$$\times \exp[-A(p^2/2m+\tfrac{1}{2}m\omega_0^2x^2)+ax]\ . \qquad (\mathrm{A.}3)$$

Completing the square on x gives

$$\langle e^{ax}\rangle = \exp(a^2/2m\omega_0 A)\int dxdp f_W(p,x) \qquad (\mathrm{A.}4\mathrm{a})$$

$$= \exp(a^2/2m\omega_0^2 A)\ . \qquad (\mathrm{A.}4\mathrm{b})$$

Since $\langle x^2\rangle = \lim_{a\to 0}\frac{d^2}{da^2}\langle e^{ax}\rangle$ (A.5)

we find immediately

$$\langle x^2\rangle = (m\omega_0^2A)^{-1}\ . \qquad (\mathrm{A.}6)$$

Inserting (A.4b) and (A.6) into (A.1), we find Bloch's theorem is verified immediately (for $Q = ax$). For $Q = bp$ the proof is equally trivial.

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Screening Constants for Systems of Charged Particles*

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Based on graphical considerations a systematic approach is given for the evaluation of the screening constants for many-particle systems interacting with Coulomb forces.

1. INTRODUCTION

Classical systems of charged particles interacting with Coulomb forces have been characterized by the Debye screening constant:

$$\kappa_0 = (4\pi\beta n e^2)^{1/2} \qquad (1.1)$$

entering the Debye screening potential;

$$\phi_D = (e^2/r)\exp(-\kappa_0 r)\ . \qquad (1.2)$$

This Debye screening was obtained originally from the Poisson-Boltzmann equation. Since then, many efforts have been made to investigate and improve upon the Debye theory. We are now able to understand the meaning of the Debye screening in terms of the modern statistical methods such as those based on diagrams,[1,2] on random phase approximation,[3] on random variables,[4] or on the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy of equation.[5]

However, in spite of these efforts there seems no systematic study of the screening effects in various systems of charged particles. Therefore, we shall consider several typical systems of charged particles with our focus on the screening effects. For this purpose, we shall adopt a diagram method and evaluate the pair distribution functions (p.d.f.) for large distances. If the decay of the distribution functions is exponential, one can determine the screening constant because the pair distribution functions are related to the potentials of average force.

It seems that the Debye screening does not require discussions since it is well understood. Therefore, we shall start our discussion with the case of a classical electron gas in a uniform magnetic field. We shall then be able to find the Debye screening by bringing the magnetic field to zero. In Sec. 3 we shall give critical comments on recent theories concerning correcting the Debye screening constant. In Sec. 4 discussions are given for a classical charged hard-sphere gas as a simplified model for polyelectrolyte solutions. In Sec. 5 we shall treat a degenerate electron gas, and in Sec. 6 a charged Bose gas will be considered. In all these cases we shall assume the presence of a cloud of positive charges in the background. For simplicity's sake, we shall adopt the units such that $\hbar = 1$ and $2m = 1$, where m is the mass of the charged particles.

2. ELECTRON GAS IN A MAGNETIC FIELD

The propagator of a charged particle from $(\vec{r}\,', \beta')$ to $(\vec{r}, \beta)$ in the coordinate-reciprocal thermal energy space is given by[6]

$$K(\vec{r}\beta, \vec{r}\,'\beta') = \sum_n e^{-(\beta-\beta')E_n}\psi_n(|\vec{r})\psi_n^*(\vec{r}\,'), \tag{2.1}$$

where in our units the wave function is given by

$$\psi_n(\vec{r}) = (A_n/2\pi)e^{i(p_x x + p_z z)}e^{-\frac{1}{2}a^2(y-y_0)^2}H_n(a(y-y_0)), \tag{2.2}$$

$$A_n = [a/\pi^{\frac{1}{2}}\,2^n n!]^{\frac{1}{2}}, \quad y_0 = p_x/a^2, \quad \omega_0 = 2eH/c = 2a^2,$$

where $H_n(y)$ is the Hermite polynomial. The corresponding energy is given by

$$E_n = (n+\tfrac{1}{2})\omega_0 + p_z{}^2. \tag{2.3}$$

Using Eqs. (2.2) and (2.3) in (2.1), performing the summation over n and integrating the result over p_x and p_z, one finds

$$K(\vec{r}, \beta; \vec{r}\,'\beta') = \frac{a^2}{(2\pi)^{5/2}}\frac{\pi}{(\beta-\beta')^{1/2}}[\alpha(\beta,\beta')\sinh(\beta-\beta')\omega_0]^{-1/2}$$

$$\times \exp\left(-\frac{1}{4}\frac{(z-z')^2}{\beta-\beta'} - \frac{a^2}{4\alpha(\beta,\beta')}[(y-y')^2+(x-x')^2] + i\,\frac{a^2}{2}(y+y')(x-x')\right), \tag{2.4}$$

$$\alpha(\beta,\beta') = \tanh[(\beta-\beta')\omega_0/2]. \tag{2.5}$$

We now consider a propagation from $(\vec{r}_1, \beta_1)$ to $(\vec{r}\,', \beta_2)$, where an interaction takes place, and from $(\vec{r}\,', \beta_2)$ to $(\vec{r}_1, \beta+\beta_1)$ (see Fig. 1). Correspondingly, we introduce a new propagator

$$F(\vec{r}_2\beta_2; \vec{r}_1\beta_1) = Z\int d\vec{r}\,'K(\vec{r}_1, \beta+\beta_1; \vec{r}\,'\beta_2)\phi(|\vec{r}_2 - \vec{r}\,'|)K(\vec{r}\,'\beta_2; \vec{r}_1\beta_1), \tag{2.6}$$

where z outside of the integrand is the fugacity and $\phi(r)$ is the Coulomb interaction. To evaluate the right-hand side it is convenient to rewrite $K(\vec{r}\beta; \vec{r}\,'\beta')$ such that

$$K(\vec{r}\beta; \vec{r}\,'\beta') = B(\beta-\beta')K'(\vec{r}-\vec{r}\,', \beta-\beta')\exp[i\,\tfrac{1}{2}a^2(y+y')(x-x')], \tag{2.7}$$

where $B(\beta-\beta') = \dfrac{a^2}{(2\pi)^{5/2}}\dfrac{\pi}{(\beta-\beta')^{1/2}}\{\alpha(\beta,\beta')\sinh[(\beta-\beta')\omega_0]\}^{-1/2}$,

$$K'(\vec{r}-\vec{r}\,', \beta-\beta') = \exp\left(-\frac{1}{4}\frac{(z-z')^2}{\beta-\beta'} - \frac{a^2}{4\alpha(\beta,\beta')}[(y-y')^2+(x-x')^2]\right). \tag{2.8}$$

Then, we find

$$F(\vec{r}_2\beta_2; \vec{r}_1\beta_1) = ZB(\beta+\beta_1-\beta_2)B(\beta_2-\beta_1)\int d\vec{r}\,'\int\frac{d\vec{q}}{(2\pi)^3}\,d\vec{p}\,G_0(p)e^{-i\vec{p}\cdot(\vec{r}_1-\vec{r}\,')}u(q)e^{i\vec{q}\cdot(\vec{r}_2-\vec{r}\,')}, \tag{2.9}$$

where $u(q)$ is the Fourier transform of $\phi(r)$, and $G_0(p)$ is that for

$$G_0(r) = ZK'(\mathrm{r}, \beta+\beta_1-\beta_2)K'(-\mathrm{r}, \beta_2-\beta_1)$$
$$= Z\exp\left(-\frac{1}{4}\frac{z^2}{\beta+\beta_1-\beta_2} - \frac{a^2(x^2+y^2)}{4\alpha(\beta+\beta_1,\beta_2)}\right)\exp\left(-\frac{1}{4}\frac{z^2}{\beta_2-\beta_1} - \frac{a^2(x^2+y^2)}{4\alpha(\beta_2,\beta_1)}\right) \tag{2.10}$$

and is given by

$$G_0(p) = \frac{1}{(2\pi)^3}\int d\vec{\mathrm{r}}\, G_0(r)\exp(i\vec{\mathrm{p}}\cdot\vec{\mathrm{r}})$$
$$= \frac{Z}{(\pi)^{3/2}}[(\beta_2-\beta_1)(\beta-\beta_2+\beta_1)/\beta]^{1/2}\left(\frac{a^2}{\alpha(\beta+\beta_1,\beta_2)}+\frac{a^2}{\alpha(\beta_2,\beta_1)}\right)^{-1}\exp[-\beta^{-1}(\beta_2-\beta_1)(\beta-\beta_2+\beta_1)p_z^{\,2}$$
$$-\left(\frac{a^2}{\alpha(\beta+\beta_1,\beta_2)}+\frac{a^2}{\alpha(\beta_2,\beta_1)}\right)^{-1}(p_x^{\,2}+p_y^{\,2})]. \tag{2.11}$$

Thus we arrive at

$$F(\vec{\mathrm{r}}_2\beta_2, \vec{\mathrm{r}}_1\beta_1) = \frac{1}{(2\pi)^3}\int G(q,\beta_2-\beta_1)u(q)d\vec{\mathrm{q}}\ , \tag{2.12}$$

where $$G(q,\beta_2-\beta_1) = \frac{Za^2\beta}{(4\pi\beta)^{3/2}}(\sinh\tfrac{1}{2}\beta\omega_0)^{-1}\exp\left(-\frac{q_z^{\,2}}{d}-\frac{q_x^{\,2}+q_y^{\,2}}{t}\right), \tag{2.13}$$

and where

$$d = \frac{\beta}{\alpha(\beta-\alpha)},\quad t = a^2\frac{\sinh(\frac{1}{2}\beta\omega_0)}{\sinh(\frac{1}{2}\alpha\omega_0)\sinh[\frac{1}{2}(\beta-\alpha)\omega_0]},\quad \alpha=\beta_2-\beta_1. \tag{2.14}$$

Let us now consider simple chain diagrams which correspond analytically superposing the $F(\vec{\mathrm{r}}_2\beta_2, \vec{\mathrm{r}}_1\beta_1)$ propagators. To sum the contributions of such chain diagrams to the pair distribution function it is convenient to introduce the Fourier transform

$$\lambda_j(q) = \int_0^\beta d\alpha\, G(q,\alpha)\, e^{2\pi i j\alpha/\beta} d\alpha\,. \tag{2.15}$$

In terms of $\lambda_j(q)$ and using convolution we find the contribution of chain diagrams to the pair distribution function to be[1]

$$\rho_2(|\vec{\mathrm{r}}_2-\vec{\mathrm{r}}_1|)-n^2 = \frac{1}{\beta(2\pi)^3}\sum_j\int\sum_{l=2}^{\infty}[-u(q)]^{l-1}\lambda_j^{\,l}(q)\,e^{i\vec{\mathrm{q}}\cdot(\vec{\mathrm{r}}_2-\vec{\mathrm{r}}_1)}d\vec{\mathrm{q}} \tag{2.16}$$
$$= \frac{-1}{\beta(2\pi)^3}\sum_j\int\frac{u(q)\lambda_j^{\,2}(q)}{1+\lambda_j(q)u(q)}\,e^{i\vec{\mathrm{q}}\cdot(\vec{\mathrm{r}}_2-\vec{\mathrm{r}}_1)}d\vec{\mathrm{q}}\ , \tag{2.17}$$

where n is the number density.

The evaluation of the eigenvalues $\lambda_j(q)$ for all values of q is difficult. However, for a classical electron gas and for large distances in which we are interested, we find

$$\lambda_j(q) = \frac{a^2Z\beta^2}{\lambda^3\sinh(\beta\omega_0/2)}\left(1+\frac{\beta}{360}(\beta\omega_0)^2(q_x^{\,2}+q_y^{\,2})+\cdots\right)\delta_{j0}\ , \tag{2.18}$$

where $\lambda=(4\pi\beta)^{1/2}$ is the de Broglie thermal wavelength.

Using Eq. (2.18) in Eq. (2.17) and performing calculations to order $\omega_0^{\,2}$ we arrive at (see Appendix for calculations)

$$\rho_2(r)-n^2 = -\frac{Z\kappa^2}{\lambda^3}\left\{\frac{e^{-\kappa r}}{4\pi r}[1-\tfrac{1}{6}(\beta\omega_0/2)^2]+\frac{\beta}{(2\pi)^3}\frac{(\beta\omega_0)^2}{180}\right.$$
$$\left.\times\left[-\left(\frac{e^{-\kappa r}}{r^3}+\frac{\kappa}{r^2}e^{-\kappa r}\right)+3|z|^2\left(\frac{e^{-\kappa r}}{r^5}+\frac{\kappa e^{-\kappa r}}{r^4}+\frac{\kappa^2 e^{-\kappa r}}{3r^3}\right)\right]\right\}\ , \tag{2.19}$$

where the screening constant is given by

$$\kappa^2 = 4\pi e^2 Z a^2 \beta^2 / \lambda^3 \sinh(\beta\omega_0/2) . \qquad (2.20)$$

For classical systems the fugacity $Z = n\lambda^3$. Therefore the screening constant κ is related to the Debye screening constant as follows

$$\kappa^2/\kappa_0{}^2 = a^2\beta/\sinh(\beta\omega_0/2) = 1 - \tfrac{1}{24}(\beta\omega_0)^2 + \cdots . \qquad (2.21)$$

For the evaluation of the equation of state we need to find the fugacity more accurately. We arrive at

$$Z = n\lambda^3\{1 - n^{1/2}\pi^{1/2} e^3\beta^{3/2}[1 + \tfrac{1}{24}(\beta\omega_0)^2] + \cdots\} , \qquad (2.22)$$

and obtain the equation of state in the form:

$$P\beta = n[1 - \tfrac{1}{3}\pi^{1/2} e^3\beta^{3/2} n^{1/2} - \tfrac{1}{24}(\omega_0 H/kT)^2 + \cdots]. \qquad (2.23)$$

3. CORRECTIONS TO THE DEBYE SCREENING

As have been discussed by Hirt, DeWitt, Bowers and Salpeter, Mitchell and Ninham[7,8] (MN) the corrections to the Debye results may be obtained by considering composite chains. These authors were mainly interested in the p.d.f. but we shall concentrate in the screening constant for the order next to the Debye approximation. For this purpose, we shall examine the asymptotic behavior of the p.d.f. and elucidate some controversial points.

The controversial points concerning the asymptotic behavior of the p.d.f. may be summarized as follows. In 1965 DeWitt discussed that the Debye screening term may be dominated by a higher-order term when the reduced distance x is larger than $8/\epsilon \ln 3$.[8] In 1966 Lie and Ichikawa[5] (LI) rejected the DeWitt observation based on a perturbation solution of the BBGKY hierarchy. They then proposed a new asymptotic formula

$$[\rho_2(r) - n^2]/n^2 = g(x) \sim -\epsilon x^{-1}\exp[-x - \psi(x)] , \qquad (3.1)$$

where $x = \kappa_0 r$, $\epsilon = \beta e^2 \kappa_0$,

$$\psi(x) = \tfrac{1}{8}\epsilon \ln 3x \exp(-\tfrac{1}{8}\epsilon \ln 3x) . \qquad (3.2)$$

More recently, Mitchell and Ninham[7] concluded that the above LI asymptotic expression was not correct and should be replaced by

$$g(x) = -(A/x)e^{-Bx} , \qquad (3.3)$$

where

$$\begin{aligned} A &= \epsilon + (\tfrac{3}{8}\ln 3 + \tfrac{1}{6})\epsilon^2 + O(\epsilon^3 \ln\epsilon); \\ B &= 1 + \tfrac{1}{8}\epsilon \ln 3 + \tfrac{1}{12}\epsilon^2 \ln\epsilon + c\epsilon^2 + O(\epsilon^3 \ln\epsilon), \end{aligned} \qquad (3.4)$$

and c is a constant. Moreover, they claimed that Eq. (3.3) is valid for all $x > 1$.

We remark first of all that the MN consideration of diagrams Fig. 6(c)–6(h) is not necessary as far as the screening constant to order ϵ^2 is concerned. Second, the MN claim concerning the x domain is subject to accepting an analytical continuation. The summation of the series such as appeared in their Eq. (3.7) can be performed only for Ω values satisfying

$$|(\epsilon/2\Omega)\tan^{-1}\tfrac{1}{2}\Omega| < |1 + \Omega^2| . \qquad (3.5)$$

This inequality limits a minimum for Ω or a maximum for x. Only when the result of such a summation is accepted for all q, can one obtain the p.d.f. for all x.

In this respect, the LI asymptotic expression may also be considered to be valid for all $x > 1$ by an analytical continuation. For x larger than $8/\epsilon \ln 3$ the function $\psi(x)$ vanishes, however, resulting in the Debye screening term.

It is remarked that both g_{MN} and g_{LI} agree with each other for small ϵ and for $1 < x < 8/\epsilon \ln 3$ in the following way:

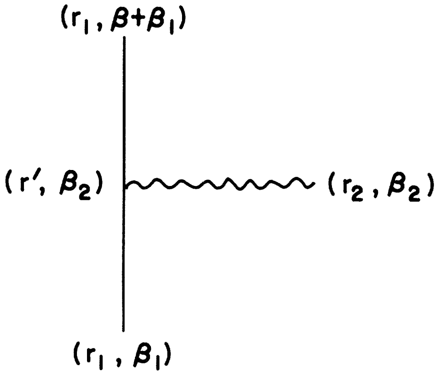

FIG. 1. Propagation with an interaction.

$$g_{\mathrm{LI}}(x) = -(\epsilon/x)e^{-x} + (\epsilon^2/8)(\ln 3)e^{-x} + \cdots . \quad (3.6)$$

$$\begin{aligned} g_{\mathrm{MN}}(x) &= -(\epsilon/x)e^{-x} + (\epsilon^2/8)\ln e^{-x} \\ &\quad - \epsilon^2(\tfrac{3}{8}\ln 3 + \tfrac{1}{6})(e^{-x}/x) + \cdots \\ &\sim -(\epsilon/x)e^{-x} + (\epsilon^2/8)\ln 3\, e^{-x} + \cdots . \quad (3.7) \end{aligned}$$

Nevertheless, the LI asymptotic expression is of undesirable form. The MN result also needs a modification since they did not consider many composite chains between two representative particles 1 and 2 which enter the p.d.f. In other words, by taking into consideration of watermelon-type diagrams such as shown in Fig. 2 one expects

$$g(x) = \exp[-A(\epsilon)e^{-B(\epsilon)x}/x] - 1 . \quad (3.8)$$

Let us now examine more closely the evaluation of the screening constant of a classical electron gas to order ϵ. The contribution of various diagrams may be estimated following the rules discussed elsewhere.[9] Generally, we consider replacing a simple chain by an effective interaction of the Debye screening potential. Thus a single interaction line gives a contribution of order ϵ. The next order diagrams are illustrated in Fig. 3 and their contributions to the p.d.f. are found to be

$$\begin{aligned} \rho^{(a)}(r) &= -(\kappa_0/2\pi)^6 \int \{(1+s^2) \\ &\quad \times (1+s'^2)[1+(\vec{s}-\vec{s}')^2]\}^{-1} \\ &\quad \times e^{i(\vec{s}-\vec{s}')\cdot\vec{x}} d\vec{s}d\vec{s}' ; \quad (3.9) \end{aligned}$$

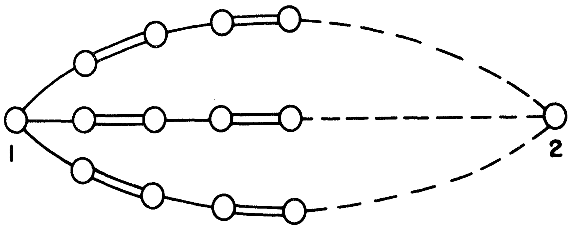

FIG. 2. A watermelon-type diagram for composite chains of the type (I) in Fig. 4.

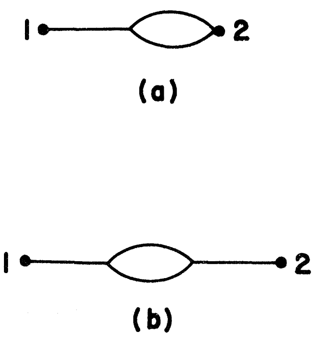

FIG. 3. Diagrams of order ϵ^2.

$$\begin{aligned} \rho^{(b)}(r) &= (\kappa_0/2\pi)^6 \int \\ &\quad \times \{(1+s^2)(1+s'^2)[1+(\vec{s}-\vec{s}')^2][1+(\vec{s}'-\vec{s})^2]\}^{-1} \\ &\quad \times e^{i(\vec{s}-\vec{s}')\cdot\vec{x}} d\vec{s}d\vec{s}' , \quad (3.10) \end{aligned}$$

where x and s are dimensionless variables defined by

$$x = \kappa_0 r, \quad s = q/\kappa_0 . \quad (3.11)$$

To simplify Eqs. (3.9) and (3.10) we introduce a new set of variables such that

$$\vec{Q} + \vec{q}/2 = \vec{s}, \quad Q - \vec{q}/2 = \vec{s}' . \quad (3.12)$$

Then after a straightforward but lengthy calculation we find

$$\rho^{(a)}(r) = -\frac{n^2\epsilon^2}{2\pi^2}\int \frac{1}{(q^2+1)} \frac{\tan^{-1}q/2}{q} e^{i\vec{q}\cdot\vec{x}} d\vec{q} ; \quad (3.13)$$

$$\rho^{(b)}(r) = \frac{n^2\epsilon^2}{4\pi^2}\int \frac{1}{(q^2+1)^2} \frac{\tan^{-1}q/2}{q} e^{i\vec{q}\cdot\vec{x}} d\vec{q} , \quad (3.14)$$

where $\epsilon = \beta e^2 \kappa_0$ as before.

We note in Eqs. (3.13) and (3.14) that the power of $1/(q^2+1)$ corresponds to the number of single effective bonds. Also one can easily see from the above derivation that the number of double bonds in a composite chain should be reflected in the power of $(\tan^{-1}q/2)/q$. We also note that three different types of composite chain can be generated by connecting alternatively single bonds and double bonds (Fig. 4). The contributions of these chains to ρ_2/n^2 can be easily found as follows:

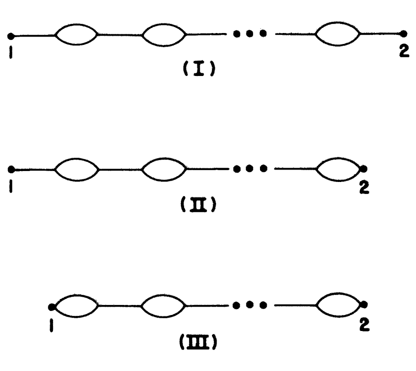

FIG. 4. Composite chains for $g(x)$ of order ϵ^2.

$$g_I(x) = -(\epsilon/\pi i x)\int_{-\infty}^{\infty} dq\, e^{iqx} \frac{q}{q^2+1+(\epsilon/2q)\tan^{-1}(q/2)}\,; \tag{3.15}$$

$$g_{\mathrm{II}}(x) = -(\epsilon^2/2\pi i x)\int_{-\infty}^{\infty} dq\, e^{iqx} \times \frac{2\tan^{-1}(q/2)}{q^2+1+(\epsilon/2q)\tan^{-1}(q/2)}\,; \tag{3.16}$$

$$g_{\mathrm{III}}(x) = (\epsilon^2/2\pi i x)\int_{-\infty}^{\infty} dq\, e^{iqx} \times \frac{(q^2+1)\tan^{-1}(q/2)}{q^2+1+(\epsilon/2q)\tan^{-1}(q/2)}\,. \tag{3.17}$$

Following Mitchell and Ninham one can evaluate the right-hand side integrals by contour integrals. The results are then determined by the residues at the pole determined by

$$q = i\omega, \quad (\epsilon/2i\omega)\tan^{-1}\tfrac{1}{2}i\omega = 1-\omega^2\,. \tag{3.18}$$

In the first integral the residue R must be evaluated to order ϵ. We find

$$R = \frac{1}{2}\left[1+\frac{\epsilon}{8\omega^2}\left(\frac{1}{\omega}\ln\frac{2-\omega}{2+\omega}+\frac{4}{4-\omega^2}\right)+\cdots\right] = \tfrac{1}{2}\left[1+\epsilon(-\tfrac{1}{8}\ln 3+\tfrac{1}{6})+\cdots\right]. \tag{3.19}$$

Thus we arrive at

$$g_{\mathrm{I}}(x) = -\frac{\epsilon}{x}e^{-\omega x}\left[1+\epsilon(-\tfrac{1}{8}\ln 3+\tfrac{1}{6})+\cdots\right]+O(e^{-2x})\,. \tag{3.20}$$

In g_{II} we need the residue to the zeroth order and get the result

$$g_{\mathrm{II}}(x) = -(\epsilon^2/2)\ln 3(e^{-\omega x}/x)+O(e^{-2x})\,. \tag{3.21}$$

To second order in ϵ, g_{III} does not contribute. As a result we arrive at the total contribution

$$g(x) = -\epsilon/x\, e^{-\omega x}\left[1+\epsilon(\tfrac{3}{8}\ln 3+\tfrac{1}{6})+O(\epsilon^2)\right], \tag{3.22}$$

$$\text{where} \quad \omega = 1+(\epsilon/8)\ln 3\,. \tag{3.23}$$

We remark that Eq. (3.22) coincides with what MN reported. They evaluated the screening constant to higher orders by taking into consideration of more complicated diagrams, but $g(x)$ to order ϵ^2 does not require such higher-order terms.

4. HARD-SPHERE CHARGED PARTICLES

A hard-sphere model for a macro-ion has been used often in the theory of polyelectrolyte solutions. In this model, macro-ions are replaced essentially by hard spheres of certain surface charges. The potential of average force for such a system has traditionally been determined by the linearized Debye-Hückel equation

$$\Delta\psi = \kappa_0^2\psi\,, \tag{4.1}$$

with the boundary condition at the hard-sphere diameter a:

$$\left(\frac{\partial\psi}{\partial r}\right)_{r=a} = -\frac{e^2}{a}\,. \tag{4.2}$$

The combination of these two equations yields

$$\psi = e^2\exp[-\kappa_0(r-a)]/(1+\kappa_0 a)r\,. \tag{4.3}$$

This result shows that the Debye screening constant κ_0 for point ions still characterizes the system.

It is to be remembered, however, that the hard-sphere potential enters this treatment only through the condition (4.2). Therefore, Eq. (4.2) is very essential to the solution. Unfortunately it is the condition at the hard-sphere boundary, namely at the shortest distance, while the solution of Eq. (4.1) corresponds to large distances. Therefore it seems to be more appropriate to avoid the short distance condition (4.2) and also to remove the assumption (4.1) that the system has the same screening constant κ as for point ions. Indeed, it must be a task of statistical mechanical investigation to find the potential of average force.

We note in this concern that the potential of average force $\Psi(r)$ is related to the p.d.f. by

$$\rho_2(r) = n^2\exp[-\Psi(r)/kT]\,. \tag{4.4}$$

We recall that $\Psi(r)$ evaluated from watermelon-type diagrams yields the Debye screening potential in the case of point charges. Thus for hard-sphere ions we may use the same approach based on watermelon diagrams.

We assume that the system is dilute as in the case of point ions and that the dimensionless parameter $n^{1/3}a$ is small, where a is the hard-sphere diameter. We may then superpose the pseudopotential which has been introduced by Lee and Yang[10] to the Coulomb potential. In momentum space we obtain

$$u(q) = 8\pi a + 4\pi e^2/q^2 \ . \qquad (4.5)$$

Using Eq. (4.5) in Eq. (2.17) we arrive at

$$\rho_2(r) = n^2 - (n\mu^2/4\pi r)[e^{-\mu r}/(1+8\pi a n\beta)] \ , \qquad (4.6)$$

where μ is a new screening constant defined by

$$\mu = \kappa_0(1+8\pi a n\beta)^{-1/2} \ . \qquad (4.7)$$

The formula (4.6) is based on a single chain between the representative particles 1 and 2. In case there are many separate chains we get a power series of which the first term is given by Eq. (4.6), its closed form being given by Eq. (4.4) with

$$\Psi(r) = (e^2/r)[e^{-\mu r}/(1+8\pi a n\beta)^2] \ . \qquad (4.8)$$

This result can also be proved by solving a Vlasov-type equation for a one-body phase-space distribution function $f(\vec{r},\vec{v})$ and using the relation

$$\Psi(q) = u(q)\int f(\vec{q},\vec{v})d\vec{v} + u(q) \ , \qquad (4.9)$$

where $f(\vec{q},\vec{v})$ is the Fourier transform of $f(\vec{r},\vec{v})$.

Our result (4.7) shows that the hard-sphere repulsion and the Coulomb force couple to each other to characterize the particle correlation at large distances. The hard-sphere repulsion plays the role of letting the Coulomb repulsion be more effective for large distances. Of course, there is no screening if there is no charge. Corresponding to the screening all thermodynamic functions show such a coupling between the two forces.[11]

5. CHARGED FERMIONS

In this section we consider a system of charged and degenerated fermions. Our aim is to find their screening effects at low temperatures. The eigenvalues λ_j for such a system to be used in Eq. (2.17) for the p.d.f. are given by[6]

$$\lambda_j(q) = \frac{1}{(2\pi)^3}\int d\vec{p}\, f(p)[1-f(\vec{p}+\vec{q})] \times \int_0^\beta e^{\alpha[p^2-(\vec{p}+\vec{q})^2]}\, e^{2\pi i j\alpha/\beta}\, d\alpha \ , \qquad (5.1)$$

where $f(p)$ is the Fermi distribution function. In our case

$$\begin{aligned} f(p) &= 0, \quad p > p_0 \,, \\ &= 1, \quad p < p_0 \,, \end{aligned} \qquad (5.2)$$

where p_0 is the Fermi momentum which is given in our units by

$$p_0 = (3\pi^2 n)^{1/3} \ . \qquad (5.3)$$

It is convenient to introduce dimensionless variables s, x, and y by

$$s = q/p_0, \quad x = p_0 r, \quad y = 2\pi j/\beta p_0^2. \qquad (5.4)$$

Then, the λ_j as a function of s and y are obtained as follows (Appendix B):

$$\lambda(s,y) = (p_0/8\pi^2)F(s,y) \qquad (5.5)$$

$$F(s,y) = 1 - \frac{1}{8}\left(s - \frac{4}{s} - \frac{y^2}{s^3}\right)\ln\left|\frac{(s^2+2s)^2+y^2}{(s^2-2s)^2+y^2}\right| - \frac{y}{2s}\left[\tan^{-1}\left(\frac{s^2+2s}{y}\right) - \tan^{-1}\left(\frac{s^2-2s}{y}\right)\right]. \qquad (5.6)$$

As before, the eigenvalues are of the dimension of reciprocal length.

We now consider fermions with spins. In this case the eigenvalues should be multiplied by a factor of 2. The summation over j of the eigenvalues may be replaced by integration over y at low temperatures. We arrive at

$$\rho_2(r)/n^2 - 1 = -(p_0^5/2\pi^6 n^2 i a_0) \times \frac{1}{x}\int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} ds\, \frac{sF^2(s,y)\,e^{isx}}{s^2+s_0^2F(s,y)} \ , \qquad (5.7)$$

where $s_0 = (2/a_0 p_0 \pi)^{1/2} = \mu_0/2^{1/2}p_0 \,,$ (5.8)

μ_0 is the Thomas-Fermi screening constant, and a_0 is the Bohr radius.

The evaluation of the double integrals in the right-hand side of Eq. (5.7) is difficult because of the form of $F(s,y)$. However, for very high density s_0 is small, and we arrive at an approximate result

$$\frac{\rho_2(r)}{n^2} - 1 = -\frac{p_0^4}{\pi^3 a_0 n^2}\left(1 + \frac{1}{3\pi p_0 a_0}\right)\frac{e^{-\mu r}}{r} \ , \qquad (5.9)$$

which improves the Thomas-Fermi screening. Here

$$\mu = \mu_0(1 + 1/6p_0 a_0) \ . \qquad (5.10)$$

The screening effects in a degenerated electron gas have been discussed by Langer and Vosko and others.[12] It is remarked that their result can be obtained easily by replacing $F(s,y)$ by $F(s,0)$ and expanding the denominator of Eq. (5.7) around $s=2$. The result is an oscillating potential instead of a screening potential, but the oscillation is not very effective at metallic densities. It is effective for low densities and appears only after the correlation function has decayed practically to zero. It is also to be remarked that both the screening and the oscillating potentials are not correct at very short distances. The correlation is finite but decreases quadratically with the distances.

6. CHARGED BOSONS

As one can see in our previous equations such as Eqs. (2.17), (3.15), (3.17), (4.6), and (5.8) the screening effects are caused by the repulsive character of the Coulombic forces. The repulsive character is reflected in the negativeness of the correlation function. Both the hard-sphere potential and Fermi statistics alter the screening property, but under certain conditions we have observed new screening effects. These results are understandable because the hard-sphere potentials and Fermi statistics are both of repulsive character.

When, however, Bose statistics is introduced we expect some basic changes because it amounts to introducing attractive pseudo-forces. Of course, the changes are dependent on the conditions and the systems of our concern. In this section we shall treat a typical example of a system of charged bosons.

The eigenvalues λ_j for degenerate bosons are given by[6]

$$\lambda_j(q) = 2n[q^2 + (2\pi j/\beta q^2)]^{-1} , \qquad (6.1)$$

where n is the density. We assume that the particles interact with each other with Coulomb forces and use Eq. (6.1) in Eq. (2.17). We arrive at

$$\rho_2(r) - n^2 = -[4nA^4/(2\pi)^3 r] \int_{-\infty}^{\infty} dx \int_0^{\infty} dq \times \frac{q^3 \sin qr}{(q^4+x^2)^2 + A^4(q^2+x^2)} , \qquad (6.2)$$

where $x = 2\pi j/\beta$ and

$$A^4 = 8\pi n e^2 . \qquad (6.3)$$

The screening property of this system may be investigated by looking at small q region. We first note

$$\rho_2(r) - n^2 = 2n/(2\pi)^2 r \int_0^{\infty} dq\, q^3 \sin qr \left(\frac{1}{q^2} - \frac{1}{(q^4+A^4)^{1/2}}\right)$$

$$= \frac{n}{(2\pi)^2} \int_0^{\infty} dq \cos qr \left[q^2 - (q^4+A^4)^{1/2}\right] , \qquad (6.4)$$

and make use of the approximation

$$q^2 - (q^4+A^4)^{1/2} \sim -\frac{2A^6}{q^4 + 2A^2 q^2 + 2A^4} .$$

We arrive at

$$\rho_2(r) - n^2 = -2^{-\frac{5}{2}} nA^2 e^{-Dr} \times [B \cos Br + D \sin Br] , \qquad (6.5)$$

where

$$2D^2 = (2^{1/2}+1)A^2, \quad 2B^2 = (2^{1/2}-1)A^2 . \qquad (6.6)$$

On the other hand, if we do not let β be infinite we find

$$\rho_2(r) = n^2 \left(1 + \frac{4e^2}{\rho} \sum_j \frac{F(a_j, r) - F(b_j, r)}{a_j - b_j}\right) , \qquad (6.7)$$

where

$$a_j = b_j + A^4, \quad b_j = (2\pi j/\beta)^2, \quad \tau = 2^{-1/2} a^{1/4} ,$$

$$F(a,r) = -\left(\frac{2a}{\pi}\right) \int_0^{\infty} (q^4+a)^{-1} \frac{\sin qr}{qr} dq \qquad (6.8)$$

$$= [e^{-\tau(a) r} \cos \tau(a) r - 1]/r .$$

7. CONCLUDING REMARKS

We have derived characteristic screening constants for several charged particle systems. It should be remembered that in arriving at our results some simplifications of the respective physical system have been made. For instance, in the case of a classical electron gas we assumed that the system is not very dense. It is certainly important to consider the cases of higher densities, but theoretical complications increase enormously. Also, if such a system is at very high temperatures quantum corrections become necessary due to the small mass of the electrons.

Superpositions of chains are not generally simple in the case of quantum systems. The exponential form such as appeared in Eq. (3.8) is valid only for a classical limit. Thus as we try to introduce higher-order corrections the resulting expressions will not be simple. We shall discuss the p.d.f. of an electron gas explicitly in more detail in a later article.

In the case of a fermion gas we have used the eigenvalues $\lambda_j(q)$ valid for small q. This approximation is acceptable since our interest is in large distance behavior of the p.d.f. Generally, the p.d.f. for a quantum system depends on a reduce distance r/λ, where $\lambda = (4\pi\beta)^{1/2}$ is the thermal de Broglie wavelength. Therefore at short distances quantum effects should be fully taken into consideration.

APPENDIX A

Equation (2.19) can be obtained from Eq. (2.17) by using cylindrical coordinates as follows:

$$q^2 = p^2 + q_z{}^2, \quad r^2 = \rho^2 + z^2;$$

$$I = \int [(q_x{}^2 + q_y{}^2)/(q^2+\kappa^2)]\, e^{i\vec{q}\circ\vec{r}} d\vec{q} = \int_{-\infty}^{\infty} dq_z \int_0^{2\pi} d\theta_1 \int_0^{\infty} dp\, [p^3/(p^2+q_z{}^2+\kappa^2)] \exp[ip\rho\cos(\theta_1-\theta)+iq_z z]$$

$$= \pi \int_{-\infty}^{\infty} dp \int_0^{2\pi} d\theta_1 p^3 \exp[-(p^2+\kappa^2)^{1/2}|z|](p^2+\kappa^2)^{-1/2}\exp[ip\rho\cos(\theta_1-\theta)]$$

$$= 2\pi^2 \{ \int_0^{\infty} dp\, p(p^2+\kappa^2)^{1/2}\exp[-(p^2+\kappa^2)^{1/2}]|z|J_0(p\rho) - \kappa^2 \int_0^{\infty} dp(p^2+\kappa^2)^{-1/2}\exp[-(p^2+\kappa^2)^{1/2}|z|]pJ_0(p\rho)\} .$$

The right-hand side integrals may be evaluated by using the formulas:

$$\int_0^{\infty} \frac{\exp[-|z|(p^2+\kappa^2)^{1/2}]}{(p^2+\kappa^2)^{1/2}} pJ_0(p\rho)dp = \frac{\exp[-\kappa(z^2+\rho^2)^{1/2}]}{(z^2+\rho^2)^{1/2}} ,$$

$$\int_0^{\infty} (p^2+\kappa^2)\exp[-|z|(p^2+\kappa^2)^{1/2}]\, pJ_0(p\rho)dp = \frac{\partial^2}{\partial |z|^2}\left(\frac{\exp[-\kappa(z^2+\rho^2)^{1/2}]}{(z^2+\rho^2)^{1/2}}\right)$$

$$= -\left(\frac{\exp[-\kappa(z^2+\rho^2)^{1/2}]}{(z^2+\rho^2)^{3/2}} + \frac{\kappa\exp[-\kappa(z^2+\rho^2)^{1/2}]}{(z^2+\rho^2)}\right) + z^2\left(\frac{3\exp[-\kappa(z^2+\rho^2)^{1/2}]}{(z^2+\rho^2)^{5/2}}\right.$$

$$\left. + \frac{\kappa\exp[-\kappa(z^2+\rho^2)^{1/2}]}{(z^2+\rho^2)^2} + \frac{2\kappa\exp[-\kappa(z^2+\rho^2)^{1/2}]}{(z^2+\rho^2)^2} + \frac{\kappa^2\exp[-\kappa(z^2+\rho^2)^{1/2}]}{(z^2+\rho^2)^{3/2}}\right) .$$

One can then obtain the desired result by using $z^2+\rho^2=r^2$.

APPENDIX B

The fermion eigenvalues given by Eq. (5.6) can be derived as follows:

$$\lambda_j(q) = \frac{1}{(2\pi)^3}\int d\vec{p} f(p)[1-f(\vec{p}+\vec{q})] \int_0^{\beta} e^{\alpha[p^2-(\vec{p}+\vec{q})^2]} e^{2\pi ij\alpha/\beta} d\alpha = \frac{1}{(2\pi)^3}\int [f(\vec{p}+\vec{q})-f(p)] \frac{d\vec{p}}{p^2-(\vec{p}+\vec{q})^2+2\pi ij/\beta}$$

$$\mathrm{Re}\lambda_j(q) = \frac{1}{(2\pi)^3}\int \frac{2(q^2+2\vec{p}\cdot\vec{q})f(p)}{(q^2+2\vec{p}\cdot\vec{q})^2+(2\pi j/\beta)^2} d\vec{p} = \frac{1}{2(2\pi)^2 q}\int_{-\infty}^{\infty} p\,dp\, f(p)\ln[(q^2+2pq)^2+(2\pi j/\beta)^2]$$

$$= \frac{1}{2(2\pi)^2 q}\,\frac{1}{(2q)^2}\int_{-2p_0q}^{2p_0q} x\,dx\,\ln[(x+q^2)^2+(2\pi j/\beta)^2] = \frac{1}{(2\pi)^2(2q)^3}\int_{-2p_0q+q^2}^{2p_0q+q2} (y-q^2)dy\,\ln[y^2+(2\pi j/\beta)^2]$$

$$= \frac{1}{(2\pi)^2(2q)^3}\left(-\tfrac{1}{2}[q^4-4p_0{}^2q^2-(2\pi j/\beta)^2]\ln\{[(q^2+2p_0q)^2+(2\pi j/\beta)^2]/[(q^2-2p_0q)^2+(2\pi j/\beta)^2]\}\right.$$

$$\left. -2q^2|2\pi j/\beta|\{\tan^{-1}[|\beta/2\pi j|(q^2+2p_0q)]-\tan^{-1}[|\beta/2\pi j|(q^2-2p_0q)]+4p_0q^3\}\right) .$$

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Phase Transition in the Pair-Hamiltonian Model for Liquid Helium*

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The thermodynamic properties of two models for degenerate Bose liquids have been investigated. The models are found to give a first-order phase transition. This aspect of the models is related to the collapse of the long-wavelength excitation spectrum as the condensate density vanishes.

I. INTRODUCTION

A number of models for the superfluid state of a Bose fluid have been proposed which are a version of the Bogoliubov model[1] generalized to include: (1) the Hartree-Fock part of the Hamiltonian, (2) Cooper pairing of particles in the nonzero momentum states, (3) the effect of temperature. In these models a phase transition takes place between a low-temperature state characterized by the presence of Bose-Einstein condensation and a normal state which is the ideal gas or the Hartree-Fock state, depending on the model. This transition has been compared[2] to the λ transition of liquid He^4, in spite of the fact that the reliability of these models decreases as the temperature increases and approaches the transition temperature. Such a comparison is tempting, however, because these models are among the few that are exactly soluble. Few numerical calculations have been attempted and thus some features of these models have been overlooked. In this paper we report numerical studies that have been made of the pair Hamiltonian of Luban[3] and of the closely related model of Shohno,[4] with particular emphasis on the phase transition.

It has been shown previously[5,6] that the condensate density for these models is multiple valued as a function of temperature; we have computed the relevant thermodynamic functions and find that the phase transition is of first order. This phenomenon is probably a general character of models of this sort; it can be traced directly to the behavior of the long-wavelength part of the single-particle excitation spectrum as the condensate vanishes.

II. THE MODELS

We have considered two models: The pair