## Electric Microfield Distributions in Plasmas<sup>\*</sup>

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A new method for calculating the distribution of electric microfields (high-frequency components) in a plasma is developed. Distributions are calculated at both a neutral and a charged point. The plasma is taken to be a system of N charged particles moving in a uniform neutralizing background. It is shown that this development allows for the inclusion of all correlations to a high degree of accuracy. This theory is then compared with the Holtsmark and Baranger-Mozer theories. A detailed analysis of all approximations is included, together with a Monte Carlo study. Numerical results are shown both graphically and in tabulated form.

#### I. INTRODUCTION

N recent years considerable effort has been expended on the problem of spectral line broadening in plasmas.<sup>1-4</sup> In relation to this problem, various theories of the electric microfield distributions have been formulated.5,6 The primary aim of these efforts has been to include particle-particle correlations to various orders and thus to improve the original work done by Holtsmark.<sup>7</sup> The microfield problem may be separated into two categories; in the first of these, the primary concern is with the treatment of extremely dense plasmas (solar cores). One approach to such plasmas has used collective coordinates to calculate the microfield distribution at an ion.<sup>5</sup> While this calculation may have been valid for that particular temperaturedensity region, its applicability to high temperature, dilute plasmas has been held in doubt, since it did not result in the Holtsmark distribution when the infinite temperature limit was taken.<sup>6</sup> The second category has been primarily concerned with less dense plasmas, such as those produced in the laboratory. The most successful of these was presented by Baranger and Mozer (hereafter referred to as B-M). Their papers considered two cases which they referred to as the highand low-frequency components. B-M maintained that their theory was of "unquestionable accuracy" in the high temperature, low density limit, and while this assertion is definitely valid, it remains unspecified as to how one quantitatively defines that region of applicability. In view of the fact that only pair correlations were considered, and that these were handled through

the Debye-Hückel pair-correlation function (and sometimes the linearized version of that function), it seems desirable to re-examine the problem with a view toward generating an alternative approach which would extend into the higher density, lower temperature regions.

With these goals in mind, the present theory is constructed. In this first paper, the plasma treated is assumed to consist of N-charged particles moving in a uniform neutralizing background; this corresponds to the B-M high-frequency case. The problem of the low frequency case will be the subject of a later communication.

Each of these N particles is assumed to interact with one another through a Coulomb potential. When treating the problem of the electric field distribution at a charged particle, an additional (N+1)st particle, conveniently placed at the origin of the reference frame, must be included. It will be shown that the field distribution at a neutral point is just a special case of the charged-point development.

Section II of this paper deals with the development of the formalism. The numerical results and analysis, including a comparison with the B-M theory, are discussed in Sec. III. Final conclusions are presented in the fourth and last section. Supplementary to the main text is an extensive Appendix. Where at all practicable, detailed calculations have been relegated to this Appendix.

#### **II. FORMALISM**

Define  $Q(\mathbf{\epsilon})d\mathbf{\epsilon}$  as the probability of finding an electric field  $\mathbf{\epsilon}$ , at a singly charged or neutral point, due to a collection of N-charged particles moving in a uniform neutralizing background, and contained in a volume  $\mathcal{V}$ . Then if Z represents the configurational partition function, we may write

$$Q(\mathbf{\epsilon}) = Z^{-1} \int \cdots \int \exp[-\beta V(\mathbf{r}_1 \cdots \mathbf{r}_N)] \\ \times \delta(\mathbf{\epsilon} + \sum_j (e\mathbf{r}_j/r_j^3)) \prod_{j=1}^N d\mathbf{r}_j, \quad (1)$$

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<sup>&</sup>lt;sup>1</sup>M. Baranger, Phys. Rev. 111, 494 (1958); 111, 481 (1958); 112, 855 (1958).

<sup>&</sup>lt;sup>2</sup> A. C. Kolb and H. R. Griem, Phys. Rev. 111, 514 (1958); 116, 4 (1959).

<sup>&</sup>lt;sup>8</sup> H. R. Griem, M. Baranger, A. C. Kolb, and G. Oertel, Phys. Rev. **125**, 177 (1962).

<sup>&</sup>lt;sup>4</sup> H. R. Griem, Phys. Rev. 140, 129 (1965).

<sup>&</sup>lt;sup>5</sup> A. A. Broyles, Phys. Rev. 100, 1181 (1955); Z. Physik 151, 187 (1958).

<sup>&</sup>lt;sup>6</sup> M. Baranger and B. Mozer, Phys. Rev. 115, 521 (1959); 118, 626 (1960).

<sup>&</sup>lt;sup>7</sup> J. Holtsmark, Ann. Physik 58, 577 (1919).

where  $\mathbf{r}_{j}$  represents the coordinates of the *j*th particle,  $\beta \equiv 1/kT$ , and  $V(\mathbf{r}_i \dots \mathbf{r}_N)$  represents the potential energy of the system. Using the identity,

$$\delta(\mathbf{x}) = (2\pi)^{-3} \int \int \int \exp[i\mathbf{l} \cdot \mathbf{x}] d\mathbf{l}, \qquad (2)$$

in Eq. (1), and performing the integration over angles, Eq. (1) becomes

$$Q(\mathbf{\epsilon}) = (2\pi^2 \epsilon)^{-1} \int_0^\infty T(l) \sin(\epsilon l) l \, dl \,, \tag{3}$$

where

$$T(l) = Z^{-1} \int \cdots \int \exp[-\beta V + i \sum_{j} \mathbf{l} \cdot (e\mathbf{r}_{j}/r_{j}^{3})] \prod_{j} d\mathbf{r}_{j}.$$
 (4)

Assuming that our system is isotropic, we let  $P(\epsilon)$  be the probability for finding an electric field  $\epsilon$  at a specified point. It satisfies the relation,

$$4\pi Q(\mathbf{\epsilon})\epsilon^2 d\epsilon \equiv P(\epsilon)d\epsilon. \tag{5}$$

Using Eq. (3), we find

$$P(\epsilon) = 2\pi^{-1}\epsilon \int_0^\infty T(l)\sin(\epsilon l)l\,dl.$$
(6)

This expression has been derived by a number of authors.5,6

Exclusive of the uniform neutralizing background, the potential energy of the system is expressed as

$$V' = \sum_{0=i (7)$$

It has been shown that the effect of the neutralizing background may be included by writing V' in terms of its Fourier expansion and excluding the zero index term.<sup>5</sup> The resulting expression is

$$V = \frac{4\pi e^2}{\mathcal{V}} \sum_{\mathbf{k}}' \sum_{i < j} \frac{1}{k^2} e^{-i\mathbf{k} \cdot \mathbf{r}_{ij}}.$$
 (8)

The prime implies that the term k=0 must be excluded from the summation over k. Now set

$$V = V_0 + \sum_i w_{i0},$$
 (9)

where

$$w_{i0} = \frac{e^2}{r_{i0}} e^{-\alpha r_{i0}/\lambda}, \qquad (10)$$

 $\alpha$  is an arbitrary, real, positive parameter which will be independently determined, and  $\lambda$  is the Debye length. If n is the particle density of our system, then

$$\lambda = (kT/4\pi ne^2)^{1/2}.$$
 (11)

Substituting Eq. (9) into our expression for T(l), we find

$$T(l) = Z^{-1} \int \cdots \int \exp[-\beta V_0 + i(\mathbf{l}/e) \cdot \nabla_0 V_0]$$
$$\times \prod_{j=1}^N \exp[-\beta w_{j0} + i(\mathbf{l}/e) \cdot \nabla_0 w_{j0}] d\mathbf{r}_j. \quad (12)$$

To proceed further, the product term of this integral is treated by a cluster expansion technique similar to that employed by Mayer<sup>8</sup> and Baranger.<sup>6</sup> We define a function  $\chi(l, j)$  as

$$\boldsymbol{\chi}(l,j) = \left[ \exp(-\beta w_{j0} + i(\mathbf{l}/e) \cdot \boldsymbol{\nabla}_{0} w_{j0}) - 1 \right].$$
(13)

It should be stressed that although the general technique is similar, the functions, in terms of which the expansion is made in the present development, are very different from those used by Mayer and Baranger. Specifically, the argument of the exponential term in x(l,j) differs considerably from the corresponding expressions in other cluster expansions. In terms of these x functions, Eq. (12) becomes

$$T(l) = Z^{-1} \int \cdots \int \exp\left[-\beta V_0 + i(\mathbf{l}/e) \cdot \nabla_0 V_0\right] \left[1 + \sum_i \chi(l,i) + \sum_{i < j} \chi(l,i) \chi(l,j) + \cdots \right] \prod_j d\mathbf{r}_j$$
$$= Z^{-1} \int \cdots \int \exp\left[-\beta V_0 + i(\mathbf{l}/e) \cdot \nabla_0 V_0\right] \prod_j d\mathbf{r}_j + NZ^{-1} \int \cdots \int \exp\left[-\beta V_0 + i(\mathbf{l}/e) \cdot \nabla_0 V_0\right] \chi(l,1) \prod_j d\mathbf{r}_j$$
$$+ \frac{1}{2} N(N-1) Z^{-1} \int \cdots \int \exp\left[-\beta V_0 + i(\mathbf{l}/e) \cdot \nabla_0 V_0\right] \chi(l,1) \chi(l,2) \prod_j d\mathbf{r}_j + \cdots; \quad (14)$$

if we define  $T_j$  as an integration over N-j particle and further define coordinates of the form

$$T_{j}(l) \equiv \int \cdots \int \exp[-\beta V_{0} + i(\mathbf{l}/e) \cdot \nabla_{0} V_{0}] \prod_{i=j+1}^{N} d\mathbf{r}_{i}, \quad (15)$$

$$Q_j(l) \equiv T_j(l) / T_0(l)$$
, (16)

<sup>8</sup> J. E. Mayer and M. G. Mayer, *Statistical Mechanics* (John Wiley & Sons, Inc., New York, 1940), Chap. 13.

we may write

$$T(l) = (T_0(l)/Z) \left[ 1 + N \int Q_1 \chi(l,1) d\mathbf{r}_1 + \frac{1}{2} N(N-1) \right]$$
$$\times \int \int Q_2 \chi(l,1) \chi(l,2) d\mathbf{r}_1 d\mathbf{r}_2 + \cdots \left]. \quad (17)$$

We then expand each of the  $Q_i$  functions in an Ursell expansion,<sup>9</sup> according to the prescription

$$\begin{aligned} & \forall Q_1(l,1) = g_1(l,1), \\ & \forall^2 Q_2(l,1,2) = g_1(l,1)g_1(l,2) + g_2(l,1,2), \\ & \forall^3 Q_3(l,1,2,3) = g_1(l,1)g_1(l,2)g_1(l,3) \\ & + g_1(l,1)g_2(l,2,3) + g_1(l,2)g_2(l,1,3) \\ & + g_1(l,3)g_2(l,1,2) + g_3(l,1,2,3), \text{ etc.} \end{aligned}$$
(18)

In the limit  $N \to \infty$ ,  $\mathfrak{V} \to \infty$ , such that  $N/\mathfrak{V} \to n$ = constant,

$$T(l) = (T_0(l)/Z) \left\{ 1 + n \int g_1(l) \chi(l,1) d\mathbf{r}_1 \right\}$$
$$+ \frac{n^2}{2!} \left[ \int g_2(l) \chi(l,1) \chi(l,2) d\mathbf{r}_1 d\mathbf{r}_2 + \left( \int g_1(l) \chi(l,1) d\mathbf{r}_1 \right)^2 \right] + \frac{n^3}{3!} \left[ ] + \cdots \right\}. \quad (19)$$

Further, if we define a new function  $h_j$  as

$$h_j(l) = \int \cdots \int g_j(l) \chi(l,1) \cdots \chi(l,j) \prod_{i=1}^j d\mathbf{r}_i, \qquad (20)$$

then

$$T(l) = (T_0(l)/Z) \{ 1 + n[h_1(l)] + (n^2/2!)[h_2(l) + h_1^2(l)] + \cdots \}.$$
 (21)

Recognizing that in Eq. (21), each expression in brackets has the form of a term in a systematic Ursell cluster expansion, we may write<sup>10</sup>

$$T(l) = (T_0(l)/Z) \left[ \prod_j \sum_m \frac{1}{m!} \left( \frac{n^{jh_j}}{j!} \right)^m \right].$$

This may be put into the more convenient form

$$T(l) = (T_0(l)/Z) \exp[\sum_j (n^j/j!)h_j(l)].$$
(22)

While this expression for T(l) is similar to one derived by Baranger,<sup>6</sup> it should be noted that the  $h_i(l)$  functions appearing in the two theories are significantly different, and that the  $(T_0(l)/Z)$  factor does not appear in the Baranger expression.

Splitting up the potential appearing in Z in the same manner as that previously described when treating T(l), we are able to carry out a similar expansion program with the result that we find

$$Z = T_0(0) \exp[\sum_j (n^j / j!) h_j(0)], \qquad (23)$$

which further implies that

$$T(l) = [T_0(l)/T_0(0)] \exp\{\sum_j (n^j/j!) [h_j(l) - h_j(0)]\}.$$
 (24)

Consider the individual terms appearing in this expression. By the method developed in Appendix A, we may show that the first factor,  $T_0(l)/T_0(0)$ , becomes

$$\frac{T_0(l)}{T_0(0)} = \exp\left[-\frac{\alpha^3 a L^2}{4(\alpha+1)^2}\right] = e^{-\gamma L^2}.$$
 (25)

In Eq. (25),

$$L \equiv l \epsilon_0$$
 and  $a \equiv r_0 / \lambda; \quad \epsilon_0 \equiv (e/r_0^2),$  (26)

where  $r_0$  is the ion-sphere radius defined by the expression

$$\frac{4}{3}\pi r_0{}^3n = 1. \tag{27}$$

Now we consider the factors resulting from terms in the series exponent. For j=1,

$$n[h_{1}(l)-h_{1}(0)] = \int \left\{ \frac{\int \cdots \int \exp[-\beta V_{0}+i(\mathbf{l}/e) \cdot \nabla_{0} V_{0}] [\exp[i\beta w_{10}+i(\mathbf{l}/e) \cdot \nabla_{0} w_{10}] - 1] \prod_{j=2}^{N} d\mathbf{r}_{j}}{\int \cdots \int \exp[-\beta V_{0}+i(\mathbf{l}/e) \cdot \nabla_{0} V_{0}] \prod_{j=1}^{N} d\mathbf{r}_{j}} - \frac{\int \cdots \int \exp[-\beta V_{0}] [\exp[-\beta w_{10}] - 1] \prod_{j=2}^{N} d\mathbf{r}_{j}}{\int \cdots \int \exp[-\beta V_{0}] \prod_{j=1}^{N} d\mathbf{r}_{j}} \right\} d\mathbf{r}_{1}. \quad (28)$$

<sup>9</sup> H. D. Ursell, Proc. Cambridge Phil. Soc. 23, 685 (1927).
 <sup>10</sup> K. Huang, *Statistical Mechanics* (John Wiley & Sons, Inc., New York, 1963), Chap. 14, Secs. 14.1, 14.2.



FIG. 1. A comparison of two T(l)approximations as applied to the present theory of the electric microfield distribution function  $P(\epsilon)$  (charged point case). [See Eqs. (A50), (A51).]  $\epsilon$  is in units of  $\epsilon_0$ .

Although these integrals appear formidable, they may be readily reduced, through the use of collective coordinates, to an approximate expression involving only a one-dimensional integral. The accuracy of this approximation is discussed later in this section. Collective coordinates are defined, and the nature of the evaluation indicated, in Appendix A. The final result is just stated here

$$I_{1}(l) = n [h_{1}(l) - h_{1}(0)] = 3 \int_{0}^{\infty} dx \, x^{2} e^{F(x)} \left[ \frac{\sin[LG(x)]}{[LG(x)]} - 1 \right] - 3 \int_{0}^{\infty} dx \, x^{2} e^{s(x)} \left[ \frac{\sin[Lq(x)]}{[Lq(x)]} - 1 \right].$$
(29)

The functions which appear in the integrands are defined as follows:

$$x = r/r_{0}, \qquad F(x) = \frac{a^{2}}{3x} \frac{1}{1-\alpha^{2}} \{ \alpha^{2}e^{-ax} - e^{-\alpha ax} \}, \qquad (30)$$

$$G(x) = \frac{1}{1-\alpha^{2}} \{ \frac{1}{x^{2}} [e^{-\alpha ax} - \alpha^{2}e^{-ax}] + \frac{a}{x} [\alpha e^{-\alpha ax} - \alpha^{2}e^{-ax}] \}, \quad q(x) = \frac{\alpha^{2}}{1-\alpha^{2}} \{ \frac{1}{x^{2}} [e^{-\alpha ax} - e^{-ax}] - \frac{a}{x} [e^{-ax} - \alpha e^{-\alpha ax}] \}.$$

The second term in the series exponent is given explicitly as

$$I_{2}(l) = \frac{1}{2}n^{2} \left[h_{2}(l) - h_{2}(0)\right] = \frac{1}{2}n^{2} \left\{ \int \int g_{2}(l) \chi(l,1) \chi(l,2) d\mathbf{r}_{1} d\mathbf{r}_{2} - \int \int g_{2}(0) \chi(0,1) \chi(0,2) d\mathbf{r}_{1} d\mathbf{r}_{2} \right\}.$$
(31)

When the  $g_2(l)$  and  $g_2(0)$  functions appearing in this equation are evaluated in Appendix A, it is found that they have a particularly interesting form. Eq. (A44) gives the following expression for  $g_2(l)$ :

$$g_2(l) = \mathcal{U}^2 Q_1(l,1) Q_1(l,2) \left[ \exp\left[ -\frac{a^2}{3x_{12}} e^{-ax_{12}} \right] - 1 \right];$$
(32)

a similar expression is found for  $g_2(0)$ . The exponential term in brackets is just the nonlinearized Debye-Hückel pair-correlation function, while the entire content of the bracket is just the two-body "cluster" function in an Ursell cluster expansion.<sup>11</sup> This is not a surprising result in view of the fact that studies of the radial-distribution function by collective coordinate techniques have indicated that when the entire potential energy of such a system is treated by collective coordinates, the result is the nonlinearized Debye-Hückel pair-correlation function.<sup>12</sup> This has special significance in this theory in that it implies that noncentral, two-body correlations, included through the mechanism of collective coordinates, are of the same accuracy as the nonlinear Debye-Hückel result. This

 <sup>&</sup>lt;sup>11</sup> E. E. Salpeter, Ann. Phys. (N. Y.) 5, 214 (1958).
 <sup>12</sup> H. L. Sahlin, dissertation, Department of Physics, University of Florida, 1963 (unpublished).

procedure allows one to use a simplified cluster expansion such as that employed in this paper. That the expansion converges very rapidly may be observed by noting that each term consists of the *difference* between two  $h_j$  functions; each of these is a *j*-dimensional integral over a product of (1) a term representing the *j*th "cluster" function, (2) *j* of the  $\chi$  functions, and (3) *j* of the  $Q_1$  terms [see for example Eq. (32)].

Each of these factors not only aids convergence of the integrals themselves, but also contributes to making the series of  $h_j$  terms rapidly convergent. The validity of this assertion is further indicated by a direct numerical comparison of the relative importance of the first and second terms in the expansion (see Fig. 1).

Using the result shown in Eq. (32) in Eq. (31), and performing a collective coordinate calculation (see Appendix A), we find

Two of the functions in the integrands, G(x) and q(x), have already been defined. Functions remaining to be specified are

$$\beta w_{i0} = \frac{a^2}{3x_{i0}} e^{-\alpha a x_{i0}}, \quad s(x_i) = \frac{\alpha^2}{1 - \alpha^2} \left(\frac{a^2}{3x_i}\right) \left[e^{-a x_i} - e^{-\alpha a x_i}\right]. \tag{34}$$

I and K refer to modified Bessel functions of the first and third kind, respectively, while  $j_k(-)$  specifies a spherical Bessel function of order k.<sup>13</sup>

Thus

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$$T(l) = \exp[-\gamma L^2 + I_1(l) + I_2(l)], \qquad (35)$$

where  $I_1(l)$  is given by Eq. (29), and  $I_2(l)$  by Eq. (33). This result is used in Eq. (6) to calculate  $P(\epsilon)$  at a charged point.

In the event that  $P(\epsilon)$  is desired at a neutral point, the charged point equations are easily adapted to accomplish this purpose. Modifications are necessitated by the fact that we no longer have any central interactions to include in the potential energy of the system. Although this fact does not alter the expression for  $T_0(l)/T_0(0)$ , it is reflected in the final equation for  $I_1(l)$  since both F(x) and  $h_1(0)$  must be set equal to zero. Therefore,

$$I_1(l)_{\text{neutral}} = nh_1(l)_{\text{neutral}} = 3 \int_0^\infty dx x^2 \left[ \frac{\sin[LG(x)]}{[LG(x)]} - \frac{\sin[Lq(x)]}{[Lq(x)]} \right].$$
(36)

Applying the same physical arguments to  $I_2(l)$  we find that

At this point it is possible to observe that in the infinite temperature limit, T(l) and hence  $P(\epsilon)$  go to the correct Holtsmark limit. From Eq. (26) we see that

as the temperature becomes infinite, a goes to zero. Applying this result to the equation for T(l), in Eq. (24), we find that only the factor  $\exp\{n[h_1(l)-h_1(0)]\}$  remains. In this limit, all other terms in the series exponential go to zero, since  $g_i(j>1)$  goes to zero, while the factor  $T_0(l)/T_0(0)$  becomes unity. It may be

<sup>&</sup>lt;sup>13</sup> The Bateman Manuscript Project, *Higher Transcendental Functions* (California Institute of Technology, Pasadena, California, 1953), Vol. II, Chap. VII.



FIG. 2. An estimate of the importance of the Jacobian correction term,  $a_3$ .  $P(\epsilon)$  curves calculated for any of the  $\alpha$  values lying in the heavy section of a given line will agree to within several percent (at worst) over the entire range of  $\epsilon$  values considered in this paper. For further explanation, see Sec. III of the text.

verified by direct substitution that in this case,

$$T(l) = \exp\left\{-3\int_{0}^{\infty} dx x^{2} \left[\frac{\sin(L/x^{2})}{(L/x^{2})} - 1\right]\right\}$$
$$= \exp\left\{-\frac{2(2\pi)^{1/2}}{5}L^{3/2}\right\}.$$
 (38)

This last relation is just the Holtsmark expression for T(l).

Two approximations have been made in this theory. The first of these is the termination of the series appearing in the exponential, with the second term. Justification for this step has been given previously, and numerical affirmation of its validity will be presented in Sec. III. The second approximation, which we will now consider, is concerned with the collective coordinate evaluation of the many-dimensional integrals occurring in this theory.

As is shown in Appendix A, Eq. (A16), the evaluation of the many-dimensional integrals involved in the calculation of T(l) may be transformed into integrals over collective coordinates which have a rather simple form. These collective-coordinate integrals, along with their solutions are given below

$$I = \int \cdots \int \exp\{-\frac{1}{2} \sum_{k} [A_{k}X_{k}^{2} + 2b_{k}X_{k}]\} J \prod_{k} dX_{k}$$
$$= \operatorname{const} \times \exp\{\frac{1}{2} \sum_{k} b_{k}^{2} / (1 + A_{k})\} \times [1 - a_{3} + a_{4} - \cdots], \quad (39)$$

where  $A_k$  and  $b_k$  are specific functions of k, the  $X_k$ 's represent collective coordinates, and J is the Jacobian of the  $\mathbf{r} \rightarrow \mathbf{X}$  transformation. The series of terms in brackets represents the possible higher order corrections to the first Jacobian approximation. In the calculations made thus far,  $a_3$ , as well as all other Jacobian correction terms, have been neglected. The assumption is of course that they really are negligible. However, if these calculations are to be taken seriously, the correctness of this last assumption must be verified. This has been done in several ways.

The first step in using, and in evaluating the present theory, is to determine the adjustable parameter  $\alpha$ . Perhaps the best choice of  $\alpha$  is the one which results in a minimum error due to the combined effect of the clusterexpansion termination error and the Jacobian error. An even better choice of  $\alpha$  would be one which resulted in the error due to each of the two major sources being negligible, if this is possible. A clear indication that such a circumstance had occurred would be the existence of a distinct and extended range of  $\alpha$  values over which the T(l) curve, and hence the  $P(\epsilon)$  curve, would remain stationary; the requirement of such a range would virtually rule out any possibility that the two errors had merely cancelled one another. The latter choice was shown to be possible, and was the one chosen to determine the best value of  $\alpha$ ; specifically, an  $\alpha$  value lying at the approximate center of the stationary range was the one chosen.

Rather than rely solely on the above argument, this criterion was subjected to several tests. First, the second term in the cluster expansion was calculated, and is shown in Fig. 1 to contribute less than 2% to any point on the  $P(\epsilon)$  curve in a "worst case" situation. Similarly, the  $a_3$  term in the Jacobian correction series was evaluated. It is seen in Fig. 2 that, in the  $\alpha$  region chosen for the calculation, this term, which indicates skewness of the collective coordinate distribution, is negligible. From the related structure of  $a_4$ , the kurtosis,<sup>14</sup> it may be deduced that the same choice of  $\alpha$  will also make  $a_4$  negligible. In an effort to also rule out the possibility that although  $a_3$  and  $a_4$  are small, the entire series is appreciable, a special case is considered.

Since the theory of B-M should indeed be valid for dilute systems at sufficiently high temperatures,  $P(\epsilon)$ curves predicted by both theories at a=0.2, should agree quite well (a=0.0 corresponds to the Holtsmark case). It is shown graphically in the next section that, in this instance, the present theory without Jacobian corrections yields a  $P(\epsilon)$  curve almost identical to that predicted from the B-M theory. The assertion is that in this case,  $a_3$ ,  $a_4$ , and the entire Jacobian correction series are really negligible. Figure 2 indicates that freedom to choose the correct  $\alpha$  value corresponding to a given a results in  $a_3$  having at least the same order of

<sup>&</sup>lt;sup>14</sup> R. Van Mises, *Mathematical Theory of Probability and Statistics* (Academic Press Inc., 1964), Chap. III-A, p. 129.



FIG. 3. A comparison of the electric microfield distribution  $P(\epsilon)$  calculated by the present theory, with that predicted by a Monte Carlo calculation (50 000 particle configurations).

FIG. 4. The electric microfield distribution function  $P(\epsilon)$ , at a charged point, for several values of a;  $\epsilon$  is in units of  $\epsilon_0$ .

FIG. 5. The electric microfield distribution function  $P(\epsilon)$ , at a neutral point, for several values of a;  $\epsilon$  is in units of  $\epsilon_0$ .

magnitude for a > 0.2 as it did when a = 0.2. If the  $\alpha$ variation affects  $a_3$  and  $a_4$  in this manner, it is plausible to expect the entire series to be similarly affected. Thus, by this argument too, we expect the present theory without Jacobian correction to be valid for rather highdensity, low-temperature regions (e.g., a=0.8).

A final attempt at verifying the procedure is shown in Fig. 3. Here we see a comparison of the results of a Monte Carlo calculation of  $P(\epsilon)$  for a=0.8 (the largest deviation from the Holtsmark distribution considered in this paper) and the corresponding curve for this theory. It is seen that while the curve predicted by the present theory peaks at the same  $\epsilon$  value as does the Monte Carlo curve, it is approximately 3% higher at this point. The qualitative features of this difference appear to be indicative of the difficulties, inherent in any Monte Carlo calculation concerned with long-range potentials<sup>15,16</sup>: In such calculations, it is necessary to choose a finite cell size and hence to neglect some of the more distant contributions to the total field strength at a point; this fact, together with the normalization requirement, will result in the probability of weaker fields being underestimated, which is the observed effect. Regardless, the agreement is sufficiently close to further substantiate the present theory.

Actual numerical results are discussed in detail in the next section.

## III. NUMERICAL RESULTS AND ANALYSIS

It should again be emphasized that all studies of the  $\alpha$  flatness region indicate that in this range the disregarded corrections due to both major sources of error are indeed negligible. Figures 1 and 2 show these results. While Fig. 1 is self-explanatory, Fig. 2 may be understood as follows: We may write<sup>5</sup>

$$a_3 = a_3^0 - \gamma' L^2. \tag{40}$$

Since  $a_3^0$  is not a function of *l* and since, in addition, it is very small compared to unity ( $\approx 10^{-5}$ ) for all cases considered, it is set equal to zero in all further discussions. In order to gain some impression of the importance of the  $a_3$  correction, we consider its influence on the calculated values of  $T_0(l)/T_0(0)$ . In view of the fact that  $\gamma'$  is quite small, it is permissible to write

$$T_0(l)/T_0(0) \cong \exp\{-\gamma L^2\} [1+\gamma' L^2]$$

$$\cong \exp\{-(\gamma-\gamma')L^2\}.$$
(41)

A measure of the importance of the correction due to  $a_3$ in this instance may be given by plotting the ratio of  $\gamma'/\gamma$  versus  $\alpha$  for a values of interest. It is clearly seen from Fig. 2 that in the regions of flatness,  $a_3$  amounts to an insignificant correction.

Figures 4 and 5 show graphs of  $P(\epsilon)$  versus  $\epsilon$  for several values of a, while Figs. 6 and 7 indicate the

TABLE I. Probability distributions  $P(\epsilon)$  at a charged point for several values of a. The electric field strength  $\epsilon$  is in units of  $\epsilon_0$ .<sup>a</sup>

E	a=0.2	a = 0.4	a=0.6	a = 0.8
0.1	0.00522	0.00718	0.00932	0.01190
0.2	0.02171	0.02813	0.03633	0.04616
0.3	0.04745	0.06110	0.07834	0.09878
0.4	0.08102	0.10344	0.13129	0.16383
0.5	0.12026	0.15185	0.19036	0.23450
0.6	0.16274	0.20284	0.25060	0.30408
0.7	0.20602	0.25299	0.30745	0.36684
0.8	0.24778	0.29932	0.35727	0.41858
0.9	0.28603	0.33946	0.39749	0.45686
1.0	0.31922	0.37181	0.42677	0.48089
1.1	0.34627	0.39552	0.44482	0.49128
1.2	0.36656	0.41044	0.45221	0.48958
1.3	0.37997	0.41698	0.45017	0.47792
1.4	0.38673	0.41599	0.44025	0.45862
1.5	0.38738	0.40858	0.42418	0.43393
1.6	0.38265	0.39597	0.40363	0.40587
1.7	0.37342	0.37942	0.38013	0.37610
1.8	0.36059	0.36008	0.35496	0.34597
1.9	0.34503	0.33898	0.32920	0.31643
2.0	0.32757	0.31700	0.30366	0.28818
2.5	0.23322	0.21325	0.19401	0.17549
3.0	0.15617	0.13876	0.12285	0.10794
3.5	0.10443	0.09176	0.08007	0.06911
4.0	0.07166	0.06275	0.05184	0.04600
4.5	0.05113	0.04493	0.03871	0.03266
5.0	0.03787	0.03355	0.02908	0.02465
6.0	0.02248	0.02012	0.01717	0.01411
7.0	0.01442	0.01288	0.01092	0.00882
8.0	0.00990	0.00826	0.00741	0.00589
9.0	0.00717	0.00637	0.00530	0.00415
10.0	0.00539	0.00476	0.00392	0.00302

\*  $P(\epsilon)$  values for  $\epsilon = 7.0, 8.0, 9.0$  and 10.0 were calculated using the first approximation to T(l) which is given by Eq. (A51); the largest error in these values should not exceed 5%. For a discussion of asymptotic expressions for  $P(\epsilon)$ , see Refs. 5 and 6.

differences occurring between the B-M theory and the present theory for cases characterized by a=0.2 and a=0.8. It will be noticed that the difference between the two theories increases as the magnitude of aincreases, and that the B-M theory favors weaker fields than does the proposed theory. One possible explanation for the direction of the difference between the two may lie in the fact that in Baranger's second correction term to T(l),  $\exp[L^{3/2}\psi_2(aL^{1/2})]$ , the linearized pair-correlation function is used instead of the non-linearized form. It has been argued by B-M that the difference between the two functional forms should not really matter since the procedure was "also in the spirit of the Debye-Hückel theory."<sup>17</sup> However Fig. 8 illustrates that the effect of a reduction in  $\psi_2(aL^{1/2})$  on the final  $P(\epsilon)$  curve may be very large. A similar reduction in the second correction term in the present theory leads to an almost imperceptible change in the  $P(\epsilon)$  curve under identical conditions; this may be deduced from Fig. 1. A reduction in the magnitude of  $\psi_2$  is what one would expect if the nonlinearized Debye-Hückel function were used instead of the linearized version; this is because the linearized form underestimates the contribution to the pair-correlation function from strong fields and hence

<sup>&</sup>lt;sup>15</sup> D. D. Carley, J. Chem. Phys. **43**, 3489 (1965). <sup>16</sup> S. G. Brush, H. L. Sahlin, and E. Teller, University of California Radiation Laboratory Report No. UCRL-14467-T, 1965 (unpublished).

<sup>&</sup>lt;sup>17</sup> B. Mozer, dissertation, Department of Physics, Carnegie Institute of Technology, 1960 (unpublished).

FIG. 6. A comparison of the electric microfield distribution function (at a charged point) determined by B-M, with that predicted by the present theory;  $\epsilon$  is in units of  $\epsilon_0$ .



FIG. 8. A comparison of two T(l) approximations as applied to the B-M theory of the electric microfield distribution function  $P(\epsilon)$  (charged point case). [See Eqs. (A50), (A51).]  $\epsilon$  is in units of  $\epsilon_0$ .



TABLE II. Probability distributions  $P(\epsilon)$  at a neutral point for several values of *a*. The electric field strength  $\epsilon$  is in units of  $\epsilon_0$ .<sup>a</sup>

e	a = 0.2	a=0.4	a=0.6	a=0.8
0.1	0.00533	0.00647	0.00758	0.00877
0.2	0.02097	0.02538	0.02965	0.03419
0.3	0.04587	0.05524	0.06424	0.07373
0.4	0.07840	0.09377	0.10838	0.12358
0.5	0.11649	0.13816	0.15845	0.17922
0.6	0.15785	0.18534	0.21062	0.23598
0.7	0.20012	0.23230	0.26127	0.28964
0.8	0.24109	0.27631	0.30729	0.33676
0.9	0.27882	0.31519	0.34632	0.37498
1.0	0.31178	0.34737	0.37687	0.40301
1.1	0.33889	0.37191	0.39829	0.42060
1.2	0.35952	0.38850	0.41064	0.42829
1.3	0.37349	0.39736	0.41458	0.42719
1.4	0.38098	0.39911	0.41113	0.41876
1.5	0.38248	0.39464	0.40156	0.40455
1.6	0.37865	0.38501	0.38720	0.38613
1.7	0.37033	0.37132	0.36933	0.36487
1.8	0.35837	0.35461	0.34913	0.34120
1.9	0.34362	0.33587	0.32760	0.31847
2.0	0.32688	0.31593	0.30556	0.29504
2.5	0.23474	0.21795	0.20476	0.19343
3.0	0.15816	0.14454	0.13431	0.12595
3.5	0.10622	0.09670	0.09005	0.08441
4.0	0.07313	0.06715	0.06250	0.05863
4.5	0.05229	0.04853	0.04553	0.04302
5.0	0.03879	0.03649	0.03463	0.03309
6.0	0.02322	0.02257	0.02191	0.02132
7.0	0.01493	0.01462	0.01431	0.01401
8.0	0.01028	0.01012	0.00995	0.00980
9.0	0.00746	0.00738	0.00728	0.00719
10.0	0.00552	0.00546	0.00541	0.00535

\*  $P(\epsilon)$  values for  $\epsilon = 7.0, 8.0, 9.0$  and 10.0 were calculated using the first approximation to T(l) which is given by Eq. (A51); the largest error in these values should not exceed 5%. For a discussion of asymptotic expressions for  $P(\epsilon)$ , see Refs. 5 and 6.

overemphasizes the  $\psi_2$  term. It would be necessary to carry out a calculation of  $\psi_2$  using the nonlinearized function before the actual magnitude of the reduction could be ascertained.

Tables I and II list some tabulated values of  $P(\epsilon)$  for reference.

### **IV. CONCLUSION**

The main text of this paper has attempted for the sake of clarity to describe the procedure and results of a new theory of electric microfield distributions in plasmas without interjecting too many detailed calculations. However, in all instances the author has endeavored to give complete references, and many of these are to the attached Appendix. It is hoped that this procedure has proved to be both acceptable and helpful to the reader.

The theory developed here has been shown to be effective in determining electric microfield distributions in plasmas of the type described, over a wide temperature-density range; it goes to the Holtsmark limit as  $T \rightarrow \infty$ , and at a=0.8 it has been shown to predict a reliable result. A comparison of this method with that of B-M clearly indicates that while the latter theory is good at high temperatures and low densities (a=0.2) it becomes progressively inaccurate as a is raised from 0.2

to 0.8. The net result of these calculations is that for the charged-point and the neutral-point cases, the distribution curves generated by the present theory favor stronger fields than does the theory of B-M.

Perhaps equally as important as the actual numerical results revealed in this paper, is the method of including noncentral forces through the mechanism of collective coordinates. Exactly how good this method is, is evidenced when the second term in the cluster expansion is calculated; here one finds that the noncentral, twoparticle correlations are included, through the use of collective coordinates, to the approximation of the nonlinear Debye-Hückel result. Since this second term is only a small correction to the theory, even in the case of high a values, such an approximation must be considered highly accurate. Furthermore, during the derivation of the general formalism, especially that part relating to the cluster expansion, the fact that it was not necessary to explicitly mention noncentral interactions resulted in much simplification. This method of development should also be applicable to other problems involving long-range forces; perhaps the partition function for a Coulomb system would be amenable to such a treatment.

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### APPENDIX A

In this Appendix we are concerned with evaluating the expression [Eq. (24)]

$$T(l) = [T_0(l)/T_0(0)] \exp\{\sum_j (n^j/j!) [h_j(l) - h_j(0)]\}$$

through the second term in the series exponent.

The evaluation is accomplished by introducing a variation of the Broyles' collective-coordinate technique.<sup>5</sup> We write

$$V = V_0 + \sum_{i \mathcal{W}_{i0}},\tag{A1}$$

where, as indicated in Sec. II,

$$V = \frac{4\pi e^2}{\mathcal{V}} \sum_{\mathbf{k}}' \sum_{i < j} \frac{1}{k^2} e^{-i\mathbf{k} \cdot \mathbf{r}_{ij}}$$
(A2)

and

$$w_{i0} = \frac{e^2}{r_{i0}} e^{-\alpha r_{i0}/\lambda}.$$
 (A3)

Again, the prime indicates the exclusion of the k=0 term in the summation over **k**. In all subsequent formulas, the prime will be dropped, with the understanding that the k=0 term will always be excluded in

all subsequent  $\mathbf{k}$  summations. Using the identity

$$\sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{r}_{ij}} = \sum_{\mathbf{k}} \left[ \cos(\mathbf{k}\cdot\mathbf{r}_{i})\cos(\mathbf{k}\cdot\mathbf{r}_{j}) \right]$$

$$+\sin(\mathbf{k}\cdot\mathbf{r}_i)\sin(\mathbf{k}\cdot\mathbf{r}_j)$$
], (A4)

and further defining a function

$$S(\mathbf{k} \cdot \mathbf{r}_i) = \cos(\mathbf{k} \cdot \mathbf{r}_i), \quad k_z \ge 0;$$
  
= sin(\mathbf{k} \cdot \mathbf{r}\_i), \quad k\_z < 0, (A5)

we write

$$V = \frac{2\pi N e^2}{\upsilon} \sum_{\mathbf{k}} \frac{1}{k^2} \left[ \frac{2}{N} \sum_{i,j=1}^N S_i S_j + \frac{4}{N} \sum_{i=1}^N S_i S_0 - 2 \right].$$
(A6)

 $\mathbf{If}$ 

$$X_k \equiv (2/N)^{1/2} \sum_i S_i,$$
 (A7)

$$X_k^2 = (2/N) \sum_{i,j} S_i S_j.$$
 (A8)

In terms of these  $X_k$ ,

$$V = \frac{\theta}{2} \sum_{\mathbf{k}} A_k X_k^2 + \theta \left(\frac{2}{N}\right)^{1/2} \sum_{\substack{\mathbf{k} \\ k_k \ge 0}} A_k X_k - \theta \sum_{\mathbf{k}} A_k, \quad (A9)$$

where

$$A_k = (k\lambda)^{-2}$$
, and  $\theta = kT$ .

By similarly Fourier expanding both  $\sum_i w_{i0}$  and  $V_0$ , and by introducing the  $X_k$  notation, we may write

$$\sum_{i} w_{i0} = \theta \left(\frac{2}{N}\right)^{1/2} \sum_{\substack{\mathbf{k} \\ k_{i} \ge 0}} \left[\frac{X_{k}}{(\lambda k)^{2} + \alpha^{2}}\right], \quad (A10)$$

and

$$V_{0} = \frac{\theta}{2} \sum_{\mathbf{k}} A_{k} X_{k}^{2} + \theta \left(\frac{2}{N}\right)^{1/2} \sum_{\substack{\mathbf{k} \\ k_{z} \ge 0}} \left[f(k) A_{k} X_{k}\right] - \theta \sum_{\mathbf{k}} A_{k}, \quad (A11)$$

where

$$f(k) = \frac{\alpha^2}{(k\lambda)^2 + \alpha^2}.$$

The evaluation of the gradients of V,  $V_0$ , and  $\sum_i w_{i0}$  with respect to the coordinates of the origin, can also be expressed in terms of the  $X_k$ ; thus,

$$\boldsymbol{\nabla}_0 V = \theta \left(\frac{2}{N}\right)^{1/2} \sum_{\mathbf{k}} \mathbf{k} \frac{1}{(k\lambda)^2} X_k, \qquad (A12)$$

$$\boldsymbol{\nabla}_{0}\boldsymbol{V}_{0} = \theta \left(\frac{2}{N}\right)^{1/2} \sum_{\substack{\mathbf{k} \\ k_{x} < 0}} \mathbf{k} \frac{f(k)}{(k\lambda)^{2}} \boldsymbol{X}_{k}, \qquad (A13)$$

and

$$\boldsymbol{\nabla}_{0}\left[\sum_{i} w_{i0}\right] = \theta\left(\frac{2}{N}\right)^{1/2} \sum_{\substack{\mathbf{k} \\ k_{s} < \mathbf{0}}} \mathbf{k} \frac{1}{\left[(k\lambda)^{2} + \alpha^{2}\right]} X_{k}. \quad (A14)$$

We now use this collective-coordinate notation to calculate T(l). Consider first the factor  $T_0(l)/T_0(0)$ .

$$\frac{T_{0}(l)}{T_{0}(0)} = \frac{\int \cdots \int \exp[-\beta V_{0} + i(\mathbf{l}/e) \cdot \nabla_{0} V_{0}] \prod_{j=1}^{N} d\mathbf{r}_{j}}{\int \cdots \int \exp[-\beta V_{0}] \prod_{j=1}^{N} d\mathbf{r}_{j}}.$$
 (A15)

Recasting this equation in terms of collective coordinates, we find

$$\frac{T_0(l)}{T_0(0)} = \frac{\int \cdots \int \exp\{-\frac{1}{2} \sum_{\mathbf{k}} [A_k X_k^2 + 2b_k(l) X_k] \} J \prod_k d\mathbf{x}_k}{\int \cdots \int \exp\{-\frac{1}{2} \sum_{\mathbf{k}} [A_k X_k^2 + 2b_k(0)] \} J \prod_k d\mathbf{x}_k},$$
(A16)

where

$$A_{k} = \frac{1}{(k\lambda)^{2}},$$

$$b_{k}(0) = \left(\frac{2}{N}\right)^{1/2} \frac{f(k)}{(k\lambda)^{2}} \times 1, \quad k_{z} \ge 0,$$

$$\times 0, \quad k_{z} < 0$$
(A17)

$$b_k(l) = \left(\frac{2}{N}\right)^{1/2} \frac{f(k)}{(k\lambda)^2} \times 1, \qquad k_z \ge 0,$$
$$\times [-i(\mathbf{l}/e) \cdot \mathbf{k}], \quad k_z < 0$$

and J represents the Jacobian of the transformation from  $\mathbf{r}$  coordinates to  $\mathbf{X}$  coordinates.

The nature of this Jacobian is considered in detail in Ref. 5, as is the nature of this integral evaluation. Here we just outline the results pertinent to this calculation. Integrals of the form

 $= \int \dots \int \exp\{-\frac{1}{2} \sum \left[A_{\mu} X_{\mu}^{2} + 2b_{\mu} X_{\mu}\right]\} I \prod dx_{\mu}$ (A18)

$$I = \int \cdots \int \exp\{-\frac{1}{2} \sum_{k} [A_k X_k^2 + 2b_k X_k] \} J \prod_{k} dx_k \text{ (A18)}$$

can be evaluated by collective coordinates to give

$$I = \operatorname{const} \times \exp\{\frac{1}{2} \sum_{\mathbf{k}} b_k^2 / (1 + A_k)\} [1 - a_3 + a_4 - \cdots],$$
(A19)

where

and

$$a_3 = \left[\frac{2}{3} \mathcal{O}(2N)^{1/2}\right] \int q^3 d\mathbf{r}$$

$$q = \sum_{\mathbf{k}} \left[ b_k S(\mathbf{k} \cdot \mathbf{r}) / (1 + A_k) \right].$$

It can be shown that  $a_4$  also involves integrals over powers of q.

Using this method to evaluate Eq. (A16) we find

$$\frac{T_0(l)}{T_0(0)} = \exp\left\{\frac{1}{2} \sum_{\mathbf{k}} \left[\frac{b_k^2(l) - b_k^2(0)}{1 + A_k}\right]\right\}.$$
 (A20)

From the definitions of  $b_k(l)$  and  $b_k(0)$ , this may be and that shown to reduce to

$$\frac{T_0(l)}{T_0(0)} = \exp\left\{-\frac{\theta^2}{Ne^2} \sum_{\substack{\mathbf{k}\\k_z < 0}} \frac{f^2(k)\mathbf{l}\cdot\mathbf{k}}{(k\lambda)^2 [1+(1/k\lambda)^2]}\right\}.$$
 (A21)

If we replace the sum over  $\mathbf{k}$  by an integral, and carry out this integration, we find that the exponent becomes

$$\left\{ \begin{array}{c} \\ \\ \end{array} \right\} = \left\{ \frac{\alpha^{3l^2}}{(\alpha+1)^2} \times \frac{\theta^{2} \upsilon}{48\pi N \lambda^5 e^2} \right\} . \tag{A22}$$

This may be further simplified by recognizing that

$$(\theta/4\pi ne^2) = \lambda^2$$

$$(3e^2/\theta\lambda)=a^3$$
.

We make use of these identities, with the result that

$$\frac{T_0(l)}{T_0(0)} = e^{-\gamma (l\epsilon_0)^2} \equiv e^{-\gamma L^2}$$
(A23)

where  $\epsilon_0 = e/r_0^2$ , and where  $\gamma = \alpha^3 a/4(\alpha+1)^2$ .

In the evaluation of both the second and third factors in T(l), integrals of the type  $Q_m$  appear

$$Q_{m}(l) = (\mathfrak{V}^{m}/T_{0}(l))$$

$$\times \int \cdots \int \exp[-\beta V_{0} + i(\mathbf{l}/e) \cdot \nabla_{0} V_{0}] \prod_{j=m+1}^{N} d\mathbf{r}_{j}. \quad (A24)$$

Again, introducing collective coordinates, we have

$$Q_{m}(l) = \frac{\bigcup^{m} \int \cdots \int \exp\{-\frac{1}{2} \sum_{k} [A_{k}X_{k}^{2} + 2b_{k}X_{k}]\} \prod_{j=m+1}^{N} d\mathbf{r}_{j}}{\int \cdots \int \exp\{-\frac{1}{2} \sum_{k} [A_{k}X_{k}^{2} + 2b_{k}X_{k}]\} \prod_{j=1}^{N} d\mathbf{r}_{j}}.$$
(A25)

In this expression we must deal with an N-m dimensional integral, as well as with one of dimension N. In order to adapt the collective coordinate formalism to this case, we change from the collective variables  $X_k$  to a new set,  $X_k'$ . The  $X_k'$  are related to the  $X_k$  by the equation

$$X_{k}' = X_{k} - a_{k}$$

$$a_{k} = \left(\frac{2}{N}\right)^{1/2} \sum_{j=1}^{m} S(\mathbf{k} \cdot \mathbf{r}_{j}).$$
(A26)

where

By making this change of variables we remove from collective consideration all terms involving the coordinates of particles 1 through *m*. Thus the collective coordinate exponentials take the form

$$-\frac{1}{2}\sum_{k}\left[A_{k}X_{k}^{2}+2b_{k}X_{k}\right]=-\frac{1}{2}\sum_{k}\left[A_{k}X_{k}^{\prime2}+2(a_{k}A_{k}+b_{k})X_{k}^{\prime}+a_{k}^{2}A_{k}+2a_{k}b_{k}\right].$$
(A27)

Now we use this procedure in both the numerator and denominator of  $Q_m(l)$ . Hence

$$Q_{m}(l) = \frac{\bigcup^{m} \int \cdots \int \exp\{-\frac{1}{2} \sum_{k} \left[A_{k}X_{k}^{\prime 2} + 2(a_{k}A_{k} + b_{k})X_{k}^{\prime}\right]\} \sum_{j=m+1}^{N} d\mathbf{r}_{j}}{\int \cdots \int \exp[-\sum_{k} a_{k}b_{k}]\{\int \cdots \int \exp[-\frac{1}{2} \sum_{k} \left[A_{k}X_{k}^{\prime 2} + 2(a_{k}A_{k} + b_{k})X_{k}^{\prime}\right]] \prod_{j=m+1}^{N} d\mathbf{r}_{j}\} \prod_{j=1}^{m} d\mathbf{r}_{j}}$$
(A28)

Carrying out the collective coordinate integration, we find

$$Q_{m}(l) = \frac{\mathbb{U}^{m} \exp\{+\frac{1}{2} \sum_{k} \left[ \left[ (a_{k}A_{k} + b_{k})^{2} / (1 + A_{k}) \right] - a_{k}^{2}A_{k} - 2a_{k}b_{k} \right] \}}{\int \cdots \int \exp\{+\frac{1}{2} \sum_{k} \left[ \left[ (a_{k}A_{k} + b_{k})^{2} / (1 + A_{k}) \right] - a_{k}^{2}A_{k} - 2a_{k}b_{k} \right] \} \prod_{j=1}^{m} d\mathbf{r}_{j}}$$
(A29)

This may be reduced to

$$Q_m(l) = \frac{\exp\{-\sum_{\mathbf{k}} [a_k b_k / (1+A_k)]\}}{\mathcal{V}^{-m} \int \cdots \int \exp\{-\sum_{\mathbf{k}} [a_k b_k / (1+A_k)]\} \prod_{j=1}^m d\mathbf{r}_j},$$
(A30)

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which, in the limit  $N \to \infty$ ,  $\mathcal{V} \to \infty$  with  $N/\mathcal{V} \to n$ , can be shown to equal

$$Q_m(l) = \exp\{-\sum_k [a_k b_k / (1+A_k)]\}.$$
(A31)

In order to proceed further, it is necessary to insert the appropriate expressions for  $a_k$ ,  $b_k$ , and  $A_k$ , to replace the sum by an integral, and to carry out the integration. We now deal with specific cases.

Consider the second factor in the T(l) expression

$$\exp[I_1(l)] = \exp[n[h_1(l) - h_1(0)]],$$

$$I_{1}(l) = n \int \mathfrak{V}\{Q_{1}(l,1)[\exp[-\beta w_{10} + (\mathbf{l}/e) \cdot \nabla_{0}w_{10}] - 1] - Q_{1}(0,1)[\exp[-\beta w_{10}] - 1]\}d\mathbf{r}_{1}, \qquad (A32)$$
$$Q_{1}(l,1) = \exp\left\{-\left(\frac{2}{N}\right)^{1/2} \sum_{\mathbf{k}} \left[\frac{S(\mathbf{k} \cdot \mathbf{r}_{1})b_{k}}{1 + A_{k}}\right]\right\}.$$

If we carry out explicit evaluation of the exponent by the method previously discussed, we find that

$$-\left(\frac{2}{N}\right)^{1/2}\sum_{\mathbf{k}}\frac{S(\mathbf{k}\cdot\mathbf{r}_{1})b_{k}}{1+A_{k}} = -\frac{\alpha^{2}}{2\pi^{2}n}\int_{0}^{\infty}\frac{dk\ k^{2}}{\left[\alpha^{2}+(k\lambda)^{2}\right]\left[1+(k\lambda)^{2}\right]}\left\{\int_{0}^{+1}\cos(kr_{1}\mu)d\mu+i\theta\int_{0}^{-1}\left[(\mathbf{l}/e)\cdot\mathbf{k}\right]\sin(kr_{1}\mu)d\mu\right\}$$
(A33)

which, expressing  $r_1$  in units of  $r_0(x_1=r_1/r_0)$  and evaluating the integrals, becomes

$$-\left(\frac{2}{N}\right)^{1/2}\sum_{\mathbf{k}}\frac{S(\mathbf{k}\cdot\mathbf{r}_{1})b_{k}}{1+A_{k}} = s(x_{1})+iLq(x_{1}) = \frac{\alpha^{2}}{1-\alpha^{2}} \times \frac{a^{2}}{3x_{1}}\left[e^{-ax_{1}}-e^{-\alpha ax_{1}}\right]+iL\frac{\alpha^{2}}{1-\alpha^{2}}\left\{\right\}\cos\theta,$$
(A34)

where the  $\cos\theta$  term comes from the  $\mathbf{l} \cdot \mathbf{k}$  factor, and where

$$\left\{ \right\} = \left\{ \frac{1}{x_1^2} \left[ e^{-\alpha a x_1} - e^{-a x_1} \right] - \frac{a}{x_1} \left[ e^{-a x_1} - \alpha e^{-\alpha a x_1} \right] \right\}.$$

Thus we may write

$$Q_1(l,1) = \exp[s(x_1) + iLq(x_1)\cos\theta].$$
(A35)

Expressing  $\beta w_{10}$  and  $\nabla_0 w_{10}$  in terms of  $x_1$ , we may evaluate  $I_1(l)$ . Thus

$$I_{1}(l) = n [h_{1}(l) - h_{1}(0)] = 3 \int_{0}^{\infty} dx_{1} x_{1}^{2} e^{F(x_{1})} \left[ \frac{\sin[LG(x_{1})]}{[LG(x_{1})]} - 1 \right] - 3 \int_{0}^{\infty} dx_{1} x_{1}^{2} e^{s(x_{1})} \left[ \frac{\sin[Lq(x_{1})]}{[Lq(x_{1})]} - 1 \right], \quad (A36)$$

where

$$F(x_{1}) = s(x_{1}) - \beta w_{10} = \frac{a^{2}}{3x_{1}} \times \frac{1}{1 - \alpha^{2}} [\alpha^{2} e^{-ax_{1}} - e^{-\alpha ax_{1}}],$$

$$G(x_{1}) = q(x_{1}) + e^{-1} w_{10}' = \frac{1}{1 - \alpha^{2}} \left\{ \frac{1}{x_{1}^{2}} [e^{-\alpha ax_{1}} - \alpha^{2} e^{-ax_{1}}] + \frac{1}{x_{1}} [\alpha e^{-\alpha ax_{1}} - \alpha^{2} e^{-ax_{1}}] \right\},$$

$$s(x_{1}) = \frac{\alpha^{2}}{1 - \alpha^{2}} \times \frac{a^{2}}{3x_{1}} [e^{-ax_{1}} - e^{-\alpha ax_{1}}], \quad q(x_{1}) = \frac{\alpha^{2}}{1 - \alpha^{2}} \left\{ \frac{1}{x_{1}^{2}} [e^{-\alpha ax_{1}} - e^{-\alpha ax_{1}}] - \frac{a}{x_{1}} [e^{-ax_{1}} - \alpha e^{-\alpha ax_{1}}] \right\},$$

$$\beta w_{10} = \frac{a^{2}}{3x_{1}} e^{-\alpha ax_{1}}, \quad e^{-1} w_{10}' = \frac{1}{x_{1}^{2}} e^{-\alpha ax_{1}} [1 + \alpha ax_{1}].$$
(A37)

Equation (A36) is just Eq. (29) appearing in Sec. II. The second factor then becomes  $\exp[I_1(l)]$ . The third, and last factor which we consider is of the form  $\exp[I_2(l)]$ , where  $I_2(l)$  is given by

$$I_{2}(l) = \frac{1}{2}n^{2} [h_{2}(l) - h_{2}(0)], \qquad h_{2}(l) = \int \int g_{2}(l)\chi(l,1)\chi(l,2)d\mathbf{r}_{1}d\mathbf{r}_{2},$$

$$\chi(l,i) = [\exp[-\beta w_{i0} + i(\mathbf{l}/e) \cdot \nabla_{0}w_{i0}] - 1], \quad g_{2}(l) = \mathbb{U}^{2} [Q_{2}(l,1,2) - Q_{1}(l,1)Q_{1}(l,2)].$$
(A38)

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We first consider  $g_2(l)$ , and here we concentrate on  $Q_2(l)$  since  $Q_1(l)$  has already been calculated.

$$Q_2(l) = \frac{1}{T_1(l)} \int \cdots \int \exp[-\beta V_0 + i(\mathbf{l}/e) \cdot \nabla_0 V_0] \prod_{j=3}^N d\mathbf{r}_j.$$
(A39)

Introducing collective coordinates again, it can be shown in a straightforward manner that

$$Q_2(l,1,2) = \exp\left\{-\sum_{\mathbf{k}} \left[\frac{a_k b_k}{1+A_k}\right] - \frac{a^2}{3x_{12}}e^{-ax_{12}}\right\}.$$
 (A40)

Now

$$a_k = (2/N)^{1/2} [S(\mathbf{k} \cdot \mathbf{r}_1) + S(\mathbf{k} \cdot \mathbf{r}_2)], \qquad (A41)$$

therefore

$$Q_{2}(l,1,2) = \exp\left\{-\left(\frac{2}{N}\right)^{1/2} \sum_{\mathbf{k}} \left[\frac{S(\mathbf{k}\cdot\mathbf{r}_{1})b_{k}}{1+A_{k}}\right] - \left(\frac{2}{N}\right)^{1/2} \sum_{\mathbf{k}} \left[\frac{S(\mathbf{k}\cdot\mathbf{r}_{2})b_{k}}{1+A_{k}}\right] - \frac{a^{2}}{3x_{12}}e^{-ax_{12}}\right\}.$$
(A42)

This clearly implies that we may finally write

$$Q_2(l,1,2) = Q_1(l,1)Q_1(l,2) \exp\left[-\frac{a^2}{3x_{12}}e^{-ax_{12}}\right].$$
(A43)

Thus,

$$g_2(l) = \mathcal{U}^2 Q_1(l,1) Q_1(l,2) \left[ \exp\left[ -\frac{a^2}{3x_{12}} e^{-ax_{12}} \right] - 1 \right].$$
(A44)

This result was written down as Eq. (32) in Sec. II, and its significance discussed.

If this expression is substituted back into the equation for  $h_2(l)$  in [Eq. (A38)] we note that the integrand of the double integral is a product of functions of  $(l,r_2)$ , and those of  $(l,r_1)$ , that is with the exception of the  $x_{12}$  coupling term in  $g_2(l)$ . In order to readily continue our calculation, and in view of the fact that this third factor should be a small correction, we proceed to linearize the Debye-Hückel pair-correlation function. Then

$$\exp\left[-\frac{a^2}{3x_{12}}e^{-ax_{12}}\right] - 1 \approx -\frac{a^2}{3x_{12}}e^{-ax_{12}}.$$
(A45)

In order to uncouple the  $x_1$ ,  $x_2$  or  $r_1$ ,  $r_2$  dependence in this coupling term, we expand it in spherical harmonics<sup>18</sup>

$$V(\mathbf{r}_{12}) = -\sum_{k=0}^{\infty} (2k+1) V_k(\mathbf{r}_1, \mathbf{r}_2) P_k(\cos\theta_k), \qquad (A46)$$

where  $V_k$  is given by

$$V_{k} = (a^{3}/3)\lambda K_{k+1/2}(r_{1}/\lambda)I_{k+1/2}(r_{2}/\lambda)/(r_{1}r_{2})^{1/2}$$
(A47)

with  $r_1 > r_2$  and  $k = 0, 1, 2 \cdots$ . This method of handling  $V(r_{12})$  allows the expression for

$$I_2(l) = \frac{1}{2}n^2 [h_2(l) - h_2(0)]$$
(A48)

to be reduced to a particularly tractable type of double integral

<sup>18</sup> W. J. Swiatecki, Proc. Roy. Soc. (London) A205, 238 (1951).

With this expression for  $I_2(l)$ , the third factor becomes  $\exp[I_2(l)]$ . Finally, terminating the series exponential in Eq. (24) with the second term, we get

$$T(l) = \exp[-\gamma L^2 + I_1(l) + I_2(l)].$$
(A50)

If we omit the  $I_2(l)$  term from this expression the result

$$T(l) \cong \exp\{-\gamma L^2 + I_1(l)\}$$
(A51)

is referred to as the first approximation to T(l). Then in this sense, the second approximation to T(l) is given by Eq. (A50).

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# Investigation of Electronic Recombination in Helium and Argon Afterglow Plasmas by Means of Laser Interferometric Measurements\*

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Two helium-neon laser interferometers were used to obtain the electron and neutral-atom densities in an afterglow plasma. The interferometric technique utilized allows one to obtain both the spatial and temporal dependence of the electron decay. The two gases studied were helium and argon at 2-8 Torr and 0.3-0.8Torr, respectively. The electron density was in the range of  $2 \times 10^{13} < N_e < 10^{15}$  cm<sup>-3</sup> and the electron temperature in the range  $1000 < T_e < 7000$  °K. The electron temperature was measured by comparing the relative atomic line intensities and by inference from the recombination coefficient. The electronic recombination in helium, argon, and helium-argon mixtures was found to be consistent with the predictions of Bates, Kingston, and McWhirter for collisional-radiative recombination. The electron temperature inferred from the measured recombination coefficient indicates a pronounced electron temperature gradient across the tube which is believed to be due to electron heating effects in the afterglow.

# INTRODUCTION

 $\mathbf{E}_{\mathrm{has}\ \mathrm{been}\ \mathrm{the}\ \mathrm{subject}\ \mathrm{of}\ \mathrm{numerous\ studies\ dating}}$ back to the early part of the twentieth century. In spite of the tremendous amount of attention focused on this phenomenon, there are still many questions that remain to be answered. One of the major advancements made in the understanding of electronic recombination was the proposal by Bates<sup>1</sup> that dissociative recombination may play a leading role in the recombination process. Whereas the importance of this phenomenon is well documented, it has become increasingly apparent that other processes may be of significance. One of these is the three-body collision of two free electrons and a positive ion resulting in an excited neutral atom. Also of great importance is the effect of electron collision which excited atoms. It has been shown that inclusion of such collisions enhances recombination.<sup>2,3</sup> The net effect has been coined collisional radiative recombination.

Collisional-radiative recombination was put on a firm theoretical foundation by Bates et al.3 It was subsequently shown, within a limited range of plasma parameters, that their results described the recombination process in helium,<sup>2</sup> hydrogen,<sup>4</sup> and cesium.<sup>5</sup>

In this work we extended the range of plasma parameters over which collisional-radiative recombination is expected to be the dominant recombination process in helium plasmas. The results of Bates are also shown to apply to argon and helium-argon plasmas.

In the work described here, the plasmas were formed in helium and argon gases in the pressure ranges 3-8 Torr and 0.2-0.8 Torr, respectively, by an electrode type of capacitor discharge. This resulted in a plasma with an electron density  $N_e \approx 10^{15} \text{ cm}^{-3}$  and  $T_e \approx 7000^{\circ} \text{K}$ immediately after cessation of the active discharge. Both  $N_e$  and  $T_e$  subsequently decay during this afterglow.

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