From: STRONGLY COUPLED PLASMA PHYSICS
 Edited by Forrest J. Rogers
 and Hugh E. Dewitt
 (Plenum Publishing Corporation, 1987)

ELECTRIC MICROFIELD DISTRIBUTIONS IN STRONGLY COUPLED PLASMAS FROM
 INTEGRAL EQUATION SOLUTIONS

F. Lado

Department of Physics
 North Carolina State University
 Raleigh, NC 27695-8202, U.S.A.

Ions radiating from a dense plasma reveal important information about plasma conditions through the detailed structure of their spectral lineshapes (Griem, 1974). This coupling of lineshape and plasma conditions is brought about by the local electric microfield distribution at the radiating ion due to all other charges in the plasma, a quantity first studied by Holtmark (1919) by neglecting all correlations between plasma particles. More recently, Iglesias (1983) has shown that the calculation of the electric microfield distribution in a plasma is equivalent to the determination of the structure of a fictitious "fluid" whose intermolecular potential has both real and imaginary parts. This new formulation of the problem is the point of departure for the work presented below, which is based on the application of a straightforward generalization of the standard methods of liquid state theory coupled with a novel representation of the generalized bridge function.

The model to be studied is the one-component-plasma (OCP), consisting of $N+1$ ions, labeled 0 through N , each of charge e and all contained in a volume V at temperature T ; a uniform background of opposite charge serves to neutralize the collection. The goal is to determine the distribution of electric field magnitudes at ion 0 due to the other N charges and the background. For a particular configuration, the field at $\vec{r}_0$ is

$$\vec{E}(\vec{r}^{N+1}) = \sum_{j=1}^N \frac{e}{r_{j0}^2} \hat{r}_{j0} - e\rho \int d\vec{r} \frac{\vec{r}_0 - \vec{r}}{|\vec{r}_0 - \vec{r}|^3}, \quad (1)$$

where $\rho = N/V$ and the integral term is the background contribution. The probability density for finding the value $\vec{E}$ for $\vec{E}(\vec{r}^{N+1})$ is then

$$W(\epsilon) = (2\pi^2 \epsilon)^{-1} \int_0^\infty dK \, KT(K) \sin(K\epsilon), \quad (2)$$

where

$$T(K) = \langle \exp[i\vec{K} \cdot \vec{E}(\vec{r}^{N+1})] \rangle \quad (3)$$

is the characteristic function corresponding to ϵ . The angular brackets denote a canonical ensemble average with the OCP potential.

Iglesias (1983) has shown Eq. (3) to be formally equivalent to

$$\ln T(K) = i\epsilon\rho \int_0^K d\lambda \int d\vec{r} [g(\vec{r}, \vec{\lambda}) - 1] \hat{K} \cdot \hat{r} / r^2, \quad (4)$$

where $g(\vec{r}_{01}, \vec{\lambda})$ is the generalized pair distribution function (PDF) for a fluid with "potential energy" given by

$$U(\vec{r}^{N+1}, \vec{\lambda}) = U_{\text{OCP}}(\vec{r}^{N+1}) - i\vec{\lambda} \cdot \vec{E}(\vec{r}^{N+1}) / \beta. \quad (5)$$

Here, $\beta = (k_B T)^{-1}$ and $\hat{r}$ and $\hat{K}$ are unit vectors in the direction of $\vec{r}$ and $\vec{K}$ respectively, with $\vec{\lambda} = \lambda \hat{K}$. This reformulation of the problem has already been used to motivate an empirical but remarkably successful approximation dubbed APEX (Iglesias, Lebowitz, and MacGowan, 1983).

As noted by Iglesias (1983), the generalized PDF can be studied with the appropriate generalizations of the standard equations of liquid state theory: a generalized Ornstein-Zernike (OZ) equation

$$h(\vec{r}_{01}, \vec{K}) = C(\vec{r}_{01}, \vec{K}) + \rho \int d\vec{r}_2 h(\vec{r}_{02}, \vec{K}) C(\vec{r}_{21}) \quad (6)$$

and a generalized closure relation

$$C(\vec{r}, \vec{K}) = h(\vec{r}, \vec{K}) - \ln\{g(\vec{r}, \vec{K}) \exp[\beta\phi(r) - i\epsilon\vec{K} \cdot \hat{r} / r^2]\} + B(\vec{r}, \vec{K}). \quad (7)$$

In these equations, $h = g - 1$, $\phi(r)$ is the Coulomb potential, and $B(\vec{r}, \vec{K})$ is the generalized bridge function for the "fluid", for which an approximation must be supplied. This is discussed below.

It is first necessary to simplify Equations (6) and (7) before they can be numerically manipulated. In extracting the angular dependence of complex functions such as $g(\vec{r}, \vec{K})$, we first note from its definition that it satisfies

$$g^*(\vec{r}, \vec{K}) = g(\vec{r}, -\vec{K}), \quad (8)$$

so that expansion in Legendre polynomials $P_\ell(x)$ automatically produces a separation of real and imaginary parts,

$$\begin{aligned} g(\vec{r}, \vec{K}) &= g(r, K, \cos\theta) = \sum_{\ell \text{ even}} g_\ell(r, K) P_\ell(\cos\theta) + i \sum_{\ell \text{ odd}} g_\ell(r, K) P_\ell(\cos\theta) \\ &= \sum_{\ell=0}^{\infty} i^\sigma g_\ell(r, K) P_\ell(\cos\theta), \end{aligned} \quad (9)$$

where for brevity in Eq. (9) and below we are using $\sigma = 0$ for ℓ even and $\sigma = 1$ for ℓ odd. Other generalized functions of $\vec{r}$ and $\vec{K}$ have similar expansions.

As for simple fluids, it is convenient to deconvolute Eq. (6) using Fourier transforms. The transform of a generalized function such as $C(\vec{r}, \vec{K})$,

$$\tilde{C}(\vec{k}, \vec{K}) = \int d\vec{r} C(\vec{r}, \vec{K}) e^{i\vec{k} \cdot \vec{r}}, \quad (10)$$

can be readily performed by orienting the z axis of the coordinate frame along $\vec{K}$, representing $C(\vec{r}, \vec{K})$ as in Eq. (9), and using the Rayleigh expansion (Gray and Gubbins, 1984)

$$e^{i\vec{k} \cdot \vec{r}} = 4\pi \sum_{\ell, m} i^\ell j_\ell(kr) Y_{\ell m}(\theta, \phi) Y_{\ell m}^*(\theta', \phi'), \quad (11)$$

where the primed and unprimed angles specify the orientations of $\vec{k}$ and $\vec{r}$ respectively. Inserting (11) into (10), we then find

$$\tilde{C}(\vec{k}, \vec{K}) = \sum_{\ell=0}^{\infty} \tilde{C}_{\ell}(k, K) P_{\ell}(\cos\theta), \quad (12)$$

with the transform coefficients given by

$$\tilde{C}_{\ell}(k, K) = 4\pi i^{\ell+\sigma} \int_0^{\infty} dr r^2 C_{\ell}(r, K) j_{\ell}(kr), \quad (13)$$

where $j_{\ell}(x)$ is the spherical Bessel function of order ℓ . Note that the $\tilde{C}_{\ell}$ are real for all ℓ .

These ingredients suffice to define an iterative algorithm for the solution of the coupled equations (6) and (7) in terms of $S(\vec{r}, \vec{K}) = h(\vec{r}, \vec{K}) - C(\vec{r}, \vec{K})$ as the unknown:

- i. Using the current (finite) set of coefficients $S_{\ell}(r, K)$, form

$$S(\vec{r}, \vec{K}) = \sum_{\ell} i^{\sigma} S_{\ell}(r, K) P_{\ell}(\cos\theta) \quad (14)$$

and similarly for $B(\vec{r}, \vec{K})$. (See below.) Then numerically evaluate the Legendre inversion integral of the closure equation (7) for

$$i^{\sigma} h_{\ell}(r, K) = (\ell + \frac{1}{2}) \int_{-1}^1 d(\cos\theta) \{ \exp[-\beta\phi(r) + i e \frac{\vec{K} \cdot \hat{r}}{2} + S(\vec{r}, \vec{K}) + B(\vec{r}, \vec{K})] - 1 \} P_{\ell}(\cos\theta) \quad (15)$$

to get the DCF coefficients

$$C_{\ell}(r, K) = h_{\ell}(r, K) - S_{\ell}(r, K). \quad (16)$$

- ii. Fourier transform these using Eq. (13) to yield the transform coefficients $\tilde{C}_{\ell}(k, K)$.

- iii. Use the transform of the OZ equation to get

$$\tilde{S}_{\ell}(k, K) = \tilde{C}_{\ell}(k, K) \tilde{C}(k) / [1 - \rho \tilde{C}(k)]. \quad (17)$$

- iv. Invert these to find the new set of coefficients

$$S_{\ell}(r, K) = (2\pi^2 i^{\ell})^{-1} \int_0^{\infty} dk k^2 \tilde{S}_{\ell}(k, K) j_{\ell}(kr). \quad (18)$$

This completes an iteration. Here a test is made for self consistency of the input and output S_{ℓ} and the cycle is repeated until convergence is reached, whereupon Eq. (4) for $T(K)$ is evaluated as

$$\ln T(K) = -\frac{4}{3} \pi \rho e \int_0^K d\lambda \int_0^{\infty} dr h_1(r, \lambda), \quad (19)$$

the orthogonality of the Legendre polynomials having reduced $h(\vec{r}, \vec{\lambda})$ in Eq. (4) to just the $\ell = 1$ coefficient.

Finally, we turn to the question of representing the generalized bridge function $B(\vec{r}, \vec{K})$, about which essentially nothing is known. Trial calculations show that its omission, as in the Hypernetted-Chain equation, or approximation with no K dependence, leads to mediocre results. Guided by the exact solution of the Mean Spherical Model (MSM) for this problem (Lado, 1986), we have adopted for $B(\vec{r}, \vec{K})$ the MSM analytic form of $g(\vec{r}, \vec{K})$ and $C(\vec{r}, \vec{K})$ and have thus used in this calculation the two-term expansion

$$B(\vec{r}, \vec{K}) = B_{\text{OCP}}(r) + i \frac{K}{\beta e} B'_{\text{OCP}}(r) P_1(\cos\theta), \quad (20)$$

where the prime denotes differentiation and the OCP bridge function is itself approximated by that of hard spheres (Rosenfeld and Ashcroft, 1979; Lado, Foiles, and Ashcroft, 1983).

Correlation functions of imaginary fluids having some novelty interest, it seems worthwhile to comment briefly on their behavior before presenting the final results for the microfield distributions, though space here allows display of only one key feature. The leading real coefficient g_0 of $g(\vec{r}, \vec{K})$ is similar to the PDF of simple fluids, with some additional oscillatory structure between the core region and the usual first peak. Higher coefficients are all oscillatory in the same range, going asymptotically to zero as g_0 goes to one. Imaginary terms show the same latter behavior. Both the magnitudes and frequencies of these oscillations increase rapidly with K , so that it becomes apparent that a sum of any practical number of terms would poorly reproduce the full $g(\vec{r}, \vec{K})$. Note however that such a sum is not needed in the solution algorithm.

What is summed is the function $S(\vec{r}, \vec{K})$ and here the story is quite different. We show in Fig. 1 the first three coefficients of both the real and imaginary parts of $S(\vec{r}, \vec{K})$ for $\Gamma = \beta e^2/a = 10$ and $K\epsilon_0 = 10$, where $\epsilon_0 = e/a^2$ and a is the usual ion sphere radius. It is clear from these figures that both S_0 and S_1 are overwhelmingly the dominant terms of their respective sets; the expansion of Eq. (14) is very rapidly convergent. Further, halving K does not change this qualitative picture: S_0 decreases modestly only for small r while, significantly, S_1 roughly diminishes by half its magnitude. If we further note that S_1 has the form of the slope of S_0 , we find in these features solid internal support for the $B(\vec{r}, \vec{K})$ ansatz of Eq. (20).

The ultimate test of Eq. (20), which is the sole approximation in this calculation, must lie however in the final computed forms of the microfield distributions. These are shown for $\Gamma = 10$ and 100 in Fig. 2, along with the corresponding APEX results (Iglesias et al., 1983) and normative computer

Figure 1. Coefficients of the real and imaginary parts of $S(\vec{r}, \vec{K})$ for $\Gamma = 10$ and $K\epsilon_0 = 10$.

Figure 2. Electric microfield distributions $P(\epsilon) = 4\pi\epsilon^2 W(\epsilon)$ at an ion for $\Gamma = 10$ and 100 obtained from the present work (I.E.), APEX, and computer simulation (stars).

simulation data (DeWitt, unpublished). It seems clear from these figures that the integral equation method initiated by Iglesias (1983), coupled with a realistic form for the generalized bridge function, is a fruitful approach to the calculation of the electric microfield distribution in a plasma.

This work was supported by the National Science Foundation under Grant No. CHE-84-02144.

REFERENCES

- DeWitt, H. E., unpublished.
 Gray, C. G., and Gubbins, K. E., 1984, "Theory of Molecular Fluids," Vol. 1, Clarendon, Oxford.
 Griem, H. R., 1974, "Spectral Line Broadening by Plasmas," Academic, New York.
 Holtzmark, J., 1919, Ann. Phys. (Leipzig), 58:577.
 Iglesias, C. A., 1983, Phys. Rev. A, 27:2705.
 Iglesias, C. A., Lebowitz, J. L., and MacGowan, D., 1983, Phys. Rev. A, 28:1667.
 Lado, F., 1986, Phys. Rev. A, 34:(November 1 issue).
 Lado, F., Foiles, S. M., and Ashcroft, N. W., 1983, Phys. Rev. A, 28:2374.
 Rosenfeld, Y., and Ashcroft, N. W., 1979, Phys. Rev. A, 20:1208.