Integral-equation method for electric microfield distributions

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The Fourier transform of the electric microfield distribution function is expressed, without approximations, in terms of a two-body function. The two-body function may be interpreted as a "generalized" radial distribution function and therefore is amenable to integral-equation techniques. In particular, the formalism is shown to simplify considerably in the hypernetted-chain approximation.

I. INTRODUCTION

The Holtsmark theory of line broadening involves the electric microfield probability distribution $Q(\vec{\epsilon})$ that the plasma will produce an electric field $\vec{\epsilon}$ at the radiating atom or ion. The microfield distribution was first calculated by Holtsmark,[1] who assumed all particles to be statistically independent. Since then, various attempts[2-6] have been made to include correlations between the particles. So far none of the above methods provides reliable numerical results for the strongly coupled plasmas.

In this paper we propose a new method for calculating the microfield distributions. Our approach is based on recognizing[7] the similarity between the formal expressions for the excess chemical potential and the Fourier transform of $Q(\vec{\epsilon})$. The Fourier transform of $Q(\vec{\epsilon})$ is then expressed, without any approximation, in terms of a two-body function which may be interpreted as a "generalized" radial distribution function (RDF) and therefore it is amenable to integral-equation techniques. In particular, the expressions for the Fourier transform of $Q(\vec{\epsilon})$ simplify considerably in the hypernetted-chain[8-10] (HNC) approximation to the generalized RDF.

The system we deal with consists of N charged particles immersed in a uniform neutralizing background. In addition, when treating the problem of the electric field distribution at a charged point, a "zeroth" particle must be included. The $N+1$ particles interact through the Coulomb interaction. The total system is assumed to be in thermal equilibrium and macroscopically neutral.

Section II of this paper deals with the development of the formalism. In Sec. III we consider some simple approximations to the generalized RDF and some numerical results are presented. The HNC approximation is discussed in Sec. IV with conclusions given in Sec. V.

II. FORMALISM

Define $Q(\vec{\epsilon})$ as the probability of finding an electric field $\vec{\epsilon}$, at a singly charged point located at $\vec{r}_0$, due to N charged particles moving in a uniform neutralizing background and contained in a volume Ω. Then, if Z represents the configurational partition function of the $N+1$ particle system, we may write

$$Q(\vec{\epsilon})=Z^{-1}\int\cdots\int d\vec{r}_0 d\vec{r}_1\cdots d\vec{r}_N e^{-\beta V}\times\delta(\vec{\epsilon}-\vec{E}) , \tag{2.1}$$

where $\vec{r}_j$ represents the coordinate of the jth particle $\beta=(kT)^{-1}$, V the potential energy of the system, and $\vec{E}$ is the electric field at $\vec{r}_0$ due to the N charged particles in a given configuration.

The potential energy of the system is expressed as

$$V=\sum_{0=i<j} v_{ij}+V_B \tag{2.2}$$

and

$$v_{ij}=e^2/|\vec{r}_i-\vec{r}_j| ,$$

where V_B represents the contributions to the potential energy due to the background.

An expression for V in terms of a Fourier expansion results in

$$V=\frac{4\pi e^2}{\Omega}\sum_{\vec{k}\neq 0}\sum_{0=i<j} e^{-i\vec{k}\cdot|\vec{r}_i-\vec{r}_j|}/k^2 , \tag{2.3}$$

where the exclusion of the $\vec{k}=0$ term in Eq. (2.3) accounts for the neutralizing background.[2]

Assuming that our system is isotropic we may rewrite[2] Eq. (2.1) as

$$P(\epsilon)=(2\epsilon/\pi)\int_0^\infty dl\, lT(l)\sin(\epsilon l)\ , \tag{2.4}$$

where $P(\epsilon)$ is related to $Q(\vec{\epsilon})$ by

$$4\pi Q(\vec{\epsilon})\epsilon^2 d\epsilon = P(\epsilon)d\epsilon\ . \tag{2.5}$$

$T(l)$ is defined by

$$T(l)=Z(l)/Z\ , \tag{2.6}$$

$$Z(l)\equiv \int\cdots\int d\vec{r}_0 d\vec{r}_1\cdots d\vec{r}_N e^{-\beta V(l)}\ , \tag{2.7}$$

$$V(l)\equiv V+i\,\vec{l}\cdot\vec{E} = \sum_{0=i<j}\left[1-\frac{i\,\vec{l}}{e\beta}\cdot\vec{\nabla}_0\right]v_{ij}\ , \tag{2.8}$$

where $\vec{\nabla}_0$ is the gradient with respect to $\vec{r}_0$. The function $Z(l)$ may be interpreted[6] as a generalized configurational partition function for a system with "potential energy" $V(l)$, defined in Eq. (2.8).

It was first noted by Morita[7] that the virial expansion for $T(l)$ is formally similar to that of the excess chemical potential. Since it is possible to express[11] the latter in terms of the RDF, it follows that $T(l)$ may be expressed in terms of a generalized RDF. To accomplish this, we introduce the parameter λ which is defined as the magnitude of the vector $\vec{l}$,

$$\lambda\equiv|\vec{l}|\ . \tag{2.9}$$

We may write for $Z(l)$ and $V(l)$,

$$Z(\lambda)=\int\cdots\int d\vec{r}_0 d\vec{r}_1\cdots d\vec{r}_N e^{-\beta V(\lambda)}\ , \tag{2.10}$$

$$V(\lambda)=V+\frac{i\lambda\hat{l}\cdot\vec{E}}{\beta}\ , \tag{2.11}$$

where $\hat{l}$ is a unit vector in the direction of $\vec{l}$.

From the definition of $T(l)$ in Eq. (2.6) we may write

$$\begin{aligned}\ln T(l)&=\ln[Z(\lambda=l)/Z(\lambda=0)]\\ &=\int_0^l d\lambda\frac{\partial\ln Z(\lambda)}{\partial\lambda}\\ &=\rho\int_0^\infty d\lambda\int d\vec{r}\,\phi(\vec{r})g(\vec{r},\lambda)\end{aligned} \tag{2.12}$$

with

$$\rho=N/\Omega\ , \tag{2.13}$$

$$\phi(\vec{r})=ie\hat{l}\cdot\vec{r}/r^3\ , \tag{2.14}$$

$$g(\vec{r},\lambda)=\Omega^2\int d\vec{r}_2\cdots d\vec{r}_N e^{-\beta V(\lambda)}/Z(\lambda)\ . \tag{2.15}$$

The two-body function $g(\vec{r},\lambda)$ may be interpreted as a generalized RDF for the zeroth particle and any other particle where the potential energy of the system is given by $V(\lambda)$.

In Eq. (2.12) the effect of the neutralizing background has not been included. With the background term Eq. (2.12) becomes

$$\ln T(l)=\rho\int_0^l d\lambda\int d\vec{r}\,\phi(\vec{r})h(\vec{r};\lambda)\ , \tag{2.16}$$

where we have introduced the generalized total correlation function

$$h(\vec{r};\lambda)=g(\vec{r},\lambda)-1\ . \tag{2.17}$$

Equation (2.16) is the main result of this paper; we have expressed $T(l)$ in terms of a two-body function. This form has the advantage that knowledge of a two-body function gives $T(l)$ exactly. This is in contrast to the previous developments[4-6] which require knowledge of many-body functions. Of course, the price to be paid for this advantage is the integration over the parameter λ in Eq. (2.16) which requires $h(\vec{r},\lambda)$ for all values of λ between 0 and l.

Before closing this section we remark that the results for $T(l)$ in Eq. (2.16) contains the correct high-temperature or Holtsmark limit. At extreme high temperatures we have

$$\lim_{T\to\infty} h(\vec{r};\lambda)=e^{\lambda\phi(\vec{r})}-1\ . \tag{2.18}$$

This expression may be substituted into Eq. (2.16) and we find

$$\lim_{T\to\infty} T(l)=\exp\left[\rho\int d\vec{r}(e^{l\phi(\vec{r})}-1)\right] \tag{2.19}$$

which is the correct Holtsmark limit.[1]

III. SIMPLE APPROXIMATIONS

In this section we make some approximations to $h(\vec{r};\lambda)$. The first and simplest approximation suitable for a Coulomb system is the Debye-Hückel theory[11] (DH). In this approximation we have

$$h(\vec{r};\lambda)\simeq\exp\left[-\beta\left[1+\frac{i\lambda\hat{l}}{e\beta}\cdot\vec{\nabla}_0\right]W^{(1)}(r)\right]-1, \tag{3.1}$$

where $W^{(1)}(r)$ is the potential of mean force evaluated to first order in the plasma parameter

$$-\beta W^{(1)}(r)=-\left[\frac{\Lambda}{x}\right]e^{-x}\ , \tag{3.2}$$

where the plasma parameter is

$$\Lambda=\beta e^2/\lambda_D=\frac{a^3}{3}\ ,$$

the Debye length is

$$\lambda_D=(4\pi e^2\rho\beta)^{-1/2}\ , \tag{3.3}$$

and

$$x=r/\lambda_D\ .$$

The parameter a has been introduced in Eq. (3.3) for convenience when comparing to previous calculations. It is defined by

$$a=\frac{r_0}{\lambda_D} \tag{3.4}$$

with Debye length λ_D, average interparticle distance r_0, and

$$\tfrac{4}{3}\pi r_0^3\rho=1\ . \tag{3.5}$$

Substitution of Eq. (3.1) into Eq. (2.16) yields

$$\ln T(l)\simeq\Lambda^{-1}\int_0^\infty dx\frac{x^2e^x}{(1+x)}\exp\left[-\frac{\Lambda}{x}e^{-x}\right]\times\left[\frac{\sin[lb(x)]}{lb(x)}-1\right], \tag{3.6}$$

where

$$lb(x)=\left[\frac{le}{\lambda_D^2}\right]\frac{e^{-x}(1+x)}{x^2}\ . \tag{3.7}$$

The one-dimensional integration over x and the sine transform in Eq. (2.4) were done numerically. The results are presented in Figs. 1 and 2.

In Fig. 1 we have a $P(\epsilon)$ plot for the value of $a=0.2$ and it is clear that there is good agreement of our results with those of Hooper.[5] This is not surprising since DH is valid in the small plasma parameter limit. In Fig. 2 we compare our results with those of Hooper[5] and Mozer and Baranger[4,12] for $a=0.8$. In this case the agreement with Hooper is not very good. We will defer further comments on Fig. 2 until the end of this section.

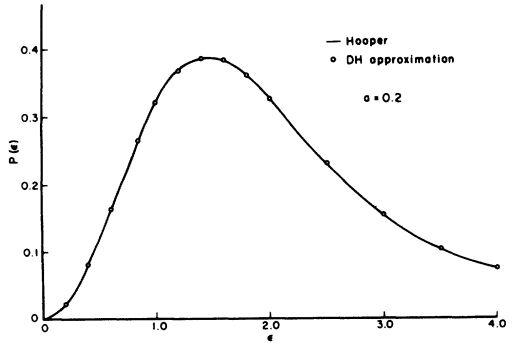

FIG. 1. A comparison of $P(\epsilon)$ curves for $a=0.2$. ϵ is in units of $\epsilon_0=e/r_0^2$.

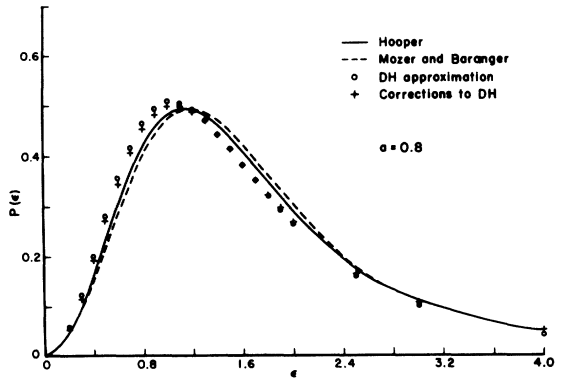

FIG. 2. A comparison of $P(\epsilon)$ curves for $a=0.8$. ϵ is in units of $\epsilon_0=e/r_0^2$.

In order to improve the Debye-Hückel results, several theories[13] have been proposed to compute higher-order terms in the parameter Λ. The application of such theories to $h(\vec{r};\lambda)$ is complicated by the angular dependence of the field terms in $V(\lambda)$. As a simplification, we assume that $h(\vec{r};\lambda)$ has the same functional form given in Eq. (3.1) but now evaluate $W(r)$, to second order in Λ,[13]

$$-\beta W^{(2)}(r)=\left[-\frac{\Lambda}{x}\right]\left[e^{-x}+\frac{\Lambda}{8}\{(3-x)[\ln 3-E_1(x)]e^{-x}+(3+x)E_1(3x)e^x+\tfrac{4}{3}(e^{-x}-e^{-2x})\}\right] \tag{3.8}$$

and

$$E_1(x)=\int_x^\infty dy\,e^{-y}/y\ . \tag{3.9}$$

Again the calculation for $T(l)$ reduces to a one-dimensional integration over x. The corrections to DH at $a=0.2$ are very small and therefore we do not show them in Fig. 1. For $a=0.8$ the corrections are not sufficiently large to make our results agree with those of Hooper. These results are presented in Fig. 2.

Our approximations above do not provide a reliable method for practical calculations of $P(\epsilon)$ in the region $a\gtrsim 0.4$. We will, however, make the following two remarks.

(i) The variations of our "simple" approximations from Mozer and Baranger[4] and Hooper[5] are less than 7%. Simple is to be interpreted here as numerically less cumbersome than the calculations in Refs. 4 and 5.

(ii) Since second-order corrections to $W(r)$ lead to better $P(\epsilon)$ results, then we conjecture that a better estimate of $h(\vec{r};\lambda)$ will lead to accurate $P(\epsilon)$ curves, not only for $a \gtrsim 0.4$ but also for the strongly coupled plasmas, $a \gtrsim 2.0$.

The second point provides the motivation for the next section.

IV. HNC APPROXIMATION

The total correlation function is amenable to integral-equation techniques. In this section we propose to evaluate $h(\vec{r};\lambda)$ in the HNC approximation. We are interested in this particular approach for two reasons. First, the HNC approximation has been successful[14] in evaluating RDF for strongly coupled plasmas. Secondly, the λ integration in Eq. (2.16) can be performed exactly in the HNC approximation.

To proceed we write $h(\vec{r};\lambda)$ in the form

$$h(\vec{r};\lambda)=\exp[-\beta v(r)+\lambda\phi(\vec{r})+\gamma(\vec{r};;\lambda)]-1 \tag{4.1}$$

which formally defines $\gamma(\vec{r};\lambda)$. The function $\gamma(\vec{r};\lambda)$ is given by the sum of nodal and bridge graphs, but in the HNC approximations the bridge graphs are neglected,[8–10,14] that is, the sum of nodal graphs is written

$$\gamma(\vec{r};\lambda)\,|_{\mathrm{HNC}}=N(\vec{r};\lambda)=h(\vec{r};\lambda)-c(\vec{r};\lambda)\ , \tag{4.2}$$

where $c(\vec{r};\lambda)$ is the generalized direct correlation function and is defined by the Ornstein-Zernike equation[15]

$$\begin{aligned} h(\vec{r}_{10};\lambda)&=c(\vec{r}_{10};\lambda)+\rho\int d\vec{r}_2 c(r_{12})h(\vec{r}_{20};\lambda)\ , \\ h(r_{12})&=c(r_{12})+\rho\int d\vec{r}_3 c(r_{13})h(r_{32})\ . \end{aligned} \tag{4.3}$$

In Eq. (4.3) $h(r)$ and $c(r)$ are the total and direct correlation functions for λ equal to zero, respectively.

It is now possible to simplify Eq. (2.16) by noting[16] that we may write from Eq. (4.1)

$$\phi(\vec{r})h(\vec{r};\lambda)=\frac{\partial h(\vec{r};\lambda)}{\partial\lambda}-\phi(\vec{r})-h(\vec{r};\lambda)\frac{\partial\gamma(\vec{r};\lambda)}{\partial\lambda}\ . \tag{4.4}$$

Substitution of Eq. (4.4) into Eq. (2.16) and making use of Eq. (4.2) leads to

$$\ln T(l)\,\Big|_{\mathrm{HNC}}=\rho[\tilde{c}(\vec{k}=0;l)-\tilde{c}(k=0)]-\frac{\rho}{2}\int d\vec{r}\,[h(\vec{r};l)N(\vec{r};l)-h(r)N(r)]\ , \tag{4.5}$$

where $\tilde{c}(\vec{k};\lambda)$ is the Fourier transform of $c(\vec{r};\lambda)$,

$$c(\vec{r};\lambda)=\int\frac{d\vec{k}}{(2\pi)^3}e^{-i\vec{k}\cdot\vec{r}}\tilde{c}(\vec{k};\lambda)\ . \tag{4.6}$$

The result in Eq. (4.5) may now be used in evaluating the microfield distribution function. The quantities c, h, and N in Eq. (4.5) are to be evaluated in the HNC framework. The quantities with $l=0$ have been calculated to high accuracy.[14] The l-dependent quantities are directionally dependent and consequently are expected to complicate the computations.

V. CONCLUSIONS

We have expressed the Fourier transform of the electric microfield distribution in terms of a generalized radial distribution function. Although simple approximations to the generalized RDF fail to provide very accurate numerical results except for weakly coupled plasmas, there are indications that our approach may prove useful for strongly coupled plasmas. In particular, it has been shown how in the HNC approximation the formalism simplifies considerably. We emphasize that RDF calculations employing integral-equation techniques or so-called computer experiments may be substituted in the formalisms of Refs. 4, 5, and 6, however, such an approach will still neglect effects due to three-or-more–body terms.

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