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CALCULATION OF FIELDS ON PLASMA IONS
BY COLLECTIVE COORDINATES

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ABSTRACT

The probability of finding a given electric field on an ion in a plasma is computed with the aid of collective coordinates. All the ions are assumed to have the same charge and the free electrons are replaced by a rigid negative smear. The Jacobian of the transformation to collective coordinates is expanded in a series of Hermite polynomials and one of the higher terms is computed as an estimate of the error. This error calculation indicates that a lower limit in the temperature probably exists below which present methods may not be used. This lower limit depends upon the form of the short range potential that is chosen. A cutoff in space at a particle separation of r_0 is employed in place of the cutoff in wave number at k_0 . An average short range potential as a function of temperature appears. The values of the probability are shown to be surprisingly insensitive to the value of r_0 at infinite temperature and to compare well with the Holtmark distribution. They also compare well with the SRNN approximation described in a previous paper in the temperature range where comparison is possible. Numerical results using the SRNN approximation are presented for temperatures too low for the method outlined here.

I. INTRODUCTION

The purpose of this paper is twofold: first, to compute the probability density $P(s)$ of finding an electric field of magnitude s on an ion in a plasma; second, to study the use of collective coordinates in a classical problem for which some comparison may be made with other means of calculation.

The problem of determining $P(s)$ has already been dealt with.^{1,2} In those

1 H. Mayer, Los Alamos Scientific Laboratory Report LA 647, 1947 (unpublished)

2 A. A. Broyles, Phy. Rev. 100, 1181, (1955). Referred to as I in the text.

calculations,² $P(s)$ seemed to be rather well determined for large values of s but considerable uncertainty remained as to the correct values in the vicinity of the maximum of $P(s)$.

Questions also arose as to the correctness of the method of employing collective coordinates. In I, the collective and particle coordinates were treated as though they were completely independent even though Eq. (1) below shows that relations do exist. The error introduced by this approximation was undetermined. It seems likely that it may be appreciable in some cases since $P(s)$ at large fields depends almost entirely upon the short range interactions; and these interactions, under the above approximation, are completely independent of the more distant ions. In this paper no such assumption is made, and it is found that the short range interaction should depend upon temperature [compare Eq. (30) here with Eq. (27) of I].

The cut-off in wave number at k_0 was employed in I in order to make small the error resulting from the assumption of the independence of collective and particle coordinates. Since this error was not computed, however, the optimum value of k_0 was uncertain. A method for determining the error is presented here. It employs an expansion of Hermite polynomials [Eq. (7)] for the Jacobian of the transformation from particle to collective coordinates. This type of an expansion was chosen so that the approximate Jacobian of I [Eq. (15) of I] is the first term. Computation of the higher terms in this expansion then gives the error made by neglecting them. Section VII describes how these higher terms were used to determine r_0 .

Also in I, the short range potential is not cut-off in space but has a tail that falls off rather slowly with increasing particle separation. In the present paper, this tail has been completely eliminated by forcing the short range interaction to be zero beyond a distance r_0 . This cut-off in space replaces the former cut-off in wave number at k_0 .³ The integrations performed to obtain $P(\epsilon)$ may now be

3 D. Pines and D. Bohm, Phys. Rev. 85, 338 (1952)

separated into integrations over regions according to whether the particle separations are less than r_0 or greater than r_0 .

It is quite convenient that a check exists on this work through a comparison, at infinite temperature, with the Holtmark distribution.⁴ This distribution is an accurate determination of $P(\epsilon)$.

4 J. Holtmark, Ann. Physik 58, 577 (1919); Physik Z. 20, 162 (1919); Physik Z. 25 73 (1924); S. Chandrasekhar and J. von Neumann, Astrophys. J. 95, 489 (1942).

An attempt has been made in the writing of this paper to separate the description of the method from the more tedious algebra by placing the latter in Sections III, IV, V, and VI. The cursory reader might be well advised to skip these sections.

II. OUTLINE OF THE METHOD

We shall not compute $P(s)$ for a true plasma but shall substitute instead a model where the free electrons are represented by a uniform smear of negative charge and all the ions are assumed to have the same positive charge. The system will be essentially infinite in extent. The charge on the ions will be taken as the unit charge and the "ion sphere radius" as the unit length. The ion sphere is a sphere containing, on the average, exactly one ion. Thus the unit of energy will be the potential energy of a system composed of two ions separated by a distance of one ion sphere radius, and the unit electric field strength will be that of the field exerted by one of these ions on the other. This is the model and these are the units employed in I.

$$\rho = \sum_{\underline{k}} \rho_{\underline{k}} e^{i\underline{k} \cdot \underline{r}}, \quad \rho_{\underline{k}} = \tau^{-1} \sum_j e^{-i\underline{k} \cdot \underline{r}_j} \equiv \tau^{-1} (x_{\underline{k}} + iy_{\underline{k}}), \quad (1)$$

where τ is the volume of the system and the $\underline{r}_j$'s are the positions of the ions.

The $x_{\underline{k}}$ and $y_{\underline{k}}$ merely serve to write the real and imaginary parts of $\rho_{\underline{k}}$.

The amplitude of $\rho_{\underline{k}}$'s at large values of k will be suppressed by cutting off the infinite peaks that occur in the potential energy of the system when two particles approach each other. Thus the cutting off will be done in the particle

coordinate space rather than in the collective coordinate space. This means that the collective coordinates will be required to handle a potential energy function that is equal to the potential energy of the system only when all the ions are separated by distances greater than some value r_0 . The collective coordinates may be used to describe a system of particles where the charge of each particle has been spread over a volume of radius r_0 . We may write, then, that the long range potential energy V_0 of the system is related to the correct potential energy V by the equation

$$V_0 = V - \sum_{i=0}^{N-1} \sum_{\substack{j=i+1 \\ i < j}}^N w_{ij} \quad (2)$$

where the particles are numbered from 0 to N , and w_{ij} is a function of the separation r_{ij} between ions i and j . The function w_{ij} varies like r_{ij}^{-1} for very close approach and is zero when r_{ij} is greater than r_0 . For the present calculation we shall choose

$$w_{ij} = \begin{cases} 0, & r_{ij} > r_0 \\ r_{ij}^{-1} - r_0^{-1}, & r_{ij} < r_0 \end{cases} \quad (3)$$

Later we will want to treat properly the configurations where ion number 1 is within a distance r_0 of ion number 0. Then it is necessary to add the short range interaction w_{10} back into V_0 , and so we define

$$V_1 \equiv V_0 + w_{10} \quad (4)$$

The probability density $Q(\underline{s})$ of obtaining a certain electric field $\underline{s}$ on an ion will be obtained by placing the ion numbered 0 at the origin, summing over all configurations of the other ions that give the required electric field at the origin, and dividing by the sum over all configurations; each configuration weighted by the Boltzmann factor. The result is given in Eq. (1) of I. If we transform the integrals in the numerator and denominator to collective coordinates substituting V_0 for V , we shall obtain values of $Q(\underline{s})$ that are in error because configurations where particles are closer together than r_0 are incorrectly represented. We shall correct for these configurations where one ion is within a distance of r_0 of the origin and neglect corrections for the other configurations that we have improperly treated. Thus we obtain

$$Q(\underline{s}) = Q_{00}(\underline{s}) - Q_{10}(\underline{s}) + Q_{11}(\underline{s}) \quad ,$$

$$Q_{00}(\underline{s}) = \frac{\left\{ \int \dots \int \exp(-V_0/\theta) \delta(\underline{s} + \nabla_0 V_0) \prod_{j=1}^N d\underline{r}_j \right\}}{\left\{ \int \dots \int \exp(-V_0/\theta) \prod_{j=1}^N d\underline{r}_j \right\}} \quad , \quad (5)$$

$$Q_{11}(\underline{s}) = \frac{N \int_{|\underline{r}_1| < r_0} \left\{ \int \dots \int \exp(-V_1/\theta) \delta(\underline{s} + \nabla_0 V_1) \prod_{j=2}^N d\underline{r}_j \right\} d\underline{r}_1}{\int_{\underline{r}_1} \left\{ \int \dots \int \exp(-V_1/\theta) \prod_{j=2}^N d\underline{r}_j \right\} d\underline{r}_1}$$

$$Q_{10} = Q_{11}(\underline{s}) \text{ with } V_0 \text{ replacing } V_1 \quad .$$

The subscript o on ∇_o indicates differentiation with respect to the coordinates of the particle at the origin. The integrals in braces in Eq. (5) will be treated by collective coordinates. In Q_{oo} , the collective coordinates will include particles 1 through N while for Q_{10} and Q_{11} , the collective coordinates will not include particles 1 and o . [see Eq. (1).]

Subtracting Q_{10} from Q_{oo} removes the portion of Q_{oo} coming from configurations where one particle is within a distance r_o of the origin while the addition of Q_{11} replaces this portion with one where the short range interaction between this particle and the one at the origin is included. The contributions to $Q(g)$ by configurations improperly treated is small and their effect will be indicated by a comparison with the Holtmark distribution at infinite temperature [Fig. 2.] These improperly treated configurations should be even less important at lower temperatures since the Boltzmann factor tends to separate the ions.

To evaluate integrals of the type occurring in Eq. (5) by means of collective coordinates, it is necessary to know the Jacobian J of the transformation from the particle coordinates to the collective coordinates. This Jacobian tells us how many points in particle space correspond to a given one in collective space. Some qualitative features of J may be seen easily by viewing the $\rho_{\underline{k}}$'s as the sum of vectors in the complex plane whose phases are $-\underline{k} \cdot \underline{r}_j$ and amplitudes $1/\gamma$. [see Eq. (1).] For example if all the component vectors are in the same direction for one $\rho_{\underline{k}}$, then all the particles must lie on a lattice, and the values of the other $\rho_{\underline{k}}$'s must be severely limited. If, however, none of the $\rho_{\underline{k}}$'s get very large, they will be fairly independent of each other and an approximation to the Jacobian may be obtained from the solution of the random walk problem. This was done to

obtain Eq. (15) of I.

The form of the Jacobian employed in Eq. (15) of I suggests that it may be expanded in a Gram-Charlier series.⁶ The moments required for this series may be

6 M. G. Kendall, The Advanced Theory of Statistics Vol. I p. 147. This series is an expansion in Hermite Polynomials. I am indebted to Mr. H. Kahn for suggesting this use of this series.

evaluated with the aid of the relation

$$\begin{aligned} \langle x_k^s y_k^t \rangle &= \int \dots \int x_k^s y_k^t J \prod_k dx_k dy_k \\ &= \tau^{-H} \int \dots \int \left(\sum_j \cos \underline{k} \cdot \underline{r}_j \right)^s \left(\sum_j \sin \underline{k} \cdot \underline{r}_j \right)^t \prod_j d\underline{r}_j. \end{aligned} \quad (6)$$

Thus we may obtain⁷

7 It will be understood throughout this paper that sums over vector indices do not include the index zero. Three superscripts are being employed on summation, integration and multiplication signs. A plus sign indicates that the index runs only over those vectors with positive s components and a minus sign, those with negative s components. An asterisk is used in a multiple summation to indicate the omission of terms where two indices are identical.

$$J = \prod_k^+ \left\{ (2\pi)^{-1} \exp \left[- (x_k^2/2 \langle x_k^2 \rangle) - (y_k^2/2 \langle y_k^2 \rangle) \right] \right\} \left\{ 1 + \dots \right\} \quad (7)$$

The contribution to P(s) from the second term in the expansion of J will be shown to be negligible while a part of the third term will be computed roughly as a guide

to the range of validity of the use of the first terms of the series alone.

III. THE POTENTIAL ENERGY

The potential energy of the system^{2,3} is given by the expression⁷

$$V = 2\pi\tau^{-1} \sum_{\underline{k}} k^{-2} \sum_{i,j=0}^N \exp \left[i\underline{k} \cdot (\underline{r}_i - \underline{r}_j) \right] \quad (8)$$

If the sum over $\underline{k}$ in Eq. (8) is approximated by an integral, V will equal

$\sum_{i < j} r_{ij}^{-1} + \text{constant}$ where $r_{ij} = |\underline{r}_i - \underline{r}_j|$. The difference between the values of V with the sum and with the integral is the interaction energy between the ions and the smeared negative charge. The Fourier expansion of w_{ij} gives

$$w_{ij} = 4\pi\tau^{-1} \sum_{\underline{k}} \exp \left[i\underline{k} \cdot (\underline{r}_i - \underline{r}_j) \right] \left[1 - f(k) \right] k^{-2}, \quad (9)$$

where

$$f(k) = \sin(kr_0)/(kr_0). \quad (10)$$

This $f(k)$ has the properties of being unit at $k = 0$ and going to zero faster than k^{-1} as k approaches infinity. For the short range interaction employed in I, $f(k)$ is unity for k 's less than k_0 and zero for larger k 's. From Eqs. (2), (4), (8) and (9), it is clear that

$$V_0 = 2\pi\tau^{-1} \sum_{\underline{k}} k^{-2} f \sum_{i,j=0}^N \exp \left[i\underline{k} \cdot (\underline{r}_i - \underline{r}_j) \right] + \text{const.} \quad (11)$$

and

$$V_1 = 2\pi\tau^{-1} \sum_{\underline{k}} k^{-2} \left\{ f \sum_{\substack{i,j=0 \\ i+j \neq 1}}^N \exp \left[i\underline{k} \cdot (\underline{r}_i - \underline{r}_j) \right] + \right. \\ \left. + 2 \exp \left[i\underline{k} \cdot (\underline{r}_1 - \underline{r}_0) \right] \right\} + \text{const.} \quad (12)$$

Now

$$4\pi\tau^{-1} \sum_{\underline{k}} k^{-2} \exp \left[i\underline{k} \cdot (\underline{r}_1 - \underline{r}_0) \right] \approx r_{10}^{-1} ,$$

since this expression represents the potential energy of a system having a large volume containing only two ions with two negative charges spread uniformly.

Thus we have

$$V_1 = r_{10}^{-1} + 2\pi\tau^{-1} \sum_{\underline{k}} k^{-2} \sum_{\substack{1, j = 0 \\ 1+j \neq 1}}^N \exp \left[i\underline{k} \cdot (\underline{r}_1 - \underline{r}_j) \right] + \text{const.} \quad (12')$$

IV. THE JACOBIAN OF THE TRANSFORMATION TO COLLECTIVE COORDINATES

The Gram-Charlier expansion⁶ is written in standard measure. It is necessary, then, to evaluate the quadratic moments from Eq. (6), and the result is

$$\langle \underline{x}_k^2 \rangle = \langle \underline{y}_k^2 \rangle = \frac{1}{2} N, \quad \langle \underline{x}_k \underline{y}_k \rangle = 0. \quad (13)$$

It is convenient to use the definitions

$$\underline{X}_k = (2/N)^{\frac{1}{2}} \underline{x}_k, \quad \underline{X}_{-k} = (2/N)^{\frac{1}{2}} \underline{y}_k. \quad (14)$$

No ambiguity arises from these definitions since only those $\underline{x}_k$'s and $\underline{y}_k$'s occur whose subscripts have positive z components.²

If we extend the Gram-Charlier expansion to many dimensions, we obtain through the fourth order terms⁷

$$J = 8 \pi \prod_{\underline{k}} \left[(2\pi)^{-\frac{1}{2}} \exp \left(-\frac{1}{2} \underline{X}_k^2 \right) \right] ,$$

$$S = 1 + \frac{1}{2} \sum_{\underline{k}, \underline{\ell}}^* \langle H_2(\underline{X}_{\underline{k}}) \underline{X}_{\underline{\ell}} \rangle H_2(\underline{X}_{\underline{k}}) \underline{X}_{\underline{\ell}} \quad (15)$$

$$\begin{aligned} & + (3!)^{-1} \sum_{\underline{k}, \underline{\ell}, \underline{m}}^* \langle \underline{X}_{\underline{k}} \underline{X}_{\underline{\ell}} \underline{X}_{\underline{m}} \rangle \underline{X}_{\underline{k}} \underline{X}_{\underline{\ell}} \underline{X}_{\underline{m}} + (4!)^{-1} \sum_{\underline{k}} \langle H_4(\underline{X}_{\underline{k}}) \rangle H_4(\underline{X}_{\underline{k}}) \\ & + (3!)^{-1} \sum_{\underline{k}, \underline{\ell}}^* \langle H_3(\underline{X}_{\underline{k}}) \underline{X}_{\underline{\ell}} \rangle H_3(\underline{X}_{\underline{k}}) \underline{X}_{\underline{\ell}} + (1/8) \sum_{\underline{k}, \underline{\ell}}^* \langle H_2(\underline{X}_{\underline{k}}) H_2(\underline{X}_{\underline{\ell}}) \rangle H_2(\underline{X}_{\underline{k}}) H_2(\underline{X}_{\underline{\ell}}) \\ & + (1/4) \sum_{\underline{k}, \underline{\ell}, \underline{m}}^* \langle H_2(\underline{X}_{\underline{k}}) \underline{X}_{\underline{\ell}} \underline{X}_{\underline{m}} \rangle H_2(\underline{X}_{\underline{k}}) \underline{X}_{\underline{\ell}} \underline{X}_{\underline{m}} + \\ & + (4!)^{-1} \sum_{\underline{k}, \underline{\ell}, \underline{m}, \underline{n}}^* \langle \underline{X}_{\underline{k}} \underline{X}_{\underline{\ell}} \underline{X}_{\underline{m}} \underline{X}_{\underline{n}} \rangle \underline{X}_{\underline{k}} \underline{X}_{\underline{\ell}} \underline{X}_{\underline{m}} \underline{X}_{\underline{n}} + \dots \end{aligned}$$

Terms whose coefficients are zero have been omitted. The averages contained in the coefficients of this series may be evaluated with the aid of Eq. (6) to give

$$\begin{aligned} \langle H_2(\underline{X}_{\underline{k}}) \underline{X}_{\underline{\ell}} \rangle &= (2N)^{-\frac{1}{2}} \left[\delta(2\underline{k} - \underline{\ell}) - \delta(2\underline{k} + \underline{\ell}) \right] \delta(\omega_{\underline{\ell}}) \\ \langle \underline{X}_{\underline{k}} \underline{X}_{\underline{\ell}} \underline{X}_{\underline{m}} \rangle &= (2N)^{-\frac{1}{2}} (-1)^{(\omega_{\underline{k}} + \omega_{\underline{\ell}} + \omega_{\underline{m}})/2} \left\{ \delta(\underline{k} + \underline{\ell} + \underline{m}) \delta(\omega_{\underline{k}} + \omega_{\underline{\ell}} + \omega_{\underline{m}} - 2) \right. \\ & \quad + \left[\delta(\underline{k} + \underline{\ell} - \underline{m}) (-1)^{\omega_{\underline{m}}} + \delta(\underline{k} - \underline{\ell} + \underline{m}) (-1)^{\omega_{\underline{\ell}}} + \delta(-\underline{k} + \underline{\ell} + \underline{m}) (-1)^{\omega_{\underline{k}}} \right] \times \\ & \quad \times \left[\delta(\omega_{\underline{k}} + \omega_{\underline{\ell}} + \omega_{\underline{m}}) + \delta(\omega_{\underline{k}} + \omega_{\underline{\ell}} + \omega_{\underline{m}} - 2) \right] \Big\} \quad (16) \\ \langle H_4(\underline{X}_{\underline{k}}) \rangle &= -3(2N)^{-1} \end{aligned}$$

$$\langle H_3(\underline{x}_k) \underline{x}_\ell \rangle = (-1)^{\omega_k} (2N)^{-1} \delta(3k - \ell) ,$$

$$\langle H_2(\underline{x}_k) H_2(\underline{x}_\ell) \rangle = - (2N)^{-1} \delta(k + \ell) ,$$

$$\begin{aligned} \langle H_2(\underline{x}_k) \underline{x}_\ell \underline{x}_m \rangle &= (2N)^{-1} \delta(\omega_m - \omega_\ell) \left[-\delta(2k + \ell + m) \right. \\ &\quad \left. + (-1)^{\omega_k} \delta(2k - \ell + m) + (-1)^{\omega_k} \delta(2k + \ell - m) + \delta(2k - \ell - m) \right] , \end{aligned}$$

$$\begin{aligned} \langle \underline{x}_k \underline{x}_\ell \underline{x}_m \underline{x}_n \rangle &= (2N)^{-1} \left\{ 2(N-1) \left[\delta(k - \ell) \delta(m - n) + \delta(k - m) \delta(\ell - n) + \right. \right. \\ &\quad \left. \left. + \delta(k - n) \delta(m - \ell) \right] + \frac{1}{2} \left[1 + (-1)^{\omega_k + \omega_\ell + \omega_m + \omega_n} \right] \right\} \times \\ &\quad \times \sum_{\text{sign comb.}} \delta(k + \ell + m + n) (-1)^{(\omega_k + \omega_\ell + \omega_m + \omega_n)/2} \end{aligned}$$

$$\omega_k = \begin{cases} 0, & k_s > 0 , \\ 1, & k_s < 0 , \end{cases}$$

where the last sum is taken over all the indicated sign combinations with the restriction that the sign preceding each vector ($\underline{k}$, $\underline{\ell}$, $\underline{m}$, or $\underline{n}$) in the δ function is the same as that preceding the corresponding ω in the exponent of the (-1) .

Thus there are eight terms in the sum. The delta function is such that

$$\delta(\underline{k}) = \begin{cases} 0, & \underline{k} \neq 0 , \\ 1, & \underline{k} = 0 , \end{cases}$$

and similarly when its argument is scalar.

V. EVALUATING $P(\underline{s})$

It is convenient to replace the δ function in Eq. (5) with its Fourier expansion and evaluate the transform of $Q(\underline{s})$. This transform has the form

$$T(\underline{L}) = \int \dots \int \exp \left\{ -(V/\theta) + i\underline{L} \cdot \nabla_0 V \right\} \prod_j d\mathbf{r}_j \quad (17)$$

Since $T(\underline{L})$ is independent of the direction of $\underline{L}$, the integration over these directions may be carried out. Also, since $Q(\underline{s})$ is independent of the direction of $\underline{s}$, the integration over these directions may be carried out to obtain

$$P(\underline{s}) = \lim_{\epsilon \rightarrow 0} \epsilon^2 Q(\underline{s}) \quad (18)$$

If we employ the subscripts on the Q 's appearing in Eq. (5) to their corresponding transforms, we may write

$$P(\underline{s}) = P_{00} - P_{10} + P_{11} \quad ,$$

$$P_{00} = \frac{2}{\pi} \epsilon \int_0^\infty \left[L \sin(L\epsilon) T_{00}(\underline{L})/T_{00}(0) \right] dL \quad , \quad (19)$$

$$P_{10} = N \frac{2}{\pi} \epsilon \int_0^\infty \left[L \sin(L\epsilon) T_{10}(\underline{L})/T_{10}(0) \right] dL \quad ,$$

$$P_{11} = N \frac{2}{\pi} \epsilon \int_0^\infty \left[L \sin(L\epsilon) T_{11}(\underline{L})/T_{11}(0) \right] dL \quad .$$

If we now write V_0 [Eq. (11)] in terms of X_k 's [Eq. (14)] where they include all the particle coordinates numbered from 1 to N Eq. (1) and we set $r_0 = 0$, we obtain⁷

$$V_0 = 2\pi N\tau^{-1} \sum_k f k^{-2} X_k^2 + \ln \tau^{-1} (2N)^{1/2} \sum_k X_k f k^{-2} + \text{const.}$$

and

$$-\nabla_0 V_0 = 8\pi\tau^{-1} \left(\frac{1}{2N}\right)^{1/2} \sum_k X_k k f k^{-2} \quad (20)$$

With Eqs. (15), (17) and (20), we may write

$$T_{\infty}(\delta) = \text{const.} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} S \prod_k \left\{ \exp \left[-A_k X_k^2 - 2 {}^0B_k(L) X_k \right] dX_k \right\}, \quad (21)$$

where

$$A_k = \frac{1}{2} \left[1 + g(k) \right], \quad {}^0B_k = g(k)(2N)^{-1/2} \begin{cases} 1, & k > 0 \\ 10 L \cdot k, & k < 0 \end{cases}$$

$$g(k) = \ln N f(k) (\tau k^2 \theta)^{-1}$$

Because of the series S [Eq. (15)], Eq. (21) will contain the following type of integral which may be integrated by parts to give

$$\begin{aligned} & \int_{-\infty}^{\infty} H_j(X_k) \exp \left[-A_k X_k^2 - 2 {}^0B_k(L) X_k \right] dX_k \\ & = {}^0G_j(k, L) \int_{-\infty}^{\infty} \exp \left[-A_k X_k^2 - 2 {}^0B_k(L) X_k \right] dX_k, \end{aligned} \quad (22)$$

where

$$^0a_1(\underline{k}, \underline{L}) = -^0B_{\underline{k}}(\underline{L})/A_{\underline{k}}, \quad ^0a_2(\underline{k}, \underline{L}) = \frac{1}{2} A_{\underline{k}}^{-1} + \left[^0B_{\underline{k}}(\underline{L})/A_{\underline{k}} \right]^2 - 1, \text{ etc.}$$

This enables us to write

$$T_{\infty}(\underline{L}) = \text{const.} \prod_{\underline{k}} \int_{-\infty}^{\infty} \exp \left\{ -\frac{A_{\underline{k}}}{2} X_{\underline{k}}^2 - 2 ^0B_{\underline{k}}(\underline{L}) X_{\underline{k}} \right\} dX_{\underline{k}} ^0S(\underline{L}), \quad (23)$$

where $^0S(\underline{L})$ is the series having the same coefficients as S [Eq. (15)] but with $^0a_j(\underline{k}, \underline{L})$ replacing $H_j(X_{\underline{k}})$ wherever $H_j(X_{\underline{k}})$ does not appear in an average. If we carry out the indicated integrations in Eq. (23), we obtain

$$T_{\infty}(\underline{L}) = \text{const.} \quad ^0S(\underline{L}) \exp \left[-\gamma \underline{L}^2 \right],$$

where

$$\gamma = -L^{-2} \sum_{\underline{k}} ^0B_{\underline{k}}^2/A_{\underline{k}}. \quad (24)$$

If the substitution for $^0B_{\underline{k}}$ and $A_{\underline{k}}$ from Eq. (21) are made, the sum in γ may be replaced by an integral and the integration over the indicated directions of $\underline{k}$ performed to give

$$\gamma = \frac{\theta^2 \zeta}{12\pi^2 N} \int_0^{\infty} \left[g^2/(1+g) \right] k^4 dk. \quad (25)$$

Fig. 1 shows γ as a function of θ .

To evaluate $T_{11}(\underline{L})$, we must write V_1 [Eq. (12')] in terms of $X_{\underline{k}}$'s [Eq. (14)] with the understanding that the $X_{\underline{k}}$'s include only particles numbered 2 to N .

Thus we have

$$V_1 = 2\pi(N-1)\tau^{-1} \sum_{\underline{k}} r k^{-2} \underline{x}_{\underline{k}}^2 + \ln \tau^{-1} \left[2(N-1) \right]^{1/2} \sum_{i=0}^1 \left\{ \sum_{\underline{k}}^+ r k^{-2} \underline{x}_{\underline{k}} \cos \underline{k} \cdot \underline{r}_1 - \sum_{\underline{k}}^- r k^{-2} \underline{x}_{\underline{k}} \sin \underline{k} \cdot \underline{r}_1 \right\} + r_{10}^{-1} + \text{const.} \quad (26)$$

and, with $r_0 = 0$

$$\nabla_0 V_1 = \underline{r}_1 r_1^{-3} - \ln \tau^{-1} \left[2(N-1) \right]^{1/2} \sum_{\underline{k}}^- k r k^{-2} \underline{x}_{\underline{k}}.$$

From Eqs. (15), (17), and (26), we see that

$$T_{11}(\underline{L}) = \text{const.} \int_{|\underline{r}_1| < r_0} \exp \left\{ -(\theta r_1)^{-1} + i \underline{L} \cdot \underline{r}_1 r_1^{-3} \right\} \left[\int \dots \int s \times \right. \\ \left. \times \prod_{\underline{k}} \left\{ \exp \left[-\underline{A}_{\underline{k}} \underline{x}_{\underline{k}}^2 - 2 \underline{B}_{\underline{k}}(\underline{L}) \underline{x}_{\underline{k}} \right] d\underline{x}_{\underline{k}} \right\} \right] d\underline{r}_1, \quad (27)$$

$$\underline{A}_{\underline{k}} = \frac{1}{2} \left[1 + g(k) \right], \quad \underline{B}_{\underline{k}} = g(k)(2N)^{-1/2} \begin{cases} 1 + \cos(\underline{k} \cdot \underline{r}_1), & k_x > 0 \\ -\sin \underline{k} \cdot \underline{r}_1 + i \theta \underline{L} \cdot \underline{k}, & k_x < 0 \end{cases}$$

Operations similar to those carried out to obtain Eq. (24) may now be performed and the results reduced to

$$T_{11}(\underline{L}) = \text{const.} \exp(-\gamma L^2) \int_{|\underline{r}_1| < r_0} \exp \left[-(\underline{u}_1/\theta) - i \underline{L} \cdot \nabla \underline{u}_1 \right] s(\underline{L}, \underline{r}_1) d\underline{r}_1,$$

where

$$u_1 = r_1^{-1} - 2\theta N^{-1} \sum_k \left[g^2 / (1 + g) \right] \cos(\underline{k} \cdot \underline{r}_1), \quad (28)$$

and γ is defined by Eq. (25). Replacing the sum in u_1 by an integral and integrating over the indicated directions of $\underline{k}$ gives

$$u_1 = r_1^{-1} - \theta \gamma (N^2 \pi^2 r_1)^{-1} \int_0^\infty \left[g^2 / (1 + g) \right] k \sin(kr_1) dk. \quad (29)$$

This function u_1 can be fitted, with an error less than .5 per cent in the range from $r_1 = 0$ to r_0 for θ 's within the range of validity of the calculations performed in this paper [see Section VIII], by the expression

$$u_1(r_1) \approx r_1^{-1} - \alpha(\theta) + \beta(\theta) r_1^2. \quad (30)$$

The functions $\alpha(\theta)$ and $\beta(\theta)$ are shown in Fig. 1.

A similar procedure may be carried through to obtain $T_{10}(L)$. The result will be identical to Eq. (28) except that u_1 is replaced by u_0 where

$$u_0 = u_1 - u_{10} \quad (31)$$

The evaluation of $P(s)$ becomes quite difficult when terms other than the first are included in the expansion of the Jacobian. For this reason, only the first term will be used and the error resulting from the omission of higher terms will be estimated in Section VI.

Replacing $^1S(L, \underline{r}_1)$ by unity in Eq. (28) and integrating over the directions of $\underline{r}_1$, we obtain

$$T_{11}(L) = \text{const. } L^{-1} \exp(-\gamma L^2) \int_0^{r_0} (u_1')^{-1} e^{-u_1/\theta} \sin(Lu_1') r_1^2 dr_1, \quad (32)$$

where the prime on u_1 indicates differentiation with respect to r_1 .

If we replace $^0S(L)$ in Eq. (24) by unity and substitute the result into Eq. (19) for $P_{00}(s)$, the integration over L may be performed to give

$$P_{00}(s) \approx 2(\pi\gamma)^{-1/2} (s^2/\gamma) e^{-s^2/\gamma} \quad (33)$$

Similarly, if we substitute $T_{11}(L)$ from Eq. (32) into $P_{11}(s)$ of Eq. (19) and perform the integration over L , we find that

$$P_{11}(s) \approx 2s(N/\gamma)(\pi/\gamma)^{1/2} \int_0^{r_0} (r_1^2/u_1') e^{-u_1/\theta} \left\{ \exp \left[- (s - u_1')^2 / (\gamma) \right] - \exp \left[- (s + u_1')^2 / \gamma \right] \right\} dr_1 \quad (34)$$

The expression for P_{10} may be obtained by replacing u_1 in $P_{11}(s)$ by u_0 [Eq. (31)]. Figures 3 and 4 show the results of calculations with Eq. (19), (33), and (34).

For very large values of s , only the second term in the integrand of $P_1(s)$ is important. The integrand is sharply peaked and has a maximum near $r_1^{-2} = s$. Thus u_1 may be expanded around $r_1 = s^{-1/2}$ and the integrand approximated by a Gaussian to give an expression very much like that of Harris Mayer's nearest neighbor approximation,^{1,2} namely

$$\lim_{s \rightarrow \infty} P_{11}(s) = (3/2s^{5/2}) \exp \left\{ - u_1(s^{-1/2}) / \theta \right\} \quad (35)$$

The quantity $3/\ln$ has been substituted for (N/τ) . As θ approaches infinity, this expression approaches the first term in the asymptotic expansion of the Heltsmark distribution.⁴

For small values of ϵ , it is convenient to write

$$P_{10} \approx P_{\infty}(\epsilon)(8\pi\tau N/\tau\epsilon) \int_0^{r_0} (r_1^2/u_0') \exp \left\{ -(u_0'/\theta) - \left[(u_0')^2/4\tau \right] \right\} \sinh(\epsilon u_0'/2\tau) dr. \quad (36)$$

If the sinh is expanded in a power series, $P_{10}(\epsilon)$ may be approximated by the first term of this series to give

$$\lim_{\epsilon \rightarrow \infty} P_{10}(\epsilon) \approx P_{\infty}(\epsilon)(4\pi\tau N/\tau) \int_0^{r_0} r^2 \exp \left\{ -(u_0'/\theta) - \left[(u_0')^2/4\tau \right] \right\} dr. \quad (37)$$

For small values of ϵ , $P_{\infty}(\epsilon)$ and $P_{10}(\epsilon)$ are much larger than $P_{11}(\epsilon)$ so that Eqs. (33) and (37) may be used to give $P(\epsilon)$. For large values of ϵ , $P_1(\epsilon)$ is much larger than the others so that Eq. (35) may be used as an approximation to $P(\epsilon)$. In Fig. 6, a comparison is made between these approximate expressions and the more accurate formulas of Eqs. (34) and (36) for $\theta = 1.2675$ and $\theta = \infty$.

VI. ERROR INTRODUCED BY APPROXIMATING THE JACOBIAN

To obtain an idea of the error introduced by dropping the higher terms in the series S occurring in the Jacobian [Eq. (15)], we shall look at the second and third terms in the series $^0S(L)$ [Eq. (23)]. They are

$$^0S(L) = 1 + a_2 + a_3 + \dots$$

$$a_2 = \frac{1}{2} (2N)^{-1/2} \sum_{\underline{k}} \sum_{\underline{m}}^* \left\{ \delta(2\underline{k} - \underline{m}) - \delta(2\underline{k} + \underline{m}) \right\} \left\{ (2A_{\underline{k}})^{-1} \right. \\ \left. + \left[{}^0B_{\underline{k}}(L) \right]^2 A_{\underline{k}}^{-2} - 1 \right\} \left\{ - {}^0B_{\underline{m}}(L) A_{\underline{m}}^{-1} \right\}.$$

$$a_3 = - (1/6) (2N)^{-1/2} \sum_{\underline{k}, \underline{m}, \underline{n}}^* (-1)^{(\omega_{\underline{k}} + \omega_{\underline{m}} + \omega_{\underline{n}})/2} \left\{ \delta(\underline{k} + \underline{m} + \underline{n}) \delta(\omega_{\underline{k}} + \omega_{\underline{m}} + \omega_{\underline{n}} - 2) \right. \quad (38)$$

$$+ \left[\delta(\underline{k} + \underline{m} - \underline{n}) (-1)^{\omega_{\underline{n}}} + \delta(\underline{k} - \underline{m} + \underline{n}) (-1)^{\omega_{\underline{m}}} + \delta(-\underline{k} + \underline{m} + \underline{n}) (-1)^{\omega_{\underline{k}}} \right] \times$$

$$\times \left[\delta(\omega_{\underline{k}} + \omega_{\underline{m}} + \omega_{\underline{n}}) + \delta(\omega_{\underline{k}} + \omega_{\underline{m}} + \omega_{\underline{n}} - 2) \right] \left\{ {}^0B_{\underline{k}}(L) {}^0B_{\underline{m}}(L) {}^0B_{\underline{n}}(L) (A_{\underline{k}} A_{\underline{m}} A_{\underline{n}})^{-1} \right\}.$$

If we perform the summation over $\underline{m}$, substitute the values of ${}^0B_{\underline{k}}(L)$ and $A_{\underline{k}}$ from Eq. (21), and convert the summation over $\underline{k}$ to an integration, we obtain

$$a_2 = -\gamma N^{-2} (2\pi)^{-3} \int_{\underline{k}}^* F(2\underline{k}) F^2(\underline{k}) \left[1 + \theta^2(L \cdot \underline{k})^2 \right] d\underline{k}. \quad (39)$$

$$F(\underline{k}) = \frac{g(\underline{k})}{1 + g(\underline{k})}$$

Thus a_2 is of the order of N^{-1} and can be neglected.

To evaluate a_3 , we notice that the first bracket appearing in it contains three delta functions and that the terms resulting from each delta function are the same. If we now perform the summation over $\underline{n}$, convert the other sums to integrals, and substitute for ${}^0B_{\underline{k}}$ and $A_{\underline{k}}$ from Eq. (21), we obtain

$$\begin{aligned}
a_3(L) = & \frac{1}{3} (2\pi)^{-6} (c/N)^2 \left\{ 2\theta^2 \int_{\underline{k}}^+ \int_{\underline{m}}^- I(\underline{L} \cdot \underline{m}) \left[\underline{L} \cdot (\underline{k} + \underline{m}) \right] d\underline{k} d\underline{m} \right. \\
& + 4\theta^2 \int_{\underline{k}}^+ \int_{\substack{\underline{m} \\ |\underline{m}| > |\underline{k}|}}^- V(\underline{k} \cdot \underline{m}) \left[\underline{L} \cdot (\underline{k} + \underline{m}) \right] d\underline{k} d\underline{m} \\
& - \theta^2 \int_{\underline{k}}^+ \int_{\underline{m}}^- I(\underline{L} \cdot \underline{k})(\underline{L} \cdot \underline{m}) d\underline{k} d\underline{m} \\
& \left. - 3 \int_{\underline{k}}^+ \int_{\underline{m}}^+ I d\underline{k} d\underline{m} \right\} ,
\end{aligned} \tag{42}$$

where

$$I = P(k) P(m) P(|\underline{k} + \underline{m}|) .$$

The last integral in a_3 has been evaluated roughly in order to obtain an idea of the region over which the calculations of $P(s)$ are valid. This contribution to a_3 , which is called a_3^0 , is shown in Fig. 5.

VII. THE DETERMINATION OF r_0

Presumably in a complete theory the value of $P(s)$ would be independent of the choice of r_0 . However, in the present calculations, r_0 must be selected so as to minimize the errors due to two approximations. They are (1) the neglect of higher terms in the expansion of the Jacobian and (2) the neglect of certain short range interactions. If r_0 is too small, the approximation to the Jacobian is poor. If r_0 is too large, the range of the short range forces becomes so large

that their omission is not justified.

Since the Holtmark distribution⁴ gives $P(\epsilon)$ at $\theta = \infty$, it is interesting to compare it with the method described in this paper for different values of r_0 . In Fig. 2 is plotted the values of ϵ corresponding to certain values of $P(\epsilon)$ divided by the corresponding ϵ given by the Holtmark distribution as a function of r_0 . There is surprisingly little change in $P(\epsilon)$ when r_0 changes by as much as a factor two. The changes in the separate parts, $P_{\infty} - P_{10}$ and P_{11} are quite large, however.

The value $r_0 = .65$ has a particular significance. In the expansion of the Holtmark distribution around $\epsilon = 0$, the first term is $(4/3\pi) \left[2.5(2\pi)^{-1/2} \right]^{4/5} \epsilon^2$. If this term is set equal to the first term of the expansion of $P_{\infty}(\epsilon)$ [Eq. (33)] a value of $\gamma = .763...$ is obtained. At $\theta = \infty$, Eq. (25) shows that γ equals $(2r_0)^{-1}$. Thus we find that r_0 equals .65... if the entire value of $P(\epsilon)$ is determined by $P_{\infty}(\epsilon)$ at very small fields. Figure 2 shows that an r_0 of .65 is close to the one giving the best comparison with the Holtmark distribution over its entire range. It is also interesting to note that the value of k_0 used in the calculations in I is such that $k_0 r_0 \approx \pi/2$ when r_0 is .65.

For smaller values of θ the error, made by neglecting some of the short range interactions, should decrease since the ions will be held apart by their Coulomb repulsion. Figure 5, however, indicates that the error, due to approximating the Jacobian, increases with decreasing θ . This error can be reduced by increasing r_0 . Thus it is clear that r_0 should be increased as θ is decreased in such a way as to minimize the errors due to the Jacobian as indicated by Fig. 5 and from neglecting short range interactions as indicated by Fig. 2. For the calculations of $P(\epsilon)$ shown in Figs. 3 and 4, a value of $r_0 = .65$ was chosen throughout.

VIII. DISCUSSION AND CONCLUSIONS

The formulas for computing $P(z)$ approximately by the method described in Section II are given by Eq's. (9), (10), (19), (21), (25), (30), (31), (33), (34), and (36). It may be computed approximately for small fields by Eq's. (33) and (34) and for large fields by Eq. (35). The results of calculations using these formulas are given in Figs. 3 and 4.

Errors in these calculations arise from two sources. They are (1) the neglect of higher terms in the expansion of the Jacobian [Eq. (7)] and (2) the improper treatment of certain configurations when ions approach more closely than the distance r_0 . Figure 5 indicates that, if the error due to the first approximation is to be kept below ten percent for r_0 equal to 0.65, then θ must be above 0.6. At a θ of 0.6, the ions are able to escape fairly frequently from their ion spheres. Figure 2 shows that the Holtmark distribution is rather well approximated by the present method of computing $P(z)$ for $r_0 = 0.65$. Since errors due to improper representation of close approaches of the ions should decrease as θ decrease, Fig. 2 should indicate an upper limit on the shift of the curve in z due to this error.

It is interesting to observe that an average short range potential [Eq. (29)] occurs in the course of the calculation. This is the potential energy of the system averaged over all the positions of the particles numbered 2 to N when particles 1 and 0 are separated by the distance r_1 . Particles 2 to N in this average are treated with collective coordinates so that their short range interactions are ignored. This average potential $u_1(r_1)$ is approximately determined for $r_0 = .65$ by the information in Fig. 1 with the aid of Eq. (30). The values $3/2$ and $1/2$ were assumed for α and β in the nearest neighbor approximation by H. Mayer.¹ The plot

of $\exp(3/2 - \alpha)/\theta$ in Fig. 1 indicates that the choice of $\alpha(\theta) = 3/2$ is a good one over the range of validity of present calculations.

A comparison is made between the SRNN approximation of I and the present method for $\theta = 1.2675$ in Figs. 3 and 4. Since the agreement is satisfactory, the approximations made in the SRNN approximation seem to be justified, and this method is the best now available for computing $P(e)$ for θ below 0.6.

Future calculations should show two improvements over those performed for Figs. 3 and 4. First it seems clear that the value of r_0 should be increased as θ is decreased to reduce the error arising from the approximation to the Jacobian. Second it seems evident that the choice of the form of w_{1j} [Eq. (3)] and therefore of $f(k)$ [Eqs. (9) and (10)] is not the best. Since the error terms in Section VI [Eq. (42)] contain the quantity, $1 + g(k)$, [Eq. (21)] in the denominator; they should be smaller if $g(k)$, and therefore $f(k)$, is not allowed to become negative. The form of $f(k)$ in Eq. (10) is such that $1 + g(k)$ will be zero for certain values of k if θ is less than .0118. This suggests that a form such as

$$f(k) = \frac{\sin^2 k r_0}{k^2 r_0^2} \quad (43)$$

might reduce the error due to the Jacobian. If the method described in this paper is to be used for evaluating the Jacobian of the transformation to collective coordinates, an investigation of the possible forms of $f(k)$ should be made.

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FIGURE LEGENDS

Fig. 1 The coefficients in the approximation to the average pair potential u_I as a function of θ together with the comparison of γ of Eq. (25) with γ_I of I. The quantity $e^{\frac{3/2 - \epsilon}{\theta}} - 1$ is given as a comparison of the value $3/2$ chosen for ϵ in reference 1.

Fig. 2 The value of the field strength ϵ computed from formulas in the text divided by ϵ_H of the Holtzmark distribution as a function of r_c for various values of $P(\epsilon)$. $P^L(\epsilon)$ represents $P(\epsilon)$ to the left of its maximum while $P^R(\epsilon)$ is to the right.

Fig. 3 The probability $P(\epsilon)$ of obtaining a field strength of magnitude ϵ for various values of θ and small values of ϵ . The dashed curves are for the r_c cutoff method described in the text while the solid curves are for the SRNN approximation of I.

Fig. 4 The probability $P(\epsilon)$ of obtaining a field strength of magnitude ϵ for various values of θ and large values of ϵ . The dashed curves are for the r_c cutoff method described in the text while the solid curves are for the SRNN approximation of I.

Fig. 5 Part of the contribution of the third order term in the expansion of the Jacobian to $P(\epsilon)$ a_3^0 as a function of θ . The size of a_3^0 relative to one is an

approximation to the relative error in $P(s)$ caused by the approximation to the Jacobian used in the calculations.

Fig. 6 A comparison of approximate formulas for $P(s)$ (dashed curves) as given by Eqs. (33), (34), and (35) with the more accurate formulas (solid curves) of this paper for $\theta = 1.2675$ and $\theta = \infty$

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Fig. 2

H^e

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K₀Σ

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Fig. 3

SRNN

r_c cutoff

31

- 31 -

P(e)

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Fig. 5

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