem 7.11 that particles that go outside the holes only feel the long-range part of the potential given by the factor $e^{-i(\lambda_\infty(\hat{\mathbf{v}})-\lambda_\infty(-\hat{\mathbf{v}}))}$, for large velocities. Therefore, we can model the particles that go outside the hole (in the Tonomura et al. experiments [37,38]) by particles that go inside the hole when the fluxes F_h are equal to zero and that feel the same long range effect $e^{-i(\lambda_\infty(\hat{\mathbf{v}})-\lambda_\infty(-\hat{\mathbf{v}}))}$ for large velocities. As in this model long-range magnetic potentials add a global constant phase that does not affect the interference pattern we take, for simplicity, a short-range magnetic potential. According to Theorem 7.11, for the particle that goes inside the hole with the magnetic flux present, up to an error of order $1/v$, we have that

$$S(A, V)\phi_{\mathbf{v}} = e^{i\frac{q}{\hbar c}\Phi}\,\phi_{\mathbf{v}}, \tag{8.1}$$

where we have taken physical units, with Φ the flux of the physical magnetic field $\mathbf{B}$ and $\phi_{\mathbf{v}} = e^{i\frac{M}{\hbar}\mathbf{v}\cdot x}\phi_0$. See Sect. 4. For the particle that goes outside the hole of the magnet, or equivalently inside the hole with the magnetic field set to zero,

$$S(A, V)\phi_{\mathbf{v}} = \phi_{\mathbf{v}}. \tag{8.2}$$

If we superimpose both asymptotic states we obtain the wave function,

$$\left(1 + e^{i\frac{q}{\hbar c}\Phi}\right)\phi_{\mathbf{v}}, \tag{8.3}$$

up to an error of order $1/v$. This shows the interference patterns that were observed experimentally by Tonomura et al. [37,38]. For example, if $\frac{q}{\hbar c}\Phi$ is an odd multiple of π there is a destructive interference and there is a dark zone behind the hole of the magnet, as observed experimentally.

Tonomura et al. [37,38] also considered the case when the reference beam is slightly tilted. In this case the reference beam is given by

$$\phi_{\mathbf{v}+\mathbf{v}_0} = e^{i\frac{M}{\hbar}\mathbf{v}_0\cdot x}\phi_{\mathbf{v}},$$

and (8.2) is replaced by,

$$S(A, V)\phi_{\mathbf{v}+\mathbf{v}_0} = \phi_{\mathbf{v}+\mathbf{v}_0} = e^{i\frac{M}{\hbar}\mathbf{v}_0\cdot x}\,\phi_{\mathbf{v}}.$$

In this case we obtain the wave function

$$e^{i\frac{M}{\hbar}\mathbf{v}_0\cdot x}\left(1 + e^{-i\frac{M}{\hbar}\mathbf{v}_0\cdot x}e^{i\frac{q}{\hbar c}}\right)\phi_{\mathbf{v}},$$

up to an error of order $1/v$. We see that the factor,

$$\left(1 + e^{-i\frac{M}{\hbar}\mathbf{v}_0\cdot x}e^{i\frac{q}{\hbar c}}\right)$$

produces the parallel fringes that were observed experimentally by Tonomura et al. [37,38].

9. Appendix A

In this Appendix we prove, for the reader's convenience, that $H_s(\natural\, k\, T; \mathcal{R}) = 0$, $s \geq 2$, that $H_1(\natural k T; \mathcal{R}) \cong \oplus_{i=1}^{k} \mathcal{R}$, and that $\left\{[Z_j]_{H_1(\natural k T; \mathcal{R})}\right\}_{j=1}^{k}$ is a basis of $H_1(\natural k T; \mathcal{R})$. $\mathcal{R}$ is $\mathbb{Z}$ or $\mathbb{R}$.

Recall that we defined, $\gamma_\pm : [0, 1] \to T : \gamma_\pm(t) = (e^{\pm 2\pi i t}, 0, 0)$.

Proposition 9.1. *$H_s(T; \mathcal{R}) = 0$, $s \geq 2$ and $H_1(T; \mathbb{Z}) \cong \mathbb{Z}$ and $\left\{[\gamma_\pm]_{H_1(T;\mathbb{Z})}\right\}$ are basis of $H_1(T; \mathbb{Z})$.*

Proof. We define $\tilde{\gamma}_\pm : [0, 1] \to \mathbb{S}^1 : \tilde{\gamma}_\pm(t) := e^{\pm 2\pi i t}$ and let $I_{\mathbb{S}^1} : \mathbb{S}^1 \to T$ be the inclusion given by $I_{\mathbb{S}^1}(s) := (s, 0, 0)$. Clearly, $I_{\mathbb{S}^1} \circ \tilde{\gamma}_\pm = \gamma_\pm$. It is easy to see that $\mathbb{S}^1$ is homotopically equivalent to T and that the inclusion $I_{\mathbb{S}^1} : \mathbb{S}^1 \to T$ is a homotopic equivalence. It follows that $I_{\mathbb{S}^1}$ induces an isomorphism in holomogy given by $H_s(I_{\mathbb{S}^1})$ (see Theorem 11.3, p. 59 [16]). Then, $H_s(T; \mathcal{R}) \cong H_s(\mathbb{S}^1; \mathcal{R})$ and hence, we have that $H_s(T; \mathcal{R}) = 0$, $s \geq 2$ by Corollary 15.5, p. 84 of [16]. For $s = 1$ and $\mathcal{R} = \mathbb{Z}$, the isomorphism is given in the following way (see p. 49 [16]). Let $\sigma_i : [0, 1] \to T$ be continuous functions and let $n_i \in \mathbb{Z}$. Let us assume that $\sum n_i \sigma_i$ is a cycle (its boundary is zero). Then, $H_1(I_{\mathbb{S}^1})[\sum n_i \sigma_i]_{H_1(\mathbb{S}^1;\mathbb{Z})} := [\sum n_i I_{\mathbb{S}^1} \circ \sigma_i]_{H_1(T;\mathbb{Z})}$.

As $I_{\mathbb{S}^1} \circ \tilde{\gamma}_\pm = \gamma_\pm$, it follows that $H_1(I_{\mathbb{S}^1})[\tilde{\gamma}_\pm]_{H_1(\mathbb{S}^1;\mathbb{Z})} = [\gamma_\pm]_{H_1(T;\mathbb{Z})}$. Then, to prove the proposition it is enough to prove that $H_1(\mathbb{S}^1; \mathbb{Z}) \cong \mathbb{Z}$ and that $\left\{[\tilde{\gamma}_\pm]_{H_1(\mathbb{S}^1;\mathbb{Z})}\right\}$ are basis of $H_1(\mathbb{S}^1; \mathbb{Z})$.

By Theorem 12.1, p. 63 of [16], there is a homomorphism $\Xi : \Pi_1(\mathbb{S}^1; 1) \to H_1(\mathbb{S}^1; \mathbb{Z})$ that sends a homotopy class to its homology class. In our case Ξ is an isomorphism since $\Pi_1(\mathbb{S}^1; 1)$ is abelian. Actually, $\Pi_1(\mathbb{S}^1; 1) \cong \mathbb{Z}$. See Theorem 4.4, p. 17 of [16]. Then, $\mathbb{Z} \cong \Pi_1(\mathbb{S}^1; 1) \cong H_1(\mathbb{S}^1; \mathbb{Z})$. To prove that $\left\{[\tilde{\gamma}_\pm]_{H_1(\mathbb{S}^1;\mathbb{Z})}\right\}$ are basis of $H_1(\mathbb{S}^1; \mathbb{Z})$ it is enough to prove that $\left\{[\tilde{\gamma}_\pm]_{\Pi_1(\mathbb{S}^1;1)}\right\}$ are basis of $\Pi_1(\mathbb{S}^1; 1)$. The isomorphism $\Lambda : \Pi_1(\mathbb{S}^1; \mathbb{Z}) \to \mathbb{Z}$ is given (see Theorem 4.4, p. 17 of [16]) as follows. Given a path σ with $[\sigma]_{\Pi_1(\mathbb{S}^1;1)} \in \Pi_1(\mathbb{S}^1; 1)$ let $\sigma' : [0, 1] \to \mathbb{R}$ satisfy $\sigma'(0) = 0$ and $e^{2\pi i \sigma'(t)} = \sigma(t)$. Then, $\Lambda[\sigma]_{\Pi_1(\mathbb{S}^1;1)} = \sigma'(1)$. In our case, if we take $\tilde{\gamma}'_\pm(t) := \pm t$, $\tilde{\gamma}'_\pm(0) = 0$ and $\tilde{\gamma}'_\pm(1) = \pm 1$. It follows that $\Lambda[\tilde{\gamma}_\pm]_{\Pi_1(\mathbb{S}^1;1)} = \pm 1$. As ± 1 are basis of $\mathbb{Z}$ it follows that $[\tilde{\gamma}_\pm]_{\Pi_1(\mathbb{S}^1;1)}$ are basis of $\Pi_1(\mathbb{S}^1; 1)$ and this concludes the proof that $[\gamma_\pm]_{H_1(T;\mathbb{Z})}$ are basis of $H_1(T; \mathbb{Z})$. □

Proposition 9.2. *For $s \geq 2$, $H_s(\natural k T; \mathcal{R}) = 0$. Furthermore, $H_1(\natural k T; \mathbb{Z}) \cong \oplus_{i=1}^{k} \mathbb{Z}$, and $\left\{[Z_j]_{H_1(\natural k T;\mathbb{Z})}\right\}_{j=1}^{k}$ is a basis of $H_1(\natural k T; \mathbb{Z})$.*

Proof. We prove the proposition by induction in k. For $k = 1$, $Z_1 = \gamma_+$ and the result follows from Proposition 9.1. Let us assume that $H_s(\natural\,(k-1)\,T; \mathcal{R}) \cong \oplus_{i=1}^{k-1} \mathcal{R}$ and that $\left\{[Z_j]_{H_1(\natural\,(k-1)\,T;\mathbb{Z})}\right\}_{j=1}^{k-1}$ is a basis of $H_1(\natural\,(k-1)\,T; \mathbb{Z})$. Let X_1 and X_2 be open subsets of $\natural\, k\, T$ such that

$$\cup_{j \leq k-1} l_j(T) \subseteq X_1,\ l_k(T) \subseteq X_2,\ X_1 \simeq \cup_{j \leq k-1} l_j(T) \approx \natural(k-1)T,\ X_2 \simeq l_k(T) \approx T,$$

and $X_1 \cap X_2$ is contractible, i.e. $X_1 \cap X_2 \simeq$ to a single point. The symbol $\simeq$ means homotopic equivalence and $\approx$ means homeomorphism.

By Example 17.1, p. 98 of [16] $(\natural\, k\, T, X_1, X_2)$ is an exact triad and we can apply the sequence of Mayer-Vietoris (17.7 p. 99 and 17.9 p. 100 of [16]),

$$H_s(X_1 \cap X_2; \mathcal{R}) \to H_s(X_1; \mathcal{R}) \oplus H_s(X_2; \mathcal{R}) \to H_s(\natural\, k\, T; \mathbb{Z}) \to H^\sharp_{s-1}(X_1 \cap X_2; \mathcal{R}).$$

As $X_1 \cap X_2$ is homotopically equivalent to a point -that we denote by $\{*\}$- we have that $H_s(X_1 \cap X_2; \mathcal{R}) \cong H_s(\{*\}; \mathcal{R}) = 0$, $H^\sharp_{s-1}(X_1 \cap X_2; \mathcal{R}) \cong H^\sharp_{s-1}(\{*\}; \mathcal{R}) = 0$ (see Theorem 11.3, p. 59, Example 9.4, p. 47 and Example 9.7, p. 48 of [16]). Hence, we obtain the isomorphism,

$$H_s(X_1; \mathcal{R}) \oplus H_s(X_2; \mathcal{R}) \to H_s(\natural\, k\, T; \mathbb{R}). \tag{9.1}$$

This isomorphism is given by (see 17.4, p. 99 of [16])

$$\left([c_1]_{H_s(X_1;\mathcal{R})}, [c_2]_{H_s(X_2;\mathcal{R})}\right) \to -[c_1]_{H_s(\natural\, k\, T;\mathcal{R})} + [c_2]_{H_s(\natural\, k\, T;\mathcal{R})}. \tag{9.2}$$

As $\cup_{j \le k-1} l_j(T) \simeq X_1$, $l_k(T) \simeq X_2$, the inclusions $\cup_{j \le k-1} l_j(T) \hookrightarrow X_1$, $l_k(T) \hookrightarrow X_2$ induce isomorphisms in homology (see Theorem 11.3, p. 59 of [16]). We have, then, the following isomorphisms:

$$H_s(\natural\,(k-1)\,T; \mathcal{R}) \overset{\cong}{\to} H_s(\cup_{j \le k-1} l_j(T); \mathcal{R}) \overset{\cong}{\to} H_s(X_1; \mathcal{R}), \tag{9.3}$$

$$H_s(T; \mathcal{R}) \overset{\cong}{\to} H_s(l_k(T); \mathcal{R}) \overset{\cong}{\to} H_s(X_2; \mathcal{R}). \tag{9.4}$$

By our induction hypothesis and (9.1, 9.2, 9.3, 9.4) $H_s(\natural\, k\, T; \mathcal{R}) \cong \oplus_{i=1}^k \mathcal{R}$. Hence, by Proposition 9.1 $H_s(\natural\, k\, T; \mathcal{R}) = 0$, $s \ge 2$. Moreover, by the induction hypothesis and (9.3), it also follows that $\left\{[Z_j]_{H_1(X_1;\mathbb{Z})}\right\}_{j=1}^{k-1}$ is a basis of $H_1(X_1; \mathbb{Z})$. By Proposition 9.1 and (9.4) $H_1(X_1; \mathbb{Z}) \cong \mathbb{Z}$; furthermore, by the definition of Z_k (see 2.2)) and as the homeomorphism $l_k : T \to l_k(T)$ induces an isomorphism in homology it follows from Proposition 9.1 that $[Z_k]_{H_1(l_k(T);\mathbb{Z})}$ is a basis of $H_1(l_k(T); \mathbb{Z})$ and then, by (9.4) it is also a basis of $H_1(X_2; \mathbb{Z})$. Finally, it follows from (9.2) that $H_1(\natural k T; \mathbb{Z}) \cong \oplus_{i=1}^k \mathbb{Z}$ and $\left\{[Z_j]_{H_1(\natural k T;\mathbb{Z})}\right\}_{j=1}^{k}$ is a basis of $H_1(\natural k T; \mathbb{Z})$. □

Proposition 9.3. *$H_1(\natural k T; \mathbb{R}) \cong \oplus_{i=1}^k \mathbb{R}$ and $\left\{[Z_j]_{H_1(\natural k T;\mathbb{R})}\right\}_{j=1}^{k}$ is a basis of $H_1(\natural k T; \mathbb{R})$.*

Proof. The homology group $H_1(\natural\, k\, T; \mathbb{R})$ is a module over the ring $\mathbb{R}$, i.e. it is a vector space (p. 47 of [16]). If G is an abelian group we can also define the homology groups as in p. 153 of [17]. In this case $H_1(\natural\, k\, T; G)$ is a group. As $\mathbb{R}$ is a group and a ring we can define the homology groups as modules and as groups. To differentiate them we will denote by $H_1(\natural\, k\, T; \mathbb{R})$ the homology module considering $\mathbb{R}$ as a ring, and by $\tilde{H}_1(\natural\, k\, T; \mathbb{R})$ considering $\mathbb{R}$ as a group. Actually, $H_1(\natural\, k\, T; \mathbb{R})$ and $\tilde{H}_1(\natural\, k\, T; \mathbb{R})$ are equal as sets and as groups. By the theorem of universal coefficients-Corollary 3 A.4, p. 264 of [17]-there is the exact sequence,

$$0 \to \tilde{H}_s(\natural\, k\, T; \mathbb{Z}) \otimes \mathbb{R} \to \tilde{H}_s(\natural\, k\, ; \mathbb{R}) \to \operatorname{Tor}(\tilde{H}_{s-1}(\natural\, k\, T; \mathbb{Z}), \mathbb{R}) \to 0.$$

As $\mathbb{R}$ is torsion free, $\operatorname{Tor}(\tilde{H}_{s-1}(\natural\, k\, T; \mathbb{Z}), \mathbb{R}) = 0$. See Proposition 3A.5, p. 265 of [17]. In consequence,

$$\tilde{H}_s(\natural\, k\, T; \mathbb{Z}) \otimes \mathbb{R} \overset{\cong}{\to} \tilde{H}_s(\natural\, k\, T; \mathbb{R}). \tag{9.5}$$

The isomorphism, I, is given as follows. Let σ be a singular simplex and take $r \in \mathbb{R}$. Then,

$$I([\sigma] \otimes r) = [r\sigma].$$

See Eq. (iv) and Lemma 3.A1, pp. 261, 262 of [17]. By Proposition 9.2 $H_1(\natural kT;\mathbb{Z}) \cong \oplus_{i=1}^k \mathbb{Z}$ and $\left\{[Z_j]_{H_1(\natural kT;\mathbb{Z})}\right\}_{j=1}^k$ is a basis of $H_1(\natural kT;\mathbb{Z})$. Then

$$\oplus_{i=1}^k \mathbb{R} \cong \tilde{H}_1(\natural\, k\, T;\mathbb{Z}) \otimes \mathbb{R}.$$

The isomorphism is given by

$$\oplus_{j=1}^k \mathbb{R} \longrightarrow \oplus_{j=1}^k (\mathbb{Z}\otimes\mathbb{R}) \longrightarrow (\oplus_{j=1}^k \mathbb{Z})\otimes\mathbb{R} \longrightarrow \tilde{H}_1(\natural\, k\, T;\mathbb{Z})\otimes\mathbb{R}$$

$(r_1,\dots,r_k) \to (1\otimes r_1\dots,1\otimes r_k) \to (1,0,\dots,0)\otimes r_1 + \cdots + (0,0,\dots 1)\otimes r_k \to \sum_{j=1}^k [Z_j]_{\tilde{H}_1(\natural\, k\, T;\mathbb{Z})} \otimes r_j$.

It follows that the morphism

$$I' : \oplus_{j=1}^k \mathbb{R} \to \tilde{H}_1(\natural\, k\, T;\mathbb{R}) : I'((r_1,\dots,r_k)) := \sum_{j=1}^k [r_j Z_j]_{\tilde{H}_1(\natural\, k\, T;\mathbb{R})},$$

is an isomorphism of groups.

We now prove that this implies that $\{[Z_j]_{H_1(\natural\, k\, T;\mathbb{R})}\}_{j=1}^k$ is a basis of $H_1(\natural\, k\, T;\mathbb{R})$ as a vector space. As $\tilde{H}_1(\natural\, k\, T;\mathbb{R})$ and $H_1(\natural\, k\, T;\mathbb{R})$ are equal as sets and as groups the morphism

$$I' : \oplus_{j=1}^k \mathbb{R} \to H_1(\natural\, k\, T;\mathbb{R}) : I'((r_1,\cdots,r_k)) := \sum_{j=1}^k [r_j Z_j]_{H_1(\natural\, k\, T;\mathbb{R})},$$

is an isomorphism of groups. By the structure of vector space of $H_1(\natural\, k\, T;\mathbb{R})$ we have that $\sum_{j=1}^k [r_j Z_j]_{H_1(\natural\, k\, T;\mathbb{R})} = \sum_{j=1}^k r_j [Z_j]_{H_1(\natural\, k\, T;\mathbb{R})}$. As I' is an isomorphism of groups we have that $\forall \sigma \in H_1(\natural\, k\, T;\mathbb{R})$ there are real numbers $\{r_j\}_{j=1}^k$ such that $\sigma = \sum_{j=1}^k r_j [Z_j]_{H_1(\natural\, k\, T;\mathbb{R})}$. This means that $\{[Z_j]_{H_1(\natural\, k\, T;\mathbb{R})}\}_{j=1}^k$ generates $H_1(\natural\, k\, T;\mathbb{R})$. Moreover, if $0 = \sum_{j=1}^k r_j [Z_j]_{H_1(\natural\, k\, T;\mathbb{R})} = \sum_{j=1}^k [r_j Z_j]_{H_1(\natural\, k\, T;\mathbb{R})}$ we have that $(r_1, r_2, \cdots, r_k) = 0$, and we conclude that $\{[Z_j]_{H_1(\natural\, k\, T;\mathbb{R})}\}_{j=1}^k$ is a linearly independent set and since it also generates $H_1(\natural\, k\, T;\mathbb{R})$ it is a basis. □

10. Appendix B

In this appendix we prove, for completeness, the following proposition.

Proposition 10.1. $\left\{[\hat{\gamma}_j]_{H_1(\Lambda;\mathbb{Z})}\right\}_{j=1}^m$ *is a basis of* $H_1(\Lambda;\mathbb{Z})$.

Proof. For simplicity we will omit $\mathbb{Z}$ in the homology groups in this proof.
Step 1. As in the proof of (2.9) we prove that $H_2(\mathbb{R}^3, \mathbb{R}^3\setminus K) \cong H_1(\mathbb{R}^3\setminus K)$. Moreover the isomorphism is given by (p. 75 of [16])

$$[\sigma]_{H_1(\mathbb{R}^3,\mathbb{R}^3\setminus K)} \to [\partial\sigma]_{H_1(\mathbb{R}^3\setminus K)}. \tag{10.1}$$

Step 2. Define $K_\varepsilon := \{x \in \mathbb{R}^3 : \mathrm{d}ist(x, K) \le \varepsilon\}$. Since $\overline{\mathbb{R}^3\setminus K_\varepsilon} \subset (\mathbb{R}^3\setminus \mathring{K})$ it follows from the excision theorem (p. 82 of [16]) that the inclusion $(K_\varepsilon, K_\varepsilon\setminus K) \hookrightarrow (\mathbb{R}^3, \mathbb{R}^3\setminus K)$ induces an isomorphism in homology.

Step 3. Let $K_{\varepsilon,j}$, $j = 1, 2, \ldots, L$ be the connected components of K_ε for ε small enough. Then, $K_{\epsilon,j} = \{x \in \mathbb{R}^3 : dist(x, K_j) \leq \varepsilon\}$. By Proposition 13.9, p. 72 of [16]

$$H_2(K_\varepsilon, K_\varepsilon \setminus K) \cong \oplus_{j=1}^{L} H_2(K_{\varepsilon,j}, K_{\varepsilon,j} \setminus K_j).$$

Step 4. We have the following homotopic equivalence $K_{\varepsilon,j} \setminus K_j \simeq \partial K_{\varepsilon,j}$, that induces the isomorphism in homology

$$H_k(K_{\varepsilon,j} \setminus K_j) \cong H_k(\partial K_{\varepsilon,j}).$$

Let us consider the exact homology sequences of the pairs $(K_{\varepsilon,j}, K_{\varepsilon,j} \setminus K_j)$ and $(K_{\varepsilon,j}, \partial K_{\varepsilon,j})$. The first starts at $H_k(K_{\varepsilon,j} \setminus K_j)$ and ends at $H_{k-1}(K_{\varepsilon,j})$ and the second starts at $H_k(\partial K_{\varepsilon,j})$ and ends at $H_{k-1}(K_{\varepsilon,j})$. By the five lemma (p. 77 of [16]) the inclusion $(K_{\varepsilon,j}, \partial K_{\varepsilon,j}) \hookrightarrow (K_{\varepsilon,j}, K_{\varepsilon,j} \setminus K_j)$ induces the isomorphism in homology,

$$H_k(K_{\varepsilon,j}, \partial K_{\varepsilon,j}) \cong H_k(K_{\varepsilon,j}, K_{\varepsilon,j} \setminus K_j).$$

Step 5. By the exact homology sequence for the pair $(K_{\varepsilon,j}, \partial K_{\varepsilon,j})$ we obtain the sequence

$$\to H_2(K_{\varepsilon,j}) \to H_2(K_{\varepsilon,j}, \partial K_{\varepsilon,j}) \overset{\Delta_2}{\to} H_1(\partial K_{\varepsilon,j}) \overset{I}{\to} H_1(K_{\varepsilon,j}) \to,$$

where Δ_2 is taking boundary and I is the inclusion. By Proposition 9.2 $H_2(K_{\varepsilon,j}) = 0$. Hence we obtain the exact sequence

$$0 \to H_2(K_{\varepsilon,j}, \partial K_{\varepsilon,j}) \overset{\Delta_2}{\to} H_1(\partial K_{\varepsilon,j}) \overset{I}{\to} H_1(K_{\varepsilon,j}) \to . \tag{10.2}$$

Let $\Gamma_j \subset \{1, 2, \ldots m\}$ be such that $\{[\gamma_i]_{H_1(K_{\epsilon,j})}\}_{i\in\Gamma_j}$ is a basis of $H_1(K_{\epsilon,j})$ (see Subsect. 2.4).

Let $\{\alpha_i\}_{i\in\Gamma_j}, \{\beta_i\}_{i\in\Gamma_j}$ be the curves defined in Example 2A.2, p. 168 of [17]. Note that we can choose $\alpha_i = \hat{\gamma}_i$ (see (2.6), just take $\frac{\varepsilon}{2}$ instead of ε in K_ε). Moreover as $\gamma_i \simeq \beta_i$ we have that (see Theorem 11.2, p. 59 of [16]) $[\beta_i]_{H_1(K_{\varepsilon,j})} = [\gamma_i]_{H_1(K_{\varepsilon,j})}$. Then, by Example 2A.2, p. 168 of [17],

$$\left\{[\hat{\gamma}_i]_{H_1(\partial K_{\varepsilon,j})}, [\beta_i]_{H_1(\partial K_{\varepsilon,j})}\right\}_{i\in\Gamma_j}$$

is a basis of $H_1(\partial K_{\varepsilon,j})$.

It is clear that $I([\hat{\gamma}_i]_{H_1(\partial K_{\varepsilon,j})}) = 0$, $i \in \Gamma_j$. Moreover, $I([\beta_i]_{H_1(\partial K_{\varepsilon,j})}) = [\beta_i]_{H_1(K_{\varepsilon,j})} = [\gamma_i]_{H_1(K_{\varepsilon,j})}$. Hence, Kern $I = \left\langle\left\{[\hat{\gamma}_i]_{H_1(\partial K_{\varepsilon,j})}\right\}_{i\in\Gamma_j}\right\rangle$, the free $\mathbb{Z}-$module or the free group generated by $\{[\hat{\gamma}_i]_{H_1(\partial K_{\varepsilon,j})}\}_{i\in\Gamma_j}$. We obtain then that,

$$H_2(K_{\varepsilon,j}, \partial K_{\varepsilon,j}) \overset{\Delta_2}{\to} \text{Kern}(I) = \left\langle\left\{[\hat{\gamma}_i]_{H_1(\partial K_{\varepsilon,j})}\right\}_{i\in\Gamma_j}\right\rangle.$$

It follows that to construct a basis of $H_2(K_{\varepsilon,j}, \partial K_{\varepsilon,j})$ it is enough to compute the inverse image under Δ_2 of the $\left\{[\hat{\gamma}_i]_{H_1(\partial K_{\varepsilon,j})}\right\}_{i\in\Gamma_j}$. Let us take then $[\sigma_i]_{H_1(K_{\varepsilon,j},\partial K_{\varepsilon,j})}$ such that, $\partial\sigma_i = \hat{\gamma}_i$. Hence, $\left\{[\sigma_i]_{H_1(K_{\varepsilon,j},\partial K_{\varepsilon,j})}\right\}_{i\in\Gamma_j}$ is a basis of $H_1(K_{\varepsilon,j}, \partial K_{\varepsilon,j})$.

Finally, by Steps 4 and 5 $\left\{[\sigma_i]_{H_2(K_{\varepsilon,j},K_{\varepsilon,j}\setminus K_j)}\right\}_{i\in\Gamma_j}$ is a basis of $H_2(K_{\varepsilon,j}, K_{\varepsilon,j} \setminus K_j)$. By Step 3 $\left\{[\sigma_i]_{H_2(K_\varepsilon,K_\varepsilon\setminus K)}\right\}_{i=1}^{m}$ is a basis of $H_2(K_\varepsilon, K_\varepsilon \setminus K)$. By Step 2 $\left\{[\sigma_i]_{H_2(\mathbb{R}^3,\mathbb{R}^3\setminus K)}\right\}_{i=1}^{m}$ is a basis on $H_2(\mathbb{R}^3, \mathbb{R}^3 \setminus K)$. By Step 1 $\left\{[\hat{\gamma}_i]_{H_1(\mathbb{R}^3\setminus K)}\right\}_{i=1}^{m}$ is a basis of $H_1(\mathbb{R}^3 \setminus K)$. $\square$

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