Electric microfield distributions in multicomponent plasmas

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We evaluate the electric microfield distribution in a multicomponent plasma (MCP). The method employed is an adaption of the very simple adjustable-parameter exponential approximation previously developed for one-component plasmas (OCP). We also discuss a still simpler approximation in which the MCP is replaced by an effective OCP. The results are generally close to each other and the former is in very good agreement with computer simulations.

I. INTRODUCTION

Recently we proposed a method for calculating electric microfield distributions in a plasma.[1] In that work, hereafter referred to as I, the plasma consisted of N identical point charges in a uniform neutralizing background. The method gave numerical results in excellent agreement with computer simulations for strongly coupled one-component plasmas (OCP) in two and three dimensions.[1,2] The primary objective here is to extend the adjustable-parameter exponential approximation (APEX) developed in I to multicomponent plasmas (MCP). Also discussed is a second approximation method in which the MCP is replaced by an effective OCP followed by an application of APEX as described in I. The numerical results from both schemes are compared to computer simulations.

II. FORMALISM

We consider the electric microfield distribution $W(\vec{\epsilon})$, defined as the probability density of finding a field $\vec{E}$ equal to $\vec{\epsilon}$ at a charge $Z_0 e$, located at $\vec{r}_0$, in a MCP where particles of species σ carry a charge $Z_\sigma e$. Here, e is the magnitude of the elementary charge, and Z_0 and all the Z_σ's are positive. The system, which also includes a uniform neutralizing background, is assumed to be described by classical equilibrium statistical mechanics with temperature T and number densities ρ_σ,

$$\rho_\sigma = N_\sigma/\Omega \; , \tag{2.1}$$

where N_σ is the number of particles of species σ and Ω is the total volume.

We have then,[1] in the limit of a macroscopic system,

$$W(\vec{\epsilon}) = \langle \delta(\vec{\epsilon}-\vec{E}) \rangle = \lim_{\substack{\{N_\sigma\},\Omega\to\infty \\ \{N_\sigma/\Omega=\rho_\sigma\}}} \int_\Omega \cdots \int_\Omega d\vec{r}_0 \prod_\sigma \prod_{j=1}^{N_\sigma} d\vec{r}_{j\sigma} \frac{e^{-\beta V}\delta(\vec{\epsilon}-\vec{E})}{Q(\{\rho_\sigma\},\Omega,T)} \; , \tag{2.2}$$

where $Q(\{\rho_\sigma\},\Omega,T)$ is the configurational partition function, $\vec{r}_{j\sigma}$ is the position of the jth particle of species σ, and $\beta=(k_B T)^{-1}$. The potential energy V is given by

$$V = e^2 \sum_\sigma \sum_{j=1}^{N_\sigma} \left[\frac{Z_0 Z_\sigma}{|\vec{r}_0 - \vec{r}_{j\sigma}|} + \frac{1}{2} \sum_{\sigma'} \sum_{\substack{i=1 \\ (i,\sigma' \neq j,\sigma)}}^{N_{\sigma'}} \frac{Z_\sigma Z_{\sigma'}}{|\vec{r}_{i\sigma'} - \vec{r}_{j\sigma}|} \right] + V_B \; , \tag{2.3}$$

where V_B is the contribution to the potential energy due to the background. The electric field acting on the charge $Z_0 e$ is given by the superposition of single-particle Coulomb fields plus a contribution $\vec{E}_B$ from the background,

$$\vec{E} = \sum_\sigma \sum_{j=1}^{N_\sigma} \frac{Z_\sigma e (\vec{r}_{j\sigma} - \vec{r}_0)}{|\vec{r}_{j\sigma} - \vec{r}_0|^3} + \vec{E}_B \; . \tag{2.4}$$

As in the case of the OCP, a simple and exact expression may be obtained for the second moment of the distribution $W(\vec{\epsilon})$. Following the procedure described in I, we write

$$\begin{aligned} \langle E^2 \rangle &= (Z_0 e)^{-2} \langle \vec{\nabla}_0 V \cdot \vec{\nabla}_0 V \rangle \\ &= (Z_0^2 e^2 \beta)^{-1} \langle \nabla_0^2 V \rangle \\ &= \frac{4\pi}{\beta} \sum_\sigma \frac{Z_\sigma}{Z_0} \left\langle \rho_\sigma - \sum_{j=1}^{N_\sigma} \delta(\vec{r}_{j\sigma} - \vec{r}_0) \right\rangle \; , \\ \langle E^2 \rangle &= \frac{4\pi}{\beta} \sum_\sigma \rho_\sigma Z_\sigma / Z_0 \; , \end{aligned} \tag{2.5}$$

where $\vec{\nabla}_0$ is the gradient with respect to $\vec{r}_0$ and

$$\vec{\nabla}_0 \cdot \vec{E}_B = -4\pi e \sum_\sigma Z_\sigma \rho_\sigma \tag{2.6}$$

even though $\vec{E}_B=\vec{0}$ in the thermodynamic limit; see also Lebowitz and Martin.[3]

It is convenient to introduce the dimensionless quantities

$$\vec{F}=\frac{\vec{E}}{e/a^2}, \quad \vec{x}=\vec{r}/a , \tag{2.7}$$

where a is the interparticle spacing

$$\frac{4\pi}{3}a^3\rho=1 \quad \text{and} \quad \rho=\sum_\sigma \rho_\sigma . \tag{2.8}$$

Equation (2.5) then becomes

$$\langle \vec{F}\cdot\vec{F}\rangle=\frac{3}{Z_0\Gamma}\sum_\sigma Z_\sigma X_\sigma , \tag{2.9}$$

where

$$\Gamma=\beta e^2/a \quad \text{and} \quad X_\sigma=\rho_\sigma/\rho \tag{2.10}$$

are the plasma-coupling parameter and number fraction for species σ, respectively.

At this point we introduce the Fourier transform of $W(\vec{\epsilon})$. Since the system is assumed isotropic we may write, setting $\epsilon=|\vec{\epsilon}|$,

$$P(\epsilon)=4\pi\epsilon^2 W(\vec{\epsilon})=\frac{2\epsilon}{\pi}\int_0^\infty dk\, k\sin(k\epsilon)T(k) \tag{2.11}$$

and

$$T(k)=\langle \exp(i\vec{k}\cdot\vec{E})\rangle . \tag{2.12}$$

The method in I used a coupling parameter integration technique to express $T(k)$ in terms of a (special) pair-distribution function.[1,4] This function was then approximated by a form containing a free parameter which was fixed by the exact second moment of $W(\vec{\epsilon})$. Instead we will follow a procedure suggested by the *a posteriori* interpretation of APEX in I. There, it was shown that APEX is equivalent to replacing the plasma by a system of noninteracting quasiparticles each producing a parametrized electric field at $\vec{r}_0$. The quasiparticles have a distribution about $\vec{r}_0$ which is different from the fully interacting "real" particles in the plasma and is determined by requiring that the field produced at $\vec{r}_0$ by quasiparticles contained in a volume element $d\vec{r}$ at position $\vec{r}$ be the same as for the real particles for each $\vec{r}$. This leads to a density of quasiparticles at $\vec{r}$ in terms of the real particle density $\rho g(r)$ and the parameter in the quasiparticle field. The parameter is then fixed to give the exact second moment.

To extend this APEX formalism to the MCP, it must be supplemented. First, the second-moment rule, Eq. (2.9), strictly gives only one constraint on the parameter set (one parameter per species) characterizing the quasiparticle fields. Second, the "local-field constraint" described above is not sufficient to determine all the quasiparticle distributions about $\vec{r}_0$. In order to obtain the necessary number of constraint equations we assume that both the local-field constraint and the second-moment rule are satisfied species by species. That is, if $G_\sigma(x)$ and $g_\sigma(x)$ denote the distribution of quasiparticles and real particles of species σ a distance x from the charge Z_0e, respectively, then we assume that

$$[g_\sigma(x)f(x)-G_\sigma(x)f_\sigma(x)]Z_0\rho_0\left[\frac{\vec{x}}{x}\right]=0 \tag{2.13}$$

for all σ, where $Z_\sigma ef_\sigma$ and $Z_\sigma ef$ denote the magnitude of the quasiparticle and Coulomb fields, respectively, with

$$f(x)=x^{-2} , \qquad f_\sigma(x)=\frac{e^{-\alpha_\sigma x}}{x^2}(1+\alpha_\sigma x) , \tag{2.14}$$

and the set $\{\alpha_\sigma\}$ consists of real, positive parameters. This yields,

$$G_\sigma(x)=g_\sigma(x)f(x)/f_\sigma(x) . \tag{2.15}$$

The quasiparticle interpretation together with the distributions $G_\sigma(x)$ in Eq. (2.15) are then used to obtain an expression for the Fourier transform of the microfield distribution,

$$T(L)=\exp\left[3\sum_\sigma X_\sigma\int_0^\infty dx\, x^2 g_\sigma(x)\frac{f(x)}{f_\sigma(x)}\times\{j_0[LZ_\sigma f_\sigma(x)]-1\}\right] , \tag{2.16}$$

where $L=(e/a^2)k$ and j_0 is the spherical Bessel function of order zero. A comparison of the second-moment sum rule, Eq. (2.9), and the second-moment expression obtained from Eq. (2.16) gives

$$\sum_\sigma Z_\sigma^2 X_\sigma\int_0^\infty dx\, x^2 g_\sigma(x)f(x)f_\sigma(x)=\frac{1}{Z_0\Gamma}\sum_\sigma Z_\sigma X_\sigma . \tag{2.17}$$

This is now assumed valid species by species to yield a set of equations

$$Z_\sigma^2\int_0^\infty dx\, x^2 g_\sigma(x)f(x)f_\sigma(x)=Z_\sigma/Z_0\Gamma \quad \text{for all } \sigma . \tag{2.18}$$

Equations (2.16) and (2.18) together with knowledge of the distributions $g_\sigma(x)$ provide a scheme for evaluating the parameter set $\{\alpha_\sigma\}$ and then the microfield distributions in MCP's of positive charges in a uniform negative background.

III. EFFECTIVE OCP

The multicomponent APEX scheme developed in the preceding section provides numerical results which are in excellent agreement with computer simulations (see Sec. IV). However, these calculations require an approximation procedure for obtaining the pair-distribution functions $g_\sigma(r)$. Although such calculations are feasible with present computers, they become increasingly difficult as the number of species increases. Therefore, in an effort to minimize the numerical complexity, we now consider an approximation which replaces the MCP with an effective OCP whose particles have the average charge

$$\bar{Z} \equiv \sum_\sigma Z_\sigma \chi_\sigma \, , \tag{3.1}$$

where the total number density and the charge density of the uniform background remain unchanged. We can now proceed by using the APEX scheme as described in I to obtain

$$T(L) = \exp\left[3 \int_0^\infty dx\, x^2 g^0(x) \frac{f(x)}{f_\alpha(x)} \{ j_0[L\bar{Z} f_\alpha(x)] - 1 \} \right] , \tag{3.2}$$

where

$$f_\alpha(x) = \frac{e^{-\alpha x}}{x^2}(1+\alpha x) \, , \tag{3.3}$$

and $\rho g^0(x)$ is the density of particles of charge $\bar{Z}e$ at a distance x from $\vec{r}_0$ obtained from the effective OCP. To determine the free parameter α we note that combining Eqs. (2.9) and (3.1) yields

$$\begin{aligned} \tfrac{1}{3}\langle \vec{F}\cdot\vec{F} \rangle &= \sum_\sigma Z_\sigma \chi_\sigma / Z_0 \Gamma \\ &= \bar{Z}/Z_0\Gamma \end{aligned} \tag{3.4}$$

so that a comparison of the second-moment expressions given by Eqs. (3.2) and (3.4) gives the constraint equation

$$\bar{Z}^2 \int_0^\infty dx\, x^2 g^0(x) f(x) f_\alpha(x) = \bar{Z}/Z_0\Gamma \, . \tag{3.5}$$

Equations (3.2) and (3.5) together with knowledge of $g^0(x)$ provide a second scheme for calculating microfield distributions in a MCP.

Note that in the effective OCP approximation the charge $Z_0 e$ is not changed, but instead of being immersed in the MCP it is now immersed in an OCP. As a result of Eqs. (3.4) and (3.5), the effective OCP scheme provides an approximation to $W(\vec{\epsilon})$ which satisfies the exact second moment. However, the local-field constraint described in Sec. II is not satisfied. That is, if we let $G^0(x)$ be the distribution of noninteracting quasiparticles of charge $\bar{Z}e$ a distance x from the charge $Z_0 e$, then we have [see Eq. (3.2)]

$$G^0(x) f_\alpha(x) = g^0(x) f(x) \, , \tag{3.6}$$

which means that the quasiparticles satisfy the local-field constraint when compared with the effective OCP. In the MCP, on the other hand, the right-hand side of Eq. (3.6) replaced by

$$\sum_\sigma \rho_\sigma g_\sigma(x) Z_\sigma f_\sigma(x) \, , \tag{3.7}$$

so that a comparison with the MCP requires

$$\left[\sum_\sigma Z_\sigma \rho_\sigma \right] g^0(x) = \sum_\sigma Z_\sigma \rho_\sigma g_\sigma(x) \, , \tag{3.8}$$

which is clearly satisfied only for large enough x where $g^0(x)$ and all the $g_\sigma(x)$ equal 1 and for $x=0$. Consequently, the effective OCP method does not, in general, satisfy the local-field constraint.

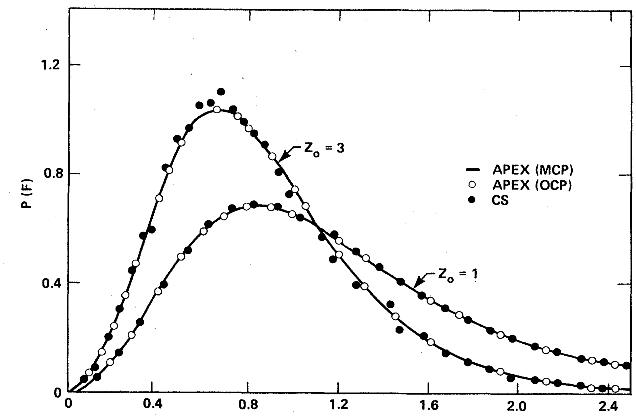

FIG. 1. Comparison of $P(F)$ curves in units defined in Eq. (2.7) for a binary mixture with charges $Z_1=3$ and $Z_2=1$, number fractions $\chi_1=0.03$ and $\chi_2=0.97$ with $\Gamma=1.0$.

IV. NUMERICAL RESULTS

In Figs. 1–4 we present $P(F)$ plots for various binary ionic mixtures with charges $Z_1 e$ and $Z_2 e$ and number fraction χ_1 and χ_2. The results are limited to cases where Z_0 is set equal to either Z_1 or Z_2 since computer simulations are impractical otherwise. The pair-distribution functions were evaluated in the hypernetted-chain approximation generalized to MCP.[5] It is clear from these figures that the multicomponent formulation of APEX [labeled as APEX(MCP) in the figures] is in excellent agreement with the computer simulations[6] (CS in the figures). We have also included the effective OCP approximation [labeled as APEX(OCP) in the figures]. The agreement for this second approximation with computer simulations and APEX(MCP) is also very good.

A discrepancy between APEX(MCP) and APEX(OCP) may arise when the effective OCP $g^0(x)$ is very different

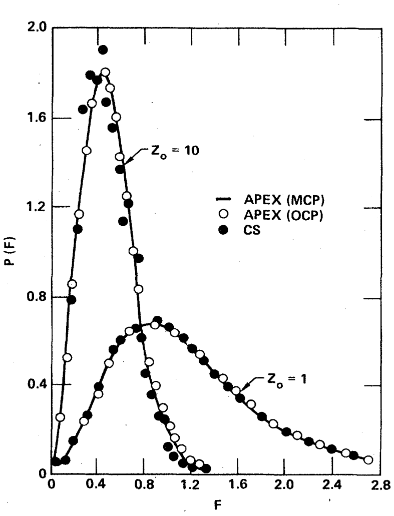

FIG. 2. Same as Fig. 1 with charges $Z_1=10$ and $Z_2=1$, number fractions $\chi_1=0.01$ and $\chi_2=0.99$ with $\Gamma=1.04$.

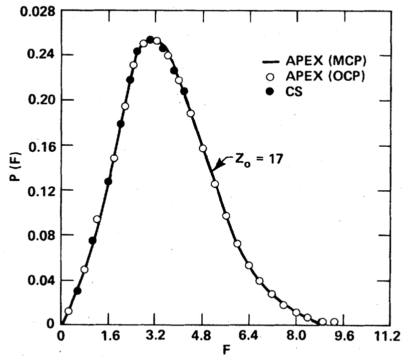

FIG. 3. Same as Fig. 1 with charges $Z_1=17$ and $Z_2=1$, number fractions $\chi_1=\chi_2=0.5$ and $\Gamma=0.1$.

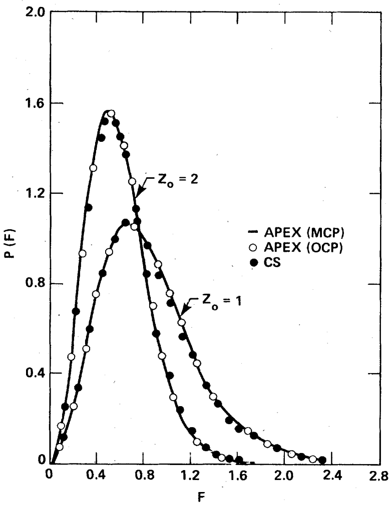

FIG. 4. Same as Fig. 1 with charges $Z_1=2$ and $Z_2=1$, number fractions $\chi_1=\chi_2=0.5$ and $\Gamma=4.88$.

from the $\{g_\sigma(x)\}$ in the MCP. For example, if APEX(OCP) has a charge distribution about $\vec{r}_0$, which on the average stays very far away from $\vec{r}_0$ when compared with the MCP, then since the local-field constraint is not satisfied (see Sec. III), the electric field produced by the effective OCP will be, on the average, too small. As a result APEX(OCP) will yield a $P(F)$ which is shifted toward smaller fields relative to APEX(MCP).

V. CONCLUSION

We have developed a method for calculating electric microfield distributions in MCP which are in excellent agreement with computer simulations. The method takes advantage of the exact second-moment sum rule and the local-field constraint described in Sec. II.

A second approximation is also developed, which although not in general as accurate as the first, is numerically simple. This second approach makes use of the second-moment sum rule but does not satisfy the local-field constraint. It was observed in I that a parametrization of the Baranger-Mozer[7] scheme which satisfied the second-moment sum rule but not the local-field constraint was not as accurate as APEX. This fact suggests that the local-field constraint plays an important role in the development of approximation schemes to calculate electric microfield distributions. Nevertheless, the effective OCP method may be of value for large-scale numerical computations in radiative transfer problems[8] or situations where only the average charge $\overline{Z}$ is known rather than the actual detailed composition of the plasma.[9,10]

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