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DINAMICA DEL CAMPO ELECTRICO EN PLASMAS

T E S I S

que para obtener el grado de

DOCTORA EN CIENCIAS (FISICA)

p r e s e n t a

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**TESIS CON  
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## INTRODUCCION

La producción reciente en laboratorio de plasmas con altas densidad y temperatura ha motivado un renovado interés en los fenómenos atómicos que ocurren en tales sistemas altamente correlacionados (Davis, 1985; DeWitt and Rogers, 1987). Debido al largo alcance de las interacciones coulombianas y a las altas densidades encontradas frecuentemente, los fuertes efectos cooperativos en el plasma pueden ejercer una influencia significativa en las propiedades radiativas y de transporte de impurezas atómicas inmersas ahí. Una descripción apropiada del acoplamiento entre el plasma y el átomo impureza puede darse en términos del campo eléctrico,  $\vec{E}$ , generado por el plasma en su posición: las ecuaciones de movimiento para el centro de masa de una impureza con carga neta  $Q_0$  son simplemente las ecuaciones de Newton, con una fuerza  $\vec{F} = Q_0 \vec{E}$ ; similarmente, las coordenadas internas del átomo obedecen las ecuaciones de Heisenberg, con un hamiltoniano para la impureza aislada más una energía de interacción dipolar,  $\vec{d} \cdot \vec{E}$ , con  $\vec{d}$  el dipolo atómico instantáneo. A través de tales interacciones, las impurezas constituyen un medio de diagnóstico muy poderoso para determinar el estado (densidad, temperatura,...) del plasma (Griem, 1974; Yaacobi et al, 1980). La observación importante aquí es que la impureza "ve" el plasma sólo a través del campo eléctrico total. Tal descripción en términos de campos eléctricos es bastante conveniente en el caso general de plasmas altamente densos (o plasmas fuertemente acoplados), en contraste con los métodos de la Teoría Cinética que se enfocan hacia secciones eficaces y trayectorias de pocas partículas (Dufty, 1981). Adicionalmente, hay razones prácticas para creer que una descripción basada en unas pocas propiedades dominantes del plasma (tal como el campo eléctrico) es también provechosa (Brissaud and Frisch, 1971, 1974; Brissaud et al, 1976; Seidel, 1977, 1979). Los beneficios de tal formulación son significativos, ya que ésta proporciona una teoría unificada tanto de procesos radiativos como de transporte (Boercker et al, 1987) en plasmas. Por lo tanto, estamos interesados aquí en las propiedades estáticas y dinámicas de esta variable, para plasmas en equilibrio. Las propiedades

estáticas han sido estudiadas ampliamente en la literatura (Dufty, 1987; Hooper, 1987), bajo una gran variedad de condiciones para los diversos parámetros en el sistema. El objetivo de esta Tesis es el desarrollar una descripción de los aspectos dinámicos del campo eléctrico generado en plasmas, con base en el formalismo teórico de la Mecánica Estadística.

Una vez que se determina la dinámica del campo eléctrico, se pueden calcular varias propiedades importantes radiativas y de transporte para la impureza atómica en el plasma. Por ejemplo, el coeficiente de autodifusión está dado en términos de la función de autocorrelación del momento,  $\langle \vec{p} \cdot \vec{p}(t) \rangle$ , la cual se relaciona fuertemente con la función de autocorrelación del campo eléctrico,  $\langle \vec{E} \cdot \vec{E}(t) \rangle$ , en el plasma (Boercker et al, 1987). Adicionalmente a las propiedades de transporte, las propiedades radiativas del átomo dependen de las características del campo eléctrico en su posición. En ese caso, la intensidad de la radiación emitida ya no ocurre a las frecuencias características de las diferencias entre los niveles de energía del átomo aislado; en lugar de eso, la radiación es distribuida sobre un continuo de frecuencias, centradas alrededor de las frecuencias atómicas características. El ensanchamiento de línea es determinado principalmente por la contribución Stark (Griem, 1974) del campo eléctrico producido a cada configuración en el plasma. El estudio de tales propiedades radiativas y de transporte para las impurezas atómicas es usualmente importante para determinar el estado del plasma (Griem, 1974; Yaacobi et al, 1980).

Adicionalmente a su importancia práctica, el estudiar las propiedades estadísticas del campo eléctrico en plasmas constituye un tópico importante desde el punto de vista del formalismo de la Mecánica Estadística. En particular, las características singulares de las interacciones eléctricas conducen a problemas especiales en la teoría de fluctuaciones, que contrastan con las de algunas otras variables (e.g. energía, densidad). En efecto, las fluctuaciones del campo eléctrico en el plasma no son gaussianas. La distribución de valores de campo eléctrico en el plasma presenta un decaimiento muy lento para valores grandes del campo, lo cual se debe a la singularidad  $1/r$  en los potenciales de Coulomb. En consecuencia, el segundo momento de esta distribución no necesariamente

existe en algunos casos<sup>1</sup>. Por otra parte, debido a que el sistema es en general altamente correlacionado, técnicas usuales en términos de interacciones de pocos cuerpos no proporcionan una descripción adecuada de efectos colectivos en el plasma. Este tipo de características, típicas en sistemas de Coulomb, hacen que éste sea un problema teórico muy interesante.

El sistema que aquí consideramos es un Plasma de Una-Componente (OCP), que consiste en  $N_1$  iones sin estructura en un "background" neutralizador uniforme, y un ión impureza con diferente masa y carga. No tomamos en cuenta los grados de libertad internos para la impureza, ya que estamos interesados básicamente en los campos eléctricos más que en procesos atómicos; además se espera que la dinámica del campo eléctrico en el plasma no dependa fuertemente de estados internos. También nos restringimos a una descripción clásica (no cuántica). El sistema se encuentra en equilibrio, con neutralidad total de carga, y todas las cargas eléctricas interactúan a través de potenciales de Coulomb. De acuerdo con la discusión anterior, nuestro interés está centrado en el campo neto instantáneo generado por el plasma en la posición de una carga dada o impureza atómica.

Se pueden distinguir dos clases de propiedades, estáticas y dinámicas, para el campo eléctrico. Las propiedades estáticas son relevantes cuando los procesos bajo consideración se llevan a cabo en tiempos que son lo suficientemente cortos para que la configuración de carga en el plasma no cambie considerablemente. Tal tiempo corto, por ejemplo, puede escogerse como el tiempo necesario para que un ión en el plasma viaje un recorrido libre medio, o también se puede definir como el inverso de la frecuencia de plasma. A esas escalas de tiempo, la distribución de valores de campo eléctrico  $\vec{E}$  a un tiempo dado, o distribución del campo microscópico,  $Q(\vec{r})$ , proporciona una descripción completa de las propiedades instantáneas del campo eléctrico. En particular, el comportamiento promedio (o macroscópico) de cualquier función arbitraria del campo eléctrico puede determinarse a partir del conocimiento de la distribución estática. A tiempos posteriores, esta información tiene que ser complementada con la

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<sup>1</sup>Un segundo momento no divergente es posible aquí sólo cuando la singularidad del campo es removida, por ejemplo, al colocar una gran carga que excluya de la posición de interés a las partículas del plasma.

probabilidad de que el campo inicial  $\vec{E}_0$  al tiempo  $t_0$  cambie a otro valor  $\vec{E}$  al tiempo  $t$ . Los aspectos dinámicos del campo son responsables, por ejemplo, de los cambios en el momento dipolar atómico, lo cual determina los perfiles de radiación. En este caso, la distribución dinámica de campos a dos tiempos diferentes, o densidad de probabilidad conjunta,  $f(\vec{E}, t; \vec{E}_0, t_0)$ , proporciona una descripción de la dinámica del campo eléctrico en el sistema. En analogía al caso estático, el comportamiento promedio de cualquier función arbitraria de los campos eléctricos a dos tiempos diferentes puede determinarse a partir de la distribución dinámica. En consecuencia, las distribuciones estática y dinámica representan la información más relevante relacionada con los campos eléctricos generados en el plasma.

Se cuenta con muy buenas técnicas de aproximación para calcular la distribución estática,  $Q(\vec{E})$ , bajo una gran variedad de condiciones para los diversos parámetros en el sistema (Dufty, 1987; Hooper, 1987). En contraste, ni siquiera existe un entendimiento fenomenológico o cualitativo de la dinámica del campo eléctrico, más allá de la función de autocorrelación para el campo eléctrico (Stamm and Smith, 1984; Pollock et al, 1985) y datos escasos de simulaciones por computadora recientes (Smith et al, 1984). De hecho, los cálculos más exitosos del ensanchamiento de líneas espectrales por plasmas se obtienen de simulaciones de dinámica molecular para el campo eléctrico, como dato a suministrarse en la ecuación de Schrödinger para el radiador (Seidel and Stamm, 1982; Stamm et al, 1984, 1986). Nuestra investigación constituye la primer tentativa para un tratamiento teórico de las propiedades dinámicas del campo eléctrico generado en plasmas.

Como se hizo notar anteriormente, la dinámica del campo eléctrico se determina a partir de la densidad de probabilidad conjunta,  $f(\vec{E}, t; \vec{E}_0, t_0)$ . A fin de estudiar las diversas propiedades y métodos de evaluación de esta distribución dinámica, el material en este trabajo ha sido básicamente dividido en dos partes. La primera parte (capítulos 2, 3 y 4) trata de las diversas propiedades y límites exactos de la distribución dinámica, así como los métodos para su evaluación. Como se detalla en discusiones posteriores, el problema puede ser reducido a cuadraturas en algunos casos límites (radiador altamente cargado, límite de tiempos cortos,...). En algunos casos, sin embargo, la evaluación de las expresiones correspondientes requiere de un trabajo numérico bastante extenso. No



obstante, muchas propiedades cualitativas importantes pueden obtenerse del estudio de estos límites. Más allá de esos límites asintóticos y aproximaciones, una descripción general presenta dificultades numéricas considerables. Dado que estamos interesados aquí en aspectos físicos más que en métodos numéricos, en la segunda parte (capítulos 5 y 6) consideramos alternativamente un enfoque semi-fenomenológico. En ese enfoque, basado en un modelaje estocástico, se consideran dos distintos aspectos del campo eléctrico en plasmas (asociados con configuraciones cercanas y lejanas, respectivamente). Las ideas físicas detrás de este planteamiento se detallan también más adelante.

En el capítulo 2 presentando una formulación general para la densidad de probabilidad conjunta,  $f(\vec{z}, t; \vec{z}_0, t_0)$ . Incluimos un breve resumen de las propiedades estáticas (§2.1), como una introducción a los aspectos dinámicos más generales del campo eléctrico. Para la evaluación y análisis de las funciones de distribución  $Q(\vec{z})$  y  $f(\vec{z}, t; \vec{z}_0, t_0)$ , en §2.2 introducimos una representación de Fourier para la función- $\delta$ , en la que ambas distribuciones quedan ahora expresadas en términos de sus funciones generadoras, estática y dinámica, correspondientes. Ahí discutimos las diversas propiedades y condiciones para la distribución dinámica y su función generadora, que se siguen de sus definiciones y de las simetrías asociadas con el estado de equilibrio. En particular, la densidad de probabilidad conjunta presenta varias invariancias (rotacional, inversión temporal, translación temporal...), y satisface condiciones de normalización que involucran la distribución estática del campo microscópico. La condición inicial es una función que presenta un pico muy pronunciado alrededor del campo relativo,  $\vec{z} - \vec{z}_0$ , y el comportamiento asintótico para  $t \rightarrow \infty$  es tal que las contribuciones de los campos  $\vec{z}$ ,  $\vec{z}_0$ , se vuelven estadísticamente independientes.

Se estudian dos límites formalmente exactos, en los cuales la densidad de probabilidad conjunta puede ser reducida a cuadraturas, a saber, el límite gaussiano y el límite de tiempos cortos. El límite gaussiano (§2.3) corresponde al caso con una carga muy intensa en el punto de interés. En este caso, los iones del OCP son empujados hacia distancias lejanas y los campos que ellos producen son débiles, lo que conduce a un límite gaussiano (Fokker-Planck) con un ancho medio determinado por la función de autocorrelación del campo eléctrico. Este límite, aunque conveniente para evaluaciones numéricas, está restringido a cargas tan intensas que pueden

resultar poco realistas. Su importancia es, por tanto, teórica más que práctica en el caso general.

Otro límite interesante es el de tiempos cortos (§2.4), el cual obtenemos aquí de dos maneras diferentes. Primero llevamos a cabo un desarrollo temporal para la función generadora dinámica (§2.4.i); a orden dominante, la probabilidad conjunta correspondiente se reduce a cuadraturas. La distribución resultante describe una difusión anisotrópica en la variable de campo relativo  $\vec{z} - \vec{z}_0$ , con un coeficiente de difusión que depende de la variable  $\vec{z} + \vec{z}_0$ . Este límite es asintóticamente exacto para  $t \rightarrow 0$ , y no se impone limitación alguna en el estado del plasma o la carga en el punto de interés. Para una evaluación de este resultado general, solamente es requerido el conocimiento de la distribución estática del campo y la función de distribución radial en el sistema. Una descripción alternativa (§2.4.ii), que no es necesariamente equivalente a la anterior, está dada en términos de un desarrollo temporal para la ecuación dinámica satisfecha por la densidad de probabilidad conjunta. Nosotros suponemos que la dependencia temporal de la función de distribución  $f(\vec{z}, t; \vec{z}_0, t_0)$  está gobernada por un operador de evolución, en el cual se impone simetría ante inversiones temporales. A tiempos cortos, este operador es similar a uno de Fokker-Planck en las variables  $\vec{z}$ ,  $t^2$ , con la solución de estado estacionario apropiada,  $Q(\epsilon)Q(\epsilon_0)$ . Debido a esto último, se espera que para tiempos largos la solución correspondiente constituya una mejor aproximación que el resultado previo. Desafortunadamente, aún no hemos sido capaces de construir una solución explícita a la ecuación diferencial construida aquí.

En el capítulo 3 presentamos un desarrollo en cúmulos (§3.1) para la función generadora dinámica, similar al de Baranger y Mozer (1959, 1960) para el caso estático. En tal desarrollo, las contribuciones de muchos cuerpos son separadas en contribuciones más manejables de uno, dos, ... cuerpos. La función generadora obtenida de este modo está dada por la del caso estático, asociada con las correlaciones estáticas en el plasma, más una serie infinita de términos que representan correlaciones dinámicas. El desarrollo correspondiente está dado en términos de potencias crecientes del así llamado "parámetro del plasma",  $\Gamma$  (energía potencial media/ energía cinética media), el cual determina el grado de acoplamiento entre las cargas en el sistema: un acoplamiento débil implica  $\Gamma \ll 1$ , y un acoplamiento fuerte,  $\Gamma \geq 1$ . Por tanto, este método está limitado a

sistemas con un acoplamiento débil. En el caso de un acoplamiento muy débil entre todas las cargas en el sistema, las correlaciones de orden superior son despreciables, de modo que sólo sobreviven en la serie los términos estático y dinámico de orden más bajo. En este caso, correspondiente a un modelo de partículas independientes y una carga muy pequeña en el punto de interés<sup>2</sup>, el problema se reduce a cuadraturas. Los detalles de esto son presentados más adelante (capítulo 4).

Otro caso interesante en el que los cálculos pueden ser reducidos a cuadraturas es el límite de campos intensos (§3.2). Un re-escalamiento apropiado en la función generadora permite factorizar potencias negativas del campo eléctrico en los diversos términos del desarrollo en cúmulos. Como resultado, el límite de campos intensos puede ser asociado con uno o dos iones cercanos al punto de interés. Las expresiones correspondientes pueden ser evaluadas numéricamente, a partir del conocimiento de la función de correlación de pares y la función de autocorrelación para la densidad en el sistema.

Para concluir este capítulo (§3.3), estudiamos un modelo renormalizado de partículas independientes (Dufty y Zogaib, 1989), que generaliza el desarrollado por Dufty et al (1985) para el caso estático. En este método sólo son retenidos los términos dominantes en el desarrollo en cúmulos, pero el campo eléctrico coulombiano es reemplazado por un campo efectivo que incluye las correlaciones de orden superior asociadas con los términos despreciados. Ese campo efectivo se escoge tal que reproduzca de modo exacto el segundo momento,  $\langle E^2 \rangle$ , o condición equivalente para el caso de puntos neutrales. La función de distribución conjunta en este modelo es por tanto reducida a cuadraturas, y reproduce exactamente la función de autocorrelación del campo eléctrico,  $\langle \vec{E} \cdot \vec{E}(t) \rangle$ . Como una consecuencia de incluir correlaciones de orden superior en un campo renormalizado, más que en un desarrollo en series para la función generadora, este método es conveniente aún para el caso general de plasmas fuertemente acoplados.

En el capítulo 4 estudiamos la función de distribución dinámica para un sistema de iones independientes y un punto neutral. En esta aproximación desaparecen las correlaciones estáticas y dinámicas de orden

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<sup>2</sup>Un punto cargado acopla las ecuaciones de movimiento de todas las cargas en el sistema, de modo que no pueden despreciarse las correlaciones dinámicas.

superior, y la función generadora para la distribución dinámica se reduce a cuadraturas. El resultado, aunque queda dado en términos de expresiones compactas, representa un desafío numérico, ya que se debe calcular una integral multi-dimensional. No es útil aquí un desarrollo de la función generadora en términos de polinomios de Legendre. En lugar de eso, nosotros consideramos algunos de los límites exactos discutidos previamente para el caso general de iones interactuantes y carga arbitraria en el punto de interés. En particular, nosotros estudiamos en detalle la distribución dinámica tanto en el límite de tiempos cortos como en el de campos intensos, que en esta aproximación son susceptibles a una evaluación numérica. El límite gaussiano discutido anteriormente no es válido en este caso, ya que el segundo momento no existe para puntos neutrales.

Primero exploramos (§4.2) el comportamiento a tiempos cortos de la distribución dinámica para un sistema de iones independientes, produciendo un campo eléctrico en la posición de un punto neutral. En particular, evaluamos numéricamente las componentes del coeficiente anisotrópico de difusión que aparece en el resultado de tiempos cortos, considerando tanto un campo de Coulomb como un campo efectivo de Debye para los iones; estas componentes son funciones monótonas crecientes del campo eléctrico. La distribución dinámica es evaluada entonces a varios tiempos y valores dados del campo inicial  $\vec{E}_0$ . En todos los casos, la distribución presenta un ensanchamiento asimétrico de la función- $\delta$  inicial, y un corrimiento monótono del pico hacia campos más pequeños. El pico decae monótonamente para valores pequeños de  $\epsilon_0$ ; para valores grandes de  $\epsilon_0$ , el pico se levanta otra vez a tiempos posteriores. Para valores de  $\epsilon_0$  con gran probabilidad de ocurrencia, el decaimiento del pico es no sólo monótono sino también lento; en contraste, para valores menos probables, el decaimiento inicial es muy abrupto. Estos hechos sugieren distinguir dos tipos distintos de procesos, uno para valores pequeños de  $\epsilon_0$ , y otro para valores grandes. Finalmente, a tiempos posteriores el pico alcanza su valor de equilibrio y continúa hacia la región negativa, lo cual refleja la limitación de este resultado a tiempos muy cortos solamente. Una comparación entre nuestros resultados y datos escasos de simulación por computadora (Smith *et al*, 1984) se muestra en §4.3, en la que los datos se comparan bien sólo de manera cualitativa. En todos los casos, el pico de nuestra distribución está recorrido a la izquierda del de los datos de simulación; el ancho es también mayor. Las discrepancias se vuelven más

significativas para valores de campo menores que la posición del pico, aunque los datos ajustan mejor cuando se consideran valores grandes de  $\epsilon_0$ . Pensamos que esas discrepancias se deben a parámetros incorrectos reportados para la simulación, ya que se puede obtener un ajuste excelente si se re-escala el tiempo de un modo apropiado.

Para concluir este capítulo, en §4.4 considerados el modelo de partícula aislada, como una aproximación para describir la dinámica de campos intensos en un sistema de iones independientes y un punto neutral. El modelo de partícula aislada para describir campos intensos es válido en general para el caso estático. En el caso dinámico, sin embargo, esta aproximación está limitada a tiempos lo suficientemente cortos para que un ión cercano (que produce un campo intenso) no se haya alejado aún. El sistema considerado en esta sección permite una evaluación numérica de los resultados correspondientes.

Las serias dificultades numéricas asociadas con el formalismo exacto en el caso general (o sea, más allá de los límites y aproximaciones discutidos aquí) justifica el buscar un enfoque alternativo más simple para este problema. Una posibilidad está dada por la Teoría de los Procesos Estocásticos, en la cual el campo es eléctrico considerado como una variable estocástica cuyas fluctuaciones presentan propiedades estadísticas similares a las de algunos otros procesos estocásticos conocidos. El objetivo de la segunda parte de este trabajo (capítulos 5 y 6) es, por tanto, el considerar modelos aproximados para la distribución dinámica  $f(\vec{z}, t; \vec{z}_0, t_0)$ , en los cuales se supone que los dos aspectos del campo eléctrico (debido a iones cercanos y lejanos) discutidos en capítulos previos satisfacen procesos estocásticos markofianos independientes.

En el capítulo 5 discutimos las ideas físicas que hay detrás tal descripción estocástica, y presentamos algunos ejemplos simples. En §5.1 presentamos algunas definiciones, e introducimos una Ecuación Maestra para la distribución dinámica, de acuerdo a la suposición markofiana. La Ecuación Maestra general es una ecuación integro-diferencial, cuyo kernel describe la probabilidad de transición por unidad de tiempo entre dos valores de campo diferentes. Se pueden distinguir dos tipos diferentes de procesos: uno con variaciones grandes, al que nos referimos como "proceso de fluctuaciones intensas", en el cual el valor del campo después de una transición es prácticamente independiente del valor inicial; otro de variaciones pequeñas, al que nos referimos como "proceso de difusión", en

el cual las transiciones se llevan a cabo a pasos pequeños. Los modelos de fluctuaciones intensas son discutidos en §5.2. Ahí, el así llamado "Proceso Canguro" es particularmente interesante, ya que fue propuesto originalmente por Brissaud y Frisch (1971, 1974) como una primer tentativa para describir formas de líneas espectrales a partir del conocimiento de solamente el campo eléctrico en la posición del átomo radiante. La distribución dinámica en el Proceso Canguro, al igual que en todos los otros modelos de esta sección, está dada por la suma de dos contribuciones: una distribución simétrica alrededor de  $\vec{E} = 0$ , que aumenta con el tiempo de cero hasta el valor de equilibrio, y una contribución de la distribución- $\delta$  original alrededor de  $\vec{E} = \vec{E}_0$ , que es simplemente se atenúa en el tiempo. Este comportamiento tan poco físico es característico de procesos sin memoria y contrasta con el resultado de tiempos cortos. Los modelos de difusión, por otra parte, son presentados en §5.3. Las distribuciones dinámicas aquí satisfacen una ecuación del tipo Fokker-Planck, que presenta tanto un término de difusión como uno de deriva. Esto es, la distribución- $\delta$  original alrededor de  $\vec{E} = \vec{E}_0$  se ensancha con el tiempo y se recorre hacia valores de campo más pequeños, tendiendo suavemente hacia el valor de equilibrio, en concordancia cualitativa con el comportamiento esperado. Esta tendencia al equilibrio, sin embargo, es muy lenta ya que no se toman en cuenta aquí procesos con grandes fluctuaciones. Los modelos de difusión son incapaces de describir transiciones a estados con valores de campo muy diferentes, como las producidas por unos cuantos iones cercanos al punto de interés. Ni los modelos de fluctuación intensa ni los de difusión proporcionan una descripción completa de la dinámica del campo eléctrico en el plasma; sin embargo, su relativa simplicidad matemática motiva el considerar modelos estocásticos alternativos, en los cuales pueda obtenerse una descripción más completa.

El espíritu del capítulo 6 es precisamente el proponer alternativas razonables hacia la construcción de modelos estocásticos más realistas. Aquí consideramos dos modelos diferentes, como una tentativa para incluir el efecto de las dinámicas rápida y lenta asociadas con iones cercanos y distantes, respectivamente. En el así llamado "Modelo Compuesto" de la §6.2, nosotros partimos de una Ecuación Maestra para la distribución dinámica y centramos nuestra atención en la intensidad de las fluctuaciones del campo eléctrico. Distinguimos dos tipos de procesos, uno de fluctuaciones intensas y uno de fluctuaciones débiles, los cuales suponemos

que son mutuamente excluyentes. En consecuencia, la evolución temporal de la distribución dinámica está gobernada por la suma de dos operadores: uno, característico de procesos con tamaño arbitrario de "saltos" para el campo eléctrico, para el que escogemos un Proceso Canguro; otro, característico de procesos con pequeños cambios en el campo eléctrico, para el que escogemos un operador de Fokker-Planck. La distribución dinámica correspondiente satisface una ecuación integro-diferencial, con coeficientes fenomenológicos asociados con los dos procesos considerados. Los resultados obtenidos constituyen una mejora sobre los de los modelos Canguro y Fokker-Planck, separadamente: ellos describen procesos *con memoria*, de modo que a  $t > 0$  ya no se tiene la poca física contribución de la distribución- $\delta$  inicial; también, la evolución dinámica asociada es más rápida aquí que en un proceso de Fokker-Planck. Estos resultados son bastante prometedores en verdad. La utilidad de este modelo, sin embargo, está limitada a aquellos casos en los cuales se puede resolver la ecuación integro-diferencial correspondiente, con relativa facilidad.

En el "Modelo de Convolución" de la §6.3, centramos nuestra atención en la intensidad del campo eléctrico mismo, en lugar de sus fluctuaciones. Nosotros consideramos el campo eléctrico en un punto dado como la suma de dos contribuciones diferentes: una debido a los iones cercanos, y una debido a los iones distantes. Estas dos contribuciones son consideradas como estadísticamente independientes para todo tiempo, de modo que su evolución dinámica está gobernada por operadores de evolución independientes. En consecuencia, la distribución de los campos eléctricos a dos tiempos diferentes es obtenida a partir de la convolución de las distribuciones dinámicas asociadas con cada uno de esos dos procesos independientes. El problema se reduce entonces a proponer modelos apropiados para tales distribuciones y a evaluar una integral de 6 dimensiones. Pensamos que una elección posible para las dos distribuciones son las correspondientes a los modelos Canguro y de Difusión; desafortunadamente, limitaciones de tiempo no nos han permitido explorar en detalle esta posibilidad. La utilidad de este modelo está limitada a aquellos casos en los cuales la integración asociada puede ser llevada a cabo numéricamente.

Los dos modelos estocásticos en este capítulo representan una generalización razonable a los del capítulo 5, en el sentido de que aquí se combinan los aspectos relevantes que los modelos existentes describen sólo

de una manera parcial. Tanto el Modelo Compuesto como el Modelo de Convolución proporcionan una descripción semi-fenomenológica de los campos eléctricos, en donde los coeficientes correspondientes tienen que ser especificados a partir de propiedades exactas (función de autocorrelación para el campo eléctrico,...) en el plasma. Se espera que la relativa simplicidad numérica asociada con tal descripción permita estudios más detallados en aquellos casos donde la formulación exacta no puede ser reducida a cuadraturas. Estudios adicionales también ayudarán a decidir uno de estos modelos en favor del otro.

Finalmente, en el capítulo 7 presentamos un resumen de los aspectos relevantes de la dinámica del campo eléctrico que hemos aprendido a través de esta investigación. A partir de esta perspectiva, formulamos algunas conclusiones generales y comentamos acerca de estudios futuros que se sugieren de nuestros resultados.



## CONCLUSIONES

El objetivo de este trabajo ha sido el desarrollar un formalismo exacto para describir las propiedades dinámicas de los campos eléctricos en plasmas, desde el punto de vista teórico de la Mecánica Estadística. El estudiar las propiedades estadísticas de los campos eléctricos generados en el plasma es importante para entender las propiedades de transporte y radiativas de impurezas atómicas inmersas ahí, lo cual constituye una herramienta muy poderosa de diagnóstico para determinar el estado del plasma; también, las características singulares de los sistemas de Coulomb conducen a algunos problemas especiales en la teoría de fluctuaciones, que contrastan con las de otras variables (e.g. energía, densidad). Por lo tanto, este problema presenta una importancia tanto práctica como teórica. Aunque las propiedades estáticas del campo eléctrico son ya bien conocidas para una gran variedad de condiciones para los diversos parámetros en el sistema, el problema dinámico ha recibido muy poca atención en la literatura. Nuestra investigación constituye una primer tentativa teórica para la descripción de las propiedades dinámicas del campo eléctrico, como una generalización al caso estático. Por simplicidad, hemos limitado nuestro estudio a un plasma clásico (no cuántico) de una componente, en equilibrio, aunque se espera que una generalización para plasmas cuánticos multi-componentes sea directa. En particular, hemos centrado nuestra atención en la distribución de probabilidad dinámica (densidad de probabilidad conjunta) para los campos eléctricos generados por los iones del plasma en la posición de un átomo impureza a dos tiempos diferentes. La información física contenida en esta distribución es, con mucho, más exhaustiva que la asociada con el conocimiento de unos cuantos de sus momentos (función de autocorrelación para el campo eléctrico...); en este sentido, nuestra investigación constituye una descripción más general y completa de los aspectos dinámicos del campo eléctrico en comparación con los estudios existentes, los cuales se limitan a unos pocos modelos semi-fenomenológicos y a la evaluación de diversas funciones promedio del

campo (tal como la función de autocorrelación para el campo eléctrico) a partir de modelos cinéticos o simulaciones por computadora.

Las propiedades estadísticas del campo eléctrico en la posición de una carga impureza en el plasma dependen fuertemente tanto del acoplamiento entre los iones del plasma (determinado por su carga, densidad y temperatura) como del acoplamiento entre esos iones y la carga impureza (determinado por el cociente entre las cargas del ion y la impureza). La naturaleza de tales acoplamientos hace que éste sea un problema numérico muy complejo en general, para el cual no pueden utilizarse técnicas usuales para sistemas de partículas neutras. A lo largo de este trabajo hemos estudiado varios límites exactos y aproximaciones útiles, que están basados en el efecto relativo de los acoplamientos anteriores en algunos casos límites donde el problema puede ser reducido a cuadraturas.

Se encontró que un caso interesante donde el acoplamiento ión-impureza juega un papel relevante era el de un punto altamente cargado, el cual rechaza a los iones del plasma hacia grandes distancias. En este caso, los campos eléctricos generados por los iones son muy débiles, lo que permite algunas simplificaciones para la función generadora asociada con la distribución dinámica del campo. Por ejemplo, si se considera la representación (2.2.11) para la función generadora, la densidad de probabilidad conjunta correspondiente presenta una forma gaussiana (Ec.2.3.3). El ancho medio asociado con esta distribución se determina a partir del conocimiento de la función de autocorrelación para el campo eléctrico, la cual puede obtenerse de modelos cinéticos o por evaluación directa. Desafortunadamente, las aproximaciones concernientes a este límite generalmente requieren una carga tan grande en el punto de interés que pueden resultar poco realistas; por tanto, su importancia es en general teórica más que práctica. No obstante, este límite proporciona una descripción cuantitativa de las propiedades dinámicas de los campos débiles producidos por configuraciones distantes, lo cual es explotado más adelante en este trabajo.

El límite gaussiano presenta la dificultad de no tender a la solución de equilibrio (tiempos largos) correcta. Como un intento para corregir esta dificultad, en Ec.(2.3.22) consideramos la posibilidad de reemplazar los factores gaussianos que aparecen en la Ec.(2.3.3) por la distribución estática del campo exacta. Sin embargo, tal reemplazo no resulta

afortunado, ya que la distribución dinámica correspondiente no satisface una de las condiciones importantes de simetría (Ec.2.2.16) que se siguen del equilibrio. Alternativamente a la representación (2.2.11) para la función generadora, también exploramos la representación (2.2.23) para el caso de campos débiles, lo que también permite reducir el problema a cuadraturas (Ec.2.3.25). El resultado correspondiente satisface todas las propiedades exactas (2.2.12)-(2.2.17), de modo que presenta un comportamiento más apropiado que el del límite gaussiano. Al igual que en el límite gaussiano, la densidad de probabilidad conjunta en este caso puede determinarse también de cantidades simples tales como la función de autocorrelación para el campo eléctrico y la función generadora (conocida) para el caso estático. Aunque la dependencia angular en este caso introduce algunas dificultades numéricas, nosotros creemos que un estudio más detallado de esta distribución redituará bastante.

El acoplamiento ión-impureza también determina la validez de aproximaciones usuales tales como la de iones independientes. Las técnicas usuales de Desarrollo en úmulos para sistemas de partículas neutrales permiten despreciar las correlaciones estáticas y dinámicas de orden superior para el caso de interacciones débiles entre las partículas, de modo que el problema puede ser reducido a cuadraturas. En nuestro caso, la validez de tal aproximación depende no sólo de la intensidad de las interacciones ión-ión sino también de sus interacciones con la carga impureza. Como hemos mostrado en §3.1, un punto con carga eléctrica acopla las ecuaciones de movimiento para los iones de modo que, en general, no pueden despreciarse las correlaciones dinámicas de orden superior. Sólo en casos limitados tales correlaciones dinámicas de orden superior se vuelven despreciables, y la cantidad desarrollada (en este caso, la función generadora) puede ser aproximada por los términos dominantes en la serie. Un ejemplo de esto es el límite de campos intensos (§3.2), el cual se encontró que estaba asociado con el efecto de uno o dos iones cerca del punto de interés. Este resultado interesante, junto con el correspondiente al límite gaussiano, sugieren el distinguir dos aspectos diferentes de los campos eléctricos en nuestro sistema: uno debido a los iones cercanos, que generan un fuerte efecto en el punto de interés, y otro debido a las configuraciones distantes, que producen un efecto débil. Así, los límites

gaussiano y de campo intenso proporcionan una interpretación física para el efecto de configuraciones cercanas y distantes en el sistema.

Debido a que la utilidad de la aproximación de partículas independientes está limitada sólo a esos casos con un acoplamiento muy débil entre todas las cargas en el plasma, hemos propuesto aquí una aproximación relacionada que se espera sea apropiada aún para plasmas fuertemente acoplados. Esta aproximación es una generalización del así llamado Modelo Renormalizado de Partículas Independientes para el caso estático, en el cual el campo de Coulomb es reemplazado por un campo eléctrico efectivo que toma en cuenta las correlaciones dinámicas de orden superior despreciadas generalmente. Este modelo presenta aún la simplicidad y estructura general del modelo simple de partículas independientes, pero proporciona una descripción más apropiada de las correlaciones de muchos cuerpos en el sistema; al introducir cantidades renormalizadas. Aunque aún no hemos explorado este modelo numéricamente, los excelentes resultados para el caso estático que han sido obtenidos en otra parte sugieren que nuestra generalización constituye una alternativa prometedora para describir la dinámica del campo eléctrico en plasmas fuertemente acoplados.

Se encontró que un límite exacto interesante donde el problema puede ser reducido a cuadraturas, sin importar el estado del plasma y la carga en el radiador, era el de tiempos cortos en §2.4.1. En este límite, la distribución dinámica de campos (Ec.2.4.6) describe difusión anisotrópica, con coeficientes que dependen de la magnitud del campo y que pueden ser determinados a partir del conocimiento de la función de correlación de pares y la distribución estática del campo. Una evaluación numérica de esta distribución (capítulo 4) ha mostrado que nuestros resultados se comparan cualitativamente bien con datos escasos de simulación por computadora, para el caso de iones independientes y un punto neutral -creemos que las discrepancias cuantitativas se deben a parámetros incorrectos reportados para la simulación-. Los resultados correspondientes muestran un ensanchamiento asimétrico del pico inicial (una función delta), con un corrimiento monótono hacia el valor de equilibrio. Otra vez se pueden distinguir dos aspectos diferentes en la evolución dinámica para la distribución de campos, de acuerdo con la magnitud del campo eléctrico inicial: para valores pequeños, la evolución

dinámica es lenta, con un decaimiento monótono para el pico; para valores grandes, la evolución es rápida, y a tiempos intermedios el pico se vuelve a levantar otra vez a partir de un valor mínimo. Para el caso de un campo eléctrico inicial muy intenso, en particular, una comparación entre esta distribución y la asociada con un ión aislado (§4.4) ha revelado concordancias excelentes a tiempos muy cortos; es posible en este modo determinar el rango de aplicabilidad del modelo de ión aislado, para describir las propiedades dinámicas de campos intensos. Finalmente, a tiempos posteriores (del orden del inverso de la frecuencia de plasma) la posición del pico alcanza su valor de equilibrio y continúa hacia la región negativa. Este hecho muestra que nuestro resultado está limitado a tiempos muy cortos ( $\approx \omega_{pi}^{-1}$ ) solamente. Una especificación precisa de la escala de tiempo asociada con este límite será posible a medida que contemos con datos más extensos de simulación para la distribución dinámica. Estudios futuros de este límite también deberían de enfocarse hacia el caso de puntos cargados, de modo que se pudiera establecer una comparación interesante con nuestros resultados en el límite gaussiano.

Una descripción alternativa, no necesariamente equivalente, para tiempos cortos fue también formulada (§2.4.ii) al imponer invariancia ante inversiones temporales en la ecuación dinámica satisfecha por la densidad de probabilidad conjunta. Se encontró que el operador de evolución correspondiente era similar a uno de Fokker-Planck, con la solución estacionaria apropiada. Debido a esto último, se espera que la solución a esta ecuación sea una mejor aproximación para tiempos posteriores que el resultado anterior. Desafortunadamente, no hemos sido capaces aún de construir una solución explícita para la ecuación diferencial correspondiente.

Los límites y aproximaciones anteriores resumen los aspectos más relevantes en la dinámica del campo eléctrico en un plasma, que se siguen de la formulación exacta que aquí presentamos. Una aplicación de nuestros resultados a problemas específicos podría requerir de una generalización para incluir una descripción cuántica, o plasmas multi-componentes. Más allá de estos límites exactos y aproximaciones, el problema es más bien numérico que físico, lo cual no es el objetivo que perseguimos en esta Tesis.

Como una alternativa a la complejidad numérica asociada con la formulación exacta, en la segunda parte de este trabajo hemos considerado algunos modelos aproximados basados en la Teoría de los Procesos Estocásticos Markovianos, los cuales presentan una relativa simplicidad matemática. Desafortunadamente, ninguno de los modelos existentes proporciona una descripción adecuada de la dinámica del campo eléctrico en plasmas, ya que ellos sólo consideran aspectos parciales del campo eléctrico: los modelos de fluctuaciones intensas (tales como el Proceso Canguro en §5.2.ii) describen procesos rápidos asociados con el efecto de las configuraciones cercanas, en los cuales el valor del campo después de una transición es prácticamente independiente del valor inicial (i.e. no existe *memoria* en el sistema); por otra parte, los modelos de difusión (tal como el Proceso de Fokker-Planck en §5.2.ii) describen procesos lentos asociados con el efecto de las configuraciones distantes, en los cuales el campo eléctrico sólo cambia a pasos muy pequeños -de tal modo que existe una *memoria* asociada con los cambios del campo eléctrico-.

Debido a la simplicidad matemática y al éxito relativo de los procesos estocásticos anteriores, hemos propuesto aquí dos generalizaciones posibles de las que se espera obtener una descripción más adecuada y completa de la dinámica del campo eléctrico en el plasma. En estos modelos hemos tratado de incorporar aquellos aspectos del campo eléctrico que parecen jugar un papel relevante en la evolución dinámica de la distribución de campos: en el primer caso (el "Modelo Compuesto" en §6.2) hemos centrado nuestra atención en el tamaño de las fluctuaciones del campo eléctrico, distinguiendo dos procesos mutuamente excluyentes, asociados con fluctuaciones débiles y fuertes; en el segundo caso (el "Modelo de Convolución" en §6.3) hemos centrado nuestra atención en el campo eléctrico mismo, en lugar de sus fluctuaciones, distinguiendo dos procesos estadísticamente independientes, asociados con configuraciones que producen campos eléctricos intensos y débiles. En cada caso asociamos uno de los modelos anteriores (i.e. Canguro y Fokker-Planck) con cada uno de los dos procesos bajo consideración.

Aunque las limitaciones de tiempo no nos han permitido aquí explorar en detalle estos dos modelos estocásticos, tenemos razones para creer que ellos constituyen una posibilidad aceptable para describir la dinámica del campo eléctrico en un modo relativamente simple. Tal esperanza se basa en

los resultados tan prometedores que se obtienen en el Modelo Compuesto, los cuales representan una mejora substancial sobre los modelos simples de fluctuaciones intensas y de difusión. Los procesos descritos aquí ciertamente presentan características más físicas que en los modelos de fluctuaciones intensas, en el sentido de que hay una memoria asociada con los cambios en el campo eléctrico; además, la evolución temporal de la distribución dinámica es más rápida aquí que en los modelos de difusión, de modo que se toma en cuenta el efecto de las configuraciones cercanas que es despreciado en esos modelos. Se esperan resultados similares para el Modelo de Convolución, en el sentido de que para todo tiempo éste "mezcla" los aspectos físicos asociados con cada uno de los procesos independientes.

En estos dos modelos, la evolución dinámica del campo eléctrico está dada en términos de los diversos coeficientes fenomenológicos asociados con los dos procesos independientes bajo consideración, los cuales deben escogerse de modo tal que reproduzcan las propiedades exactas (autocorrelación del campo eléctrico,...) en el sistema. La flexibilidad de tal enfoque semi-fenomenológico permite el probar algunos modelos simples para esos coeficientes de modo que, en principio, el problema numérico pueda ser manejable. Aunque aún no hemos sido capaces de contruir una solución exacta en el caso de algunas elecciones realistas para estos coeficientes, nuestros desarrollos (no incluidos aquí) parecen indicar que para el Modelo Compuesto pueden obtenerse soluciones aproximadas. Las dificultades numéricas asociadas con este modelo son, con mucho, menos severas que las de la descripción exacta; esto mismo se aplica para el Modelo de Convolución.

Por supuesto, todavía quedan varias preguntas por ser contestadas en estudios subsecuentes de estos modelos estocásticos para plasmas. Por ejemplo, no es claro hasta aquí qué tan apropiada resulta la suposición markofiana para describir tales sistemas tan altamente correlacionados. Una respuesta a esto requiere, por ejemplo, de una comparación entre nuestros resultados con los de simulación por computadora para la distribución dinámica (aún no disponibles en la literatura). Esto también será útil para establecer la validez y rango de aplicabilidad de cada uno de los dos modelos que hemos propuesto aquí. Mientras esos resultados de simulación llegan a ser disponibles, nuestros estudios actuales se centran en analizar las hipótesis físicas detrás de los dos modelos, el Compuesto y

el de Convolución, así como su consistencia con propiedades exactas en el sistema. Esto también habrá de darnos un criterio para decidir uno de estos modelos en favor del otro.



**ELECTRIC FIELD DYNAMICS IN PLASMAS**

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Lorena Zogaib  
March, 1990

## CHAPTER 1

### INTRODUCTION

Recent production of hot dense plasmas in the laboratory has motivated renewed consideration of atomic phenomena in such highly correlated systems (Davis, 1985; DeWitt and Rogers, 1987). Due to the long-range Coulomb interactions and high densities frequently encountered, strong cooperative effects in the plasma can have a significant influence on transport and radiative properties of atomic impurities immersed there. An appropriate description for the coupling between the plasma and the impurity atom can be given in terms of the electric field  $\vec{E}$  generated by the plasma at its position: the equations of motion for the center of mass of an impurity with a net charge  $Q_0$  are simply Newton's equations, with a force  $\vec{F} = Q_0 \vec{E}$ ; similarly, the atomic internal coordinates obey Heisenberg equations with a Hamiltonian for the isolated impurity plus a dipole interaction energy,  $\vec{d} \cdot \vec{E}$ , with  $\vec{d}$  the instantaneous atomic dipole. Through such interactions, impurities constitute a very powerful diagnosis tool for determining the state (density, temperature,...) of the plasma (Griem, 1974; Yaacobi *et al.*, 1980). The important observation at this point is that the impurity "sees" the plasma only through the total electric field. Such a description in terms of electric fields is well suited in the general case of plasmas with high densities (or Strongly Coupled Plasmas), in contrast to Kinetic Theory methods which focus on few-particle trajectories and cross sections (Dufty, 1981). In addition, there are practical reasons to believe that an approach based on a few dominant properties of the plasma (such as the electric field) is also profitable (Brissaud and Frisch, 1971, 1974; Brissaud *et al.*, 1976; Seidel, 1977, 1979). The benefits of such a formulation are significant since it provides a unified theory of both radiative and transport processes (Boercker *et al.*, 1987) in plasmas. Therefore, we are concerned here with the static and dynamical properties of this variable for plasmas in equilibrium. The static properties have been widely studied in the literature (Dufty, 1987; Hooper, 1987), under a

variety of conditions for the diverse parameters in the system. The objective of this dissertation is to develop a description of the dynamical aspects of the electric field generated in plasmas, based on the theoretical formalism of Statistical Mechanics.

Once the electric field dynamics is determined, several important transport and radiative properties of the atomic impurity in the plasma can be calculated. For example, the self diffusion coefficient is given in terms of the momentum time correlation function, which is closely related to the electric field autocorrelation function for the plasma (Boercker *et al*, 1987). In addition to the transport properties, radiative properties for the atom depend on the characteristics of the electric field at its position. In that case, the intensity of radiation emitted no longer occurs at frequencies characteristic of the differences between its isolated atom energy levels; instead, the radiation is distributed over a continuum of frequencies centered about the characteristic atomic frequencies. The spectral line broadening is mostly determined by the Stark contribution (Griem, 1974) from the electric field produced at each configuration in the plasma. Studying such transport and radiative properties of atomic impurities is usually important for determining the state of the plasma (Griem, 1974; Yaacobi *et al*, 1980).

In addition to its practical importance, studying the statistical properties of the electric field in plasmas constitutes an important subject from the point of view of the formalism of Statistical Mechanics. In particular, the singular characteristics of electric interactions lead to special problems in the theory of fluctuations, which contrast to those for some other variables (e.g. energy, density). Indeed, electric field fluctuations in the plasma are not Gaussian. The distribution of electric field values in the plasma presents a very slow decaying behavior at large values of the field, which is due to the  $1/r$  singularity of Coulomb potentials. Consequently, the second moment for this distribution does not necessarily exist in some cases. On the other hand, since the system is highly correlated in general, standard techniques in terms of few-body interactions usually fail to provide an adequate description of collective

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\* A non-divergent second moment here is possible only when the field singularity is removed, for instance, by placing a large charge that excludes the plasma particles from the position of interest.

effects in the plasma. Features like these, characteristic of Coulomb systems, make this a very interesting theoretical problem.

The system considered here is a One-Component plasma (OCP), consisting of  $N_1$  structureless ions in a uniform neutralizing background and a single impurity ion with different mass and charge. Internal degrees of freedom for the impurity are not considered here, since we are interested primarily in electric fields rather than in atomic processes and it is expected that the plasma field dynamics is not strongly dependent on internal states. We also restrict ourselves to a classical description. The system is in equilibrium, with overall charge neutrality, and all the charges interact via Coulomb potentials. According to the discussion above, we focus attention on the net instantaneous electric field generated by the plasma at the impurity.

We distinguish two kind of properties, static and dynamical, for the electric field. Static properties are relevant when the processes under consideration take place at times short enough for the charge configuration in the plasma not to change considerably. Such a short time, for instance, may be chosen to be the time necessary for an ion in the plasma to travel a mean free path, or it can be defined as the inverse ion plasma frequency. At these time scales, the distribution of electric field values  $\vec{E}$  at a given time, or microfield distribution,  $Q(\vec{E})$ , provides a complete description for the instantaneous properties of the electric field. In particular, the average (or macroscopic) behavior of any arbitrary function of the field can be determined from the knowledge of the static distribution. At later times, this information has to be supplemented with that of the probability for an initial field  $\vec{E}_0$  at time  $t_0$  to change into another value  $\vec{E}$  at time  $t$ . Dynamical aspects of the field are responsible, for instance, for changes in the atomic dipole moment which determine radiation profiles. In this case, the dynamical distribution of fields at two different times, or joint probability density,  $f(\vec{E}, t; \vec{E}_0, t_0)$ , provides a description of electric field dynamics in the system. In analogy to the static case, the average behavior of any arbitrary function of the fields at two different times can be determined from the dynamical distribution. Consequently, both the static and dynamical distributions represent the most relevant information concerning the electric fields generated in the plasma.

There are very good approximation techniques available to calculate the static distribution  $Q(\vec{z})$ , under a variety of conditions for the diverse parameters in the system (Dufty, 1987; Hooper, 1987). In contrast, there is not even a phenomenological or qualitative understanding of electric field dynamics, beyond the electric field autocorrelation function (Stamm and Smith, 1984; Pollock *et al*, 1985) and limited data from recent computer simulations (Smith *et al*, 1984). In fact, the most successful calculations of plasma-broadened spectral lines are obtained from molecular dynamics simulation of the electric field as input to the Schrödinger equation for the radiator (Seidel and Stamm, 1982; Stamm *et al*, 1984, 1986). Our research here is a first attempt at the theoretical treatment of the dynamical properties of electric fields generated in plasmas.

As noted above, electric field dynamics is determined from the joint probability density,  $f(\vec{z}, t; \vec{z}_0, t_0)$ . In order to study the various properties and methods of evaluation for such a dynamical distribution, the material in this work has been basically divided in two parts. The first part (Chapters 2, 3 and 4) deals with the diverse properties and exact limits of the dynamical distribution, as well as several approaches to its evaluation. As will be detailed in subsequent discussions, the problem can be reduced to quadratures in some limiting cases (large charge at the field point, short time limit, independent particle model, high field limit,...). The evaluation of the corresponding expressions, however, requires extensive numerical work in some cases; nevertheless, many important qualitative properties can be obtained from the study of these limits. Beyond those asymptotic limits and approximations, a general description presents considerable numerical difficulties. Since we are concerned here with physical aspects rather than numerical methods, an alternative semi-phenomenological approach is considered in the second part (Chapters 5 and 6). In that approach, which is based on a stochastic modeling, two different aspects of the electric field in plasmas (associated with nearby and distant configurations, respectively) are considered. The physical ideas behind such an approach are also detailed later on.

We start in Chapter 2 by presenting a general formulation for the joint probability density  $f(\vec{z}, t; \vec{z}_0, t_0)$ . We include an overview of static properties (§2.1), as an introduction to the most general dynamical aspects of the electric field. To further evaluation and analysis of the distribution functions  $Q(\vec{z})$  and  $f(\vec{z}, t; \vec{z}_0, t_0)$ , a Fourier representation for



the  $\delta$ -function is introduced (§2.2), in which both distributions are expressed now in terms of their corresponding static and dynamical generating functions. We discuss the various properties and conditions for the dynamical distribution and its generating function, which follow from their definitions and symmetries of the equilibrium state. In particular, the joint probability density presents diverse invariances (rotational, time reversal, time translational,...) and it satisfies normalization conditions involving the static microfield distribution. The initial condition is a sharply peaked function of the relative field,  $\vec{z} - \vec{z}_0$ , and the asymptotic behavior as  $t \rightarrow \infty$  is such that the contributions from the fields  $\vec{z}, \vec{z}_0$ , become statistically independent.

Two formally exact limits are studied in which the joint probability density can be reduced to quadratures, namely, the Gaussian and the short time limits. The Gaussian limit (§2.3) corresponds to the case with a very large charge at the field point. In this case, ions of the OCP are repelled to large distances and the fields are weak, leading to a Gaussian (Fokker-Planck) limit with a half width determined from the electric field time correlation function. This limit, although suitable for numerical evaluation, is in some cases restricted to an unrealistic large charge at the field point. Its importance, therefore, is rather theoretical than practical in the general case.

Another interesting limit is that for short times (§2.4), which is obtained here in two different ways. We first perform a time expansion for the dynamical generating function (§2.4.1); at leading order the corresponding joint probability density is reduced to quadratures. The resulting distribution represents anisotropic diffusion in the relative field variable  $\vec{z} - \vec{z}_0$ , with a time-independent diffusion coefficient depending on the fields through  $\vec{z} + \vec{z}_0$ . This limit is asymptotically exact as  $t \rightarrow 0$ , and no limitation is imposed on the plasma state and the charge on the field point. To further evaluation of this general result, only the knowledge of the static microfield distribution and the radial distribution function in the system is required. The applicability of this result is limited to very short times. An alternative, not necessarily equivalent, description is given in terms of a time expansion in the dynamical equation satisfied by the dynamical distribution (§2.4.11). We assume here that the time dependence of the distribution function  $f(\vec{z}, t; \vec{z}_0, t_0)$  is governed by an evolution operator, in which time reversal symmetry is imposed. At short

times, this operator is similar to one of Fokker-Planck in the variables  $\vec{z}$ ,  $t^2$ , with the appropriate steady-state solution,  $Q(\vec{z})Q(\epsilon_0)$ . Because of this latter fact, the corresponding solution is expected to be a better approximation to longer times than the previous result. Unfortunately, we have not been able yet to construct an explicit solution to the differential equation constructed here.

In Chapter 3 we present a cluster expansion (§3.1) for the dynamical generating function, similar to that performed by Baranger and Mozer (1959, 1960) for the static case. In such an expansion, many-body contributions are separated into more manageable one-body, two-body, ..., contributions. The generating function obtained in this way is given by that for the static case, which accounts for static correlations in the plasma, plus an infinite series of terms representing dynamical correlations. The corresponding expansion is given in terms of increasing powers of the so called plasma parameter,  $\Gamma$  (average potential energy/average kinetic energy), which determines the degree of coupling for the charges in the system: weak coupling implies  $\Gamma \ll 1$ , and strong coupling,  $\Gamma \geq 1$ . Hence, this method is limited to systems with a weak coupling. For very weak coupling between all the charges, high-order correlations become negligible, so that only the leading, static and dynamical, terms in the series survive. In this case, corresponding to an independent particle model and a very small charge at the field point<sup>\*</sup>, the problem is reduced to quadratures. The details are presented later on (Chapter 4).

Another interesting case in which the calculation can be reduced to quadratures is that for high fields (§3.2). A suitable scaling in the generating function allows to factorize negative powers of the electric field in the various terms of the cluster expansion. As a result, the high field limit can be associated with one or two ions close to the field point. The corresponding expressions can be evaluated numerically from the knowledge of the pair correlation function and the density-density time correlation function for the system.

To conclude this chapter (§3.3), a renormalized independent particle model is studied (Dufty and Zogaib, 1989), generalizing that developed by Dufty et al (1985) for the static case. In this method, only the leading

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\* A charged point couples the equations of motion for all the charges in the system, so that dynamical correlations are non-vanishing.

terms in the cluster expansion are retained, but the Coulomb electric field is replaced by an effective field accounting for the high-order correlations associated with the neglected terms. Such an effective field is chosen to give the exact second moment,  $\langle E^2 \rangle$ , or related condition for neutral points. The joint distribution function from this model is therefore reduced to quadratures, and it yields the exact electric field time correlation function  $\langle \vec{E} \cdot \vec{E}(t) \rangle$ . As a consequence of including high-order correlations in a renormalized field, rather than in a series expansion for the generating function, this method is suitable even for the general case of strongly coupled plasmas.

In chapter 4 we study the dynamical microfield distribution for a system of non-interacting ions and a neutral field point. In this approximation, high-order static and dynamical correlations vanish, and the generating function for the dynamical distribution is reduced to quadratures. The result, although given in terms of compact expressions, is numerically challenging since a multi-dimensional integral must be computed. A Legendre Polynomial expansion for the generating function is not helpful here. Instead, we consider some of the exact limits previously discussed for the general case of interacting ions and arbitrary charge on the impurity or field point. In particular, we study in detail the dynamical distribution at both short time and high field limits, which are susceptible of numerical evaluation in this approximation. The Gaussian limit discussed above is not valid in this case, since the second moment for a neutral point does not exist.

We first explore (§4.2) the short time behavior of the dynamical distribution for a system of non-interacting ions producing an electric field at a neutral point. In particular, we evaluate numerically the components of the anisotropic diffusion coefficient appearing in the short time result, assuming both a Coulomb and an effective Debye field for the ions; these components are monotonically increasing functions of the electric field. The dynamical distribution is evaluated then at different times and given values for the initial field  $\vec{e}_0$ . In all cases, the distribution presents an asymmetric broadening of the initial delta function and a monotonic shift of the peak towards smaller fields. The decay of the peak is monotonic for small  $\epsilon_0$ ; for large  $\epsilon_0$ , it raises again at longer times. For values of  $\epsilon_0$  with high probability to occur, the decay of the peak is not only monotonic but also slow; in contrast, for

less probable values the initial decay is very abrupt. These facts suggest distinguishing between two different processes, one for small  $\epsilon_0$  and another one for large  $\epsilon_0$ . Ultimately, at later times the peak reaches its equilibrium value and it continues towards the negative region, which reflects the limitation of this result to very short times only. A comparison of our results to some limited computer simulation data (Smith *et al.*, 1984) is shown in §4.3, in which only qualitative agreements are obtained. In all cases, the peak of our distribution is shifted to the left of that from the simulation data; the width is also broader. The discrepancies become more significant for field values below the peak, although the fitting improves when large values of the initial field are considered. We believe that those discrepancies are due to incorrect parameters reported for the simulation, since an excellent fit may be obtained if the time is scaled appropriately.

To conclude this chapter, we consider the single particle model (§4.4) as an approximation to describe high field dynamics, for a system of non-interacting ions and a neutral point. The single particle model to describe large fields is valid in general for the static case, in which only the contributions at a given time are important. For the dynamical case, however, this approximation is limited to times short enough for a close ion (producing a large field) not to move far away. The system considered in this section allows numerical evaluation of the corresponding results.

The serious numerical difficulties associated with the exact formalism in the general case (*i.e.* beyond the limits and approximations discussed here) justify looking for an alternative, simpler approach to the problem. A possibility is provided by the Theory of Stochastic Processes, in which the electric field is regarded as a stochastic variable whose fluctuations present statistical properties similar to those from some known stochastic processes. The objective of the second part of this work (Chapters 5 and 6) is, therefore, to consider approximate models for the dynamical distribution  $f(\vec{E}, t; \vec{E}_0, t_0)$ , in which the two aspects of electric fields (due to close and distant ions) discussed in previous chapters are assumed to satisfy independent Markov stochastic processes.

In chapter 5 we discuss the physical ideas behind such an stochastic approach and present some simple examples. In §5.1 we present some definitions and introduce a general Master Equation for the dynamical

distribution, as follows from the Markov assumption. The general Master Equation is an integro-differential equation whose kernel describes transition rates between two different field values. We distinguish two different kind of processes: one of large variations, referred to as a Strong Fluctuation process, in which the value of the field after a transition is practically independent of the initial value; another one of small variations, referred to as a Diffusion process, in which the transitions take place only at small steps. Strong Fluctuation models are discussed in §5.2. There, the so called Kangaroo Process is particularly interesting since it was originally proposed by Brissaud and Frisch (1971, 1974) as a first attempt to describe spectral line shapes from the knowledge of only the electric field at the radiating atom, which they called the Model Microfield Method. The dynamical distribution in the Kangaroo Process, the same as in all the other models in this section, is given by the sum of two contributions: a symmetric distribution about  $\vec{E} = 0$  that increases with time from zero to the equilibrium value, and a contribution from the original  $\delta$ -distribution about  $\vec{E} = \vec{E}_0$  that is simple attenuated in time. Such an unphysical behavior is characteristic of processes with *no memory* and it contrasts to the exact short time result. Diffusion Models, on the other hand, are presented in §5.3. The dynamical distributions here satisfy a Fokker-Planck-like equation, which presents both a diffusive and a drift term. That is, the original  $\delta$ -distribution at  $\vec{E} = \vec{E}_0$  broadens with time and shifts towards smaller fields, smoothly approaching the equilibrium value, in qualitative agreement to the expected behavior. This approaching, however, is very slow since processes with large fluctuations are disregarded here. Diffusion models are unable to describe transitions of states with very different field values, as those produced by a few close ions passing the field point. Neither the Strong Fluctuation models nor the Diffusion models provide a complete description of electric field dynamics in the plasma; nevertheless, their relative mathematical simplicity motivates consideration of alternative stochastic models in which a more complete description can be obtained.

The spirit of chapter 6 is precisely to propose reasonable alternatives towards the construction of more realistic stochastic models. Two different approaches are considered here, as an attempt to include the effect of both a fast and a slow dynamics associated with close and distant ions, respectively. In the so called Composite model of §6.2, we assume a

Master Equation for the dynamical distribution and focus attention on the strength of electric field fluctuations. We distinguish two kind of processes, one of strong and one of weak fluctuations, which we assume to be mutually exclusive. Consequently, the time evolution for the dynamical distribution is governed by the sum of two operators: one that is characteristic of processes with arbitrary size of electric field jumps, which is chosen to be that from a Kangaroo process; another one that is characteristic of processes with small electric field changes, which is chosen to be a Fokker-Planck operator. The corresponding dynamical distribution satisfies an integro-differential equation, with phenomenological coefficients associated with the two processes consider  $\downarrow$ . The results here constitute an improvement over those from simple Kangaroo or Fokker-Planck models: they describe processes with *memory*, so that there no longer remains at  $t > 0$  an unphysical contribution from the initial  $\delta$ -distribution; also, the associated dynamical evolution is faster here than in a Fokker-Planck process. These results are quite promising, indeed. The utility of this model, however, is limited to those cases in which the integro-differential equation can be solved with a relative simplicity.

In the Convolution model of §6.3, we focus attention on the strength of the electric field itself, instead of in its fluctuations. We regard the electric field at a given position as the sum of two different contributions: one due to close ions, and another one due to distant ions. These two components of the field are assumed to be statistically independent for all times, so that their corresponding dynamical evolution is governed by independent evolution operators. Consequently, the distribution of fields at two different times is obtained from the convolution of the dynamical distributions associated with each of the two independent processes. The problem reduces here to propose suitable models for such distributions and evaluate a six-dimensional integration. We believe that a tenable choice is given by the distributions from the Kangaroo and Diffusion models; unfortunately, limitations of time have not allowed us to explore this possibility into detail. The utility of this model is limited to those cases in which the associated integration can be performed numerically.

The two stochastic models in this chapter represent a reasonable generalization to those in chapter 5, in the sense that they combine the

relevant aspects described partially by the existing models. Both the Composite and Convolution models provide a semi-phenomenological description of electric fields, where the corresponding coefficients have to be specified from exact properties (electric field autocorrelation, ...) in the plasma. The relative numerical simplicity associated with such an approach is expected to allow more detailed studies in those cases where the exact formulation can not be reduced to quadratures. Further studies will also decide one of these models in favor of the other one.

Finally, we present in chapter 7 an overview of the relevant aspects of electric field dynamics that we have learned throughout this research. From this perspective, we formulate some general conclusions and comment on undergoing studies suggested by our results.

## CHAPTER 2

### GENERAL FORMULATION

#### 2.1. Introduction

We consider a system of particles with overall charge neutrality and identify a specific particle with total charge, center of mass position and momentum  $(Q_0, \vec{R}_0, \vec{P}_0)$ , referred to as the radiator. The system is in equilibrium. In the general case, the radiator may be an atomic impurity or charge distribution, interacting with each of the remaining charges, or perturbers, through Coulomb potentials. In that case, transport properties of the radiator are determined from the net instantaneous electric force exerted on it by the plasma; similarly, radiative properties are modified by the interactions of its internal degrees of freedom with the field due to the perturbers (Stark effect). A detailed microscopic analysis of such highly correlated systems is difficult, and it is often useful to formulate atomic properties in terms of a very few dominant properties of the plasma. We assume that the relevant effect of the perturbers on the radiator is appropriately represented by the total electric field  $\vec{E}(t)$  at its center of mass. This assumption is equivalent to considering only the leading terms, monopole and dipole, in a multipole expansion for the interaction potential. Accordingly, we focus our attention here on the statistical properties of the electric field at the radiator due to the perturbers in the plasma.

We distinguish here two kind of properties, static and dynamical, for the electric field. Static properties of the field are relevant at time scales short enough for the charge configuration in the plasma not to change considerably. An adequate choice for this latter may be an inverse plasma frequency, or alternatively, it can be chosen to be the time necessary for a particle to travel a mean free path. At these time scales, the processes under consideration may be appropriately described in terms of the net instantaneous electric field generated at the position of



interest. In this case, the distribution of electric field values at a given time, or static microfield distribution, provides a complete description for the instantaneous electric field. On the other hand, dynamical properties of the field play a relevant role when longer times are considered. Variations in the electric field generated by a changing charge configuration in the system produce, for instance, variations in the dipole moment of an impurity atom, which modify its corresponding radiation profile. The dynamical distribution of fields at two different times, or joint probability density, provides a description of electric field variations in the plasma. Consequently, both static and dynamical distributions represent the most relevant information concerning the electric fields generated in the plasma. Although we are primarily interested here in dynamical properties, we first include a brief discussion about the most relevant characteristics of the static microfield distribution.

The distribution of field values in equilibrium is defined by

$$Q(\vec{\epsilon}) = \langle \delta(\vec{\epsilon} - \vec{E}) \rangle, \quad (1)$$

where the brackets denote an equilibrium canonical average. The microfield distribution (1) represents the probability density to find a field value  $\vec{E} = \vec{\epsilon}$  for the total electric field at the radiator. As a consequence of considering states of equilibrium, the distribution  $Q(\vec{\epsilon})$  is time independent. Also rotational invariance implies  $Q(\vec{\epsilon}) = Q(\epsilon)$ . Consequently, it is useful to introduce the probability density for the magnitude of the field,

$$P(\epsilon) = 4\pi\epsilon^2 Q(\epsilon). \quad (2)$$

The functions  $Q(\vec{\epsilon})$  and  $P(\epsilon)$  satisfy the normalization conditions

$$\int d\vec{\epsilon} Q(\epsilon) = \int_0^{\infty} d\epsilon P(\epsilon) = 1. \quad (3)$$

A typical graph for the distribution  $P(\epsilon)$  is shown in Fig.1, obtained from molecular dynamics simulations.

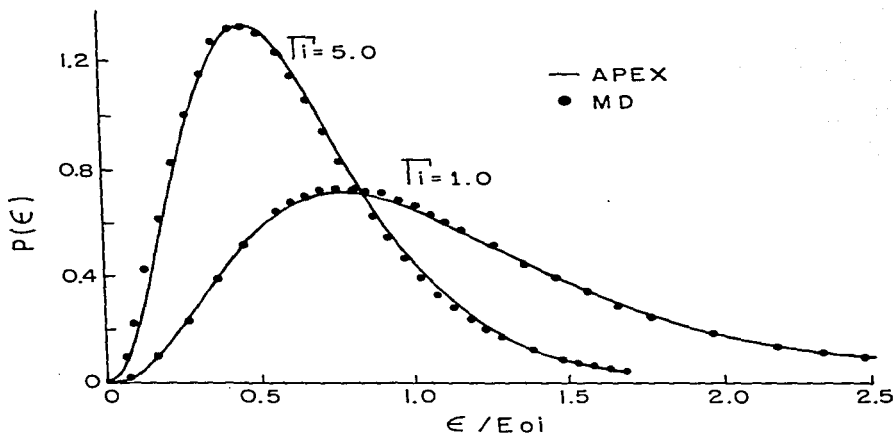


Fig. 1. Microfield distribution from molecular dynamics (MD) and the APEX model (defined later on) for two different values of the plasma parameter,  $\Gamma_i = 1$  and 5. A dimensionless field,  $\epsilon/E_{0i}$ , has been introduced here, with  $E_{0i}$  defined in page 16. (Adapted from the paper by Iglesias et al, 1983).

Some remarks are important here. The average (1) over all possible configurations in phase space spreads the microscopic  $\delta$ -distribution over a continuous range of values for  $\vec{\epsilon}$ , getting its maximum value at  $\vec{\epsilon} = 0$  and monotonically decaying to zero as the field increases. Compared to a Gaussian distribution, this decay is much slower due to the singular behavior of electric interactions, which diverge at short distances. In other words, the slow decay of the microfield distribution is associated with fields produced by close configurations. For the particular case of a neutral point, the second moment  $\langle E^2 \rangle$  of the distribution is divergent; close configurations can be excluded only when there is a charged point rejecting the perturbers. The former property limits the application of some standard techniques discussed in subsequent sections. Ultimately, the distribution of the magnitudes,  $P(\epsilon)$ , is expected to reach its maximum at a mean field value  $\epsilon_m = q/r_o^2$ , where  $q$  is the charge and  $r_o$  is a mean distance determined from the density  $n$  ( $4\pi r_o^3/3 = n^{-1}$ ), which accounts for the degree of coupling of the particles in the system.

The knowledge of the microfield distribution  $Q(\epsilon)$  provides a complete description of the static properties of the electric field in the plasma. In particular, for any arbitrary function  $A(\vec{E})$  of the field we have

$$\langle A(\vec{E}) \rangle = \int d\vec{\epsilon} A(\vec{\epsilon}) \langle \delta(\vec{\epsilon} - \vec{E}) \rangle = \int d\vec{\epsilon} A(\vec{\epsilon}) Q(\epsilon). \quad (4)$$

This fact has motivated extensive studies of this distribution, available in the current literature (Dufty, 1987; Hooper, 1987). The standard way to express such a distribution in terms of non-singular functions is provided by the Fourier representation of the  $\delta$ -function. Thus, Eq.(1) may be written as

$$Q(\vec{\epsilon}) = \int \frac{d\vec{\lambda}}{(2\pi)^3} e^{-i\vec{\lambda} \cdot \vec{\epsilon}} e^{I(\lambda)}, \quad (5)$$

with  $I(\lambda)$  the static generating function defined by

$$I(\lambda) \equiv \ln \langle e^{i\vec{\lambda} \cdot \vec{E}} \rangle. \quad (6)$$

For further evaluation of the average in (6), specification of the plasma is necessary. The simplest realistic case consists of a

two-component plasma of  $N_1$  ions and  $N_e$  electrons in equilibrium with an atomic impurity or radiator. Internal degrees of freedom for this latter can be suppressed if one is interested in the electric field rather than atomic processes. All the charges interact through Coulomb potentials. The corresponding Hamiltonian for this system is

$$H = \sum_{\alpha=0}^N \frac{p_{\alpha}^2}{2m_{\alpha}} + \sum_{\alpha} \sum_{\beta=0}^N \frac{Z_{\alpha} Z_{\beta} e^2}{|\vec{q}_{\alpha} - \vec{q}_{\beta}|} \quad (7)$$

with  $(\vec{q}_{\alpha}, \vec{p}_{\alpha})$  the phase coordinates of the  $\alpha$ th-particle,  $(\vec{q}_0, \vec{p}_0) \equiv (\vec{R}_0, \vec{P}_0)$  standing for the radiator,  $N = N_e + N_1$  the total number of perturbers, and

$$m_{\alpha}, Z_{\alpha} e = \begin{cases} m_0, Z_0 e = Q_0 & \alpha = 0 \\ m_1, Z_1 e & 1 \leq \alpha \leq N_1 \\ m_e, -e & N_1 + 1 \leq \alpha \leq N \end{cases} \quad (8)$$

are the mass and charge on the radiator, ions and electrons, respectively. In addition, overall charge neutrality implies

$$N_e = Z_0 + Z_1 N_1 \quad (9)$$

Ultimately, the net electric field  $\vec{E}$  at the radiator is given by

$$\vec{E} = \sum_{\alpha=1}^N (Z_{\alpha} e) \hat{x}_{\alpha} / x_{\alpha}^2 \quad (10)$$

with  $\vec{x}_{\alpha}$  the relative position  $\vec{x}_{\alpha} = \vec{q}_{\alpha} - \vec{R}_0$ . The generalization for the case of a multi-component plasma is straightforward.

An alternative simpler model is also considered, in which the role of the electrons is replaced by that of a uniform neutralizing background. This seems to be reasonable if one takes into account the following. Because of the relatively large mass ratio  $m_1/m_e$ , the thermal speed of the electrons is larger than that of the ions ( $v_e \approx 40v_1$ ); for the time scale associated with ion dynamics, the fast electrons may be regarded as uniform static clouds of negative charge surrounding the slow positive charges. Consequently, the electrons act as a shield, lowering the range and intensity of electric interactions between all the other particles.

Coulomb fields and potentials for the ions are replaced, therefore, by effective screened interactions. This model, known as a one-component plasma (OCP), is the one we consider throughout this work. The corresponding Hamiltonian is given by

$$H = \frac{p_0^2}{2m_0} + \sum_{\alpha=1}^{N_1} \frac{p_\alpha^2}{2m_\alpha} + \sum_{\alpha=1}^{N_1} u_{\alpha 0} + \sum_{\alpha > \beta = 1}^{N_1} \sum_{\alpha > \beta = 1}^{N_1} u_{\alpha\beta} + \sum_{\alpha=0}^{N_1} V_\alpha + V_B, \quad (11)$$

where the various potential energy terms represent ion-radiator ( $u_{\alpha 0}$ ), ion-ion ( $u_{\alpha\beta}$ ), background-radiator and ions ( $V_\alpha$ ) and background-background ( $V_B$ ) effective screened interactions. Associated with this Hamiltonian, the total electric field at the radiator due to the OCP is given by

$$\vec{E} = \sum_{\alpha=1}^{N_1} \vec{E}(\vec{x}_\alpha) + \vec{E}_B, \quad (12)$$

where  $\vec{E}_B$  is the contribution from the background, and  $\vec{E}(\vec{x}_\alpha)$  is the Debye field

$$\vec{E}(\vec{x}_\alpha) = (Z_\alpha e) f(x_\alpha) \hat{x}_\alpha / x_\alpha^2, \quad f(x_\alpha) = (1 + a_D x_\alpha) e^{-a_D x_\alpha}. \quad (13)$$

The parameter  $a_D^{-1}$  characterizes the effective range of the electric interactions between the particles. It will be useful to consider  $a_D \rightarrow 0$  sometimes, to incorporate the long-ranged nature of Coulomb interactions in the OCP.

Diverse characteristic parameters can be defined for the OCP, in terms of state variables and ionic charge. Among the most relevant we have: the ion plasma frequency,  $\omega_{p1} = (4\pi n_1 (Z_1 e)^2 / m_1)^{1/2}$ , with  $n_1$  the ion density; the ion sphere radius, or mean distance for the ions,  $r_{01}$ , defined from the condition  $4\pi r_{01}^3 / 3 = n_1^{-1}$ ; the field strength,  $E_{01} = Z_1 e / r_{01}^2$ , representing a mean field generated by ions at a distance  $r_{01}$ ; the coupling constant or plasma parameter,  $\Gamma_1$ , defined as the ratio mean potential energy/mean kinetic energy,  $\Gamma_1 = (Z_1 e)^2 / r_{01} k_B T$ , with  $T$  the temperature of the system. In terms of the plasma parameter, weak coupling for the ions means  $\Gamma_1 \ll 1$ , whereas strong coupling implies  $\Gamma_1 \approx 1$ . The first case is equivalent to a

system of weakly-interacting ions, since the plasma parameter can be thought of a factor multiplying the dimensionless potential energy. For strongly coupled plasmas, the screening effects due to the electrons become quite considerable. In particular, the range of electric interactions between the remaining charges is expected to become shorter as the plasma parameter increases. As a consequence, the microfield distribution  $P(\epsilon)$  tends to shift toward values closer to zero (see Fig.1), becoming a  $\delta$ -function around  $\epsilon = 0$  in an extreme case. A similar situation occurs for highly charged radiators, which tend to reject nearby perturbers, favoring configurations associated with very weak fields only.

All of the former constitutes an exact formalism to study the static properties of the electric field in the plasma. As mentioned before, diverse approximations and limits for the microfield distribution or its generating function have been widely studied in the literature, under a variety of conditions for the diverse parameters in the system. In this sense, we regard this matter as known and focus our attention on the dynamical properties of the microfield, instead.

As the charge configuration changes in the plasma, the fields produced by those charges at a given position also change in time. Dipole interactions, for instance, modify the orientation and shape of the charge distribution in an atomic impurity; its radiative properties are, therefore, affected by those changes in configuration. Hence, a complete description of the electric field has to include the dynamical aspect, as well, to give an answer to questions such as how probable it is for a given field to change into another given value at a different time. In contrast to the static case, very limited studies have been done in this respect. Those studies are basically in the context of spectral line shapes. An example is provided by the so called "Kangaroo Process" introduced by Brissaud and Frisch (1971, 1974), which is based on the Theory of Stochastic Processes; in addition, there exist some limited computer simulation data of the dynamical distribution for the particular case of non-interacting particles (Smith et al, 1984).

In the following, we present an exact general formalism to study the dynamics of the electric field in a plasma in equilibrium. We also study some limits and approximations, which characterize diverse aspects of the time evolution in the dynamics of this variable.

## 2.2. Definitions and exact properties

As an extension of the definition for the static microfield distribution, dynamical properties of the fields can be determined from the joint distribution function

$$f(\vec{E}, t; \vec{E}_0, t_0) = \langle \delta(\vec{E} - \vec{E}(t)) \delta(\vec{E}_0 - \vec{E}(t_0)) \rangle. \quad (1)$$

Eq.(1) gives the probability density to find an electric field  $\vec{E}(t) = \vec{E}$  at time  $t$  and a value  $\vec{E}(t_0) = \vec{E}_0$  at time  $t_0$ . Equivalently, we introduce here the conditional probability density

$$P(\vec{E}, t | \vec{E}_0, t_0) = f(\vec{E}, t; \vec{E}_0, t_0) / Q(\vec{E}_0), \quad (2)$$

which gives the probability to find a value  $\vec{E}$  for the field at time  $t$  given that there was a value  $\vec{E}_0$  at  $t_0$ . Based on stationarity, in all the following we set  $t_0 = 0$ , without loss of generality. We also define  $\vec{E}(0) \equiv \vec{E}$ .

In analogy to the static case, the knowledge of the distribution function (1) provides a description of the microfield dynamics in a plasma. In particular, for any arbitrary functions A, B, of the electric field we have

$$\begin{aligned} \langle A(\vec{E}(t)) B(\vec{E}) \rangle &= \int d\vec{E} \int d\vec{E}_0 A(\vec{E}) B(\vec{E}_0) \langle \delta(\vec{E} - \vec{E}(t)) \delta(\vec{E}_0 - \vec{E}) \rangle \\ &= \int d\vec{E} \int d\vec{E}_0 A(\vec{E}) B(\vec{E}_0) f(\vec{E}, t; \vec{E}_0, 0). \end{aligned} \quad (3)$$

Equivalently, from the knowledge of the conditional probability density (2) it is possible to calculate the conditional average

$$\langle A(\vec{E}(t)) \rangle_{\vec{E}_0} = \int d\vec{E} A(\vec{E}) P(\vec{E}, t | \vec{E}_0, 0), \quad (4)$$

which represents an average restricted to those configurations with initial field  $\vec{E} = \vec{E}_0$ ; that is, for an arbitrary function  $A(\vec{E}(t))$  of the field,

$$\langle A(\vec{E}(t)) \rangle_{\epsilon_0} = \frac{\langle A(\vec{E}(t)) \delta(\vec{\epsilon}_0 - \vec{E}) \rangle}{Q(\epsilon_0)}. \quad (5)$$

The results (3) and (4) are related by

$$\langle A(\vec{E}(t)) B(\vec{E}) \rangle = \int d\vec{\epsilon}_0 Q(\epsilon_0) \langle A(\vec{E}(t)) \rangle_{\epsilon_0} B(\epsilon_0). \quad (6)$$

As an application of the conditional average  $\langle \rangle_{\epsilon}$  above, an interesting case is that with  $A(\vec{E}(t)) = \vec{E}(t)$ . In particular, for a system of non-interacting ions (neutral point) the average  $\langle \vec{E}(t) \rangle_{\epsilon}$  calculated from Eq. (5) becomes

$$\langle \vec{E}(t) \rangle_{\epsilon} = n \int d\vec{r} \vec{F}(\vec{r}, t) \frac{Q(\vec{\epsilon} - \vec{E}(\vec{r}))}{Q(\epsilon)}, \quad (7)$$

with  $Q$  the static microfield distribution and  $\vec{F}(\vec{r}, t)$  the average

$$\vec{F}(\vec{r}, t) = \langle \vec{E}(\vec{r} + \vec{v}t) \rangle_{\nu}, \quad (8)$$

which satisfies  $\vec{F}(\vec{r}, 0) = \vec{E}(\vec{r})$  and  $\vec{F}(\vec{r}, \infty) = 0$ . This latter function can be easily expressed in terms of quadratures

$$\vec{F}(\vec{r}, t) = -4\pi\hat{r} \frac{e^{-(r/ut)^2}}{\pi^{3/2} (ut)^2} \int_0^{\infty} dy y^2 f(uty) e^{-y^2} j_1(2ry/ut), \quad (9)$$

with  $u = (2k_B T/m_i)^{1/2}$  the thermal speed,  $j_1$  the spherical Bessel function of order 1 (Arfken, 1985) and  $f$  the screening factor in the Debye field (1.13). The conditional average  $\langle \vec{E}(t) \rangle_{\epsilon}$  obtained in this way is, therefore, given in terms of the static distribution  $Q$  and a simple quadrature.

This interesting result constitutes one of the limited cases in which a dynamical property of electric fields in the plasma can be computed from the knowledge of only the static distribution. In the general case, knowledge of the dynamical distribution is also required to determine dynamical properties in the system, according to Eqs. (3) and (4).

Similarly to the representation (1.5) for the microfield distribution, the joint probability density may be written as



$$f(\vec{c}, t; \vec{c}_0, 0) = \int \frac{d\vec{\lambda}}{(2\pi)^3} \frac{d\vec{\lambda}'}{(2\pi)^3} e^{-i\vec{\lambda} \cdot \vec{c}} e^{-i\vec{\lambda}' \cdot \vec{c}_0} G(\vec{\lambda}, \vec{\lambda}'; t) \quad (10)$$

where  $G(\vec{\lambda}, \vec{\lambda}'; t)$  is the corresponding dynamical generating function,

$$G(\vec{\lambda}, \vec{\lambda}'; t) = \ln \langle e^{i\vec{\lambda} \cdot \vec{c}(t)} e^{i\vec{\lambda}' \cdot \vec{c}_0} \rangle \quad (11)$$

In particular, note that the generating function (11) reduces to the static generating function (1.6) when one of the variables  $\lambda$  or  $\lambda'$  vanishes.

Several additional properties of the joint probability density follow from its definition and the symmetries of the equilibrium state, namely,

i) Normalization conditions

$$\int d\vec{c} f(\vec{c}, t; \vec{c}_0, 0) = Q(c_0) \quad ; \quad \int d\vec{c}_0 f(\vec{c}, t; \vec{c}_0, 0) = Q(c) \quad (12)$$

ii) Initial conditions

$$f(\vec{c}, 0; \vec{c}_0, 0) = Q(c_0) \delta(\vec{c} - \vec{c}_0) \quad ; \quad G(\vec{\lambda}, \vec{\lambda}'; 0) = I(|\vec{\lambda} + \vec{\lambda}'|) \quad (13)$$

iii) Mixing

$$f(\vec{c}, \infty; \vec{c}_0, 0) = Q(c)Q(c_0) \quad ; \quad G(\vec{\lambda}, \vec{\lambda}'; \infty) = I(\lambda) + I(\lambda') \quad (14)$$

iv) Time reversal invariance

$$f(\vec{c}, t; \vec{c}_0, 0) = f(\vec{c}, -t; \vec{c}_0, 0) \quad ; \quad G(\vec{\lambda}, \vec{\lambda}'; t) = G(\vec{\lambda}, \vec{\lambda}'; -t) \quad (15)$$

v) Time translational invariance

$$f(\vec{c}, t; \vec{c}_0, 0) = f(\vec{c}_0, t; \vec{c}, 0) \quad ; \quad G(\vec{\lambda}, \vec{\lambda}'; t) = G(\vec{\lambda}', \vec{\lambda}; t) \quad (16)$$

vi) Rotational invariance

$$f(\vec{c}, t; \vec{c}_0, 0) = f(c, c_0, \hat{e} \cdot \vec{c}_0; t); \quad G(\vec{\lambda}, \vec{\lambda}'; t) = G(\lambda, \lambda', \hat{\lambda} \cdot \hat{\lambda}'; t) \quad (17)$$

Conditions (13) and (14) show that for short and long times  $G(\vec{\lambda}, \vec{\lambda}'; t)$  is simply related to the corresponding (known) generating function for the static distribution,  $I$ . This fact suggests writing  $G(\vec{\lambda}, \vec{\lambda}'; t)$  as

$$G(\vec{\lambda}, \vec{\lambda}'; t) = I(\lambda) + I(\lambda') + H_{\infty}(\vec{\lambda}, \vec{\lambda}'; t), \quad (18)$$

with  $H_{\infty}(\vec{\lambda}, \vec{\lambda}'; t)$  defined by

$$H_{\infty}(\vec{\lambda}, \vec{\lambda}'; t) \equiv \ln \left\{ \frac{\langle e^{i\vec{\lambda} \cdot \vec{E}(t)} e^{i\vec{\lambda}' \cdot \vec{E}} \rangle}{\langle e^{i\vec{\lambda} \cdot \vec{E}} \rangle \langle e^{i\vec{\lambda}' \cdot \vec{E}} \rangle} \right\}. \quad (19)$$

According to this,  $H_{\infty}(\vec{\lambda}, \vec{\lambda}'; \infty) = 0$ , so that (14) is automatically satisfied as  $t \rightarrow \infty$ . An alternative representation for  $G(\vec{\lambda}, \vec{\lambda}'; t)$ , more convenient when considering short times, is

$$G(\vec{\lambda}, \vec{\lambda}'; t) = I(|\vec{\lambda} + \vec{\lambda}'|) + H_0(\vec{\lambda}, \vec{\lambda}'; t), \quad (20)$$

with

$$H_0(\vec{\lambda}, \vec{\lambda}'; t) = H_{\infty}(\vec{\lambda}, \vec{\lambda}'; t) - H_{\infty}(\vec{\lambda}, \vec{\lambda}'; 0). \quad (21)$$

Using this latter representation for  $G(\vec{\lambda}, \vec{\lambda}'; t)$ , the initial condition (13) can be obtained easily if the integrals in (10) are expressed in terms of new variables  $\vec{\ell} \equiv \vec{\lambda} + \vec{\lambda}'$  and  $\vec{\eta} \equiv (\vec{\lambda} - \vec{\lambda}')/2$ , that is,

$$f(\vec{e}, t; \vec{e}_0, 0) = \int \frac{d\vec{\eta}}{(2\pi)^3} \frac{d\vec{\ell}}{(2\pi)^3} e^{-i\vec{\eta} \cdot (\vec{e} - \vec{e}_0)} e^{-i\vec{\ell} \cdot (\vec{e} + \vec{e}_0)/2} G_e. \quad (22)$$

Here the variables  $\vec{\eta}, \vec{\ell}$  have been introduced to preserve the  $\vec{e} \leftrightarrow \vec{e}_0$  symmetry.

The former equivalent representations are exact. They are quite convenient when either long or short times are considered. Unfortunately, this is not the case at intermediate times, in which  $G(\vec{\lambda}, \vec{\lambda}'; t)$  varies from  $I(|\vec{\lambda} + \vec{\lambda}'|)$  to  $I(\lambda) + I(\lambda')$  as time evolves. Both expressions for the generating function, (18) and (19), fail to show such an evolution in a

clear, simple way. A more convenient alternative representation, suitable for all times, is given by

$$G(\vec{\lambda}, \vec{\lambda}'; t) = (1-\alpha) [I(\lambda) + I(\lambda')] + \alpha I(|\vec{\lambda} + \vec{\lambda}'|) \quad (23)$$

where  $\alpha = \alpha(\vec{\lambda}, \vec{\lambda}'; t)$  is a function that varies from 1 to 0 as  $t$  goes from 0 to  $\infty$ ,

$$\alpha(\vec{\lambda}, \vec{\lambda}'; t) = \frac{G(\vec{\lambda}, \vec{\lambda}'; t) - G(\vec{\lambda}, \vec{\lambda}'; \infty)}{G(\vec{\lambda}, \vec{\lambda}'; 0) - G(\vec{\lambda}, \vec{\lambda}'; \infty)} \quad (24)$$

The utility of this representation is, however, limited to having a simple dependence of  $\alpha(\vec{\lambda}, \vec{\lambda}'; t)$  on  $\vec{\lambda}$  and  $\vec{\lambda}'$ . Although this condition does not hold in general, it may be satisfied in some limiting cases; an example of this will be discussed in the following section (§2.3). The advantage of expressions such as (18), (20) and (23) is to provide a more manageable, simpler way to evaluate the dynamical generating function (11). In all cases,  $G(\vec{\lambda}, \vec{\lambda}'; t)$  is obtained from the well known static generating function,  $I(\lambda)$ , and a time dependent function where to introduce useful approximations preserving the exact properties (12)-(17).

Before getting involved in a numerical evaluation of the dynamical generating function (11), some formally exact limits can be extracted easily, namely, the Gaussian limit and the limit for short times, which are described as follows.

### 2.3. Gaussian limit

When there is a large charge on the field point, close ions are rejected and the main contributions are due to distant ions. Under these conditions, the electric field  $\vec{E}(t)$  takes only small values and the generating function (2.11) may be expanded in powers of  $\vec{\lambda}$  and  $\vec{\lambda}'$ . In that case, the leading contribution is quadratic in these variables,

$$G(\vec{\lambda}, \vec{\lambda}'; t) = -\frac{1}{2} [\lambda_1 \lambda_j + \lambda'_1 \lambda'_j] C_{1j}(0) - \lambda_1 \lambda'_j C_{1j}(t), \quad (1)$$

with

$$C_{ij}(t) \equiv \langle E_i(t) E_j \rangle. \quad (2)$$

For reasons of symmetry, this tensor is diagonal ( $C_{ij}(t) = C_{kk}(t) \delta_{ij}/3$ ).

Substitution of the generating function (1) in the form (2.10) for the joint probability yields the product of two Gaussian distributions,

$$f(\vec{z}, t; \vec{z}_0, 0) = (1 - \alpha^2(t))^{-3/2} Q_g \left\{ \frac{\vec{z} - \alpha(t) \vec{z}_0}{(1 - \alpha^2(t))^{1/2}} \right\} Q_g(\epsilon_0), \quad (3)$$

where  $\alpha(t) \equiv \alpha(\vec{0}, \vec{0}; t) = \langle E_i(t) E_i \rangle / \langle E^2 \rangle$  is the equilibrium electric field autocorrelation function, and  $Q_g(\epsilon)$  is the Gaussian limit of  $Q(\epsilon)$ ,

$$Q_g(\epsilon) = [3/2\pi \langle E^2 \rangle]^{3/2} \exp[-3\epsilon^2/2 \langle E^2 \rangle]. \quad (4)$$

It may be shown that this result satisfies the conditions (2.12)-(2.17). Note also that the limit (3) can be thought of as being the solution to a non-Markovian Fokker-Planck equation<sup>\*</sup>,

$$\frac{\partial}{\partial t} f(\vec{z}, t; \vec{z}_0, 0) = \frac{\partial}{\partial \epsilon_1} \gamma(t) \left[ \frac{\partial}{\partial \epsilon_1} + 3\epsilon_1 / \langle E^2 \rangle \right] f(\vec{z}, t; \vec{z}_0, 0), \quad (5)$$

where  $\gamma(t) = -\langle E^2 \rangle \dot{\alpha}(t) / 3\alpha(t)$ . We will return to this point in a subsequent chapter (§5.3).

This limit is only applicable for electric field distributions at charged points for which the second moment,  $\langle E^2 \rangle$ , exists. Furthermore, it requires that configurations corresponding to weak fields dominate to justify small  $\vec{\lambda} \cdot \vec{E}$ . This restricts the result to small  $\vec{z}$ ,  $\vec{z}_0$  and large charge on the particle at which the field is calculated. These criteria lead to some restrictions for the diverse parameters in terms of which  $\langle E^2 \rangle$  and  $\alpha(t)$  are expressed, which are detailed as follows.

<sup>\*</sup>This equation describes a Markov process only when  $\gamma$  is independent of time, or equivalently, when  $\alpha(t)$  is exponential (Chaturvedi, 1983).

Consider first the dimensionless screened field

$$\vec{E}(\vec{x}) = \{1 + (r_{01}/\lambda_D)x\} e^{-\{r_{01}/\lambda_D\}x} \vec{x}/x^2, \quad (6)$$

expressed in ion units, that is,  $\vec{x}/r_{01} \rightarrow \vec{x}$ ,  $\vec{E}(\vec{x})/E_{01} \rightarrow \vec{E}(\vec{x})$ . Here the screening length  $\lambda_D = (k_B T/4\pi n_0 e^2)^{1/2}$  is chosen to be the electron Debye length. For the sake of convenience, introduce now the definitions

$$A \equiv \Gamma_1/Z_1, \quad B \equiv Z_0 \Gamma_1/Z_1 \quad (7)$$

with  $\Gamma_1$  the ion plasma parameter. The condition for small fields implies  $x > x_0$ , with  $x_0(A)$  determined from

$$\frac{(1 + \sqrt{3A} x_0)}{x_0^2} e^{-\sqrt{3A} x_0} = 1. \quad (8)$$

On the other hand, the condition for distant configurations may be obtained by approximating the radial distribution function by  $g(x) = \exp\{-\beta u(x)\}$ , with  $u(x)$  the effective screened potential energy for the interaction ion-radiator and  $\beta = (k_B T)^{-1}$ . In terms of the former dimensionless variables we have

$$g(x) = \exp\left\{-\frac{B}{x} e^{-\sqrt{3A} x}\right\}, \quad (9)$$

Note that the parameter A accounts for screening effects due to electrons (regardless of the presence of the radiator), whereas B is simply related to the strength of naked interactions ion-radiator. We therefore regard A and B as independent parameters. From the radial distribution (9), the condition for distant ions implies  $x > x_1$ , with  $x_1(A,B)$  determined from

$$\frac{B}{x_1} \exp\{-\sqrt{3A} x_1\} = 1. \quad (10)$$

From the former analysis, we expect for the Gaussian limit to be valid when  $x > x_1 \approx x_0$ . In particular, we look for conditions on the parameters A and B such that  $x_1 > x_0$ , or configurations generating fields weaker than

a characteristic value  $E(x_0)$ . To that end, we take  $x_1 = nx_0$  ( $n = 1, 2, \dots$ ), so that the conditions (8) and (10) imply

$$B = n \frac{(1 + \sqrt{3A} x_0)}{x_0} e^{-\sqrt{3A} (1-n)x_0}. \quad (11)$$

The graphs corresponding to the condition (11), for several curves  $x_1 = nx_0$  ( $n = 1, 2, \dots$ ) are shown in Figure 2. It is clear from these graphs that for a given ratio  $\Gamma_1/Z_1$  the Gaussian limit is satisfied with more accuracy as  $n$  (and therefore  $Z_0\Gamma_1/Z_1$ ) becomes larger. For Coulomb fields,  $A = 0$ ,  $x_0 = 1$  and the condition (11) simply implies large  $Z_0\Gamma_1/Z_1$  values.

To study the Gaussian limit into some detail, we consider here the simplest case of Coulomb interactions. In particular, we focus attention on the conditional probability density that follows from the joint probability (3) and the Gaussian microfield distribution (4), namely,

$$P(\vec{E}, t | \vec{E}_0, 0) = \left( \frac{3}{2\pi \langle E^2 \rangle (1-\alpha(t)^2)} \right)^{3/2} \exp \left\{ - \frac{3(\vec{E} - \alpha(t)\vec{E}_0)^2}{2 \langle E^2 \rangle (1-\alpha(t)^2)} \right\}. \quad (12)$$

The exact second moment  $\langle E^2 \rangle$  for this case (see, for instance, Iglesias et.al., 1983a) is given by

$$\langle E^2 \rangle = 4\pi n_1 k_B T Z_1 / Z_0. \quad (13)$$

We introduce now dimensionless units (ion units), in terms of which

$$\langle E^2 \rangle = 3Z_1 / Z_0 \Gamma_1. \quad (14)$$

In addition, a simple model for the electric field autocorrelation function (Boercker et.al., 1987) is considered here. This model is based on kinetic calculations for the exact self-structure factor, in which the collision operator is chosen to be similar to that from the linearized Boltzmann equation (BGK model) with time independent frequency  $\nu$ . In this case, the corresponding electric field autocorrelation  $\alpha(t)$  is expressed in terms of two relaxation times,

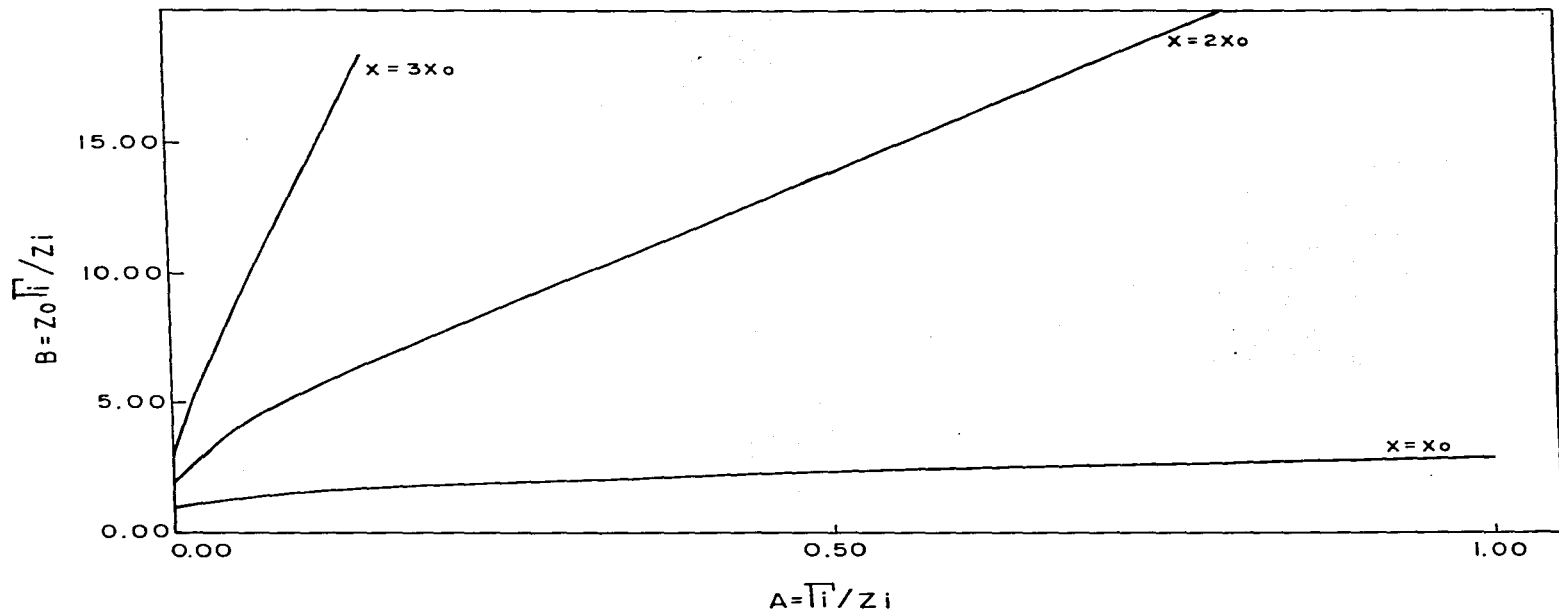


Fig.2. Graphs of the parameter  $B = Z_0 \Gamma_1 / Z_1$  vs.  $A = \Gamma_1 / Z_1$  (Eq.2.2.11), for  $x_1 = nx_0$  ( $n = 1,2,3$ ), to determine the validity of the Gaussian limit.

$$\alpha(t) = (w_+ e^{-w_+ t} - w_- e^{-w_- t}) / (w_+ - w_-), \quad (15)$$

where the characteristic frequencies  $w_+$  and  $w_-$  are given by

$$w_{\pm} = \frac{1}{2} \left( \nu \pm (\nu^2 - 4\gamma)^{1/2} \right) w_{p1}, \quad (16)$$

with  $w_{p1}$  the ion plasma frequency and  $\gamma = Z_0 m_i / 3Z_1 m_0$ . Here,

$$\nu = \frac{D}{3} (Z_0 \Gamma_1 / Z_1)^2 \langle E^2 \rangle, \quad (17)$$

with  $\langle E^2 \rangle$  from (14) and  $D$  the self diffusion constant in units of  $r_{01}^2 w_{p1}$ . For sufficiently large values for the plasma parameter ( $\Gamma_1 \geq 1$ ), and  $Z_1 = Z_0 = 1$ , the diffusion constant may be approximated (Hansen et.al., 1975) by

$$D \approx 2.95 \Gamma_1^{-4/3}. \quad (18)$$

Note then that for large values of  $\Gamma_1$  the characteristic frequencies in (16) become imaginary, in such a way that the autocorrelation function (15) at these values is oscillatory.

The electric field autocorrelation  $\alpha(t)$  from (15) is plotted in Fig.3 for the case  $Z_1 = Z_0 = 1$ ,  $m_1 = m_0$  at two different values  $\Gamma_1 = 10$  and 100. As shown in these graphs, the function  $\alpha(t)$  starts in 1 at  $t = 0$  and decays to zero after sufficiently long times ( $t \approx 15w_{p1}^{-1}$ ). This process is not monotonic, though. Indeed, at a time of the order  $w_{p1}^{-1}$  the function  $\alpha(t)$  reaches its equilibrium value ( $\alpha(\infty) = 0$ ), but it continues towards negative regions. This first crossing determines a shorter time scale in the process. After this characteristic time, the autocorrelation function reaches its minimum and tends to zero monotonically in the case with  $\Gamma_1 = 10$ . In contrast, this function presents a few more oscillations at  $\Gamma_1 = 100$ . The change of sign for the function  $\alpha(t)$  is necessary for a charged point\*, since in this case the momentum is related to the electric field ( $d\vec{p}/dt = Q_0 \vec{E}$ ) in such a way that the area under the function  $\langle \vec{E} \cdot d\vec{p}(t)/dt \rangle$  vanishes (Pollock and Weisheit, 1985). Additional graphs for the result (15) are presented in Fig.4, where it is shown a comparison with molecular

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\* For a neutral point  $\alpha(t) > 0$ .



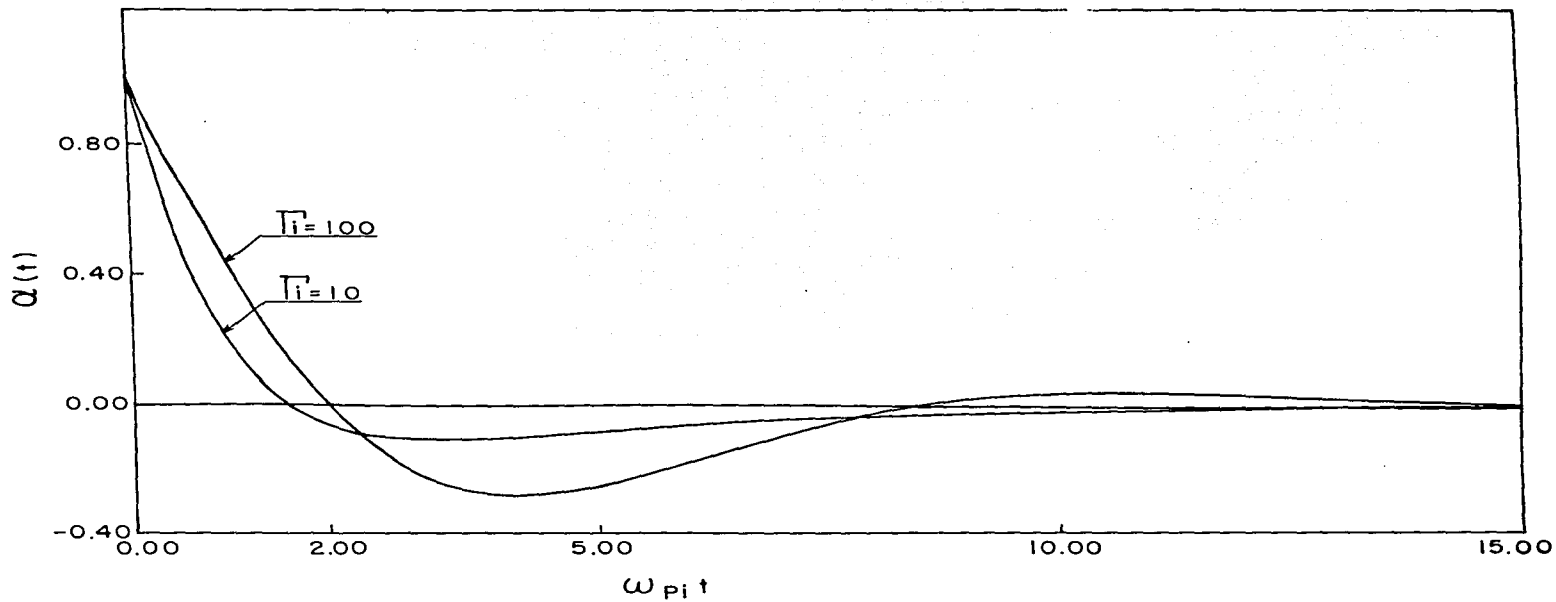


Fig.3. Electric field autocorrelation function from Eq.(2.3.15) for two different values of the plasma coupling parameter,  $\Gamma_i = 10$  and 100. Here,  $Z_0 = Z_i = 1$  and  $m_i = m_0$ .

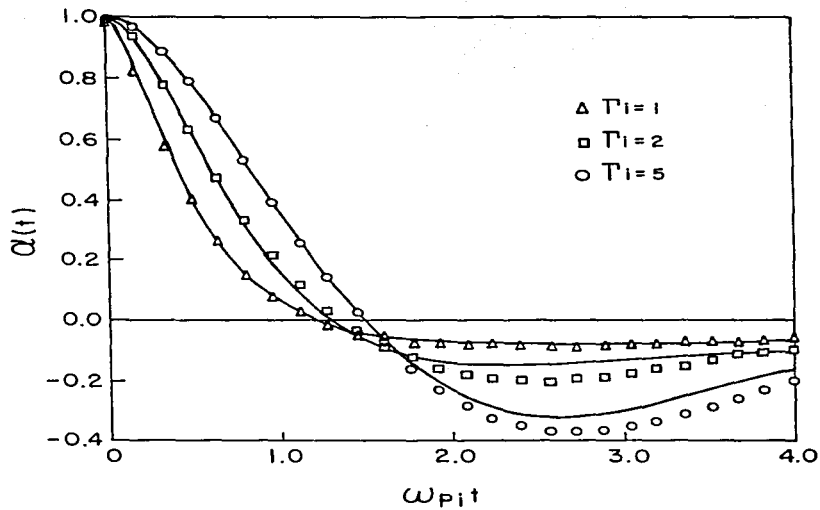


Fig. 4. Electric field autocorrelation function from Eq. (2.3.15) (—) and molecular dynamics ( $\Delta, \square, \circ$ ), for  $\Gamma_1 = 1, 2, 5$  and  $Z_0 = Z_1$ . (Adapted from the paper by Boercker *et al.*, 1987).

dynamics computer simulation at some  $\Gamma_1$  values. The agreement is quite good over the entire frequency range, suggesting that the model is reasonable to our purposes.

More generally, alternative models for the electric field autocorrelation function may be obtained from the knowledge of functions such as the charge density autocorrelation, or its Fourier transform  $S(\vec{k}, \vec{k}', t)$ . In terms of this latter, we have

$$\langle E_1(t) E_1 \rangle = \int \frac{d\vec{k}}{(2\pi)^3} \frac{d\vec{k}'}{(2\pi)^3} \vec{f}^*(\vec{k}) \cdot \vec{f}(\vec{k}') S(\vec{k}, \vec{k}', t), \quad (19)$$

where  $\vec{f}(\vec{k})$  is the form factor representing the Fourier transform of the single particle field amplitude,

$$\vec{f}(\vec{k}) = (Z_1 e)^{-1} \int d\vec{r} e^{i\vec{k} \cdot \vec{r}} \vec{E}(\vec{r}); \quad (20)$$

In particular, the form factor for the Debye field (1.13) is given by

$$\vec{f}(\vec{k}) = 4\pi i \vec{k} / (k^2 + a_D^2). \quad (21)$$

Thus, the electric field autocorrelation (19) can be calculated if good approximations to  $S(\vec{k}, \vec{k}', t)$  are known\*.

For evaluation of the conditional probability (12), we consider here the two relaxation time model defined in (15). We chose the values  $\Gamma_1 = 10$  and  $Z_1 = Z_0 = 1$ ; we also take  $m_1 = m_0$ . The corresponding microfield distribution  $P_g(\epsilon) = 4\pi \epsilon^2 Q_g(\epsilon)$  is plotted in Fig.5. As shown in this graph, the most probable value for the magnitude of the field in this case occurs at  $\epsilon \approx 0.5$ . Based on this, we have chosen for the initial field the value  $\epsilon_0 = 1$ .

To study the dynamical aspects of the conditional probability in this limit, we consider first that component of the field parallel to the initial value  $\vec{\epsilon}_0$ , that is, we set  $\theta = 0$  in (12). The corresponding graphs at several times are shown in Fig.6. As expected, the initial  $\delta$ -distribution about  $\epsilon = 1$  broadens and the peak position shifts towards

\* To our knowledge, such approximations for the general case of strongly coupled plasmas are limited to neutral points only (Ichimaru, 1982).

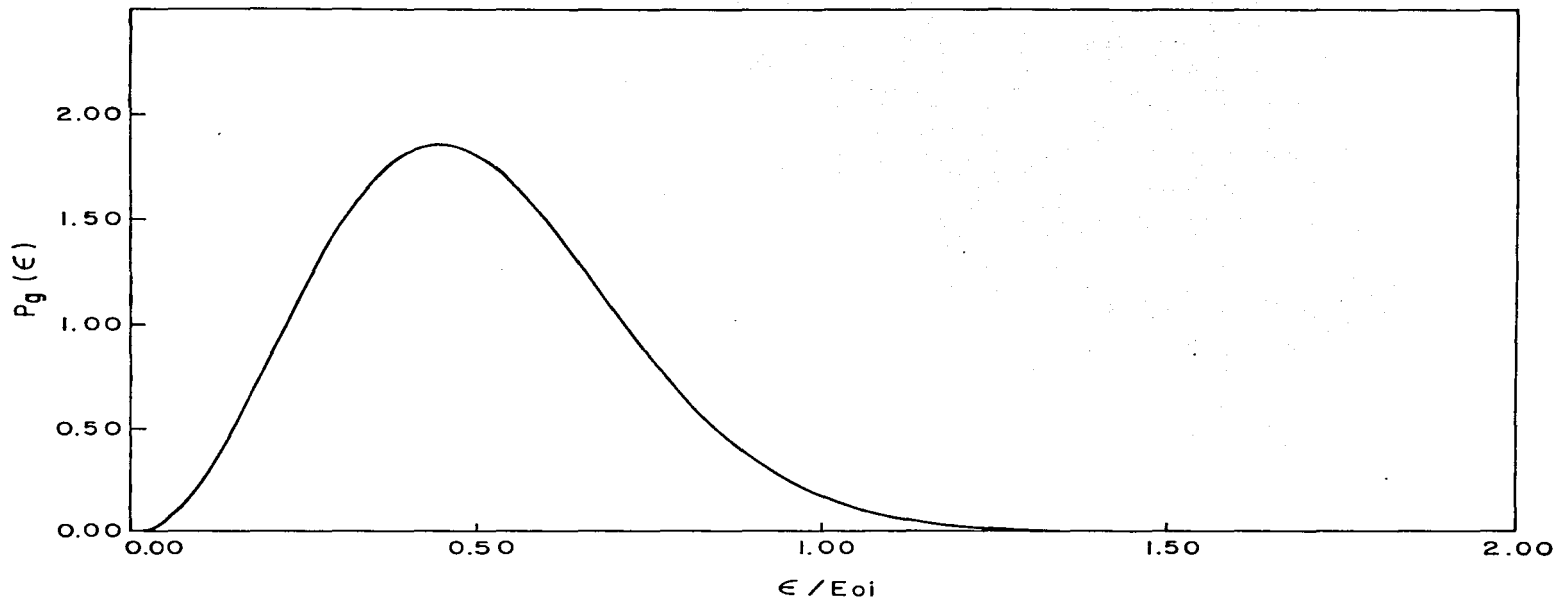


Fig.5. Microfield distribution associated with the Gaussian distribution (2.3.4), for a plasma parameter  $\Gamma_1 = 10$  ( $Z_0 = Z_1 = 1$ ).

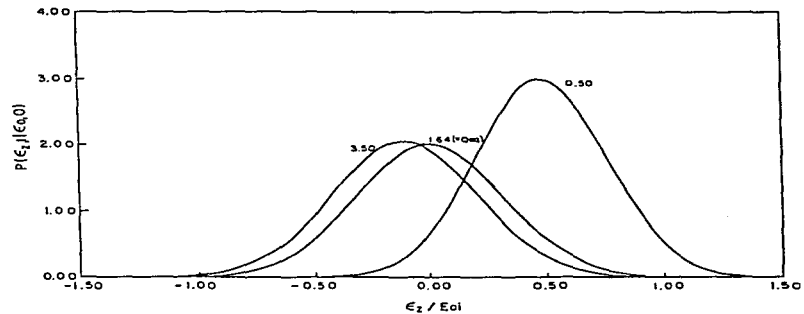
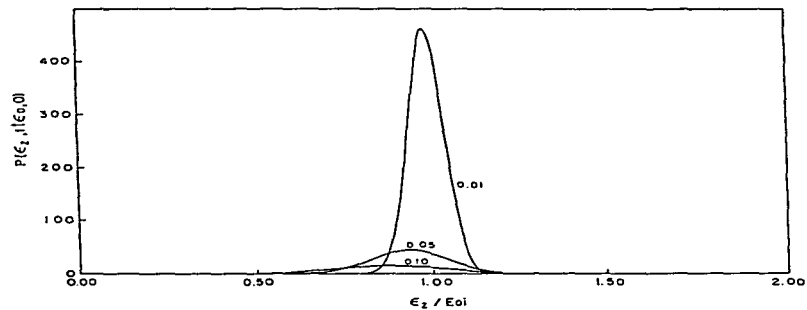
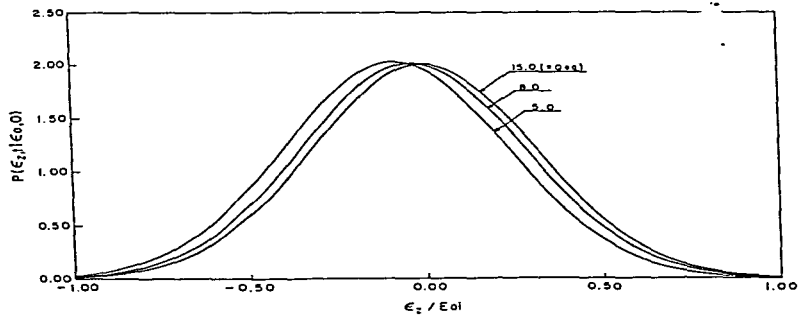


Fig. 6. Conditional probability density (2.3.12) for the case  $\hat{c} \parallel \hat{c}_0$ , with  $c_0 = 1$ , at (a)  $w_{p1} t = 0.01, 0.05, 0.10$ , (b)  $w_{p1} t = 0.50, 1.64, 3.50$ , and (c)  $w_{p1} t = 5.0, 8.0, 15.0$ .



smaller field values as time increases; the height of the peak also changes to preserve normalization. The distribution is symmetric. The conditional probability reaches its equilibrium value at a time  $t_0 \approx 1.64w_{p1}^{-1}$ , but it continues moving towards the negative region. This latter is a consequence of the change of sign in the autocorrelation function  $\alpha(t)$  (see Fig.3). During the time interval  $1.64 \leq w_{p1} t \leq 3.5$ , in which the absolute value of  $\alpha(t)$  increases again, the peak of the distribution becomes narrower and rises over its equilibrium value. At  $t > 3.5w_{p1}^{-1}$ , the peak decreases and broadens again, moving slowly towards  $\epsilon = 0$ . The equilibrium distribution  $Q_g(\epsilon)$  is finally reached at  $t \approx 15w_{p1}^{-1}$ . Finally, the angular dependence for the conditional probability (12) is studied by evaluating this function at  $\theta = 0, \pi/2$  and  $\pi$ , at an intermediate time ( $t = 3.5w_{p1}^{-1}$ ). This dependence is shown in Fig.7. Note that the conditional probability associated with that component of the field anti-parallel to  $\vec{e}_0$  is only a reflexion about  $\epsilon = 0$  of that for the parallel component. In contrast, the distribution for the perpendicular fields is always centered about  $\epsilon = 0$ ; it differs from the equilibrium distribution  $Q_g$ , except at those times when  $\alpha(t) = 0$ .

The Gaussian limit can be partially improved by the ad hoc replacement of  $Q_g$  by  $Q$  in Eq. (3), that is

$$P(\vec{e}, t | \vec{e}_0, 0) = \frac{1}{(1-\alpha(t)^2)^{3/2}} Q\left(\frac{\vec{e}-\alpha(t)\vec{e}_0}{(1-\alpha(t)^2)^{1/2}}\right). \quad (22)$$

In this way the dependence on the exact static distribution is preserved for both long and short times. However, the corresponding joint probability density does not satisfy the symmetry condition  $\vec{e} \leftrightarrow \vec{e}_0$  from (2.16). Note that this result does not satisfy Eq.(5). A related approximation has been considered by Smith, *et al* (1983, 1984) as a diffusion model. In that model, the conditional probability density is given by

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\* In both papers, the authors have written a wrong normalization factor, that is,  $(1+\Gamma)^{-3}$  instead of  $(1-\Gamma)^{-3}$ .

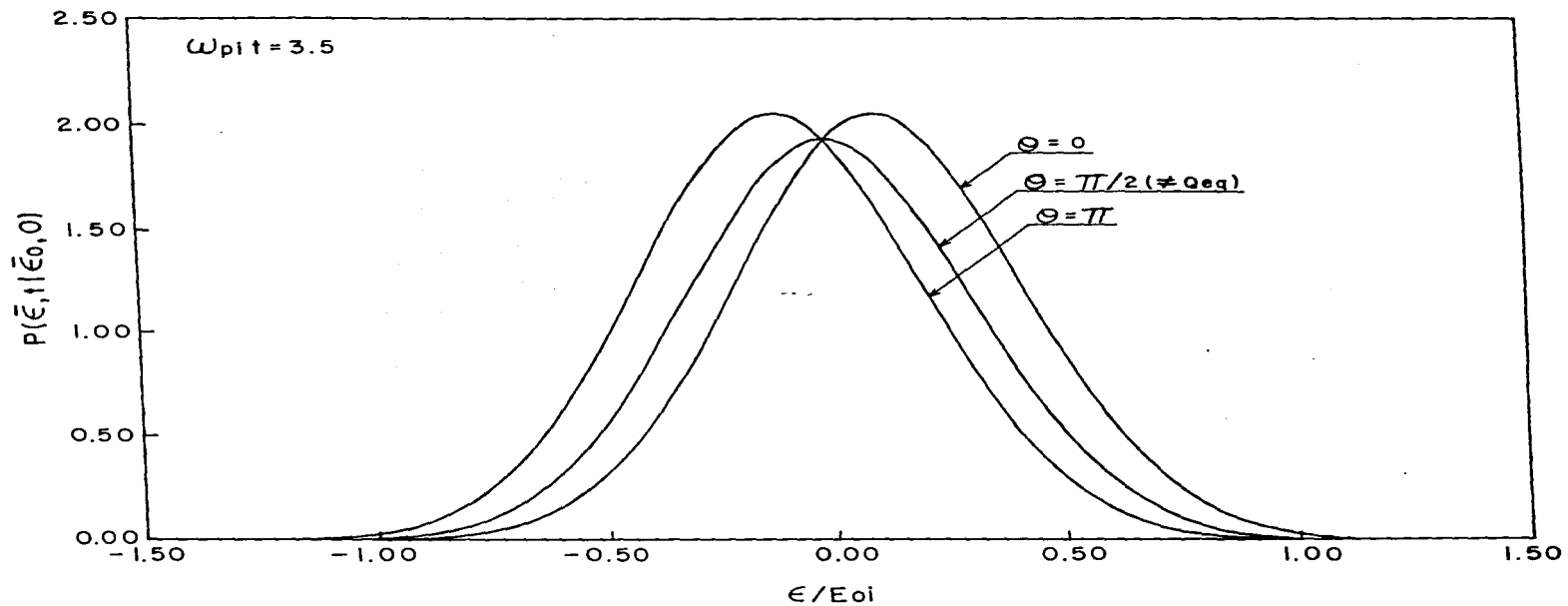


Fig.7. Conditional probability density (2.3.12) for  $\epsilon_0 = 1$  and  $\omega_{pi} t = 3.5$ , evaluated at  $\theta = 0, \pi/2, \pi$ .

$$P(\vec{E}, t | \vec{E}_0, 0) = \frac{1}{\{1-\Gamma(\epsilon_0, t)\}^3} Q\left(\frac{\vec{E}-\Gamma(\epsilon_0, t)\vec{E}_0}{1-\Gamma(\epsilon_0, t)}\right), \quad (23)$$

with  $\Gamma(\epsilon_0, t)$  a function of the initial field  $\epsilon_0$ , which decreases monotonically from 1 to 0 as time increases from 0 to  $\infty$ , and it is related to the autocorrelation  $\langle \vec{E}(t) \cdot \vec{E} \rangle$  by

$$\langle \vec{E}(t) \cdot \vec{E} \rangle = \int d\vec{c} \epsilon^2 Q(\epsilon) \Gamma(\epsilon, t). \quad (24)$$

The distribution (23) presents similar characteristics to (22), with some additional difficulties. For instance, for the particular case with  $\Gamma$  independent of  $\epsilon_0$ , the normalization condition is not satisfied appropriately. In addition, even for the case when  $Q$  is replaced by  $Q_g$ , the corresponding joint probability density  $f(\vec{E}, t; \vec{E}_0, 0)$  does not satisfy the symmetry condition  $\vec{E} \leftrightarrow \vec{E}_0$ , which contrast with our result (3).

A more systematic extension in the same spirit is obtained by expanding only  $\alpha(\vec{\lambda}, \vec{\lambda}'; t)$  in the representation (2.23). Then the joint probability density is found to be,

$$f(\vec{E}, t; \vec{E}_0, 0) = \int d\vec{\epsilon}_1 Q(\epsilon_1; \alpha(t)) Q(|\vec{E}-\vec{E}_1|; 1-\alpha(t)) Q(|\vec{E}_0-\vec{E}_1|; 1-\alpha(t)), \quad (25)$$

where  $Q(\epsilon; x)$  is simply related to the generating function for  $Q(\epsilon)$  in Eq. (1.5) by

$$Q(\epsilon, x) = \int \frac{d\vec{\lambda}}{(2\pi)^3} e^{-i\vec{\lambda} \cdot \vec{E}} \times I(\lambda). \quad (26)$$

The result (25) for the joint probability density reproduces the exact static distributions in the limits  $t \rightarrow 0$  and  $t \rightarrow \infty$ , and reduces to the Gaussian form (3) if  $Q$  is replaced by  $Q_g$ . We have not explored yet the range of validity for this result.

In all the cases in this section, the joint distribution can be completely determined from the static electric field distribution and the time dependent electric field autocorrelation function.



## 2.4. Short time limit

A description of early stages of the microfield dynamics is possible by studying the corresponding exact limit for the joint distribution function (Zogaib and Dufty, 1988). We present as follows two different ways of taking such a limit: from a time expansion of the dynamical generating function, and from the short time behavior of the dynamical equation satisfied by the joint distribution function.

### 2.4.1. Short time expansion of the generating function.

Here, an expansion in powers of  $t$  is performed for the generating function  $G(\vec{\lambda}, \vec{\lambda}'; t)$ . In this case, the leading terms in the representation (2.11) are

$$G(\vec{\lambda}, \vec{\lambda}'; t) = I(|\vec{\lambda} + \vec{\lambda}'|) + \frac{1}{2} \lambda_i \lambda'_j F_{ij}(|\vec{\lambda} + \vec{\lambda}'|) t^2 + (\text{order } t^4), \quad (1)$$

where  $F_{ij}(\lambda)$  is related to the conditional average for the initial time derivative of the electric field,  $\dot{E}_i$ ,

$$F_{ij}(\lambda) e^{I(\lambda)} = \int d\vec{e} Q(\vec{e}) \langle \dot{E}_i \dot{E}_j \rangle_{\vec{e}} e^{i\vec{\lambda} \cdot \vec{e}}. \quad (2)$$

Use now the generating function (1) to calculate  $f(\vec{e}, t; \vec{e}_0, 0)$  from (2.22). To this end, define a function  $\mathcal{F}(\vec{e}, \vec{\eta}; t)$ ,

$$\mathcal{F}(\vec{e}, \vec{\eta}; t) = \ln \left\{ \frac{1}{Q(\vec{e})} \int \frac{d\vec{\ell}}{(2\pi)^3} e^{-i\vec{\ell} \cdot \vec{e}} e^{I(\ell) + H(\vec{\ell}, \vec{\eta}; t)} \right\}, \quad (3)$$

with

$$H(\vec{\ell}, \vec{\eta}; t) = -\frac{t^2}{2} (\eta_1 + \ell_1/2)(\eta_j - \ell_j/2) F_{ij}(\ell); \quad (4)$$

\*If the expansion is performed on  $f(\vec{e}; t; \vec{e}_0)$  instead, a less physical series with singular coefficients ( $\delta$ -functions) is obtained.

thus, the joint probability density becomes

$$f(\vec{\epsilon}, t; \vec{\epsilon}_0, 0) = Q((\vec{\epsilon} + \vec{\epsilon}_0)/2) \int \frac{d\vec{\eta}}{(2\pi)^3} e^{-i\vec{\eta} \cdot (\vec{\epsilon} - \vec{\epsilon}_0)} e^{\mathcal{F}((\vec{\epsilon} + \vec{\epsilon}_0)/2, \vec{\eta}; t)} \quad (5)$$

Hence, to leading order in  $t$ ,

$$\begin{aligned} f(\vec{\epsilon}, t; \vec{\epsilon}_0, 0) &= Q(a) \int \frac{d\vec{\eta}}{(2\pi)^3} e^{-i\vec{\eta} \cdot \Delta\vec{\epsilon}} e^{t^2 [A_3(a) - \eta_i \eta_j \langle \dot{E}_i \dot{E}_j \rangle_a] / 2} \\ &= Q(a) e^{A_3(a)t^2/2} \frac{e^{-(\Delta\epsilon)_\perp^2 / 2A_1 t^2}}{(2\pi t^2 A_1)} \frac{e^{-(\Delta\epsilon)_\parallel^2 / 2A_2 t^2}}{(2\pi t^2 A_2)^{1/2}}. \end{aligned} \quad (6)$$

Here  $\Delta\vec{\epsilon} = \vec{\epsilon} - \vec{\epsilon}_0$  and  $\vec{a} = (\vec{\epsilon} + \vec{\epsilon}_0)/2$ ; also,  $\Delta\vec{\epsilon}_\perp$  and  $\Delta\vec{\epsilon}_\parallel$  are the components of  $\Delta\vec{\epsilon}$  perpendicular and parallel to  $\vec{a}$ , respectively. The coefficients  $A_m(a)$  are related to  $\langle \dot{E}_i \dot{E}_j \rangle_a$  by,

$$\begin{aligned} A_1(a) &= \frac{1}{2} \langle [\dot{E}^2 - (\hat{a} \cdot \dot{E})^2] \rangle_a, & A_2(a) &= \langle (\hat{a} \cdot \dot{E})^2 \rangle_a \\ A_3(a) &= -[4Q(a)]^{-1} \frac{\partial^2}{\partial a_i \partial a_j} Q(a) \langle \dot{E}_i \dot{E}_j \rangle_a = -[4Q(a)]^{-1} \frac{\partial}{\partial a_i} Q(a) \langle \dot{E}_i \rangle_a. \end{aligned} \quad (7)$$

In the last identity for  $A_3(a)$  we have used that

$$Q(a) \langle \dot{E}_i \rangle_a = \frac{\partial}{\partial a_j} Q(a) \langle \dot{E}_i \dot{E}_j \rangle_a. \quad (8)$$

as follows from stationarity.

The joint probability (6) is asymptotically exact as  $t \rightarrow 0$ . It satisfies the conditions (2.13), (2.15)-(2.17), but does not yield the long time limit (2.14); the normalization condition (2.12) is satisfied only asymptotically, as  $t \rightarrow 0$ . It is Gaussian in the field difference,  $\Delta\vec{\epsilon}$ , but has a more complex dependence on the field  $\vec{a}$  through the conditional correlation function  $\langle \dot{E}_i \dot{E}_j \rangle_a$ . This latter may be calculated in an approximation suitable for strongly coupled plasmas as follows. First, it is expressed in terms of the conditional pair correlation function  $g(\vec{r}; \vec{a})$  as

$$\langle \dot{E}_i \dot{E}_j \rangle_a = k_B T m_i n_i \int d\vec{r} \left( \frac{\partial E_i(\vec{r})}{\partial r} \right) \left( \frac{\partial E_j(\vec{r})}{\partial r} \right) g(\vec{r}; \vec{a}); \quad (9)$$

here,  $g(\vec{r}; \vec{a})$  is the pair correlation function for a particle at a position  $\vec{r}$  relative to the field point, given that the field there has the value  $\vec{a}$ ,

$$n_i g(\vec{r}_1; \vec{a}) = N_i \int d\vec{r}_2 \dots d\vec{r}_{N_i} \frac{\delta(\vec{a} - \vec{E})}{Q(a)} \frac{e^{-U/k_B T}}{Q(N_i, \Omega, T)}. \quad (10)$$

with  $U$  the total potential energy and  $Q(N_i, \Omega, T)$  the configurational partition function in the canonical ensemble.

The conditional pair correlation  $g(\vec{r}; \vec{a})$  in (10) can also be calculated from a suitable functional derivative of the generating function,  $I(\lambda)$ , for the static distribution. Since accurate approximations for  $I(\lambda)$  are known (Dufty, 1987), suitable for strongly coupled plasmas, they may be used to determine  $g(\vec{r}; \vec{a})$  as well. The details of such a calculation for various approximations to  $I(\lambda)$  are discussed in Lado, Dufty (1987). In particular, for the APEX approximation to  $I(\lambda)$  (Iglesias et.al, 1983a), which will be discussed in §3.3, the coefficients (9) reduce to,

$$\langle \dot{E}_i \dot{E}_j \rangle_a = k_B T m_i n_i \int d\vec{r} \left( \frac{\partial E_i(\vec{r})}{\partial r_\ell} \right) \left( \frac{\partial E_j(\vec{r})}{\partial r_\ell} \right) g(\vec{r}) Q(\vec{a} - \vec{E}^*(\vec{r})) / Q(a). \quad (11)$$

where  $g(\vec{r})$  is the usual equilibrium radial distribution function for a particle at a distance  $r$  from the field point, and  $\vec{E}^*$  is the APEX effective field for that particle. The short time distribution (6) can therefore be calculated to a good approximation for strongly coupled plasmas from knowledge of  $Q(\epsilon)$  and the radial distribution function. The applicability of this interesting result could be established if extensive computer simulations were available in the literature.

The short time result (6) is evaluated in detail later on (§4.2), for the particular case of non-interacting ions and a neutral point.

#### 2.4.ii. Short time expansion of the dynamical equation

An alternative description is given here, in terms of the short time

behavior of the dynamical equation satisfied by the joint probability density  $f(\vec{c}, t; \vec{c}_0, 0)$ . We assume here that this function satisfies the equation

$$\frac{\partial}{\partial t} f(\vec{c}, t; \vec{c}_0, 0) = -\hat{\mathcal{L}}(\vec{c}, t) f(\vec{c}, t; \vec{c}_0, 0), \quad (12)$$

with  $\hat{\mathcal{L}}(\vec{c}, t)$  an operator governing the time dependence. The solution to this equation is required to satisfy the initial condition (2.13). Since time reversal invariance implies  $\hat{\mathcal{L}}(\vec{c}, t) = -\hat{\mathcal{L}}(\vec{c}, -t)$ , then

$$\hat{\mathcal{L}}(\vec{c}, t) \xrightarrow{t \rightarrow 0} t\hat{\mathcal{L}}(\vec{c}) + (\text{order } t^3). \quad (13)$$

Consider now the average  $\langle A(\vec{E}(t))B(\vec{E}) \rangle$ , with A, B two arbitrary functions of the field. From (2.3), (12) and (13) we have

$$\frac{d^2}{dt^2} \langle A(\vec{E}(t))B(\vec{E}) \rangle \Big|_{t=0} = - \int d\vec{c} A(\vec{c}) \hat{\mathcal{L}}(\vec{c}) [Q(\vec{c}) B(\vec{c})]. \quad (14)$$

On the other hand, a short time expansion of the integrand in (2.6) gives

$$\langle A(\vec{E}(t))B(\vec{E}) \rangle \xrightarrow{t \rightarrow 0} \int d\vec{c} Q(\vec{c}) \left\{ A(\vec{c}) + \frac{t^2}{2} \left[ \frac{\partial A}{\partial \epsilon_1} \langle \dot{\epsilon}_1 \rangle_{\vec{c}} + \frac{\partial^2 A}{\partial \epsilon_1 \partial \epsilon_j} \langle \dot{\epsilon}_1 \dot{\epsilon}_j \rangle_{\vec{c}} \right] \right\} B(\vec{c}). \quad (15)$$

This latter equation with the condition (8) implies

$$\frac{d^2}{dt^2} \langle A(\vec{E}(t))B(\vec{E}) \rangle \Big|_{t=0} = \int d\vec{c} A(\vec{c}) \frac{\partial}{\partial \epsilon_1} [\langle \dot{\epsilon}_1 \dot{\epsilon}_j \rangle \left( \frac{\partial}{\partial \epsilon_j} - \frac{\partial \ln Q}{\partial \epsilon_j} \right) Q(\vec{c}) B(\vec{c})]. \quad (16)$$

A comparison of (14) and (16) gives

$$\hat{\mathcal{L}}(\vec{c}) = - \frac{\partial}{\partial \epsilon_1} \left[ \langle \dot{\epsilon}_1 \dot{\epsilon}_j \rangle_{\vec{c}} \left( \frac{\partial}{\partial \epsilon_j} - \frac{\partial \ln Q(\vec{c})}{\partial \epsilon_j} \right) \right], \quad (17)$$

so that Eq. (12) becomes

$$\frac{\partial}{\partial s} f(\vec{c}, s; \vec{c}_0, 0) = \frac{\partial}{\partial \epsilon_1} [D_{1j}(\vec{c}) \left( \frac{\partial}{\partial \epsilon_j} - V_j(\vec{c}) \right)] f(\vec{c}, s; \vec{c}_0, 0), \quad (18)$$

with  $s \equiv t^2$  and

$$D_{ij}(c) = \frac{1}{2} \langle \dot{E}_i \dot{E}_j \rangle_c, \quad V_i(c) = \frac{\partial}{\partial c_i} \ln[Q(c)]. \quad (19)$$

It can be shown that the solution to this equation, with initial condition (2.13), is asymptotically exact as  $t \rightarrow 0$  and has the properties (2.12), (2.14)-(2.17) as well. For finite times, the short time forms (18) and (6) are not equivalent. Equation (18) has the advantage of approaching the correct long time limit and therefore may extrapolate better to longer times than (6). On the other hand, we have an explicit form for (6) whereas we have not been able to construct the solution to (18).

## 2.5. Discussion

The results in this chapter allow us to gain some understanding of electric field dynamics in some particular cases where the problem can be reduced to quadratures. In general, although the angular dependence of the generating function  $G(\lambda, \lambda', \hat{\lambda} \cdot \hat{\lambda}'; t)$  reduces the number of integrals to be performed, the remaining integrations usually requires extensive numerical work. This fact could suggest to consider an expansion of the distribution  $f(\vec{c}, t; \vec{c}_0, 0)$  in terms of Legendre Polynomials. As shown in Appendix A, that expansion is not useful here: on the one hand, the leading terms contain only partial information about the angular dependence at both short and long times; on the other hand, numerical evaluation of those first few terms also requires extensive numerical work.

In the following chapter we present an alternative representation for the dynamical distribution in terms of a cluster expansion, which usually constitutes a useful technique for systems with many-body interactions. As shown there, the corresponding results can be also reduced to quadratures in some interesting cases.

## CHAPTER 3

### CLUSTER EXPANSION

#### 3.1. A Cluster expansion for the case of interacting particles

Approximations for the dynamical distribution  $f(\vec{U}, t; \vec{r}_0, 0)$  may be obtained from a cluster expansion similar to that performed by Baranger and Mozer (1959, 1960) for the static case. In a cluster expansion, many-body contributions are separated into one-body, two-body, ..., contributions, which can be more suitable for theoretical analysis. These few-body contributions are the leading terms in the expansion, and they play a relevant role when high-order correlations are negligible.

To this end, write first the generating functions  $I(\lambda)$  and  $G(\vec{\lambda}, \vec{\lambda}'; t)$  as

$$I(\lambda) = \ln \left\langle \prod_{\alpha=1}^{N_1} e^{i\vec{\lambda} \cdot \vec{E}_{\alpha}} \right\rangle, \quad (1)$$

$$G(\vec{\lambda}, \vec{\lambda}'; t) = \ln \left\langle \prod_{\alpha=1}^{N_1} e^{i\vec{\lambda} \cdot \vec{E}_{\alpha}} e^{-\hat{L}t} \prod_{\beta=1}^{N_1} e^{i\vec{\lambda}' \cdot \vec{E}_{\beta}} \right\rangle, \quad (2)$$

where  $\vec{E}_{\alpha} \equiv \vec{E}(\vec{r}_{\alpha})$  is the field due to the  $\alpha$ th-ion at a distance  $\vec{r}_{\alpha}$  from the radiator and  $\hat{L}$  is the Liouville operator  $\hat{L}\psi = \{\psi, \hat{H}\}$ , with  $\{ , \}$  the Poisson Brackets. In analogy to Mayer functions (Pathria, 1988), define now

$$\phi_{\alpha}(\vec{\lambda}) = e^{i\vec{\lambda} \cdot \vec{E}_{\alpha}} - 1, \quad (3)$$

with  $\phi_{\alpha}(\vec{\lambda}) \equiv \phi(\vec{\lambda}, \vec{r}_{\alpha})$ . Substitution of (3) in (1) and (2) gives  $I$  and  $G$  as functionals of  $\phi$ , i.e.,  $I = I[\phi]$ ,  $G = G[\phi, \phi'; t]$ .

$$\begin{aligned}
I[\phi] &= \ln \langle \pi(1 + \phi_\alpha(\vec{\lambda})) \rangle \\
&= \langle \Sigma \phi_\alpha(\vec{\lambda}) \rangle + \frac{1}{2} \left\{ \langle \Sigma \Sigma \phi_\alpha(\vec{\lambda}) \phi_\beta(\vec{\lambda}) \rangle - \langle \Sigma \phi_\alpha(\vec{\lambda}) \rangle^2 \right\} + \dots \quad (4)
\end{aligned}$$

$$\begin{aligned}
G[\phi, \phi'; t] &= \ln \langle \pi(1 + \phi_\alpha(\vec{\lambda})) e^{-\hat{L}t} \pi(1 + \phi_\beta(\vec{\lambda}')) \rangle \\
&= \langle \Sigma \phi_\alpha(\vec{\lambda}) \rangle + \frac{1}{2} \left\{ \langle \Sigma \Sigma \phi_\alpha(\vec{\lambda}) \phi_\beta(\vec{\lambda}') \rangle - \langle \Sigma \phi_\alpha(\vec{\lambda}) \rangle^2 \right\} + \dots \\
&\quad + \langle \Sigma \phi_\alpha(\vec{\lambda}') \rangle + \frac{1}{2} \left\{ \langle \Sigma \Sigma \phi_\alpha(\vec{\lambda}') \phi_\beta(\vec{\lambda}') \rangle - \langle \Sigma \phi_\alpha(\vec{\lambda}') \rangle^2 \right\} + \dots \\
&\quad + \langle \Sigma \phi_\alpha(\vec{\lambda}) e^{-\hat{L}t} \Sigma \phi_\beta(\vec{\lambda}') - \phi_\beta(\vec{\lambda}') \rangle + \dots \quad (5)
\end{aligned}$$

The last equalities in  $I[\phi]$  and  $G[\phi, \phi'; t]$  represent the leading terms in a functional Taylor series expansion in the functions  $\phi$  and  $\phi'$ .

Evaluating the averages in (4), we have

$$\begin{aligned}
I[\phi] &= n_1 \int d\vec{r}_1 \phi_1(\vec{\lambda}) g^{(2)}(\vec{r}_1) \\
&\quad + \frac{n_1^2}{2} \int d\vec{r}_1 d\vec{r}_2 \phi_1(\vec{\lambda}) \phi_2(\vec{\lambda}') \{ g^{(3)}(\vec{r}_1, \vec{r}_2) - g^{(2)}(\vec{r}_1) g^{(2)}(\vec{r}_2) \} + \dots \quad (6)
\end{aligned}$$

with  $n_1$  the ion density. This is the Baranger-Mozer result for the static generating function  $I(\lambda)$  of  $Q(\vec{e})$ . The functions  $g^{(k+1)}(\vec{r}_1, \dots, \vec{r}_k)$  are the correlation functions for  $k+1$  bodies (McQuarrie, 1976),

$$g^{(k+1)}(\vec{r}_1, \dots, \vec{r}_k) = \frac{1}{n_1^k} \frac{N_1!}{(N_1 - k)!} \frac{\int d\vec{r}_{k+1} \dots d\vec{r}_{N_1} e^{-\beta U}}{\int d\vec{r}_1 \dots d\vec{r}_{N_1} e^{-\beta U}}, \quad (7)$$

with  $U$  the total potential energy. The variable  $\vec{r}_\alpha$  denotes the position of the  $\alpha$ th-ion relative to the field point,  $\vec{r}_\alpha = \vec{q}_\alpha - \vec{R}_0$ . For the case when the ions do not interact with each other but only with the radiator, all the correlations  $g^{(k+1)}(\vec{r}_1, \dots, \vec{r}_k)$ ,  $k \geq 2$ , factorize into simpler two-body

correlations,  $g^{(2)}(\vec{r}_1)$ . In this case, all the high-order terms in (6) vanish, so that  $I[\phi]$  becomes

$$I[\phi] \rightarrow n_1 \int d\vec{r}_1 \phi_1(\vec{\lambda}) g_0^{(2)}(\vec{r}_1), \quad g_0^{(2)}(\vec{r}_\alpha) = \frac{N_1}{n_1} \frac{e^{-\beta U(r_\alpha)}}{\int d\vec{r} e^{-\beta U(r_\alpha)}} \quad (8)$$

where  $U(r_\alpha)$  represents the interaction between the  $\alpha$ th-ion and the radiator.

Similarly to (6), we obtain for  $G[\phi, \phi'; t]$ ,

$$G[\phi, \phi'; t] = I[\phi] + I[\phi'] + n_1 \int d\vec{r}_1 d\vec{r}_2 \phi_1(\vec{\lambda}) \phi_2(\vec{\lambda}') C(\vec{r}_1, \vec{r}_2; t) + \dots \quad (9)$$

with  $I[\phi]$  the static generating function, Eq.(6), and  $C(\vec{r}_1, \vec{r}_2; t)$  the ion density-density autocorrelation function,

$$C(\vec{r}_1, \vec{r}_2; t) = \langle n(\vec{r}_1, t) [n(\vec{r}_2) - \langle n(\vec{r}_2) \rangle] \rangle / n_1. \quad (10)$$

Here,  $n(\vec{r}, t)$  denotes the microscopic ion density at the point  $\vec{r}(t)$ ,

$$n(\vec{r}, t) = \sum_{\alpha} \delta(\vec{r} - \vec{q}_{\alpha}(t) + \vec{R}_0(t)). \quad (11)$$

Eq.(9) is the generalization of Eq.(6) for the dynamical case. The last term is the leading dynamical contribution, bilinear in the function  $\phi$ , and the dots indicate other dynamical contributions with higher order in  $\phi$ . The result (9) justifies writing  $G(\vec{\lambda}, \vec{\lambda}'; t)$  as in (2.2.18). It also provides an approximation for  $H_{\infty}(\vec{\lambda}, \vec{\lambda}'; t)$ , alternative to that in (2.2.19), namely,

$$H_{\infty}(\vec{\lambda}, \vec{\lambda}'; t) = n_1 \int d\vec{r}_1 d\vec{r}_2 \phi_1(\vec{\lambda}) \phi_2(\vec{\lambda}') C(\vec{r}_1, \vec{r}_2; t) + \dots \quad (12)$$

For very weak coupling between the ions, high-order correlations are expected to be negligible, so that only the leading static and dynamic terms in the series survive; that is,



$$G[\phi, \phi'; t] = n_1 \int d\vec{r}_1 [\phi_1(\vec{\lambda}) + \phi_1(\vec{\lambda}')] g^{(2)}(\vec{r}_1) \\ + n_1 \int d\vec{r}_1 d\vec{r}_2 \phi_1(\vec{\lambda}) \phi_2(\vec{\lambda}') C(\vec{r}_1, \vec{r}_2; t), \quad (13)$$

where  $g^{(2)}(\vec{r})$  and  $C(\vec{r}_1, \vec{r}_2; t)$  are calculated in the random phase (Debye-Vlasov) approximation (Baus and Hansen, 1980). Models of the form (13), *i.e.* retaining only the structure of the first two terms in the functional expansion, will be referred to as Independent Particle models. For non-interacting ions and a neutral field point the independent particle model is exact (see appendix B), with

$$g^{(2)}(\vec{r}) = 1, \quad (14)$$

$$C(\vec{r}_1, \vec{r}_2; t) \rightarrow C(\vec{r}_1 - \vec{r}_2; t) = (\pi u^2 t^2)^{-3/2} \exp \left\{ - \frac{(\vec{r}_1 - \vec{r}_2)^2}{(ut)^2} \right\}, \quad (15)$$

where  $u = (2k_B T/m_1)^{1/2}$  is the thermal speed. In contrast, even for the case of non-interacting ions, if there is a charge on the field point high-order (dynamical) terms remain in the functional expansion. That is, electric interactions with the radiator introduce dynamical correlations between the ions. The generating function (13) should properly be understood as resulting instead from the weak coupling limit.

### 3.2. High field limit

The behavior of the distribution function for very large field values is expected to be governed by the fields of one particle close to the field point at  $t = 0$  and one particle nearby at time  $t$ . To extract this contribution it is convenient to go back to the cluster expansion for  $G(\vec{\lambda}, \vec{\lambda}'; t)$  introduced in the previous section.

For particles near the field point the field is approximately Coulomb. This suggests a scaling in the joint probability (2.2.10) according to  $\lambda \epsilon \rightarrow \lambda$ ,  $r^2 \epsilon \rightarrow r^2$ , which shows that each factor of the function  $\phi$  in the generating function (1.5) introduces a factor of  $\epsilon^{-3/2}$  or  $\epsilon_0^{-3/2}$ . Formally, therefore, the high order terms not shown in the expansion (1.9) become negligible for sufficiently large  $\epsilon, \epsilon_0$ . Furthermore, the exponential of  $G$

in the dynamical distribution (2.2.10) also can be expanded to quadratic order in  $\phi$ . The terms contributing for large  $\epsilon$ ,  $\epsilon_0$ , are then found to give,

$$f(\vec{z}, t; \vec{z}_0, 0) \rightarrow Q(\epsilon)Q(\epsilon_0) + \int d\vec{r}_1 d\vec{r}_2 \delta(\vec{z} - \vec{E}(\vec{r}_1)) \delta(\vec{z}_0 - \vec{E}(\vec{r}_2)) C(\vec{r}_1, \vec{r}_2; t), \quad (1)$$

where  $Q(\epsilon)$  is given by its high field limit,

$$Q(\epsilon) \rightarrow n_1 \int d\vec{r}_1 \delta(\vec{z} - \vec{E}(\vec{r}_1)) g^{(2)}(\vec{r}_1), \quad (2)$$

which follows from the same expansion. For the large fields considered, we may replace  $\vec{E}(\vec{r})$  in (1) by Coulomb fields  $(Z_1 e/r^2)$  and perform the integration to give,

$$f(\vec{z}, t; \vec{z}_0, 0) \rightarrow Q(\epsilon)Q(\epsilon_0) + \frac{1}{4} (\epsilon \epsilon_0)^{-9/2} (Z_1 e)^3 C(\hat{\epsilon} \sqrt{Z_1 e/\epsilon}, \hat{\epsilon}_0 \sqrt{Z_1 e/\epsilon_0}; t), \quad (3)$$

with

$$Q(\vec{z}) = \frac{n_1}{2} (Z_1 e)^{3/2} \epsilon^{-9/2} g^{(2)}(\hat{\epsilon} \sqrt{Z_1 e/\epsilon}). \quad (4)$$

The high field limit is seen to be determined from the radial distribution,  $g^{(2)}(r)$ , and  $C(\vec{r}_1, \vec{r}_2; t)$ . The explicit form of the second term on the RHS of the distribution (3) will be evaluated and discussed later on (§4.4) for the case of a neutral field point and non-interacting ions.

The interpretation of (3) as the single field contribution can be made more apparent by rewriting it in the equivalent form,

$$f(\vec{z}, t; \vec{z}_0, 0) \rightarrow \sum_1 \sum_j \langle \delta(\vec{z} - \vec{E}(\vec{r}_1(t))) \delta(\vec{z}_0 - \vec{E}(\vec{r}_j)) \rangle, \quad (5)$$

where the summations range over all particles. Equation (5) represents all possible ways to produce the fields,  $\vec{z}_0$  at  $t = 0$  and  $\vec{z}$  at  $t$ , by a single particle (not necessarily the same). This limit also preserves the properties (2.2.13)-(2.2.17). We note that for short times and large

fields the second term on the right side of (3) dominates the first term, i.e. both fields are due to the same single particle.

### 3.3. Renormalized independent particle model

Here we consider a generalization to the Renormalized Independent particle model, introduced by Dufty et al (1985) for the static case. This model (Dufty and Zogaib, 1989) assumes the form (1.13) for the generating function, but replaces  $g^{(2)}(\vec{r})$  and  $C(\vec{r}_1, \vec{r}_2; t)$  by their exact values. Furthermore, an effective field,  $\vec{E}^*(\vec{r})$ , and an associated function,  $\phi^*(\vec{r}, \vec{\lambda})$  (analogous to (1.3)), are introduced. Here, the functional  $G[\phi, \phi'; t]$  is replaced by

$$G[\phi, \phi'; t] \equiv G^*[\phi^*, \phi'^*; t], \quad (6)$$

where  $\phi(\vec{r}, \vec{\lambda})$  and  $\phi^*(\vec{r}, \vec{\lambda})$  are related by the identity

$$\phi = -1 + (1 + \phi^*)^R, \quad (7)$$

with  $R$  the ratio of the field magnitudes  $E/E^*$ . Elimination of  $\phi$  on the RHS of the functional (1.5) using (7) gives the desired renormalized cluster series,

$$G^*[\phi^*, \phi'^*; t] \rightarrow I[\phi^*] + I[\phi'^*] + \int d\vec{r}_1 d\vec{r}_2 \phi^*(\vec{\lambda}) \phi^*(\vec{\lambda}') R_1 R_2 C(\vec{r}_1, \vec{r}_2; t), \quad (8)$$

where the static generating function  $I[\phi^*]$  is given by

$$I[\phi^*] = n_1 \int d\vec{r}_1 \phi^*(\vec{\lambda}) R_1 h_2(\vec{r}_1) + \frac{1}{2} \int d\vec{r}_1 d\vec{r}_2 \phi^*(\vec{\lambda}) \phi^*(\vec{\lambda}') \cdot \{h_3(\vec{r}_1, \vec{r}_2) R_1 R_2 - \delta(\vec{r}_1 - \vec{r}_2) h_2(\vec{r}_1) R_1 (1 - R_1)\} + \dots \quad (9)$$

with  $R(\vec{r}_1) \equiv R_1$  and  $h_p(\vec{r}_1, \dots, \vec{r}_{p-1})$  the Ursell cluster functions (McQuarrie, 1976) associated with the set of correlation functions  $g^{(p)}(\vec{r}_1, \dots, \vec{r}_{p-1})$ .

$$h_2(\vec{r}_1) = g^{(2)}(\vec{r}_1)$$

$$h_3(\vec{r}_1, \vec{r}_2) = g^{(3)}(\vec{r}_1, \vec{r}_2) - g^{(2)}(\vec{r}_1)g^{(2)}(\vec{r}_2). \quad (10)$$

The effective field  $\vec{E}^*$  is now chosen so that the Independent Particle model approximation for  $Q(\epsilon)$  yields the exact second moment,  $\langle E^2 \rangle$  (or related condition for neutral points). With such a choice it is possible to show that the joint distribution function calculated from (8) yields the exact time dependent second moments,  $\langle E_i(t)E_j \rangle$ . The fundamental symmetries and conditions (2.2.12)-(2.2.17) are also preserved.

In contrast to the independent particle result (1.13), the generating function (8) is suitable to describe strongly coupled plasmas and an arbitrary charge on the field point. Calculations from this model present an excellent agreement with computer simulation results for the static case, over a wide range of values for the plasma parameter (Dufty *et al*, 1985). A related Renormalized Independent Particle model is the so called APEX (Adjustable-Parameter EXponential), introduced by Iglesias *et al* (1983a) for the static generating function. In such a model,  $I[\phi^*]$  is given by the leading term in the expansion (9), and the renormalized field  $E^*$  is chosen to be a Debye screened field with an adjustable parameter to fit the exact second moment  $\langle E^2 \rangle$ . Although APEX calculations are in excellent agreement with simulation results for electric fields at highly charged points, a less accurate description is obtained for the case of a neutral point (Dufty *et al*, 1985).

Due to the lack of extensive computer simulation results for the joint probability distribution, the accuracy of the renormalized models in this section has not been established yet for the dynamical case. An analysis in this spirit is presented in chapter 4 for a system of non-interacting ions and a neutral point, for which some limited simulation data are available.

## CHAPTER 4

### DYNAMICS OF THE ELECTRIC FIELD AT A NEUTRAL POINT, IN A ONE-COMPONENT PLASMA OF NON-INTERACTING PARTICLES

#### 4.1. Introduction

As shown in Chapter 3, even for strongly coupled plasmas it is possible to renormalize the terms in the cluster expansion for the generating function, in such a way that the result resembles that for the case of independent particles. This is obtained by introducing an effective field, which accounts for the many-body correlations in the system. The advantage of an independent particle model is that the corresponding generating function can be expressed in terms of quadratures, so that the problem reduces to one of numerical methods only. Because of its importance and simplicity, in this chapter we study the electric field dynamics that follows from such a model. We consider here an extreme case of weak coupling, in which the dynamical generating function may be approximated by only the leading terms in a cluster expansion. Based on the Renormalized Independent Particle model mentioned before, we assume that the electric field is given by an effective Debye field that accounts for the effect of high-order correlations. For simplicity, we restrict ourselves to the case of a neutral point, which allows simple numerical evaluation. The corresponding results are studied in detail at some of the exact limits previously introduced for the general case (short times and high fields), in which the numerical problem becomes relatively simple.

According to the results in §3.1, for the particular case of non-interacting ions and a neutral point the terms of the generating function in the representation (2.2.18) reduce to

$$I(\lambda) = n_1 \int d\vec{r}_1 \phi(\vec{r}_1, \vec{\lambda}), \quad (1)$$

$$H_{\infty}(\vec{\lambda}, \vec{\lambda}'; t) = n_1 \int d\vec{r}_1 d\vec{r}_2 \phi(\vec{r}_1, \vec{\lambda}) \phi(\vec{r}_2, \vec{\lambda}') e^{\frac{-(\vec{r}_1 - \vec{r}_2)^2 / (ut)^2}{(\pi u^2 t^2)^{3/2}}} \quad (2)$$

with  $u^2 = 2k_B T/m_1$ . Substitution of (1) and (2) in (2.2.18) gives the exact generating function for this model, as shown in Appendix B.

Expression (2) for  $H_{\infty}(\vec{\lambda}, \vec{\lambda}'; t)$  can not be integrated in an easy way. In effect, note that the integrand there depends on the three angles  $\hat{r}_1 \cdot \vec{\lambda}$ ,  $\hat{r}_2 \cdot \vec{\lambda}'$  and  $\hat{r}_1 \cdot \hat{r}_2$ , so that the addition theorem should be used repeatedly. On the other hand, the angular dependence of this function,  $H_{\infty} = H_{\infty}(\lambda, \lambda', \hat{\lambda} \cdot \hat{\lambda}'; t)$ , could also suggest performing an expansion in terms of Legendre polynomials. As shown in Appendix C, in order for such a method to be useful an important contribution from the angular dependence should be neglected; however, neglecting those terms implies an inappropriate behavior at both short and long times. An exact numerical evaluation of the function (2) is rather associated with standard Monte Carlo techniques for multi-dimensional integrals.

The dynamical generating function obtained from Eqs. (2.2.18), (1) and (2) is susceptible to simple numerical evaluation at some of the exact limits (short times and large fields) already introduced in previous sections (§2.4.1 and §3.2, respectively) for the general case. The Gaussian limit is not valid here, since the second moment  $\langle E^2 \rangle$  is divergent for a neutral point. The corresponding results are presented as follows.

#### 4.2. Dynamical properties at short times

As already shown in §2.4.1, the limit for short times is interesting because it is exact and it is relatively easy to evaluate from the knowledge of simple functions such as the conditional radial distribution  $g(\vec{r}; \vec{E})$ . In particular, for a system of non-interacting particles the coefficients (2.4.7) can be evaluated numerically in an exact form, so that the dynamical behavior of the electric field at short times can be studied in detail. As an additional advantage, the corresponding results can be compared with some limited computer simulation data for this case.

To this end, we introduce here an alternative representation for the coefficients (2.4.7), more convenient for numerical evaluation, namely,

$$A_1(a) = \frac{1}{Q(a)} \int \frac{d\vec{\lambda}}{(2\pi)^3} e^{-i\vec{\lambda} \cdot \vec{a}} e^{I(\lambda)} \left\{ I_1 + \frac{1}{2}(1 - (\hat{a} \cdot \hat{\lambda})^2) I_2 \right\} \quad (1)$$

$$A_2(a) = \frac{1}{Q(a)} \int \frac{d\vec{\lambda}}{(2\pi)^3} e^{-i\vec{\lambda} \cdot \vec{a}} e^{I(\lambda)} \left\{ I_1 + (\hat{a} \cdot \hat{\lambda})^2 I_2 \right\} \quad (2)$$

$$A_3(a) = \frac{1}{Q(a)} \int \frac{d\vec{\lambda}}{(2\pi)^3} e^{-i\vec{\lambda} \cdot \vec{a}} e^{I(\lambda)} \frac{\lambda^2}{4} \{ I_1 + I_2 \}, \quad (3)$$

with  $I_1(\lambda)$ ,  $I_2(\lambda)$  the averages

$$I_1(\lambda) = \frac{\langle \frac{1}{2} [\hat{E}^2 - (\hat{\lambda} \cdot \hat{E})^2] e^{i\vec{\lambda} \cdot \vec{E}} \rangle}{\langle e^{i\vec{\lambda} \cdot \vec{E}} \rangle}, \quad I_2(\lambda) = \frac{\langle -\frac{1}{2} [\hat{E}^2 - 3(\hat{\lambda} \cdot \hat{E})^2] e^{i\vec{\lambda} \cdot \vec{E}} \rangle}{\langle e^{i\vec{\lambda} \cdot \vec{E}} \rangle}. \quad (4)$$

To further evaluation of these functions, it is also convenient to introduce dimensionless variables, that is,

$$\begin{aligned} \vec{r}/r_{01} &\rightarrow \vec{r}, & 4\pi r_{01}^3/3 &= n^{-1} \\ \vec{E}/E_{01} &\rightarrow \vec{E}, & E_{01} &= Z_1 e/r_{01}^2 \text{ (normal field strength)} \\ \vec{\lambda} E_{01} &\rightarrow \vec{\lambda}, & r_{01} a_D &\rightarrow a_D \end{aligned} \quad (5)$$

In terms of these variables, an angular integration for the generating function  $I(\lambda)$  of the microfield distribution  $Q(a)$  in (1)-(3) gives

$$I(\lambda) = 3 \int_0^\infty dr r^2 [j_0(\lambda r/r^2) - 1], \quad (6)$$

with  $f \equiv f(r)$  the Debye screening factor (2.1.13), and  $j_0$  the spherical Bessel function of order 0 (Arfken, 1985). In the particular case of Coulomb interactions ( $a_D = 0$ ), this integral can be evaluated analytically (Griem, 1974), giving

$$I(\lambda) = -\gamma\lambda^{3/2}, \quad (7)$$

with  $\gamma = -2(2\pi)^{1/2}/5$ . Similarly, we have for the averages (4)

$$I_1(\lambda) = 3 \int_0^\infty dr r^2 \left\{ \frac{r^2}{r^6} J_0\left(\frac{\lambda r}{r^2}\right) + G(r) \left(\frac{\lambda r}{r^2}\right)^{-1} J_1\left(\frac{\lambda r}{r^2}\right) \right\}. \quad (8a)$$

$$I_2(\lambda) = 3 \int_0^\infty dr r^2 \left\{ G(r) J_0\left(\frac{\lambda r}{r^2}\right) - 3G(r) \left(\frac{\lambda r}{r^2}\right)^{-1} J_1\left(\frac{\lambda r}{r^2}\right) \right\}. \quad (8b)$$

with  $J_0$  and  $J_1$  the spherical Bessel functions of order 0 and 1, respectively, and the function  $G(r)$  defined by

$$G(r) \equiv \frac{1}{r^6} (F^2 - 2fF), \quad F(r) \equiv 3f - r \frac{df}{dr}. \quad (9)$$

In the case of Coulomb interactions ( $a_D = 0$ ), the functions (8) reduce to

$$I_1(\lambda) = \delta\lambda^{-3/2}, \quad I_2(\lambda) = -I_1(\lambda), \quad (10)$$

with  $\delta = \frac{9}{2} \left(\frac{\pi}{2}\right)^{1/2}$ .

On the other hand, an angular integration of the functions  $A_1(a)$  in Eqs. (1) - (3) gives

$$A_1(a) = \frac{1}{2\pi^2 Q(a)} \int_0^\infty d\lambda \lambda^2 e^{I(\lambda)} \left\{ I_1(\lambda) J_0(a\lambda) + I_2(\lambda) \frac{J_1(a\lambda)}{(a\lambda)} \right\}, \quad (11)$$

$$A_2(a) = \frac{1}{2\pi^2 Q(a)} \int_0^\infty d\lambda \lambda^2 e^{I(\lambda)} \left\{ [I_1(\lambda) + I_2(\lambda)] J_0(a\lambda) - 2I_2(\lambda) \frac{J_1(a\lambda)}{(a\lambda)} \right\}, \quad (12)$$

$$A_3(a) = \frac{1}{8\pi^2 Q(a)} \int_0^\infty d\lambda \lambda^4 e^{I(\lambda)} \{ I_1(\lambda) + I_2(\lambda) \} J_0(a\lambda), \quad (13)$$

where the variable  $\vec{a}$  has been replaced by  $\vec{a} \rightarrow \vec{a}/E_{01} = (\vec{e} + \vec{e}_0)/2$  and the microfield distribution  $Q(a)$  is given by



$$Q(a) = \frac{1}{2\pi^2} \int_0^{\infty} d\lambda \lambda^2 e^{I(\lambda)} j_0(a\lambda), \quad (14)$$

with  $I(\lambda)$  from (6). The function  $A_3(a)$  in (13) is expected not to play an important role in the dynamics at short times. In particular; from (10) we have  $A_3(a) = 0$  for Coulomb fields; this result also applies at large values of the fields, since these values correspond to close configurations for which the screening is not taking place yet. The results from a numerical integration of the coefficients  $A_1$  and  $A_2$  in (11)-(12) are shown in Fig.8. There, we have chosen the value  $a_D = 0.613$  for the inverse Debye length, as it will be justified later on (§4.3). The values of  $A_1, A_2$ , computed in this way present a very good agreement with the analytical asymptotic limits. For the sake of future reference, we write here the asymptotic large field limit for these coefficients,

$$\lim_{a \gg 1} A_1(a) = a^3, \quad \lim_{a \gg 1} A_2(a) = 4a^3, \quad \lim_{a \gg 1} A_3(a) = 0. \quad (15)$$

In order to study the electric field dynamics at short times, we have chosen the conditional probability density instead of the joint probability density; both distributions are proportional to each other for a given value of the initial field. For simplicity, as well as for a future comparison with some available results from computer simulations, we analyze the case with  $\vec{E}_\perp = 0$ , where  $\vec{E}_\perp$  is that component of  $\vec{E}$  perpendicular to  $\vec{e}_0$ . Without loss of generality, we also assume that  $\vec{E}_0 = c_0 \hat{z}$ . A dimensionless time  $w_{pi} t \rightarrow t$  is introduced, with  $w_{pi}$  the ion plasma frequency ( $Z_1 = 1$ ). We denote by  $P(c_z, t | c_0, 0)$  the probability density associated with the vector  $\vec{E}$ , evaluated at fields with  $\vec{E}_\perp = 0$ . This function should not be confused with the conditional probability density for the z-component of the field regardless of the other components, and which satisfies a different normalization condition.

Thus, the conditional probability density (2.4.6) reduces to

$$P(c_z, t | c_0, 0) = \frac{Q(a)}{Q(c_0)} \frac{e^{A_3 t^2 / 2}}{4\pi t^2 A_1} \frac{e^{-(c_z - c_0)^2 / 4A_2 t^2}}{(4\pi t^2 A_2)^{1/2}}, \quad (16)$$

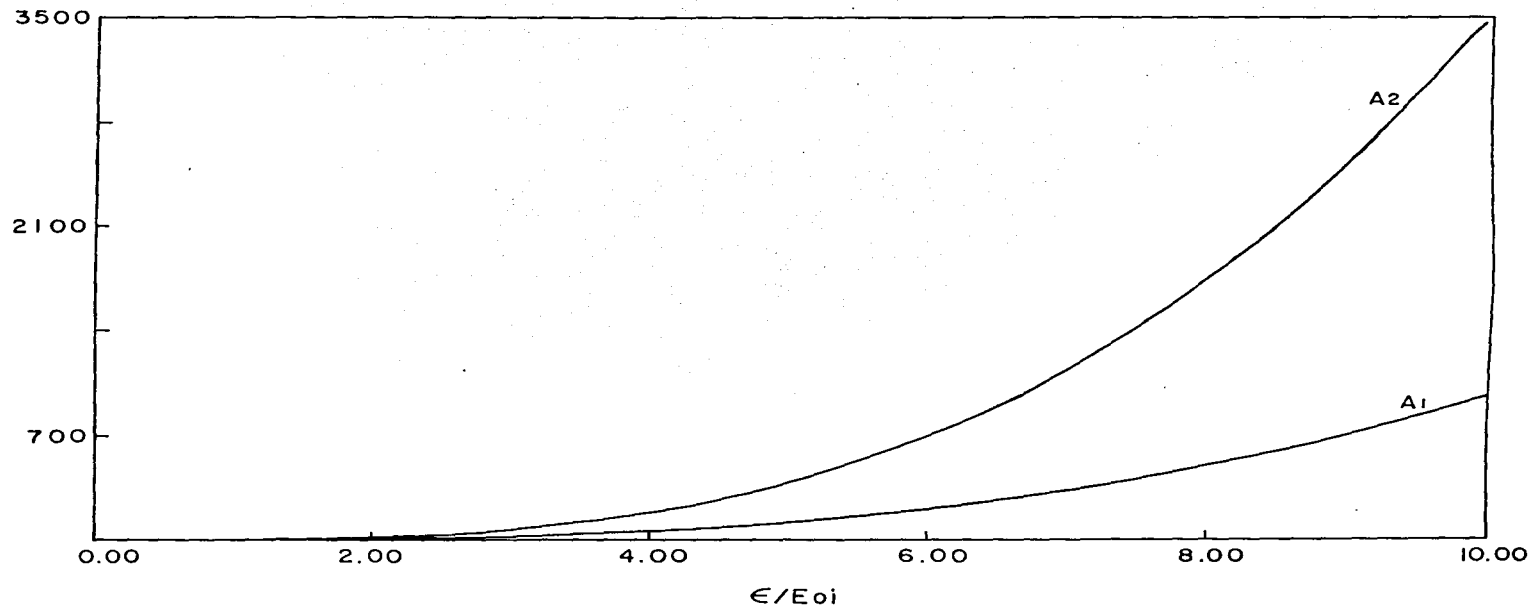


Fig.8. Coefficients  $A_1$  and  $A_2$  (Eqs.4.2.11 and 4.2.12) as a function of the field magnitude, for a system of non-interacting ions and a neutral point (Debye fields).

with  $A_1(a)$  from (11)-(13). The distribution (16) is studied here as a function of  $\epsilon_z$  at different times  $t$ , for fixed given values of the initial field  $\epsilon_0$ . In relation to this latter, the value  $\epsilon_0 = 1$  is particularly interesting since it corresponds to that field at which the microfield distribution  $P(\epsilon)$  presents its maximum (Coulomb fields), as shown in Fig.9.

The results from the conditional probability (16) for some given values of  $\epsilon_0$  are shown in Figs.10-12. In all cases,  $P(\epsilon_z, t | \epsilon_0, 0)$  presents the same qualitative behavior: an asymmetric broadening of the initial delta function and a monotonic shift of the peak towards smaller fields. The decay of the peak is monotonic for small  $\epsilon_0$ ; for large  $\epsilon_0$ , it raises again at longer times. All this is in contrast to the Model Microfield distribution (Brissaud and Frisch, 1971), for which the amplitude of the delta function is simply attenuated in time. In addition, for values of  $\epsilon_0$  with high probability to occur (see Fig.10), the decay of the peak is not only monotonic but also slow. In contrast, for less probable values of  $\epsilon_0$  the initial decay is very abrupt (see Fig.12). These facts suggest distinguishing between two different processes, one for small  $\epsilon_0$  and another one for large  $\epsilon_0$ . Ultimately, the graphs show that at later times the peak position reaches the equilibrium value and continues towards the negative region. This is an obvious limitation of the distribution (16), which has not been constraint to reach the equilibrium value as  $t \rightarrow \infty$ .

Additional interesting results arise from the comparison between Coulomb and Debye cases. Figs.13 and 14 show that at short times the differences between both cases become smaller as larger values of the field are considered. This is easily understandable if large field values are regarded as produced by close configurations, corresponding to ions inside the screening radius for Debye fields. At longer times, the free streaming of the ions makes the former no longer true.

#### 4.3. Comparison of results to some limited computer simulation data

In order to establish the limits of applicability of our short time result (2.16), we have established a comparison with some limited computer simulation data (Smith, et al., 1984). The simulation data we refer to here, were evaluated at a temperature  $T = 10^4 K$  and an ion density  $n_i = 10^{17} \text{ cm}^{-3}$ , using 125 ions in a sphere of radius  $5r_{01}$ . The corresponding plasma parameter  $\Gamma_i$  was therefore 0.125, so that the inverse Debye length

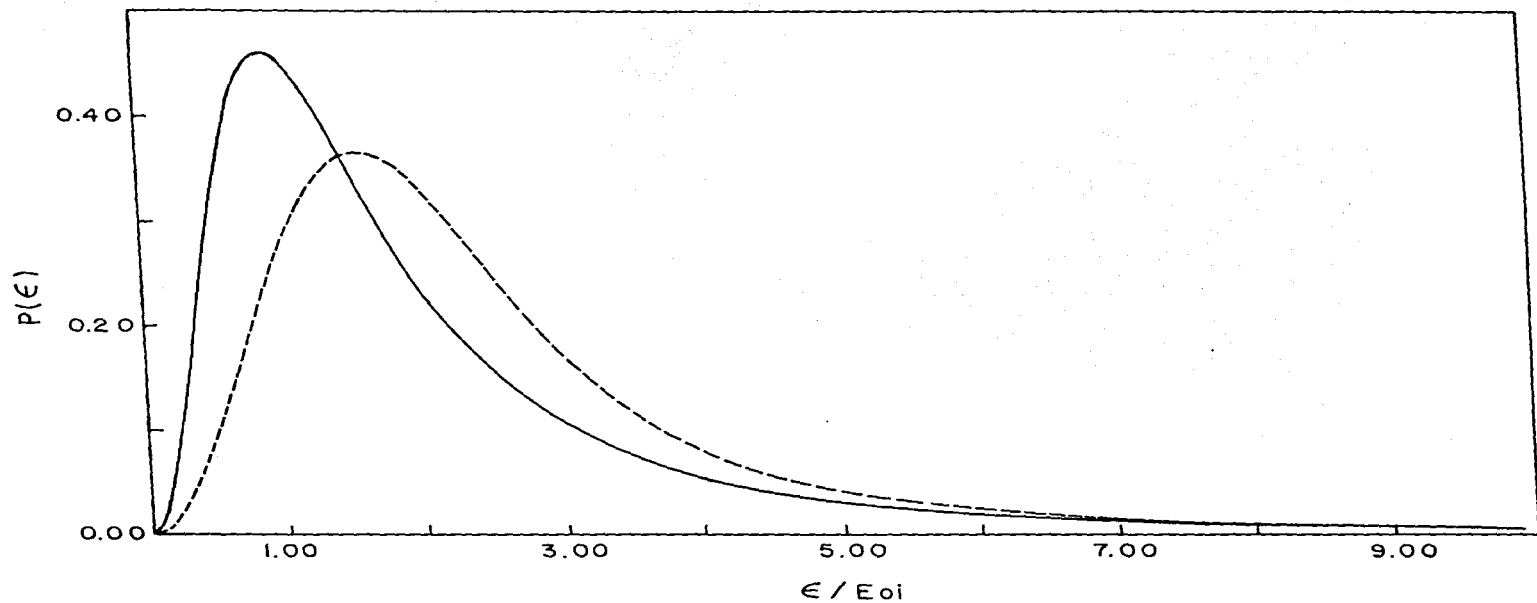


Fig.9. Microfield distribution for a system of non-interacting ions and a neutral point, for both Debye (—) and Coulomb (- - -) fields.

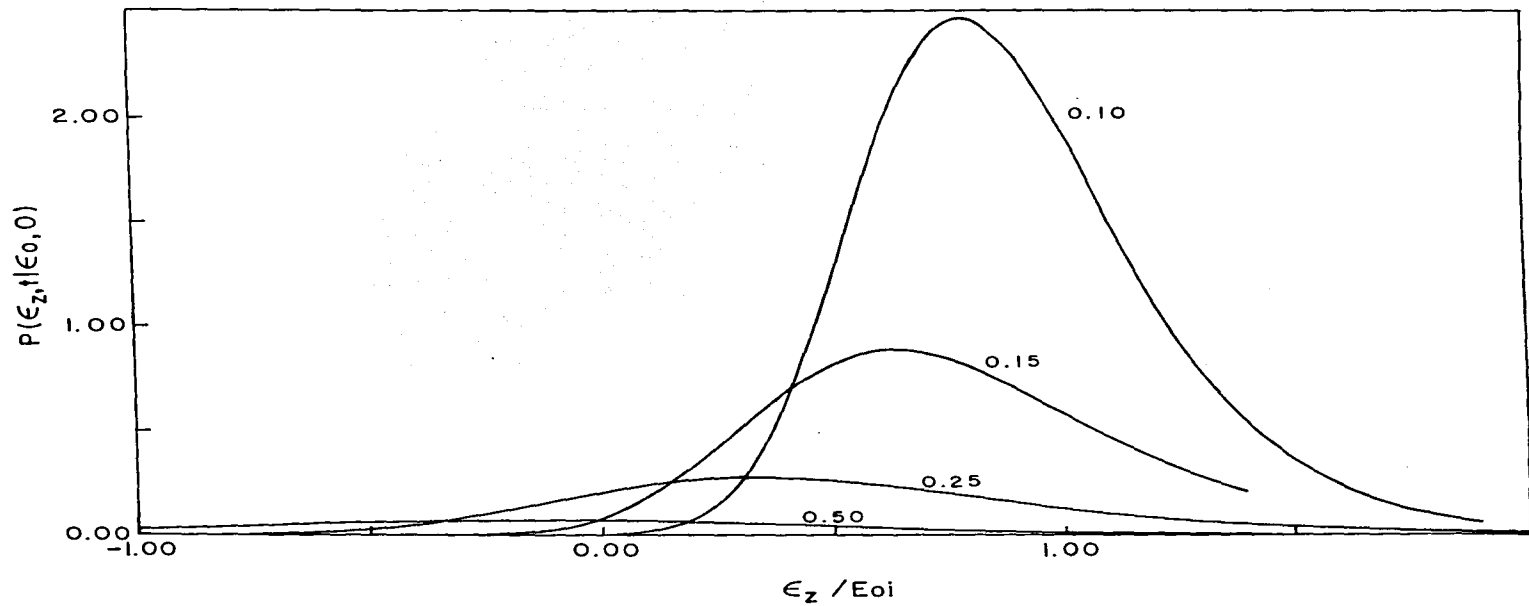


Fig. 10. Conditional probability density (4.2.16) for  $\epsilon_0 = 1$  (Debye fields) at  $w_{p1} t = 0.10, 0.15, 0.25, 0.50$ .

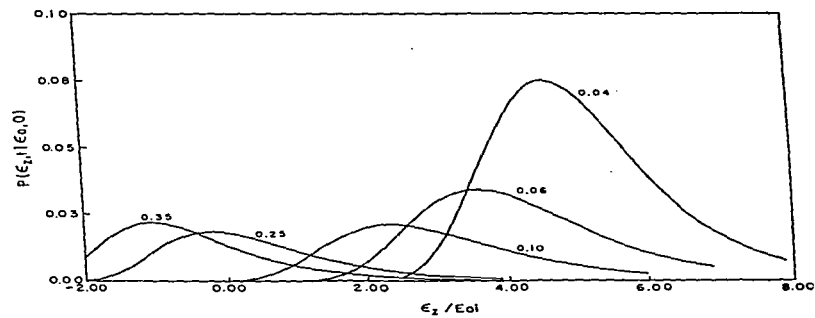
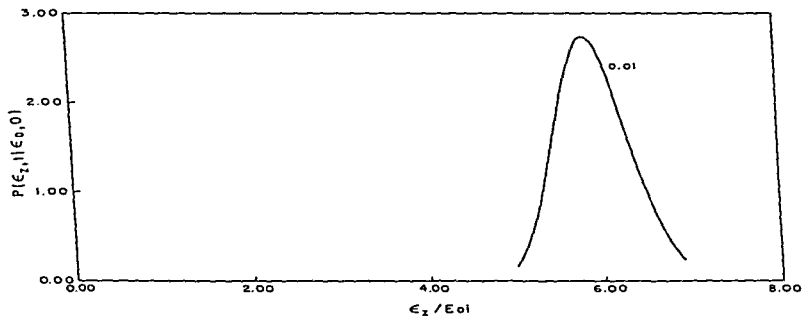


Fig. 11 - Conditional probability density (4.2.16) for  $\epsilon_0 = 6$  (Debye fields)  
 at (a)  $\omega_{p1} t = 0.01$ , and (b)  $\omega_{p1} t = 0.04, 0.06, 0.10, 0.25, 0.35$ .

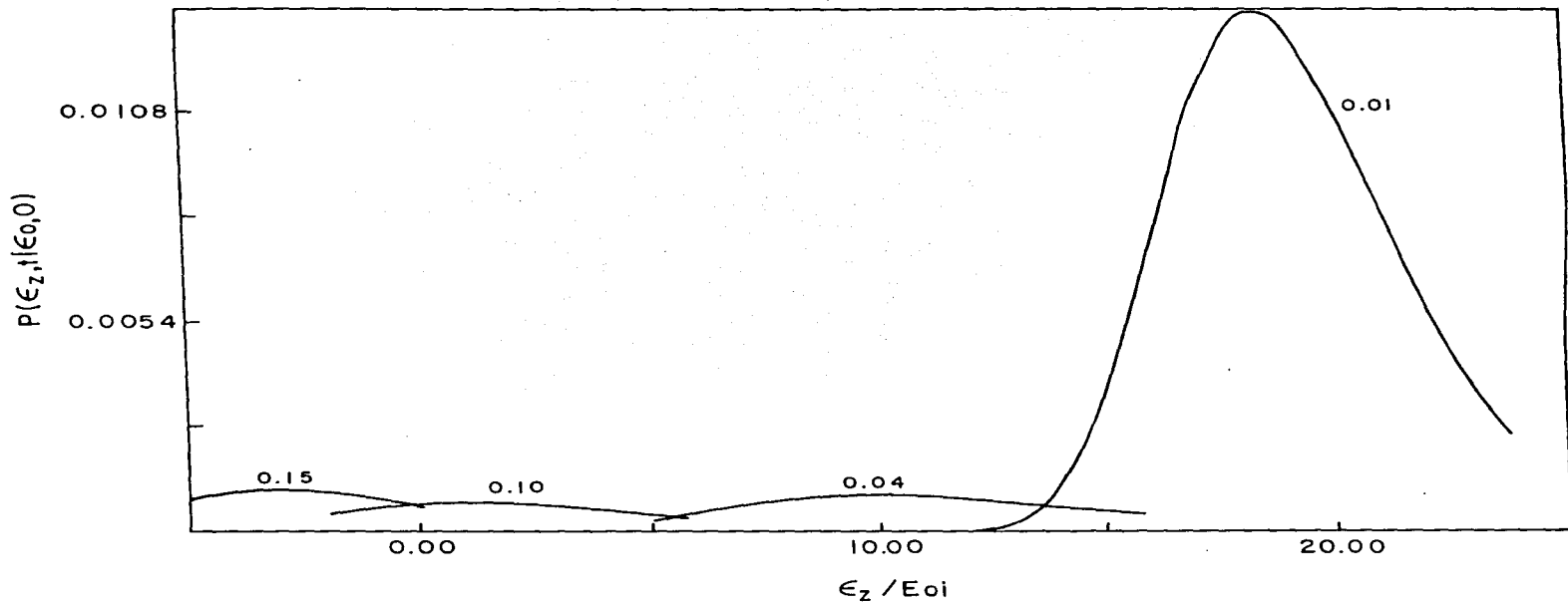


Fig. 12. Conditional probability density (4.2.16) for  $\epsilon_0 = 20$  (Debye fields) at  $w_{pi} t = 0.01, 0.04, 0.10, 0.15$ .

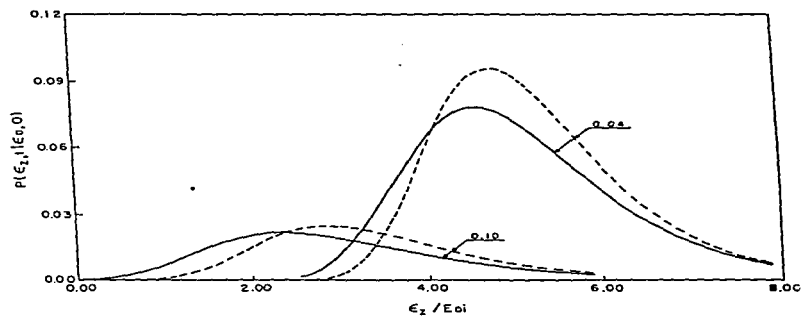
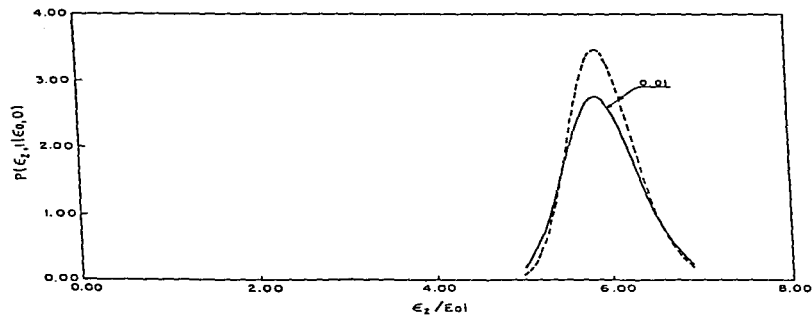


Fig.13. Conditional probability density (4.2.16) for  $\epsilon_0 = 6$ , for Debye (—) and Coulomb (- - -) fields, at (a)  $w_{p1}t = 0.01$ , and (b)  $w_{p1}t = 0.04, 0.10$ .



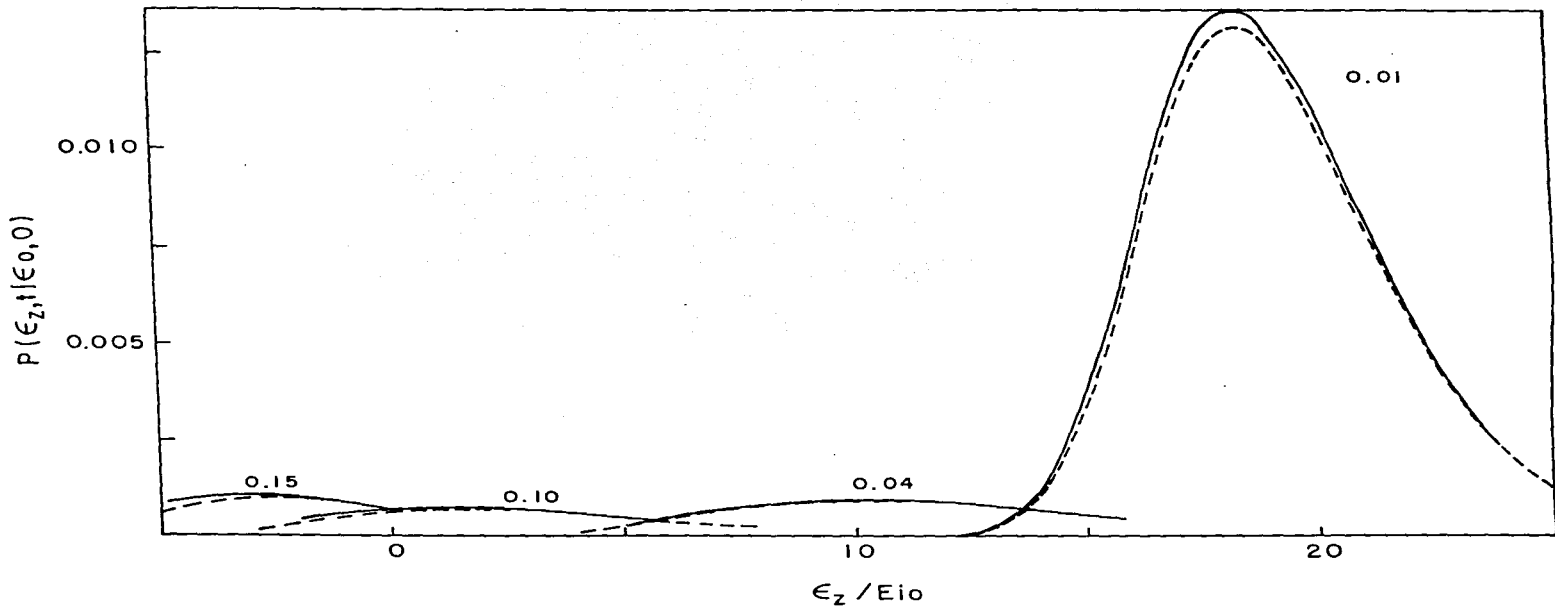


Fig. 14. Conditional probability density (4.2.16) for  $\epsilon_0 = 20$ , for Debye (—) and Coulomb (- - -) fields, at  $w_{pi} t = 0.01, 0.04, 0.10, 0.15$ .

$a_D (\sqrt{3}\Gamma_1)$  was 0.613. The details of that simulation can be found in (Stamm and Smith, 1984a).

The results from this comparison are shown in Figs.15-17. At each chosen value for the initial field, a fixed renormalization of our results was performed to fit the simulation data at the earliest time. In all the cases considered, our results present a shifting of the peak to the left of the simulation data; the width is also broader. Our results look like if they would constitute later stages in the evolution of those from simulation. The disagreement worsen as time increases (compare, for instance, Figs.11b and 12b. In contrast with this inappropriate behavior for the peak position and the width, in most of cases the  $h_{e1}, h_i$  fits well.

A possible interpretation to the former disagreements is that our approximation is limited to time intervals shorter than those considered in the simulation data. In fact, in keeping only the leading term in the time expansion (2.4.3) for  $\mathcal{F}(\vec{E}, \vec{n}; t)$ , we have assumed that the next contributions are negligible; this might be not necessarily true, since the coefficients corresponding to each order in time are also functions of the field, and hence an appropriate convergence in (2.4.3) is strongly dependent on both the time and field values. More specifically, we already know that the coefficient associated with the first non-vanishing power of  $t$  (namely,  $t^2$ ) is related to the average  $\langle \dot{E}^2 \rangle_a$ , which increases monotonically with the field; the coefficients corresponding to the next non-vanishing correction (order  $t^4$ ) are related to the averages  $\langle E^2 \rangle_a$ ,  $\langle E^4 \rangle_a$  and  $\langle \dot{E}^2 \rangle_a^2$ , which are even more singular than  $\langle \dot{E}^2 \rangle_a$ . An alternative explanation for the discrepancies above may be related with incorrect parameters reported for the simulation. This is based on the fact that excellent agreements may be obtained if the time is scaled appropriately. In addition, it is also probable that the boundary conditions used in the simulation (Stamm and Smith, 1984a) introduce additional effects not considered in our model. The lack of additional computer simulation results, as well as alternative theoretical models, makes difficult to clarify the origin of the problem.

#### 4.4. An approximation for large fields: the single-ion model

A particular case of interest is that for large fields, already discussed in §3.2 from a general perspective. Here, we particularize those results to the case of non-interacting ions and a neutral point.

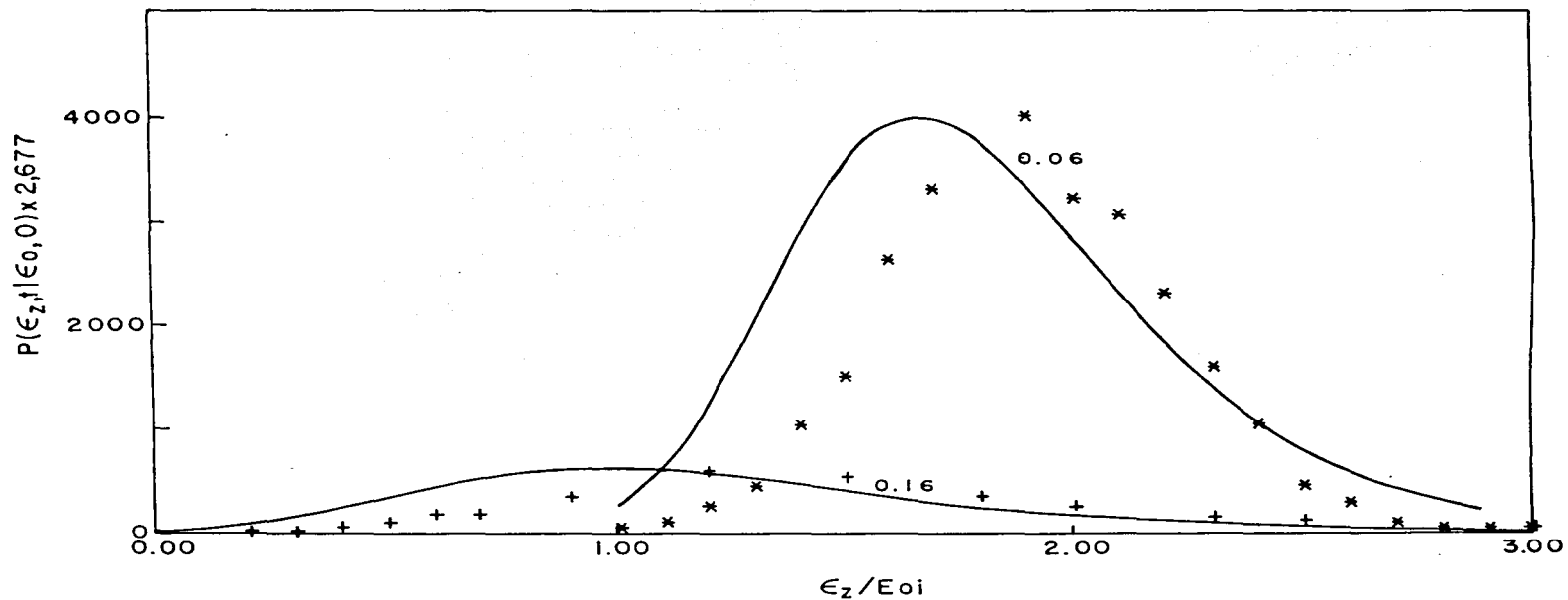


Fig.15. Conditional probability density from (4.2.16) (—) and computer simulation, for  $\epsilon_0 = 2$  at  $w_{p1} t = 0.06, 0.16$ .

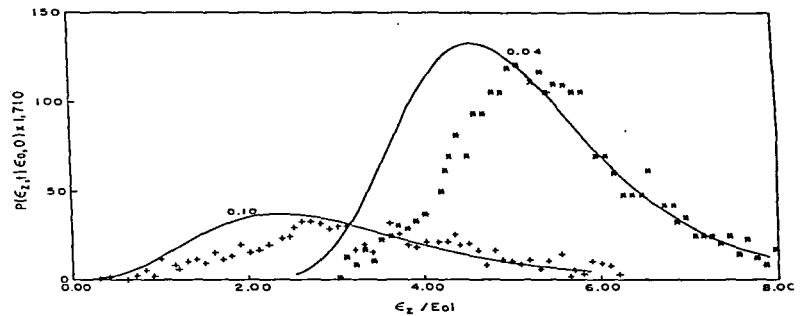
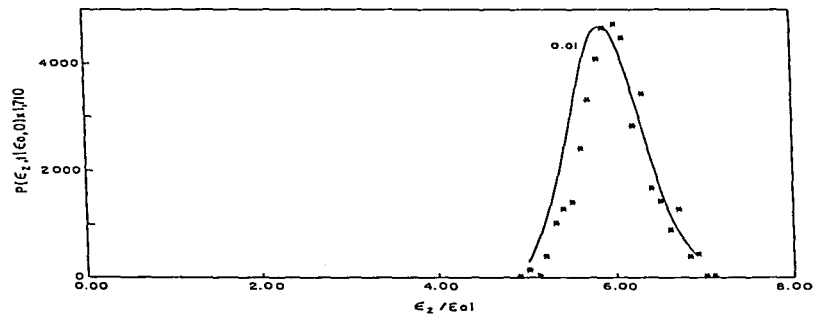


Fig. 16. Conditional probability density from (4.2.16) (—) and computer simulation, for  $\epsilon_0 = 6$  at (a)  $w_{p1}t = 0.01$  and (b)  $w_{p1}t = 0.04, 0.10$ .

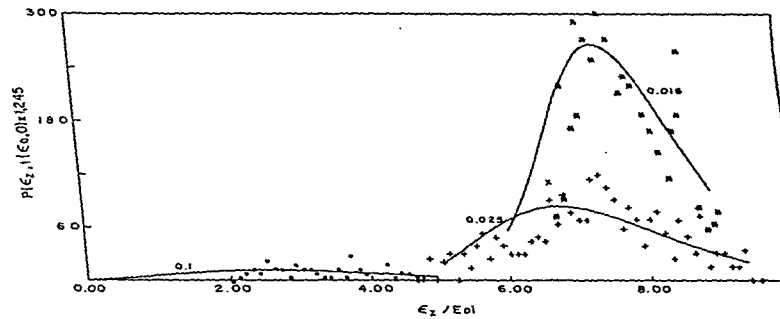
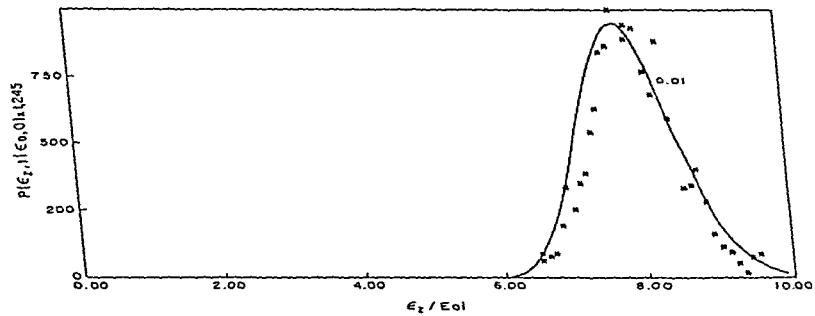


Fig. 17. Conditional probability density from (4.2.16) (—) and computer simulation, for  $\epsilon_0 = 8$  at (a)  $w_{p1} t = 0.01$  and (b)  $w_{p1} t = 0.016, 0.025$ .

Large fields are expected to be produced mainly by configurations close to the field point. According to the results obtained from the cluster expansion for the generating function (§3.2), the contributions at large fields are associated with one or two particles passing the field point. In this case, the static and dynamical properties of the electric field are properly described by Eqs. (3.2.2) and (3.2.5), respectively. In particular, for the case of non-interacting ions and a neutral point, those expressions reduce to

$$Q \rightarrow Q_1(\epsilon_0) = n_1 \int d\vec{q}_1 \delta(\vec{\epsilon}_0 - \vec{E}(\vec{q}_1)) , \quad (1)$$

$$f \rightarrow f_1(\vec{\epsilon}, t; \vec{\epsilon}_0, 0) = n_1 \int d\vec{q}_1 d\vec{v}_1 f(\vec{v}_1) \delta(\vec{\epsilon} - \vec{E}(\vec{q}_1 + \vec{v}_1 t)) \delta(\vec{\epsilon}_0 - \vec{E}(\vec{q}_1)) , \quad (2)$$

where the notation stresses the fact that the corresponding static and dynamical distributions describe the field from a single ion only. In writing (2), we have made explicit use that the ions do not interact with each other. The function  $f(\vec{v})$  in (2) is the Maxwell-Boltzmann distribution (McQuarrie, 1976),

$$f(\vec{v}) d\vec{v} = \left( \frac{m_1}{2\pi k_B T} \right)^{3/2} e^{-m_1 v^2 / 2k_B T} d\vec{v} . \quad (3)$$

Eq. (1) gives the probability density for the field due to a single ion to have a value  $\vec{\epsilon}_0$  at  $t = 0$ , and Eq. (2) the probability density for that field to change into another value  $\vec{\epsilon}$  at time  $t$ . This latter is expected to apply only at times short enough for the ion not to move far away from the initial close distance from the field point. Ultimately, a conditional probability density may be also defined from Eqs. (1) and (2),

$$P_1(\vec{\epsilon}, t | \vec{\epsilon}_0, 0) = f_1(\vec{\epsilon}, t; \vec{\epsilon}_0, 0) / Q_1(\epsilon_0) . \quad (4)$$

To further evaluation of the single particle distributions  $Q_1$  and  $f_1$ , one can consider Coulomb fields in (1) and (2). This is because the effects of screening are practically negligible at large fields. The details of such a calculation are given in Appendix D and summarized here as follows,

$$Q_1(\epsilon_0) = \frac{n_1}{2} (Z_1 e)^{3/2} \epsilon_0^{-9/2}, \quad (5)$$

$$f_1(\vec{z}, t; \vec{\epsilon}_0, 0) = \frac{n_1}{4} \frac{(Z_1 e)^3 (\epsilon \epsilon_0)^{-9/2}}{(\pi u^2 t^2)^{3/2}} \exp\left\{-\frac{Z_1 e}{(ut)^2} \left(\frac{\hat{\epsilon}}{\sqrt{\epsilon}} - \frac{\hat{\epsilon}_0}{\sqrt{\epsilon_0}}\right)^2\right\}. \quad (6)$$

In particular, note that the distribution (5) is also the asymptotic (*i.e.* large  $\epsilon_0$ ) Holtmark result (Griem, 1974). In order to compare these results with the short time limit (§4.2) at large fields, we introduce here the dimensionless variables defined in (2.5). In this case, the distributions (4) and (5) become

$$Q(\vec{\epsilon}_0) = \frac{3}{8\pi} \epsilon_0^{-9/2}, \quad (7)$$

$$P_1(\vec{z}, t | \vec{\epsilon}_0, 0) = \frac{N_1}{2} \left(\frac{a_D^2}{2\pi t^2}\right)^{3/2} \epsilon^{-9/2} \exp\left\{-\left(\frac{a_D^2}{2t^2}\right) \left(\frac{\hat{\epsilon}}{\sqrt{\epsilon}} - \frac{\hat{\epsilon}_0}{\sqrt{\epsilon_0}}\right)^2\right\}. \quad (8)$$

We also consider  $\vec{\epsilon}_0 = \epsilon_0 \hat{z}$  and  $\vec{z} \parallel \vec{\epsilon}_0$ . In terms of the variable "a" previously introduced, the single-ion conditional probability (8) at large fields and short times becomes

$$\lim_{a \gg 1} P_1(\epsilon_z, t | \epsilon_0, 0) = \frac{N_1}{2} \left(\frac{a_D^2}{2\pi t^2}\right)^{3/2} a^{-9/2} \exp\left\{-\left(\frac{a_D^2}{2t^2}\right) \left(\frac{\epsilon_z - \epsilon_0}{(4a)^3}\right)^2\right\}. \quad (9)$$

This expression is the same obtained from the short time limit (2.16) if the asymptotic large field value (2.15) for the coefficients  $A_1(a)$  is taken into account. Thus, the conditional probability (9) describes appropriately the dynamics of very large fields at short times.

To conclude, Figs. 18 and 19 show a comparison between the conditional probability corresponding to both N-particles and single-ion models, at two different values,  $\epsilon_0 = 6$  and  $\epsilon_0 = 20$ , for the initial field. Based on the discussion above, only Coulomb fields are considered. From those graphs it is clear that a very good agreement is obtained only at large field values and very short times.

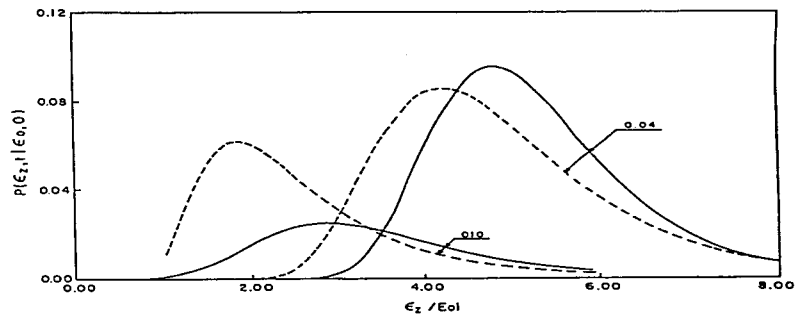
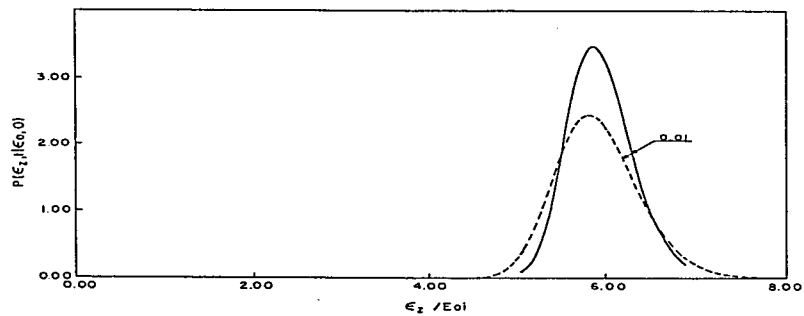


Fig. 18. Conditional probability density from N-particle model (---) and single-ion model (—), for  $c_0 = 6$ , at times (a)  $\omega_{p1} t = 0.01$ , and (b)  $\omega_{p1} t = 0.04, 0.10$  (Coulomb fields).



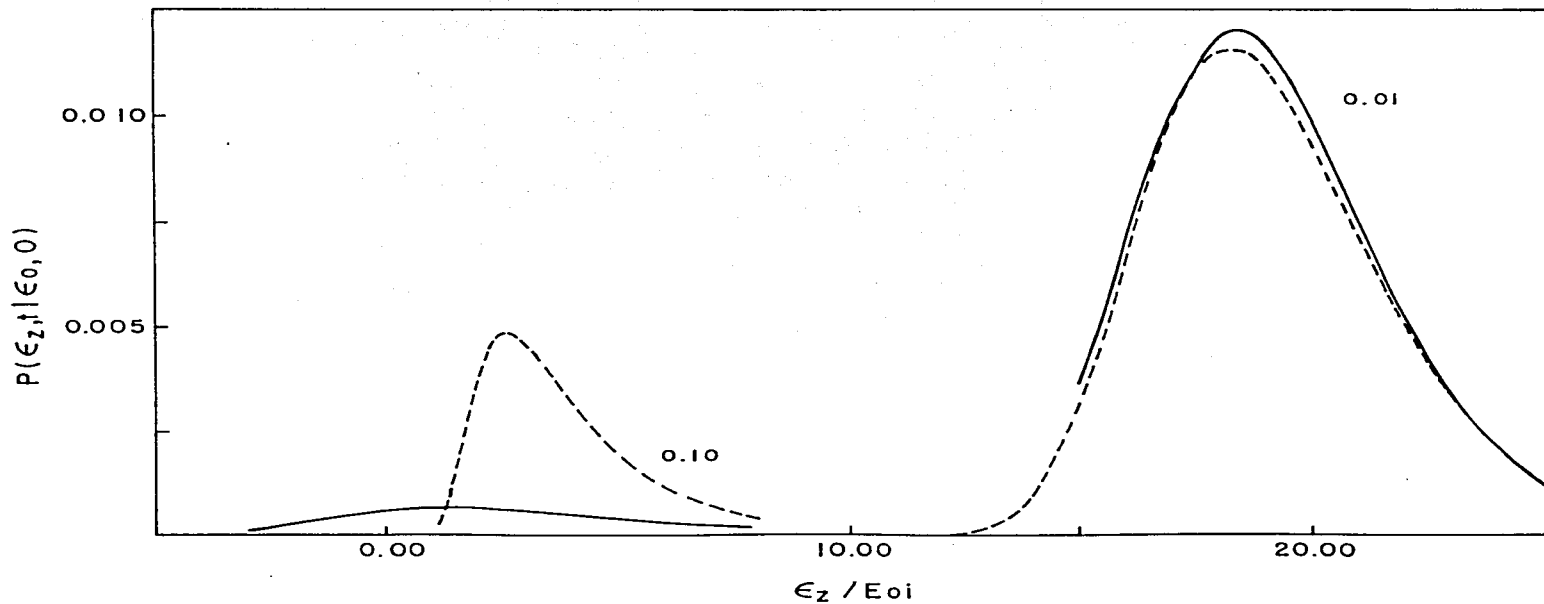


Fig.19. Conditional probability density from N-particle model (---) and single-ion model (—), for  $\epsilon_0 = 20$ , at times  $\omega_{pi} t = 0.01, 0.10$  (Coulomb fields).

## CHAPTER 5

### ALTERNATIVE APPROACHES BASED ON STOCHASTIC PROCESSES

#### 5.1. Introduction

The results in previous chapters give the exact behavior of the dynamical distribution at the various interesting asymptotic limits (Gaussian, short time, high field,...) in which the problem can be reduced to quadratures. In particular, we have learned that the conditional probability  $P(\vec{c}, t | \vec{c}_0, 0)$  at short times describes anisotropic diffusion in which the initial  $\delta$ -distribution spreads and shifts towards smaller field values. The way this distribution approaches the equilibrium value,  $Q(c)$ , at longer times is highly dependent on the intensity of the initial field  $\vec{c}_0$ : for small values of  $c_0$  the decay of the peak is monotonic, whereas for large values the distribution reaches a minimum value at an intermediate time, rising afterwards towards  $Q(c)$ . The first case is associated with the electric field produced by distant configurations; the second case, in contrast, is related to initial configurations with a few close particles producing a large field at the field point. We believe that these two aspects (due to distant and close configurations) are relevant not only at short times, but they appear throughout the entire dynamical evolution of the fields in the plasma. This expectation, as well as the serious numerical difficulties associated with the exact description, justify looking for an alternative approach in which the two former aspects of electric fields may be combined in a simpler way.

We consider here an alternative approach to the exact description, in which the electric field  $\vec{E}(t)$  is regarded as a stochastic variable whose variations characterize the statistical properties associated with the two aspects above. In particular, we assume that  $\vec{E}(t)$  changes according to a stationary Markov process, so that the dynamical properties for this variable are fully determined by the microfield distribution,  $Q(c)$ , and the conditional probability  $P(\vec{c}, t | \vec{c}_0, 0)$ . Also as a consequence of the Markov

assumption, this latter distribution satisfies a Master Equation, whose characteristics are forced to reproduce the various exact results ( $\langle \vec{E}(t) \cdot \vec{E} \rangle$ , steady-state solution, ...) for the system.

More specifically, we regard the electric field  $\vec{E}(t)$  as a stepwise constant stochastic process, which jumps at randomly chosen times (jumping times) between random step values. The electric field takes a series of values  $\vec{E}(t) = \vec{e}_1$  at the times  $t_1$  ( $i = 1, \dots, n$ ), and the random vectors  $\vec{e}_1$  are chosen independently with the same probability distribution,  $Q(\epsilon)$ . The times  $t_1$  are independently distributed in  $(-\infty, \infty)$  according to a given density frequency,  $\nu(\vec{e})$ , which is field dependent in the general case. The probability to find given values of the field at given times is described by the joint probability distribution  $f_n(\vec{e}_n t_n; \vec{e}_{n-1} t_{n-1}; \dots; \vec{e}_1 t_1)$ . For this function, the Markov assumption implies

$$f_n(\vec{e}_n t_n; \dots; \vec{e}_1 t_1) = P(\vec{e}_n t_n | \vec{e}_{n-1} t_{n-1}) \cdot \dots \cdot P(\vec{e}_2 t_2 | \vec{e}_1 t_1) f_1(\vec{e}_1 t_1), \quad (1)$$

where  $P$  is the conditional probability density and  $f_1$  is the probability density for a given value at a given time. In particular, for a stationary process the distribution  $f_1$  is time-independent\*. According to the property (1), a Markov process is fully determined by the two distributions  $P$  and  $f_1$ . These two distributions can not be chosen arbitrarily, but obey the following identities,

$$f_1(\vec{e}_2 t_2) = \int d\vec{e}_1 P(\vec{e}_2 t_2 | \vec{e}_1 t_1) f_1(\vec{e}_1 t_1), \quad (2)$$

$$P(\vec{e}_3 t_3 | \vec{e}_1 t_1) = \int d\vec{e}_2 P(\vec{e}_3 t_3 | \vec{e}_2 t_2) P(\vec{e}_2 t_2 | \vec{e}_1 t_1); \quad (3)$$

this latter is called the Chapman-Kolmogorov equation.

We now restrict ourselves to a subclass of Markov process for which

$$P(\vec{e}, t + \Delta t | \vec{e}', t) \xrightarrow{\Delta t \rightarrow 0} A \delta(\vec{e} - \vec{e}') + \Delta t W(\vec{e} | \vec{e}'), \quad (4)$$

where  $W(\vec{e} | \vec{e}')$  is called the transition rate ( $W \geq 0$ ) and  $A$  is a normalization condition.

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\* In our case  $f_1$  is the microfield distribution  $Q(\epsilon)$ .

$$A = 1 - \nu(\vec{c}')\Delta t, \quad (5)$$

with  $\nu(\vec{c}')$  the frequency density defined by

$$\nu(\vec{c}') = \int d\vec{c} W(\vec{c}|\vec{c}'). \quad (6)$$

For an isotropic plasma, the frequency (6) depends on the field through the magnitude only, that is  $\nu = \nu(c')$ . The inverse of this function is the average duration of a field of strength  $c'$ , so that for time separation much larger than  $1/\nu(c')$  the microfields are weakly correlated. Finally, since  $\nu\Delta t$  is the probability that at least one jump occurs in the time interval  $(0, \Delta t)$ , the normalization factor  $A$  in (4) gives the probability for no jumps occurring in that time interval.

Substitution of (4) and (5) into (3) gives the differential form of the Chapman-Kolmogorov equation,

$$\frac{\partial}{\partial t} P(\vec{c}t|\vec{c}'t') = -\nu(\vec{c})P(\vec{c}t|\vec{c}'t') + \int d\vec{c}'' W(\vec{c}|\vec{c}'')P(\vec{c}''t''|\vec{c}'t'), \quad (7)$$

which is better known in Physics as a Master Equation. Equivalently, using (6) this latter may be also written as

$$\frac{\partial}{\partial t} P(\vec{c}t|\vec{c}'t') = \int d\vec{c}'' \{W(\vec{c}|\vec{c}'')P(\vec{c}''t''|\vec{c}'t') - W(\vec{c}'|\vec{c}'')P(\vec{c}t|\vec{c}'t')\}. \quad (8)$$

The transition rate  $W$  here contains information about the statistical properties of electric field fluctuations in the plasma (Van Kampen, 1980). In the case of strong fluctuations, for instance, the value of the field after a jump is practically independent of the value it had before the jump. A model consistent with this is one in which the transition rate  $W(\vec{c}|\vec{c}')$  is given by the product form

$$W(\vec{c}|\vec{c}') = w_1(\vec{c}')w_2(\vec{c}), \quad (9)$$

with  $w_1$  and  $w_2$  two independent functions associated with the initial and final states, respectively. Examples of such processes with *no memory* are the Poisson Step Process and the Kangaroo Process, discussed in §5.2. They are referred to here as Strong Fluctuation models. On the other hand,

small fluctuations necessarily imply processes with *memory* for which the probability to find the value  $\vec{c}$  after the jump is peaked around the value  $\vec{c}'$  before the jump. A plausible model in one in which the transition rate  $W(\vec{c}|\vec{c}')$  is given by

$$W(\vec{c}|\vec{c}') = w_1(\vec{c}')w_2(\vec{c}-\vec{c}'), \quad (10)$$

with  $w_2(\delta\vec{c})$  a function that is peaked about  $\delta\vec{c} = 0$ . Examples of such models are discussed in §5.3. They are referred to as Diffusion models. Finally, in all the models to be considered, the steady-state solution to the corresponding Master Equation has been chosen to be the microfield distribution,  $Q(\epsilon)$ , in agreement with the expected behavior from the exact description.

## 5.2. Strong Fluctuation models

### 5.2. i. Poisson step process

In a Poisson step process (PSP) (Brissaud and Frisch, 1971) the jumping times for the stochastic field are distributed with a constant frequency  $\nu$ , according to a Poisson distribution. The transition rate for the PSP is chosen to be

$$W(\epsilon|\epsilon') = \nu Q(\epsilon), \quad (1)$$

so that the Master Equation (1.7) reduces to

$$\frac{\partial}{\partial t} P(\vec{c}, t | \vec{c}_0, 0) = -\nu P(\vec{c}, t | \vec{c}_0, 0) + \nu Q(\epsilon), \quad (2)$$

with solution

$$P(\vec{c}, t | \vec{c}_0, 0) = e^{-\nu t} \delta(\vec{c}-\vec{c}_0) + (1 - e^{-\nu t})Q(\epsilon). \quad (3)$$

The conditional probability (3) is given by the sum of two contributions: a  $\delta$ -distribution at  $\vec{c} = \vec{c}_0$  that decays away with time, and a symmetric distribution about  $\vec{c} = 0$  that increases with time and finally approaches the equilibrium distribution,  $Q(\epsilon)$ . This unphysical behavior is

characteristic of processes for which any change in  $\vec{E}$  completely destroys all memory of the initial field.

This model leads to some additional difficulties concerning the electric field autocorrelation  $\langle \vec{E}(t) \cdot \vec{E} \rangle$ . Indeed, using the conditional probability (3) to calculate the average  $\langle \vec{E}(t) \cdot \vec{E} \rangle$  we have

$$\langle \vec{E}(t) \cdot \vec{E} \rangle = \int d\vec{E} Q(\epsilon) \epsilon^2 e^{-\nu t}. \quad (4)$$

This integral is divergent for all times in the case of a neutral point, contrarily to the exact result. Thus, this model is limited to charged points only. A generalization to this model, which is also simple and provides a partial solution to the former difficulty, is the so called Kangaroo Process defined in the following.

### 5.2. ii. Kangaroo process

The Kangaroo Process (KP) is a generalization to the PSP, which was first introduced by Brissaud and Frisch (1971) in their Model Microfield Method (MMM) to describe spectral line shapes. In a KP the separation between successive electric field jumps is also distributed according to a Poisson law but with a field dependent frequency,  $\nu(\epsilon)$ . For the case of an isotropic plasma, the transition rate  $W(\epsilon|\epsilon')$  in this model is chosen to be

$$W(\epsilon|\epsilon') = \nu(\epsilon') w(\epsilon). \quad (5)$$

The function  $w(\epsilon)$  here is chosen so that the microfield distribution,  $Q(\epsilon)$ , is the steady-state solution for the corresponding Master Equation, that is,

$$w(\epsilon) = \frac{\nu(\epsilon) Q(\epsilon)}{\langle \nu \rangle}, \quad \langle \nu \rangle = \int d\vec{E} \nu(\epsilon) Q(\epsilon). \quad (6)$$

Thus the Master Equation for the KP becomes

$$\frac{\partial}{\partial t} P = -\nu(\epsilon) P(\vec{z}, t | \vec{z}_0, 0) + \frac{\nu(\epsilon) Q(\epsilon)}{\langle \nu \rangle} \int d\vec{E}' \nu(\epsilon') P(\vec{z}', t | \vec{z}_0, 0). \quad (7)$$

An exact analytical solution to Eq. (7) can be obtained by introducing the Laplace Transformed conditional probability,  $P(\vec{z}, z | \vec{z}_0, 0)$ , with

$$P(\vec{z}, t | \vec{z}_0, 0) = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} dz e^{zt} P(\vec{z}, z | \vec{z}_0, 0); \quad (8)$$

in this case, it can be shown that

$$P(\vec{z}, z | \vec{z}_0, 0) = \frac{1}{\nu(\epsilon) + z} \left\{ \delta(\vec{z} - \vec{z}_0) + \nu(\epsilon) Q(\epsilon) \frac{I(z, \epsilon_0)}{z \langle I(z) \rangle} \right\}, \quad (9)$$

with

$$I(z, \epsilon) = \frac{\nu(\epsilon)}{\nu(\epsilon) + z}, \quad \langle I(z) \rangle = \int d\vec{z} Q(\epsilon) I(z, \epsilon). \quad (10)$$

From (8)-(10) the conditional probability  $P(\vec{z}, t | \vec{z}_0, 0)$  is given by

$$P = e^{-\nu(\epsilon)t} \delta(\vec{z} - \vec{z}_0) + \frac{\nu(\epsilon) Q(\epsilon)}{\langle \nu \rangle} \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} dz \frac{e^{zt}}{z (\nu(\epsilon) + z)} \frac{I(z, \epsilon_0)}{\langle I(z) \rangle}. \quad (11)$$

To our purposes, it is enough noting here that the conditional probability (11) may be written as

$$P(\vec{z}, t | \vec{z}_0, 0) = e^{-\nu(\epsilon)t} \delta(\vec{z} - \vec{z}_0) + h(\epsilon, \epsilon_0, t) Q(\epsilon), \quad (12)$$

with  $h(\epsilon, \epsilon_0, t)$  an isotropic function of the magnitude of the electric field  $\vec{z}$  which depends parametrically on  $\epsilon_0$  and  $t$ .

The conditional probability (12) presents the same qualitative features as the distribution (3); in particular, there still remains the unphysical  $\delta$ -contribution at  $t > 0$ . However, in contrast to the PSP model, the electric field autocorrelation  $\langle \vec{E}(t) \cdot \vec{E} \rangle$  here is not necessarily divergent at  $t \neq 0$ . Indeed, from (11) we have

$$\langle \vec{E}(t) \cdot \vec{E} \rangle = \int d\epsilon P(\epsilon) \epsilon^2 e^{-\nu(\epsilon)t}. \quad (13)$$

Thus, the function  $\nu(\epsilon)$  is chosen now in such a way that the RHS of (13) is equal to the exact autocorrelation  $\langle \vec{E}(t) \cdot \vec{E} \rangle$ . To that end, it is useful to assume that  $\nu(\epsilon)$  is a monotonic function with  $\nu(\infty) = \infty$ . This is a reasonable assumption since strong fields are expected to last a shorter

time than more probable small values. Taking  $\nu$  as the new integration variable we obtain

$$\langle \vec{E}(t) \cdot \vec{E} \rangle = \int_{\nu(t_0)}^{\infty} d\nu P(\epsilon) \epsilon^2 \frac{d\epsilon}{d\nu} e^{-\nu t}, \quad (14)$$

which is essentially a Laplace integral. The calculation of  $\nu(\epsilon)$  in terms of the exact autocorrelation  $\langle \vec{E}(t) \cdot \vec{E} \rangle$  requires the inversion of the Laplace transformation and the solution to a simple differential equation. Some examples of this method may be found in Brissaud and Frisch (1974). It is worth mentioning here that the former results are restricted to neutral points only, since the integral in (13) is always a positive function of time.

### 5.2. iii. Additional models

A more general non-Markovian model has been proposed by Seidel (1980) in which a class of stochastic processes known as a renewal process (Cox, 1962) has been used. We simply mention here that the corresponding conditional probability also presents the form (12), with slightly different functions. The important point is that there still remains a non-vanishing contribution from the original  $\delta$ -function. Hence, a similar discussion to that in the previous section applies here.

### 5.3. Diffusion models

#### 5.3.1. The Gaussian model

An example of a Diffusion process is provided by the Gaussian model, already introduced in §2.3 to describe the dynamical properties of weak fields. As shown there, the conditional probability density for that case is given by

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\* As already mentioned in §2.3, the electric field autocorrelation presents a negative portion for charged points.



$$P(\vec{E}, t | \vec{E}_0, 0) = \frac{1}{(1-\alpha(t)^2)^{3/2}} Q_G \left( \frac{\vec{E} - \alpha(t)\vec{E}_0}{(1-\alpha(t)^2)^{1/2}} \right), \quad (1)$$

where  $Q_G(c)$  is the Gaussian distribution (2.3.4) and  $\alpha(t) = \langle \vec{E}(t) \cdot \vec{E} \rangle / \langle E^2 \rangle$  is the equilibrium electric field autocorrelation function, with  $\alpha(0) = 1$  and  $\alpha(\infty) = 0$ . The distribution (1) satisfies the non-Markovian Fokker-Planck equation

$$\frac{\partial}{\partial t} P(\vec{E}, t | \vec{E}_0, 0) = \frac{\partial}{\partial c_1} \gamma(t) \left[ \frac{\partial}{\partial c_1} + 3c_1 / \langle E^2 \rangle \right] P(\vec{E}, t | \vec{E}_0, 0), \quad (2)$$

with steady-state solution  $Q_G(c)$ , and  $\gamma(t) = -\langle E^2 \rangle \dot{\alpha}(t) / 3\alpha(t)$ . Since we are concerned here with Markov processes only, we consider those cases with a time-independent coefficient  $\gamma$ .

The distribution (1) constitutes an improvement over the Strong Fluctuation models above, since now the original  $\delta$ -distribution spreads and shifts towards smaller field values, in qualitative agreement with the exact short time behavior. The changes in the electric field here are described by a process with *memory*, which is more physical than the corresponding *no memory* variations from Strong Fluctuation models. However, the conditional probability (1) does not provide a complete description of electric field dynamics in the plasma, since large variations for the field due to close configurations are disregarded here. The corresponding time evolution for the conditional probability is therefore very slow. Also, the distribution (1) is symmetric about the peak at  $\alpha(t)\vec{E}_0$ , in contrast to the exact short time results, and it does not approach the correct steady-state solution,  $Q(c)$ . In addition, the Gaussian distribution (1) is limited only to those cases with a finite second moment  $\langle E^2 \rangle$ .

### 5.3.ii. Generalization to the Gaussian model

As already mentioned in §2.3, the Gaussian distribution (1) can be partially improved if  $Q_G(c)$  is replaced by the exact microfield distribution  $Q(c)$  (see Eq. (2.3.22)); in this way, the correct steady-state solution is obtained as  $t \rightarrow \infty$ . However, the corresponding joint probability  $f(\vec{E}, t; \vec{E}_0, 0)$  for this case does not present the required

symmetry  $\vec{e} \leftrightarrow \vec{e}_0$  from condition (2.2.16). In addition, the same as in the Gaussian model, the distribution (2.3.22) is symmetric about the peak, and it is also limited to having a finite second moment  $\langle E^2 \rangle$ . Note that this distribution does not satisfy the differential equation (2), since this latter assumes having a quadratic dependence for the corresponding generating function.

A similar discussion applies for the related distribution by Smith *et al*, mentioned in §2.3.

### 5.3.iii. Fokker-Planck process

For the general case of a transition rate presenting the form (1.10) with  $w_2$  a sharply peaked function about  $\vec{e} = \vec{e}'$ , the Master Equation (1.8) may be written as a second order partial differential equation. To that end, write the transition rate  $W(\vec{e}|\vec{e}')$  as (Van Kampen, 1980)

$$W(\vec{e}|\vec{e}') = W(\vec{e}'; \vec{\eta}), \quad \vec{\eta} = \vec{e} - \vec{e}', \quad (3)$$

with  $W(\vec{e}'; \vec{\eta})$  a sharply peaked function of  $\vec{\eta}$  which varies slowly with  $\vec{e}'$ . Thus Eq. (1.8) becomes

$$\frac{\partial}{\partial t} P(\vec{e}, t) = \int d\vec{\eta} W(\vec{e} - \vec{\eta} | \vec{\eta}) P(\vec{e} - \vec{\eta}, t) - P(\vec{e}, t) \int d\vec{\eta} W(\vec{e} | -\vec{\eta}), \quad (4)$$

where we have used the abbreviation  $P(\vec{e}, t)$  for the conditional probability  $P(\vec{e}, t | \vec{e}_0, 0)$ . The two assumptions above for the transition rate  $W(\vec{e} | \vec{\eta})$  allow to perform a Taylor expansion for the first integral in the RHS of (4). Hence, up to second order,

$$\begin{aligned} \frac{\partial}{\partial t} P(\vec{e}, t) = & \int d\vec{e}' W(\vec{e}; \vec{\eta}) P(\vec{e}', t) - \int d\vec{\eta} \eta_1 \frac{\partial}{\partial e_1} \langle W(\vec{e}; \vec{\eta}) P(\vec{e}, t) \rangle \\ & + \frac{1}{2} \int d\vec{\eta} \eta_1 \eta_j \frac{\partial^2}{\partial e_1 \partial e_j} \langle W(\vec{e}; \vec{\eta}) P(\vec{e}, t) \rangle - P(\vec{e}, t) \int d\vec{\eta} W(\vec{e} | -\vec{\eta}). \end{aligned} \quad (5)$$

Here, the first and fourth terms cancel, and the other two terms can be written with the aid of the jump moments

$$A_1(\vec{e}) = \int d\vec{\eta} \eta_1 W(\vec{e}; \vec{\eta}), \quad D_{1j}(\vec{e}) = \frac{1}{2} \int d\vec{\eta} \eta_1 \eta_j W(\vec{e}; \vec{\eta}). \quad (6)$$

The result is

$$\frac{\partial}{\partial t} P(\vec{c}, t) = -\frac{\partial}{\partial c_1} \{A_1(\vec{c})P(\vec{c}, t)\} + \frac{\partial^2}{\partial c_1 \partial c_j} \{D_{1j}(\vec{c})P(\vec{c}, t)\}. \quad (7)$$

In addition, if the detailed balance condition (Van Kampen, 1980) is imposed for the steady-state solution,  $Q(c)$ , we have

$$\frac{\partial}{\partial t} P(\vec{c}, t) = \frac{\partial}{\partial c_1} \{D_{1j}(\vec{c})[\frac{\partial}{\partial c_j} P(\vec{c}, t) - P(\vec{c}, t) \frac{\partial}{\partial c_j} \ln Q(c)]\}. \quad (8)$$

Eq. (8), or equivalently Eq. (7), is called the Fokker-Planck equation for Markov processes. The first term in the RHS of (8) is called the "diffusion term" or "fluctuation term"; the second one "transport term", "convection term" or "drift term". An example of a Markov Fokker-Planck equation ( $D_{1j}(\vec{c}) = D\delta_{1j}$ ) is provided by the Gaussian result (1), in the case where the function  $\alpha(t)$  decays exponentially ( $\gamma(t) \rightarrow \text{constant}$ ). Finally, note that for an isotropic plasma  $D_{1j}$  depends on the magnitude of  $\vec{c}$  only, so that the solution to Eq. (8) is symmetric about its peak.

It is worth mentioning here that there is no connection between the diffusion equation (8) and the short-time result (2.4.18). It is well known that the Fokker-Planck equation only applies at mesoscopic time scales, giving incorrect results at very short times.

#### 5.4. Discussion

In the last two sections we have presented the few existing models to describe electric field dynamics in a plasma from a stochastic approach. All of those models take into account only a partial aspect of electric field variations, namely, either that related to large fluctuations (referred to as Strong Fluctuation models), or that related to small fluctuations (referred to as Diffusion models). The Strong Fluctuation models (§5.2) are basically phenomenological, and were originally introduced in the context of spectral line shapes. They all lead to a conditional probability density in which there always remains a contribution from the initial  $\delta$ -distribution at  $\vec{c} = \vec{c}_0$ ; this is in

contrast to the exact short time result, where the initial  $\delta$ -distribution broadens and shifts towards smaller field values. The Strong Fluctuation models describe processes in which any change for the electric field  $\vec{E}$  completely destroys all memory of the initial field  $\vec{E}_0$ . Because of this unphysical behavior, none of these models provides an adequate description of electric field variations in the plasma (Smith et al, 1981). On the other hand, the Diffusion models (§5.3) describe Fokker-Planck-like processes, for which the plasma electric field changes very slowly. These models disregard the effect of a few close ions passing the field point. Hence, a complete description of electric field variations in the plasma is not expected here.

The former discussion justifies looking for a more physical model, in which both small and large variations for the electric field are taken into account. Alternative models based on the results above are proposed in the following chapter (Ch.6), as an attempt to describe electric field dynamics in a more appropriate way.

## CHAPTER 6

### DYNAMICAL DISTRIBUTION FOR INDEPENDENT PROCESSES

#### 6.1. Introduction

The stochastic models in the previous chapter provide a partial description of electric field dynamics in a plasma, with a relative mathematical simplicity. The Strong Fluctuation models describe processes with *no memory*, in which the value of the stochastic field at a given time is practically independent of the value it had before the jump; this generates a fast evolution for the dynamical distribution, mainly associated with the electric field produced with a few close ions. On the other hand, Diffusion models describe processes with *memory*, in which the stochastic field changes at small steps only; this generates a slow evolution for the dynamical distribution, mainly associated with the electric field due to distant configurations. A more complete description of electric field dynamics should include the effect from both close and distant ions. Our goal here is to propose alternative stochastic models, which are still mathematically simple (compared with the exact formulation), but provide a more appropriate description of electric fields in plasmas.

Two reasonable models are proposed here. In the first case, we focus attention on the size of fluctuations for the field, and distinguish two kind of processes: one of strong fluctuations, and another one of weak fluctuations; we assume that these two processes are mutually exclusive. The dynamical distribution here satisfies a composite Master Equation, given in terms of two independent evolution operators associated with each of those processes. In the second case, we focus attention on the strength of the electric field itself, instead of in its fluctuations, and distinguish two kind of contributions: a large field produced by close ions, and a small field due to distant ions; we assume that these two

contributions are statistically independent and satisfy a different dynamical evolution. The dynamical distribution here is given by the convolution of the dynamical distributions associated with each of the two independent fields. The details are presented in the following.

## 6.2. A Master Equation for Independent processes

We consider here the Master Equation (5.1.8) for the conditional probability and propose a particular model for the transition rate,  $W(c|c')$ , in which the two aspects of electric field variations discussed in Chapter 5 are taken into account. More specifically, we assume that the processes associated with large and small variations are mutually exclusive, in such a way that the transition rate (5.3.3) is given by the sum

$$W(c'; \eta) = W_1(c'; \eta) + W_2(c'; \eta), \quad \vec{\eta} = \vec{\varepsilon} - \vec{\varepsilon}', \quad (1)$$

with  $W_1$  accounting for transitions associated with large variations for the electric field and  $W_2$  accounting for transitions corresponding to small variations. In this case, the corresponding Master Equation presents the form

$$\left(\frac{\partial}{\partial t} P\right) = \left(\frac{\partial}{\partial t} P\right)_1 + \left(\frac{\partial}{\partial t} P\right)_2, \quad (2)$$

where the terms  $\left(\frac{\partial}{\partial t} P\right)_1$  and  $\left(\frac{\partial}{\partial t} P\right)_2$  satisfy Eq. (5.3.4) with transition rates  $W_1$  and  $W_2$ , respectively. Also, associated with each of these terms there is a steady-state solution  $Q_1, Q_2$ .

A Taylor's expansion for the term  $\left(\frac{\partial}{\partial t} P\right)_2$ , similar to that in §5.3.iii, gives the Fokker-Planck equation

$$\left(\frac{\partial}{\partial t} P\right)_2 = D \frac{\partial}{\partial \varepsilon_1} \left\{ \frac{\partial}{\partial \varepsilon_j} P(\vec{\varepsilon}, t) - P(\vec{\varepsilon}, t) \frac{\partial}{\partial \varepsilon_j} \ln Q_2(\varepsilon) \right\} = -\hat{F}P(\vec{\varepsilon}, t), \quad (3)$$

where we have assumed  $D_{1j}(\varepsilon) = D\delta_{1j}$  ( $D = \text{constant}$ ). We have also introduced here the notation  $P(\vec{\varepsilon}, t) = P(\vec{\varepsilon}, t | \vec{\varepsilon}_0, 0)$ . On the other hand, a

tenable model for the term  $(\frac{\partial}{\partial t} P)_1$  is the Kangaroo process introduced in §5.2.ii, that is,

$$(\frac{\partial}{\partial t} P)_1 = -\nu(\epsilon)P(\vec{z}, t) + \frac{\nu(\epsilon)Q(\epsilon)}{\langle \nu \rangle_1} \int d\vec{z}' \nu(\epsilon') P(\vec{z}', t), \quad (4)$$

with  $\langle \rangle_1$  the average with respect to the distribution  $Q_1$ . In this model the distributions  $Q_1$  and  $Q_2$  can not be chosen arbitrarily, since the steady-state condition  $P(\vec{z}, \infty) = Q(\epsilon)$  for the composite process imposes a relation between the three distributions  $Q_1$ ,  $Q_2$ , and  $Q$ . In this case, Eqs.(2)-(4) imply

$$\frac{\nu(\epsilon)Q_1(\epsilon)}{\langle \nu \rangle_1} = \hat{L} \frac{Q(\epsilon)}{\langle \nu \rangle}, \quad (5)$$

with  $\langle \rangle$  the average with respect to the microfield distribution  $Q$  and

$$\hat{L} = \nu(\epsilon) + \hat{F}, \quad (6)$$

where  $\hat{F}$  is the Fokker-Planck operator from Eq.(3). Substitution of Eqs.(3)-(6) into Eq.(2) gives the desired Master Equation

$$\frac{\partial}{\partial t} P = -\hat{L}(P(\vec{z}, t) - \frac{Q(\epsilon)}{\langle \nu \rangle} \int d\vec{z}' \nu(\epsilon') P(\vec{z}', t)). \quad (7)$$

The solution to this equation satisfies all properties (2.2.12)-(2.2.17); in particular,  $P(\vec{z}, 0) = \delta(\vec{z} - \vec{z}_0)$ .

The time evolution for the conditional probability satisfying Eq.(7) is governed by the combination of a fast (Kangaroo) process and a slow diffusion (Fokker-Planck) process; the corresponding time scales are determined by the coefficients  $\nu(\epsilon)$  and  $D$ , respectively. A relation between these two coefficients can be obtained from the electric field autocorrelation  $\langle \vec{E}(t) \cdot \vec{E} \rangle$  computed from Eq.(7), similarly to the method in Eq.(5.2.14). An additional equation is also required for a complete specification of these coefficients. This latter can be provided, for instance, by long-time (transport) properties in the system.

Another important quantity that has to be specified in this model is the distribution  $Q_2$ . For instance, this distribution can be chosen to be the exact microfield distribution,  $Q(\epsilon)$ . In that case, Eqs. (5)-(6) imply

$$\hat{L}Q(\epsilon) \rightarrow \nu(\epsilon)Q(\epsilon), \quad Q_1 = Q_2 = Q. \quad (8)$$

That is, the choice  $Q_2 = Q$  forces each process to reach the exact steady-state solution,  $Q(\epsilon)$ , separately. In this way, a pure Kangaroo process is obtained when  $D = 0$ , and a pure Fokker-Planck process is obtained when  $\nu(\epsilon) = 0$ . Another possibility is to assume a Gaussian form for the distribution  $Q_2$ ,

$$Q_2(\epsilon) = \left(\frac{A}{\pi}\right)^{3/2} e^{-A\epsilon^2}, \quad A = \text{constant} \quad (9)$$

which is a reasonable choice for the Fokker-Planck process in Eq. (3). In that case, each process reaches its characteristic steady-state solution ( $Q_1$ ,  $Q_2$ ) and only the combination gives the exact microfield distribution  $Q$ . For the particular case with  $D = 0$ , a Kangaroo process is obtained, with  $Q_1 \rightarrow Q$ . However, the case with  $\nu(\epsilon) = 0$  does not represent a simple Fokker-Planck process for  $P(\vec{\epsilon}, t)$  but for  $P(\vec{\epsilon}, t) - Q(\epsilon)$ , instead. This latter is necessary in order to approach the correct steady-state solution  $Q$  and not the Gaussian distribution in Eq. (9). The former two choices for the distribution  $Q_2$  are expected to be equivalent for the case of a highly-charged point; for a neutral point, they are equivalent only asymptotically for very small field values.

The formal solution to the Master Equation (7) is given by

$$P(\vec{\epsilon}, t) = e^{-\hat{L}t} \delta(\vec{\epsilon} - \vec{\epsilon}_0) + \int_0^t d\tau g(\epsilon_0, \tau) e^{-\hat{L}(t-\tau)} \{\hat{L}Q(\epsilon)\}, \quad (10)$$

with

$$g(\epsilon_0, t) = \langle \nu \rangle^{-1} \int d\vec{\epsilon}' \nu(\epsilon') P(\vec{\epsilon}', t | \vec{\epsilon}_0, 0) \quad (11)$$

a formal definition that satisfies  $g(\epsilon_0, 0) = \nu(\epsilon_0) / \langle \nu \rangle$ ,  $g(\epsilon_0, \infty) = 1$ . It is also convenient to introduce the definition



$$y(\vec{c}, \vec{c}_0; t) = e^{-\hat{L}t} \delta(\vec{c} - \vec{c}_0), \quad (12)$$

in terms of which the conditional probability (10) becomes

$$P(\vec{c}, t) = y(\vec{c}, \vec{c}_0; t) + \int_0^t d\tau \int d\vec{c}' g(c_0, \tau) \{\hat{L}Q(c')\} y(\vec{c}, \vec{c}'; t-\tau), \quad (13)$$

with  $y(\vec{c}, \vec{c}_0; t)$  satisfying the equation

$$\frac{\partial}{\partial t} y(\vec{c}, \vec{c}_0; t) = -\hat{L}y(\vec{c}, \vec{c}_0; t), \quad y(\vec{c}, \vec{c}_0; 0) = \delta(\vec{c} - \vec{c}_0). \quad (14)$$

Also, it is possible to show that  $g(c_0, t)$  can be obtained from a Volterra integral equation of the second kind (Arfken, 1985) involving the function  $y(\vec{c}, \vec{c}_0; t)$ . Hence, the conditional probability (13) is simply determined from the microfield distribution  $Q(c)$  and the time-dependent function  $y(\vec{c}, \vec{c}_0; t)$ . For this latter, a simpler equation can be obtained by introducing the definition

$$y(\vec{c}, \vec{c}_0; t) = Q_2^{1/2} \varphi(\vec{c}, \vec{c}_0; t); \quad (15)$$

hence, from Eqs. (14)-(15) we have

$$\frac{\partial}{\partial t} \varphi(\vec{c}, \vec{c}_0; t) = \{D\nabla^2 - V(c)\} \varphi(\vec{c}, \vec{c}_0; t), \quad (16)$$

with  $\nabla = \partial/\partial \vec{c}$  and

$$V(c) = \frac{D}{4} (\nabla \ln Q_2)^2 + \frac{D}{2} \nabla^2 \ln Q_2 + \nu(c). \quad (17)$$

Solutions to the differential equation (16) are known in the literature for some simple choices of  $V(c)$ .

An alternative way to express the solution to the Master Equation (7), more convenient for numerical evaluation than Eq. (13), is provided by the introduction of Laplace variables. To our purposes, it is enough noting here that the conditional probability for this model presents the form

$$P(\vec{z}, t) = e^{-\hat{L}t} \delta(\vec{z} - \vec{z}_0) + h'(c, c_0; t), \quad (18)$$

with  $h'(c, c_0; t)$  an isotropic function of the field  $c$  that depends parametrically on  $c_0$ ,  $t$ . A comparison between the conditional probability (18) and that in Eq. (5.2.12) reveals that our result here represents a more physical solution than that from Strong Fluctuation models, in the sense that the operator  $\hat{L}$  generates a time evolution for the initial  $\delta$ -distribution, instead of producing a simple attenuation. Thus, our model describes processes with *memory*. In addition, the time evolution for these processes is faster than in the case of Diffusion models, since the effect of close configurations is not disregarded here.

A simple illustrative example in which the most relevant characteristics of our model are exhibited is that with a field-independent frequency,  $\nu(c) = \nu_0$ , with  $\nu_0$  a constant. In this case, the conditional probability (13) reduces to

$$P(\vec{z}, t) = e^{-\nu_0 t} y_{FP}(\vec{z}, \vec{z}_0; t) + Q(c) - e^{-\nu_0 t} \int d\vec{z}' Q(c') y_{FP}(\vec{z}, \vec{z}'; t) \quad (19)$$

with  $y_{FP}(\vec{z}, \vec{z}_0; t)$  the solution to the Fokker-Planck equation

$$\frac{\partial}{\partial t} y_{FP} = -\hat{F} y_{FP}(\vec{z}, \vec{z}_0; t), \quad y_{FP}(\vec{z}, \vec{z}_0; 0) = \delta(\vec{z} - \vec{z}_0). \quad (20)$$

The distribution (19) satisfies all properties (2.2.12)-(2.2.17). At short times, it describes a diffusion (Fokker-Planck) process with an attenuation characterized by  $\nu_0^{-1}$ . At longer times, the peak position is determined by both the diffusive part and that from the Kangaroo process. Hence, the approaching to equilibrium is faster ( $\nu_0 > 0$ ) than in a simple Fokker-Planck process. This can be made explicit, for instance, by considering the model  $Q_2 = Q$ . In this case, the conditional probability (19) reduces to

$$P(\vec{z}, t) = e^{-\nu_0 t} y_{FP}(\vec{z}, \vec{z}_0; t) + (1 - e^{-\nu_0 t}) Q(c), \quad (21)$$

with  $y_{FP}$  the (unknown) solution to Eq. (20) with steady-state solution  $Q(\epsilon)$ . An adequate choice for the constant  $\nu_0$  determines how fast the distribution (21) reaches the equilibrium value  $Q$ .

For a numerical evaluation of the conditional probability (19) it is convenient to chose the Gaussian form (9) for  $Q_2$ ; in this case, an exact solution to the Fokker-Planck equation (20) can be obtained, namely,

$$y_{FP}(\vec{z}, \vec{z}_0; t) = \left( \frac{A}{\pi \{1 - \exp(-2\beta t)\}} \right)^{3/2} \exp \left\{ - \frac{A(\vec{z} - e^{-\beta t} \vec{z}_0)^2}{1 - \exp(-2\beta t)} \right\}, \quad (22)$$

with  $\beta = 2AD$ . The distribution (22) describes a so called Ornstein-Uhlenbeck process (Van Kampen, 1980). The results from a numerical integration of the conditional probability (19) with (22) are shown in Figs. 20 and 21, where we have regarded the coefficients  $A$ ,  $\beta$  and  $\nu_0$  as simple parameters of the model. In particular, these parameters have been adjusted to fit the simulation data we referred to in the former chapter (Smith et al, 1984) at earliest time (Fig. 20); a fixed renormalization of the conditional probability (19) was necessary to this end. The results from a comparison at later times (not included here) reveal considerable disagreements between our model and the simulation data; this is a consequence of an over-simplification of our model, due to the choice  $\nu(\epsilon) = \text{constant}$ . In Fig. 21 it is shown the evolution of the former distribution at later times. Two values for the jumping frequency,  $\nu_0 = 0$  and  $\nu_0 > 0$ , are considered there. In both cases, the short time behavior is that of a simple attenuated Fokker-Planck distribution (not a  $\delta$ -distribution!). At intermediate times, a second peak raises about  $c = 0$ , resembling the behavior of the conditional probability in a simple Kangaroo process. Finally, the approaching to equilibrium for the case with  $\nu_0 > 0$  is faster than in the case with  $\nu_0 = 0$ , which shows the effect of the Kangaroo process in this composite model. The former results are promising, indeed, since they represent an improvement over those corresponding to each simple Kangaroo or Diffusion models, separately.

The results above also suggest that a more appropriate description of electric field dynamics should include a field dependence in the jumping frequency: for large fields, the value taken by this function should be

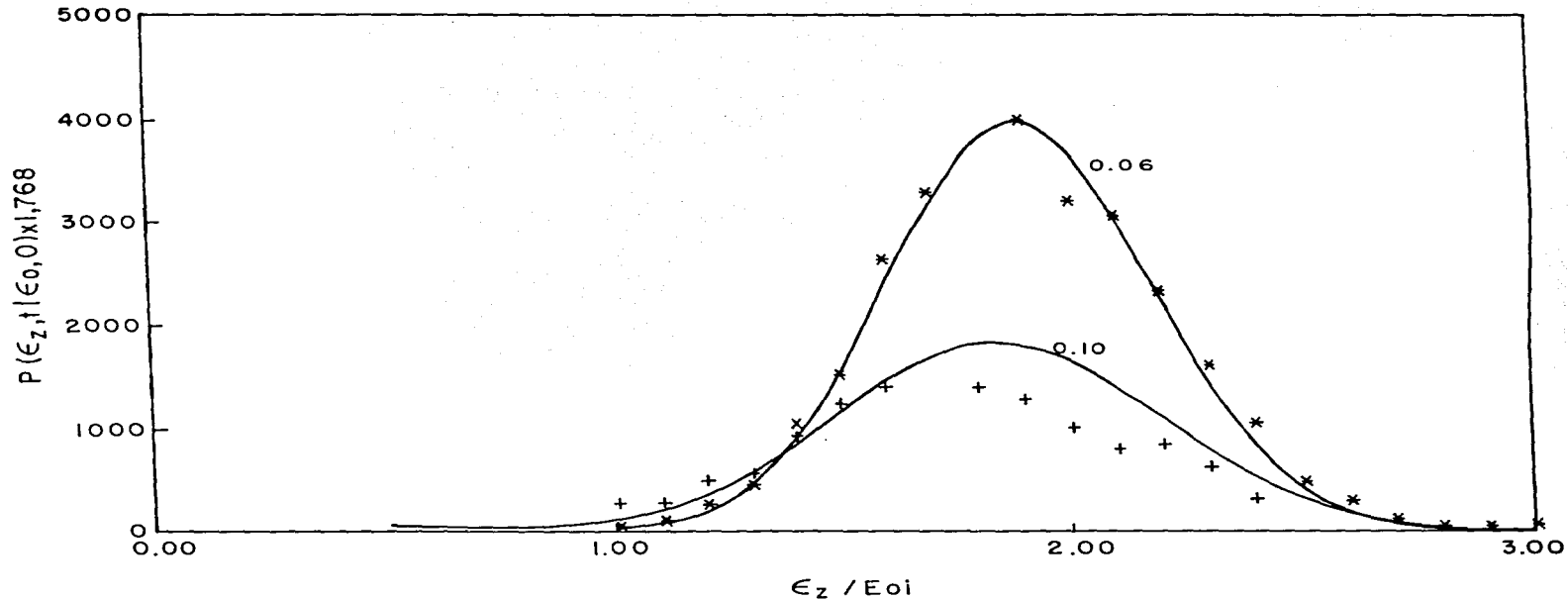


Fig.20. Conditional probability density from the Composite model and computer simulation, for  $\epsilon_0 = 2$ , at  $w_{p1} t = 0.06, 0.10$ . Here, we have chosen  $\Lambda = 0.6$ ,  $\beta = 0.8$  and  $\nu_0 = 3.45$ .

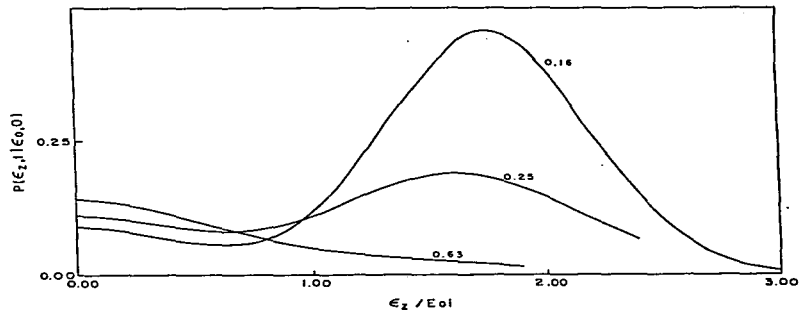
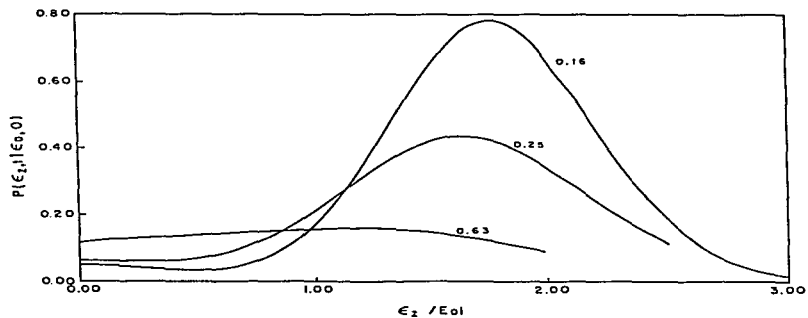


Fig.21. Conditional probability density from the Composite model,  $\epsilon_0 = 2$ , at  $w_p t = 0.16, 0.25, 0.63$ . The value chosen for the corresponding parameters is  $A = 0.6, \beta = 0.8$  and (a)  $\nu_0 = 0$ , (b)  $\nu_0 = 3.45$ .

large enough to produce a fast decay for the main peak, whereas for small fields, the jumping frequency should be small enough to avoid a very fast rising for the equilibrium peak. Unfortunately, this introduces in general some difficulties for determining the function  $y(\vec{c}, \vec{c}_0; t)$  from Eqs. (15) to (17). In relation to this latter, the choice  $\nu = \nu_0 + \nu_1 c + \nu_2 c^2$  is a good alternative, in the sense that an exact solution to Eq. (16) can be obtained. Such a choice, however, is not useful for the case of a neutral point since it leads to a divergent average  $\langle \nu \rangle$ .

The utility of the Composite model in this section is limited to having a relatively simple functional dependence for the operator  $\hat{L}$ , or equivalently the function  $\nu(c)$ , so that Eq. (14) for  $y(\vec{c}, \vec{c}_0; t)$  can be solved numerically. Thus, future studies should be addressed on determining the jumping frequency  $\nu(c)$  from suitable models for the electric field autocorrelation function. The results obtained in this way are also expected to motivate extensive computer simulations, as a helpful tool to give an answer on the validity of our model.

### 6.3. The Convolution model

An alternative model combining the effect of large and small fields is proposed here. To this end, we assume that the electric field  $\vec{E}(t)$  can be written as the sum of two statistically independent fields

$$\vec{E}(t) = \vec{E}_1(t) + \vec{E}_2(t), \quad (1)$$

whose time evolution are governed by two different operators  $\hat{L}_1$ ,  $\hat{L}_2$ , according to

$$\delta(\vec{c} - \vec{E}_k(t)) = e^{-\hat{L}_k t} \delta(\vec{c} - \vec{E}_k), \quad k = 1, 2. \quad (2)$$

The field  $\vec{E}_1$  accounts for those configurations producing a large field value, and  $\vec{E}_2$  for those configurations producing a small value. It is possible to show then that the joint probability (2.2.1) becomes

$$f(\vec{z}, t; \vec{z}_0, 0) = \iint d\vec{z}_1 d\vec{z}_2 e^{-\hat{L}_2(\vec{z}-\vec{z}_1)t} \delta(\vec{z}-\vec{z}_1-\vec{z}_0+\vec{z}_2) \cdot \\ e^{-\hat{L}_1(\vec{z}_1)t} \delta(\vec{z}_1-\vec{z}_2) \langle \delta(\vec{z}_0-\vec{z}_2-E_2) \delta(\vec{z}_2-E_1) \rangle. \quad (3)$$

We now identify

$$P_k(\vec{z}, t | \vec{z}_0, 0) = e^{-\hat{L}_k(\vec{z})t} \delta(\vec{z} - \vec{z}_0) \quad (4)$$

as the conditional probability density associated with the process  $k$ . This latter can be expressed in terms of the corresponding joint probability density  $f_k$  and the associated steady-state solution  $Q_k$ ,

$$P_k(\vec{z}, t | \vec{z}_0, 0) = f_k(\vec{z}, t; \vec{z}_0, 0) / Q_k(\epsilon). \quad (5)$$

Substitution of Eqs. (4) and (5) into Eq. (3) for the joint probability gives

$$f(\vec{z}, t; \vec{z}_0, 0) = \iint d\vec{z}_1 d\vec{z}_2 f_1(\vec{z}_1, t; \vec{z}_2, 0) f_2(\vec{z}-\vec{z}_1, t; \vec{z}_0-\vec{z}_2, 0) \cdot \\ Q(\vec{z}_0-\vec{z}_2, \vec{z}_2) / Q_2(\vec{z}_0-\vec{z}_2) Q_1(\epsilon_2), \quad (6)$$

with  $Q(\vec{z}_1, \vec{z}_2)$  the average

$$Q(\vec{z}_1, \vec{z}_2) = \langle \delta(\vec{z}_1 - \vec{E}_1) \delta(\vec{z}_2 - \vec{E}_2) \rangle. \quad (7)$$

Finally, it is possible to show that the assumption of statistical independence at time  $t$  also implies statistical independence at  $t = 0$ , so that

$$Q(\vec{z}_1, \vec{z}_2) = Q_1(\epsilon_1) Q_2(\epsilon_2). \quad (8)$$

Hence, the distribution (6) reduces to

$$f(\vec{z}, t; \vec{z}_0, 0) = \iint d\vec{z}_1 d\vec{z}_2 f_1(\vec{z}_1, t; \vec{z}_2, 0) f_2(\vec{z}-\vec{z}_1, t; \vec{z}_0-\vec{z}_2, 0). \quad (9)$$

Thus, the joint probability density for this model is the convolution of two distributions,  $f_1, f_2$ , representing the dynamics of two statistically independent fields: a large field produced by close ions, and a small field generated by distant ions.

Suitable models for the operators  $\hat{L}_1$  and  $\hat{L}_2$  are those in the Kangaroo and Diffusion models introduced previously. In that case, the distribution  $f_1$  is obtained from the conditional probability (5.2.11), with steady-state solution  $Q_1$ , and  $f_2$  from the Fokker-Planck equation (5.3.8), with steady-state solution  $Q_2$ . The distributions  $Q_1, Q_2$  are not arbitrary, but satisfy the relation

$$Q(c) = \int d\vec{c}_1 Q_1(c_1) Q_2(\vec{c} - \vec{c}_1). \quad (10)$$

This result is equivalent to neglecting static correlations between the configurations producing large and small field values at a given time. This is valid only approximately for a system of interacting particles, becoming exact in the particular case of non-interacting ions (neutral point). In addition to the distributions  $Q_1$  and  $Q_2$ , specification of the coefficients  $\nu(c)$  and  $D$  is required for an evaluation of the joint probability in (9). Suitable models for these coefficients have to be provided by knowledge of exact properties (electric field autocorrelation, ...) in the system.

In contrast to the result (10) for the static microfield distribution, the convolution (9) for the dynamical distribution is always an approximation. Indeed, even for the simplest case of non-interacting ions there always exist dynamical correlations between the configurations producing large fields and small fields; they are associated, for instance, with a close ion that moves far apart from the field point at a later time. Such dynamical correlations, therefore, are expected to play an important role only as time increases. We assume here that those correlations are negligible for all times.

The joint probability density (9) presents the advantage of being expressed in terms of two distributions,  $f_1, f_2$ , which are assumed to be known. It also provides a physical interpretation of electric field dynamics as generated by two independent processes, with well-known



dynamical properties. The flexibility of the method allows a direct substitution of suitable choices for the independent distributions, instead of solving an integro-differential equation as in the model in §6.2. The utility of the Convolution model, however, is limited to those choices of  $f_1$  and  $f_2$  for which the six-dimensional integral in (9) can be performed numerically. It is not still clear to us that the associated numerical problem is simpler here than in the Composite model above. Also, the validity of the Convolution model is still a question to be answered as extensive computer simulations are available in the literature. Limited studies in this spirit may be found in Smith et.al. (1984), for a system of non-interacting ions (neutral point).

#### 6.4. Discussion

Each of the two stochastic models in this chapter constitutes a promising alternative to describe electric field dynamics in a plasma, beyond the asymptotic limits where the exact formalism can be reduced to quadratures. These two models are semi-phenomenological, in the sense that they are based on those aspects of electric fields that seem to play a relevant role in the dynamical properties for the system. For instance, if one assumes that the dynamical distribution satisfies a Master Equation, a reasonable approach is to focus attention on the size of fluctuations for the electric field. Strong fluctuations are due to the motion of ions near the field point, and are expected to generate a fast relaxation for the dynamical properties in the system. On the contrary, weak fluctuations are due to distant ions and are associated with a slow relaxation of dynamical properties. This is basically the spirit of our Composite model in §6.2. An alternative approach that focus attention on the electric field itself, instead of on its fluctuations, is provided by the Convolution model in §6.3. We assume there that strong fields produced by close ions are statistically independent of weak fields from distant configurations. Both approaches are plausible, and summarize the physical aspects that we believe are relevant in our problem. They also constitute a generalization to existing models, which only describe those aspects partially.

Besides providing a physical interpretation of electric field dynamics in a plasma, the models here are expected to be more manageable numerically

than the exact formulation. In the first case, the problem reduces basically to solving a partial differential equation (i.e. to determine the function  $\gamma(\vec{E}, \vec{E}_0; t)$ ), and in the second case to perform a six-dimensional integration (instead of the nine-dimensional integration from the exact formulation). There is also the flexibility of trying suitable choices for the corresponding phenomenological coefficients, instead of introducing approximations in the dynamical generating function  $G$ . In particular, for the Convolution model there is the advantage of a direct substitution of some simple models for the two independent distributions that are available in the literature.

Limitations of time have not allowed us to explore the Convolution model numerically. In the case of the Composite model, we have limited to analyze a very simple, illustrative example in which we obtain substantial improvements over existing Diffusion and Strong Fluctuation models. In particular, the time evolution for the dynamical distribution is faster here than in simple Diffusion models, which are unable to describe processes with large variations for the field (as those associated with the motion of close ions); also, our results describe processes with *memory*, in contrast to the unphysical *no memory* processes from Strong Fluctuation models.

Further studies are expected to decide one of these models in favor of the other one. To that end, it is necessary to explore both models into more detail. Comparison of those results with extensive computer simulations (not available yet) would be also desired, as a helpful way to determine the validity of each of our stochastic models.

## CHAPTER 7

### CONCLUSIONS

Our goal here has been to develop an exact formalism to describe dynamical properties of electric fields in plasmas, from the theoretical point of view of Statistical Mechanics. Studying statistical properties of electric fields generated in the plasma is important for understanding dynamical transport and radiative properties of atomic impurities immersed there, which constitutes a very powerful diagnosis tool to determine the state of the plasma; also, the singular characteristics of Coulomb systems lead to some special problems in the theory of fluctuations that contrast to those for some other variables (e.g. energy, density). Hence, this problem presents both a practical and theoretical importance. Although static properties of the electric field are well-known for a variety of the conditions for the diverse parameters in the system, the dynamical problem has received very limited attention in the literature. Our research constitutes a first theoretical attempt at the description of dynamical properties for the electric field, as a generalization to that for the static case. For the sake of simplicity, we have limited our study to a classical, One-Component plasma in equilibrium, although generalization to quantum, multi-component plasmas is expected to be straightforward. In particular, we have focused attention on the dynamical probability distribution (joint probability density) for electric fields generated by the plasma ions at the position of a radiating impurity atom, or field point, at two different times. The physical information contained in this distribution is, by far, more exhaustive than that associated with the knowledge of a few of its moments (electric field autocorrelation function, ..); in this sense, our research constitutes a more general and complete description of dynamical aspects of the electric field than existing studies, which are limited to some semi-phenomenological models and

evaluation of diverse average functions of the field (such as the electric field autocorrelation) from kinetic models or computer simulations.

Statistical properties of the electric field at the position of an impurity charge in the plasma are highly dependent on both the coupling between the plasma ions (determined by their charge, density and temperature) and the coupling between these ions and the impurity charge (determined by the ion-impurity charge ratio). The nature of such couplings makes this a very complex numerical problem in general, for which standard techniques for systems of neutral particles can not be applied. Throughout this work we have studied several interesting exact limits and useful approximations, which are based on the relative effect of the former couplings in some limiting cases where the problem can be reduced to quadratures.

An interesting case where the ion-impurity coupling plays a relevant role was found to be that of a highly charged point repelling the plasma ions to large distances (§2.3). In this case, the electric fields generated by the plasma ions at the field point are very weak, which allows some simplification for the generating function associated with the dynamical microfield distribution. For instance, if the representation (2.2.11) for the generating function is assumed, the corresponding joint probability density presents a Gaussian form (Eq.2.3.3). The half-width associated with this distribution is determined from the knowledge of the electric field autocorrelation function, which can be obtained from kinetic models of direct evaluation. Unfortunately, the approximations concerning this limit generally require an unrealistic large charge at the field point; hence, its importance is theoretical rather than practical, in general. Nevertheless, this limit provides a quantitative description of dynamical properties for weak fields produced by distant configurations, which is exploited later on in this work.

The Gaussian limit presents the difficulty of not approaching the correct equilibrium (long time) limit. As an attempt to correct this difficulty, in Eq.(2.3.22) we consider the possibility of replacing the Gaussian factors in (2.3.3) by the exact (static) microfield distribution. However, such a replacement was found to be unsuccessful since the corresponding dynamical distribution did not satisfy an important symmetry condition (Eq.2.2.16) that follows from the equilibrium choice.

Alternatively to the representation (2.2.11) for the generating function, the representation (2.2.23) was also explored for the case of weak fields, which also allows reducing the problem to quadratures (Eq.2.3.25). The corresponding result satisfies all exact properties (2.2.12)-(2.2.17), so that it presents a more appropriate behavior than the Gaussian limit. The same as in the Gaussian limit, the joint probability density here can be also determined from simple quantities such as the electric field autocorrelation function and the (known) generating function for the static case. Although the angular dependence in this case introduces some numerical difficulties, we believe that a more detailed study of this distribution will be profitable.

The ion-impurity coupling also determines the validity of standard approximations such as that of non-interacting ions. Usual Cluster Expansion techniques for a system of neutral particles allow neglecting high-order static and dynamical correlations in the case of weak interactions between the particles, so that the problem can be reduced to quadratures. In our case, the validity of such an approximation depends not only on the strength of ion-ion interactions but also on their interactions with the impurity charge. As we have shown in §3.1, a charged impurity couples the equations of motion for the ions, so that high-order dynamical correlations can not be neglected in general. Only in some limited cases such high-order dynamical correlations become negligible, and the expanded quantity (in this case, the generating function) can be approximated by the leading terms. An example of this is the limit for high fields (§3.2), which was found to be associated with the effect of one or two ions close to the field point. This interesting result together with the corresponding for the Gaussian limit suggest distinguishing two different aspects of electric fields in our system: one due to close ions generating a strong effect on the field point, and another one due to distant configurations producing a weak effect. Thus, the Gaussian and high-field limit provide a physical interpretation for the effect of close and distant configurations in the system.

Since the utility of the independent particle approximation is limited only to those cases with a very low coupling between all the charges in the plasma, we have proposed here a related approximation that is expected to be suitable even for strongly coupled plasmas. This approximation is a

generalization to the so called Renormalized Independent Particle model for the static case, in which the Coulomb field is replaced by an effective electric field that accounts for high-order correlations usually neglected. This model still presents the simplicity and general structure of the simple independent particle model, but it provides a more appropriate description of many-body correlations in the system by introducing renormalized quantities. Although we have not explored yet this model numerically, the excellent results that have been obtained somewhere else for the static case suggest that our generalization constitutes a promising alternative for description of electric field dynamics in strongly coupled plasmas.

An interesting exact limit where the problem can be reduced to quadratures, regardless of the plasma state and charge at the field point, was found to be that for short times in §2.4.i: In this limit, the dynamical distribution of fields (Eq.2.4.6) describes anisotropic diffusion, with time-independent coefficients that depends on the field magnitude and can be determined from the knowledge of the pair correlation function and the static microfield distribution. A numerical evaluation of this distribution (chapter 4) has shown qualitative agreements with some limited computer simulation data for a system of non-interacting ions and a neutral point -quantitative discrepancies are believed to be due to incorrect parameters reported for the simulation-. The corresponding results show an asymmetric broadening of the initial peak (a  $\delta$ -distribution), with a monotonic shift towards the equilibrium value. Again, two different aspects in the dynamical evolution for the distribution of fields can be distinguished here, according to the magnitude of the initial field: for small values, the dynamical evolution is slow, with a monotonic decay for the peak; for large values, the evolution is fast, and the peak raises again from a minimum value, at an intermediate time. For the case of a very large initial field, in particular, a comparison between this distribution and that associated with a single ion (§4.4) has revealed excellent agreements at very short times; in this way, it is possible to determine the range of applicability of the single-ion model to describe dynamical properties of high fields. Finally, at later times (of the order of the inverse plasma frequency) the peak position reaches its equilibrium value but continues towards the negative

region. This fact shows the limitations of our result to very short times ( $\approx \omega_{pi}^{-1}$ ) only. A precise specification of the time scales associated with this limit will be possible as extensive simulation data for the dynamical distribution become available in the literature. Future studies of this limit should also be addressed to the case of charged points, so that it could be established an interesting comparison with our results for the Gaussian limit.

An alternative, not necessarily equivalent, description at short times was also formulated (§2.4.ii) by imposing time reversal invariance in the dynamical equation satisfied by the joint probability density. The corresponding evolution operator was found to be similar to one of Fokker-Planck, with the appropriate steady-state solution. Because of this latter fact, the solution to this equation is expected to be a better approximation to longer times than the result above. Unfortunately, we have not been able yet to construct an explicit solution to the corresponding differential equation.

The former limits and approximations summarize the most relevant aspects of electric field dynamics in a plasma, that follow from the exact formulation presented here. An application of our results to specific problems may require a generalization to quantal, multi-component plasmas. Beyond these exact limits and approximations the problem becomes numerical rather than physical, which is not the goal we have pursued in this dissertation.

As an alternative to the numerical complexity associated with the exact formulation, in the second part of this work we have considered some approximate models based on the Theory of Markov Stochastic Processes, that present a relative mathematical simplicity. Unfortunately, none of the existing models provides an adequate description of electric field dynamics in plasmas, since they consider only partial aspects of the electric field: Strong Fluctuation models (such as the Kangaroo process in §5.2.ii) describe fast processes associated with the effect of close configurations, in which the value of the field after a transition is practically independent of the initial value (i.e. there is *no memory* in the system); on the other hand, Diffusion models (such as the Fokker-Planck process in §5.2.ii) describe slow processes associated with the effect of distant

configurations, in which the electric field only changes at small steps -in such a way that there is *memory* associated with electric field changes-.

Because of the relative success and mathematical simplicity of those stochastic models, we have proposed here two possible generalizations that are expected to provide a more complete and adequate description of electric field dynamics in the plasma. In these models we have tried to incorporate those aspects of the field that seem to play a relevant role in the dynamical evolution for the field distribution: in the first case (the Composite model in §6.2) we have focused attention on the size of electric field fluctuations, distinguishing two mutually exclusive processes associated with weak and strong fluctuations; in the second case (the Convolution model in §6.3) we have focused attention on the electric field itself, instead of its fluctuations, distinguishing two statistically independent processes associated with configurations producing weak and strong electric fields. In each case, we associate one of the simple models above (Kangaroo and Fokker-Planck) with each of the two processes under consideration.

Although limitations of time have not allowed us to explore here these two stochastic models into detail, we have reasons to believe that they constitute a tenable possibility to describe electric field dynamics, in a relatively simple way. Such an expectation is based on the promising results obtained for the Composite model, which represent substantial improvements over simple Strong Fluctuation and Diffusion models. Indeed, the processes described here present more physical characteristics than in Strong Fluctuation models, in the sense that there is some *memory* associated with electric field changes; also, the time evolution for the dynamical distribution is faster here than in Diffusion models, which accounts for the effect of close configurations disregard there. Similar results are expected for the Convolution model, in the sense that it "mingles" the physical aspects associated with each of the two independent processes for all times.

In these two models, the dynamical evolution for the electric field is given in terms of the various phenomenological coefficients associated with the two independent processes under consideration, which have to be chosen to reproduce the exact properties (electric field autocorrelation, ...) in the system. The flexibility of such a semi-phenomenological approach



allows trying some simple models for these coefficients so that, in principle, the numerical problem can be manageable. Although we have not been able yet to construct an exact solution for some realistic choices for these coefficients, our developments (not included here) seem to indicate that approximate solutions can be obtained for the Composite model. The numerical difficulties associated with this model are, by far, less severe than those from the exact description; the same applies for the Convolution model.

Of course, there still remain several questions to be answered in subsequent studies of these stochastic models for plasmas. For instance, it is not clear at this point how appropriate the Markov assumption results for describing such highly correlated systems. An answer to this question requires, for instance, a comparison of our results with extensive computer simulations for the dynamical distribution (not available yet in the literature). This will be also helpful for establishing the validity and range of application for each of the two models proposed here. As the simulation results become available, current studies are focused on analyzing the physical hypothesis behind both the Composite and Convolution models, as well as their consistency with exact (known) properties in the system. This will also give us a criterion to decide one of these models in favor of the other one.

## APPENDIXES

### A. Legendre polynomial expansion for the joint probability density

Taking advantage of the angular dependence of the joint probability density,  $f(\epsilon, \epsilon_0, \hat{\epsilon} \cdot \hat{\epsilon}_0; t)$ , we can perform an expansion of this distribution in terms of Legendre Polynomials. To this end, introduce first the characteristic function

$$F(\vec{\lambda}, \vec{\lambda}'; t) = \langle e^{i\vec{\lambda} \cdot \vec{E}(t)} e^{i\vec{\lambda}' \cdot \vec{E}} \rangle \quad (1)$$

and expand it in terms of Legendre polynomials; in this case,

$$F(\vec{\lambda}, \vec{\lambda}'; t) = \sum_{k=0}^{\infty} \left( \frac{2k+1}{2} \right) P_k(y) F_k(\lambda, \lambda'; t), \quad (2)$$

where  $y \equiv \hat{\lambda} \cdot \hat{\lambda}'$ ,  $P_k$  is the Legendre polynomial of order  $k$  (Arfken, 1985) and the coefficients  $F_k$  are given by

$$F_k(\lambda, \lambda'; t) = \int_{-1}^1 dy P_k(y) F_k(\lambda, \lambda', y; t). \quad (3)$$

From (2.2.10), (1) and (2), we obtain for the joint probability density

$$f(\epsilon, \epsilon_0, \hat{\epsilon} \cdot \hat{\epsilon}_0; t) = \sum_{k=0}^{\infty} P_k(x) f_k(\epsilon, \epsilon_0; t), \quad (4)$$

where  $x \equiv \hat{\epsilon} \cdot \hat{\epsilon}_0$  and

$$f_k(\epsilon, \epsilon_0; t) = \frac{2k+1}{2(2\pi)^6} \int_0^{\infty} d\lambda \lambda^2 G_k(\lambda\epsilon) \int_0^{\infty} d\lambda' \lambda'^2 G_k(\lambda'\epsilon_0) F_k(\lambda, \lambda'; t). \quad (5)$$

Here, the function  $G_k(\lambda\epsilon)$  is given by

$$G_k(\lambda\epsilon) = \int_{-1}^1 dx e^{-i\lambda\epsilon x} P_k(x) = (-i)^k (4\pi) j_k(\lambda\epsilon), \quad (6)$$

with  $J_k$  the spherical Bessel function of order  $k$  (Arfken, 1985).

The expansion (4) provides an exact representation for the joint probability density. The  $k = 0$  term corresponds to an angular average, useful to describe changes in the magnitude of the field. The remaining terms ( $k \geq 1$ ) in the expansion are related to the angular dependence of the distribution; they are important, for instance, to study variations of the dipole momentum in radiators with internal degrees of freedom. Ultimately, the asymptotic limit (2.2.14) is ensured by the fact

$$\lim_{t \rightarrow \infty} f_k(\epsilon, \epsilon_0; t) = Q(\epsilon)Q(\epsilon_0)\delta_{k0}. \quad (7)$$

Although the problem of evaluating the joint probability is reduced now to performing simpler two-dimensional integrations, determining the coefficients  $F_k(\lambda, \lambda'; t)$  requires still considerable numerical work. In addition, there is no clear criterion to decide the number of terms to be kept in the expansion, in such a way that the angular dependence can still be described appropriately through the entire time range.

A Legendre polynomial expansion for the alternative representation (2.2.22) of the joint probability density can be performed in a way similar to this. It is not included here, since it leads to the same kind of discussion.

#### B. Exact formulation for non-interacting ions and a neutral point

A proof of Eqs. (3.1.13)-(3.1.15) for the dynamical generating function is given here for the case of non-interacting ions and a neutral point. To this end, consider the characteristic function  $F(\vec{\lambda}, \vec{\lambda}'; t)$  defined in Appendix A, with  $\vec{E}(t)$  the total electric field due to the  $N_1$  independent ions. In this case, Eq. (A.1) becomes

$$\begin{aligned}
F(\vec{\lambda}, \vec{\lambda}'; t) &= \langle \prod_{\alpha=1}^{N_1} e^{i\vec{\lambda} \cdot \vec{E}(\vec{q}_\alpha + \vec{p}_\alpha t/m_1) + i\vec{\lambda}' \cdot \vec{E}(\vec{q}_\alpha)} \rangle \\
&= \left\{ \frac{1}{\Omega} \int d\vec{q}_1 d\vec{p}_1 f(\vec{p}_1) e^{i\vec{\lambda} \cdot \vec{E}(\vec{q}_1 + \vec{p}_1 t/m_1)} e^{i\vec{\lambda}' \cdot \vec{E}(\vec{q}_1)} \right\}^{N_1} \quad (1)
\end{aligned}$$

with  $\Omega$  the macroscopic volume for the system and  $f(\vec{p})$  the Maxwell-Boltzmann distribution (McQuarrie, 1976),

$$f(\vec{p}) d\vec{p} = \frac{e^{-\beta p^2/2m_1} d\vec{p}}{\int e^{-\beta p^2/2m_1} d\vec{p}} \quad (2)$$

Write now the characteristic function (1) as

$$\begin{aligned}
F(\vec{\lambda}, \vec{\lambda}'; t) &= \left\{ 1 + \frac{1}{\Omega} \int d\vec{q}_1 d\vec{p}_1 \phi(\vec{p}_1) [e^{i\vec{\lambda} \cdot \vec{E}(\vec{q}_1 + \vec{p}_1 t/m_1)} e^{i\vec{\lambda}' \cdot \vec{E}(\vec{q}_1)} - 1] \right\}^{N_1} \\
&= \left\{ 1 + \frac{1}{N_1} G(\vec{\lambda}, \vec{\lambda}'; t) \right\}^{N_1} \quad (3)
\end{aligned}$$

with

$$\begin{aligned}
G(\vec{\lambda}, \vec{\lambda}'; t) &\equiv n_1 \int d\vec{q}_1 \phi(\vec{\lambda}, \vec{q}_1) + n_1 \int d\vec{q}_1 \phi(\vec{\lambda}', \vec{q}_1) \\
&\quad + n_1 \int d\vec{q}_1 d\vec{p}_1 f(\vec{p}_1) \phi(\vec{\lambda}, \vec{q}_1 + \vec{p}_1 t/m_1) \phi(\vec{\lambda}', \vec{q}_1). \quad (4)
\end{aligned}$$

the corresponding generating function. The functions  $\phi(\vec{\lambda}, \vec{q}_\alpha)$  above are defined in (3.1.13). Note that for large volumes (i.e., large  $N_1$ ,  $N_1/\Omega = \text{constant}$ ) the function  $G(\vec{\lambda}, \vec{\lambda}'; t)$  is bounded and independent of  $N_1$ , so that the characteristic function (3) becomes

$$F(\vec{\lambda}, \vec{\lambda}'; t) = e^{G(\vec{\lambda}, \vec{\lambda}'; t)}. \quad (5)$$

Finally, since

$$\phi(\vec{\lambda}, \vec{q}_1 + \vec{v}_1 t) = \int d\vec{r}_1 \phi(\vec{\lambda}, \vec{r}_1) \delta(\vec{r}_1 - \vec{q}_1 - \vec{v}_1 t) \quad (6)$$

then the generating function (4) can be also written as

$$G(\vec{\lambda}, \vec{\lambda}'; t) = n_1 \int d\vec{r}_1 \phi(\vec{\lambda}, \vec{r}_1) + n_1 \int d\vec{r}_1 \phi(\vec{\lambda}', \vec{r}_1) \\ + n_1 \int d\vec{r}_1 d\vec{r}_2 \phi(\vec{\lambda}, \vec{r}_1) \phi(\vec{\lambda}', \vec{r}_2) C(\vec{r}_1 - \vec{r}_2; t), \quad (7)$$

with  $C(\vec{r}_1 - \vec{r}_2; t)$  the density-density autocorrelation function for the system of independent ions and a neutral point,

$$C(\vec{r}_2 - \vec{r}_1; t) = \int d\vec{q}_1 d\vec{p}_1 \delta(\vec{r}_2 - \vec{q}_1) \delta(\vec{r}_1 - \vec{q}_1 - \vec{p}_1 t / m_1) \cdot f(\vec{p}_1) \\ = (\pi u^2 t^2)^{-3/2} \exp\left\{-\frac{(\vec{r}_1 - \vec{r}_2)^2}{(ut)^2}\right\}, \quad (8)$$

where  $u = (2k_B T / m_1)^{1/2}$  is the thermal speed.

C. Legendre polynomial expansion of the generating function for the case of non-interacting ions and a neutral point.

Here we take advantage of the angular dependence of the function  $H_\infty$  in (4.1.3). An expansion of  $H_\infty(\lambda, \lambda', \hat{\lambda} \cdot \hat{\lambda}'; t)$  in terms of Legendre polynomials gives

$$H_\infty(\lambda, \lambda', y; t) = \sum_{k=0}^{\infty} \frac{(2k+1)}{2} H_k^{(\infty)}(\lambda, \lambda'; t) P_k(y), \quad (1)$$

with  $y = \hat{\lambda} \cdot \hat{\lambda}'$ . The coefficients  $H_k^{(\infty)}(\lambda, \lambda'; t)$  are given by

$$H_k^{(\infty)}(\lambda, \lambda'; t) = (2\pi)^2 n_1 \int_0^\infty dr_1 r_1^2 \phi_k(\lambda, r_1) \int_0^\infty dr_2 r_2^2 \phi_k(\lambda', r_2) C_k(r_1, r_2; t), \quad (2)$$

with

$$\phi_k(\lambda, r_1) = \int_{-1}^1 dx_1 \phi(\lambda, r_1, x_1) P_k(x_1), \quad (3)$$

$$C_k(r_1, r_2; t) = \int_{-1}^1 dz C(r_1, r_2, z) P_k(z), \quad (4)$$

and  $z \equiv \hat{r}_1 \cdot \hat{r}_2$ ,  $\hat{x}_1 \equiv \hat{\lambda} \cdot \hat{r}_1$ . The functions  $P_k$  are the Legendre Polynomials of order  $k$  (Arfken, 1985).

Eqs. (3) and (4) can be integrated analytically in terms of Bessel functions. That is,

$$\phi_k(\lambda, r_1) = 2 [i^k j_k(\lambda E_1) - \delta_{k0}], \quad (5)$$

with  $j_k$  the spherical Bessel function of order  $k$  (Arfken, 1985) and  $E_1$  the electric field produced by the  $i$ th-particle. Similarly,

$$C_k(r_1, r_2; t) = 2 \frac{e^{-(r_1^2 + r_2^2)/(ut)^2}}{(\pi u^2 t^2)^{3/2}} \left( \frac{(\pi/2)(ut)^2}{2r_1 r_2} \right) I_{k+1/2} \left( \frac{2r_1 r_2}{(ut)^2} \right), \quad (6)$$

with  $I_{k+1/2}$  the Bessel modified function of order  $k+1/2$  (Arfken, 1985).

The problem of evaluating the generating function for this case is reduced now to perform two-dimensional integrations, in terms of more familiar Bessel functions. However, the same as in the case of the expansion (A.4) for the joint probability density, it is not clear how many terms should be kept here in order to preserve the correct angular dependence at both short and long times.

#### D. Microfield distribution and joint probability density for the single particle model in a system of non-interacting ions and a neutral point.

When Coulomb fields are considered, the joint probability density (4.4.2) for the single particle model becomes

$$f_1(\vec{z}, t; \vec{z}_0, 0) = \frac{n_1(Z_1 e)^3}{(\pi u^2 t^2)^{3/2}} \int d\vec{\eta} d\vec{\xi} \delta(\vec{z} - \frac{\vec{\eta}}{\xi^3}) \delta(\vec{z}_0 - \frac{\vec{\eta}}{\eta^3}) e^{-Z_1 e \left( \frac{\vec{\eta} - \vec{\xi}}{u t} \right)^2}, \quad (1)$$

where  $\vec{\eta} = \vec{q}_1 / \sqrt{Z_1 e}$ ,  $\vec{\xi} = (\vec{q}_1 + \vec{v}_1 t) / \sqrt{Z_1 e}$  and  $u^2 = 2k_B T / m_1$ . A second change of variables,  $\vec{x} = \vec{\xi} / \xi^3$  and  $\vec{x}_0 = \vec{\eta} / \eta^3$ , gives

$$f_1(\vec{z}, t; \vec{z}_0, 0) = \alpha \int d\vec{x} d\vec{x}_0 \delta(\vec{z} - \vec{x}) \delta(\vec{z}_0 - \vec{x}_0) \exp\left\{-\frac{Z_1 e}{(u t)^2} \left( \frac{\vec{x}}{\sqrt{x}} - \frac{\vec{x}_0}{\sqrt{x_0}} \right)^2\right\}, \quad (2)$$

with  $\alpha \equiv n_1(Z_1 e)^3 / 4(\pi u^2 t^2)^{3/2}$ . Finally, a direct integration of (2) gives

$$f_1(\vec{z}, t; \vec{z}_0, 0) = \alpha (\epsilon \epsilon_0)^{-9/2} \exp\left\{-\frac{Z_1 e}{(u t)^2} \left( \frac{\hat{z}}{\sqrt{\epsilon}} - \frac{\hat{z}_0}{\sqrt{\epsilon_0}} \right)^2\right\}. \quad (3)$$

Eq. (3) represents the joint probability density for the single independent particle model (neutral point) when Coulomb interactions are considered.

A similar change of variables is used to evaluate the single particle microfield distribution (4.4.1) for this case, giving

$$Q_1(\epsilon_0) = \frac{n_1}{2} (Z_1 e)^{3/2} \epsilon_0^{-9/2}. \quad (4)$$

This result is also the asymptotic (large field) Holtsmark distribution (Griem, 1974).

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