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Equilibrium properties of a two-dimensional Coulomb gas

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The canonical partition function of the two-dimensional Coulomb gas interacting through the Coulomb potential $-q_i q_j \ln r_{ij}$ is considered in detail. The equation of state $PV/2N = k_B T - q^2/4$ is shown to be meaningful above the critical temperature $T_c = q^2/2k_B$ through the use of upper and lower bounds (valid for all $T > T_c$) for the canonical partition function Q^* with $\lim Q^* \sim N!\,(Q_1^*)^N$ as $T \to T_c^+$, Q_1^* denoting the restriction of Q^* to a pair $(+\,-)$. Below T_c, the equilibrium properties are investigated with the use of the binary approximation proposed by Hauge and Hemmer for charged disks. The resolution of the two-body Schrödinger equation allows us to consider point particles and place on a firm basis preliminary conclusions about the divergent behavior of the thermodynamic functions. The pair-correlation function $g_2(r)$ is investigated above T_c for the one-component model within the framework of the Debye approximation, through a potential of average force $w_2(r)$, up to the third order in the plasma parameter $q^2/k_B T$. The short-range behavior of $w_2(r)$ appears as a renormalizable quantity, while the long-range behavior confirms and extends three-dimensional findings. The $T \to \infty$ limit of the corresponding thermodynamic functions coincides with exact results derived by Mehta for the same model restricted to the unit circumference. Finally, the Debye free energy is shown to fulfill a sufficient condition required by the existence of the thermodynamic limit.

I. INTRODUCTION

Recently a great deal of attention has been devoted[1-7] to the study of the statistical properties of the two-component and two-dimensional system of point charges interacting through the Coulomb potential $\phi(r_{ij}) = -q_i q_j \ln(r_{ij}/L)$ with $q = |q_i| = |q_j|$ and $L = 1$ fixing the zero point of the potential. The motivations for this interest are numerous. The most evident one is to seek analogies or differences with the well-known three-dimensional situation. This approach appears particularly fruitful for the Coulomb potential obtained as a solution of the Poisson equation

$$\Delta\phi = -(n-2)S_n\delta, \quad n \geq 3$$
$$= -S_n\delta, \quad n \leq 2 \tag{1.1}$$

with $S_n = 2\pi^{n/2}/\Gamma(\frac{1}{2}n)$, thus making evident that in this problem the equilibrium properties are strongly dimensional dependent, while the generality of the results is guaranteed by the Fourier transform expression $-S_n p^{-2}$ valid for all n. More specific motivations to consider this problem in plasma physics are due to its close analogy with the strongly magnetized real plasma, for which it could provide a good model. For instance, this model has allowed Taylor and McNamara to put on a firm basis the linear Bohm conjecture ($D \sim B^{-1}$) for the diffusion coefficient.[7]

In contradistinction to the one-dimensional Coulomb problem solved by Lenard and Prager,[8] it allows for a transparent and relatively simple study of the pair condensation process in the canonical ensemble, so that we may hope to gain some insights into the behavior of a real-dense-classical plasma with a moderate temperature. As is well known, it does not appear possible to evaluate the classical partition function for a two-component three-dimensional Coulomb gas

$$Q = \int \cdots \int \exp\left(\frac{q^2}{k_B T} \sum_{1 \leq i < j \leq 2N} |r_{ij}|^{-1}\right) \cdots d\vec{r}_i\, d\vec{r}_j \cdots \tag{1.2}$$

which diverges catastrophically when $r_{ij} \to 0$. In two dimensions, the situation appears more fortunate with

$$Q = \int_V \cdots \int_V \exp\left(\beta \sum_{i \leq i < j \leq 2N} q_i q_j \ln|r_{ij}|\right) \prod_{i=1}^{2N} d^2\vec{r}_i\,,$$
$$\beta = (k_B T)^{-1} \tag{1.3}$$

where the volume dependence may be separated out with the aid of the scaling procedure[1-3]

$$|\vec{s}_i| = |\vec{r}_i| V^{-1/2} \tag{1.4}$$

and we get

$$Q = V^{2N + \Sigma_{i<j}\beta q_i q_j/2} Q^* \text{ (independent of } V) \tag{1.5}$$

where

$$Q^* = \int \cdots \int \prod_{i \leq i < j \leq 2N} |\hat{s}_i - \hat{s}_j|^{\beta q_i q_j} d^2\hat{s}_1 \cdots d^2\hat{s}_N \tag{1.6}$$

with $\hat{s}_i = s_i e^{i\theta_i}$, $0 \leq \theta_i \leq 2\pi$ and $0 \leq s_i \leq 1$ in the unit circle.

The canonical pressure[1-5]

$$P = k_B T \frac{\partial \ln Q}{\partial V} = k_B T (1 - \tfrac{1}{4}\beta q^2) \frac{2N}{V} \tag{1.7}$$

yields immediately the equation of state. Equation (1.7) is meaningful only if the conditions

$$\int_0^\infty dr_{ij}\, r_{ij}^{1-\beta q^2} < +\infty, \quad k_B T > \tfrac{1}{2} q^2 \tag{1.8}$$

are fulfilled. Our investigations started with a conjecture[5] which will be demonstrated later[6] about the sufficiency of this inequality. Then, we were able to conclude that the many-body interactions are dominated by the two-body ones in the vicinity of the transition temperature at least. The investigation of the equation of state below the transition temperature requires technical tools different from those used for the study of the canonical equilibrium at $T \geq T_c = q^2/2k_B$. However, as demonstrated below, it appears possible to set on a firm ground the Hauge and Hemmer conjecture[4]

$$PV = N k_B T, \quad k_B T < \tfrac{1}{2} q^2 \tag{1.9}$$

for a perfect gas of noninteracting pairs of the opposite charges. Equation (1.7) stands unchanged[4] for the one-component system in the presence of a neutralizing background, and it may be extended in a straightforward way[4] to the form

$$PV = (N_+ + N_-) k_B T \left[1 - \frac{\beta q^2}{4} \left(1 - \frac{(N_+ - N_-)^2}{N_+ N_-} \right) \right] \tag{1.10}$$

for a system without charge neutrality ($N_+ \neq N_-$). Although it is possible to derive some interesting properties from accurate bounds and estimates for the interacting part of the canonical partition function Q^*, we did not find it possible to estimate the corresponding pair-correlation functions. This explains why we devote considerable attention to the high-temperature Debye approximation for the one-component pair-correlation function in the presence of a neutralizing background. This quantity is of a great interest for further studies in real magnetized plasmas, and it also allows deeper understanding and appreciation of the various approaches used for the corresponding three-dimensional problem. As a by-product, general trends about the expansion of the potential of average force with respect to the plasma parameter may be obtained. The present paper is organized as follows: in Sec. II we transform the integrand of Q^* into a more compact expression yielding upper and lower bounds for all $T > T_c$. Thus, we establish the sufficiency of the condition (1.8). These bounds are further extended to the canonical thermodynamic functions. We obtain in Sec. III an explicit equivalent of Q^* for $T \to T_c^+$ exhibiting in a transparent form the preeminence of binary interactions in the vicinity of the critical temperature. The low-temperature properties are investigated in Sec. IV with the approximation of N noninteracting quantum pairs of opposite charges. The eigenvalues of the corresponding two-body Schrödinger equation are used to establish that the corresponding partition function and its derivatives remain meaningful when $k_B T < \frac{1}{2} q^2$. C_V is shown to diverge quadratically at T_c, thus confirming an earlier conjecture due to Hauge and Hemmer[4] for charged classical disks. We start in Sec. V a thorough analysis of the high-temperature Debye approximation for the pair-correlation function $g_2(r) = e^{+w_2(r)}$ of the one-component system in terms of a potential of mean force up to the third order in the plasma parameter $q^2/k_B T$. As a by-product of this study, the short-range behavior $\lim g_2(r)$ as $r \to 0$ appears as an easy renormalizable quantity, in contradistinction to the three-dimensional analog. The third-order graphs contributing to $w_2(r)$ are detailed in Sec. VI, while the Debye thermodynamic functions are given in Sec. VIII through a first-order estimate in the plasma parameter for $g_2(r)$. The high-temperature limits of these functions allow one to make contact with previous results obtained by Mehta[9] for the one-component model restricted to the unit circumference. The Debye free energy is seen to exhibit a functional form compatible with a finite expression in the thermodynamic limit ($N \to \infty$, $V \to \infty$, $N/V < +\infty$).

II. CANONICAL PARTITION FUNCTION

A. Compact expression

Although it does not appear possible to us to obtain an explicit expression for Q^*, we are looking for information derived from it through uniform upper and lower bounds valid for all $T > T_c$. This is a standard procedure if one recalls that only a very few partition functions may be evaluated exactly. To reach this goal it appears useful to rewrite the integrand of Eq. (1.6) in a more compact form, thus making contact with a technique already used by Dyson, Gaudin, and Mehta[10] and others for the one-component version of the present model restricted to the unit circumference where the particles interact through $\phi(\theta_{ij}) = -q^2 \ln|e^{i\theta_i} - e^{i\theta_j}|$ and simulate the behavior of the highly excited nuclear levels whose spacing proves to be independent of the nucleon-nucleon potential. The authors considered above obtained an exact expression for Q^* by writing

$$\exp\left(\beta\sum_{i<j}\ln|e^{i\theta_i}-e^{i\theta_j}|\right)$$

as a Van der Monde determinant. Therefore we consider Eq. (1.6) under the form

$$Q^*=\int_0^1\cdots\int_0^1 dr_1\cdots dr_{2N}\int_0^{2\pi}d\theta_1\cdots d\theta_{2N}\left(\prod_{i=1}^{2N}r_i\right)\times\frac{\prod_{1\le i<j\le N}|z_i-z_j|^{\beta q^2}|\xi_i-\xi_j|^{\beta q^2}}{\prod_{i,j=1}^{N}|z_i-\xi_j|^{\beta q^2}}, \quad (2.1)$$

$$z_i\equiv\hat{r}_i=r_ie^{i\theta_i},\quad 1<i<N$$

$$\xi_i\equiv\hat{r}_i=r_ie^{i\theta_i},\quad N+1<i<2N,$$

and make use of the relation

$$\Delta=\frac{\prod_{1\le i<j\le N}(z_i-z_j)(\xi_i-\xi_j)}{\prod_{i,j=1}^{N}(z_i-\xi_j)}=(-1)^{N(N-1)}\operatorname*{Det}_{i,j=1,N}\left(\frac{1}{z_i-\xi_j}\right), \quad (2.2)$$

a variant of Cauchy lemma.[10] It may be checked in a straightforward way with the aid of a recurrence by substracting line 1 from lines $2\cdots n$ in the determinant on the right-hand side, and substracting column 1 from columns $2\cdots n$ in the resulting determinant. Equation (2.2) introduced in Eq. (2.1) yields the required compact expression

$$Q^*=\int_0^1\cdots\int_0^1 dr_1\cdots dr_{2N}\int_0^{2\pi}\cdots\int_0^{2\pi}d\theta_1\cdots d\theta_{2N}\times\left(\prod_{i=1}^{2N}r_i\right)\left|\operatorname{Det}\left(\frac{1}{z_i-\xi_j}\right)\right|^{\beta q^2}. \quad (2.3)$$

B. Upper and lower bounds

An accurate upper bound may be given to Eq. (2.3) through the inequalities (the first one is Minkowski)

$$\left\{\int(f+g+\cdots+l)^k dx\right\}^{1/k}<\left(\int f^k dx\right)^{1/k}+\cdots+\left(\int l^k\right)^{1/k},\quad k>1 \quad (2.4a)$$

$$\int(f+g+\cdots+l)^k dx<\int f^k dx+\cdots+\int l^k dx,\quad 0<k<1 \quad (2.4b)$$

applied to

$$\operatorname*{Det}_{i,j}\left(\frac{1}{z_i-\xi_j}\right)=\sum_{P=1}^{N!}\frac{\delta_P}{\prod_{i=1}^{N}(z_i-\xi_{P_i})}\cdots \quad (2.5)$$

with P: $(1,2,\ldots,N)\to(P_1,P_2,\ldots,P_N)$ and δ_P, signature of the permutation P, which gives

$$Q^*\le(N!)^{\max(\beta q^2,1)}\sum_{P=1}^{N!}\int_0^1 dr_1\cdots\int_0^1 dr_{2N}\times\int_0^{2\pi}d\theta_1\cdots\int_0^{2\pi}d\theta_{2N}\prod_{i=1}^{N}\frac{r_i r_{N+P_i}}{|z_i-\xi_{\alpha_i}|^{\beta q^2}}. \quad (2.6)$$

The permutation of $\sum_P$ with $\int_0^1\cdots\int_0^1$ allows us to factor each multiple integral as a product of N two-body quadratures for a pair $(+-)$, and Eq. (2.6) becomes

$$Q^*\le(N!)^{\max(\beta q^2,1)}(Q_1^*)^N, \quad (2.7)$$

where[3] $(4\gamma=\beta q^2)$

$$Q_1^*=\int_0^1 dr_1\int_0^1 dr_2\int_0^{2\pi}d\theta_1\int_0^{2\pi}d\theta_2\frac{r_1r_2}{|z_1-z_2|^{4\gamma}}=\frac{\pi^2\Gamma(2-4\gamma)}{(1-\gamma)(1-2\gamma)\Gamma(1-2\gamma)\Gamma(2-2\gamma)}. \quad (2.8)$$

Equations (2.7) and (2.8) prove that Q^* has no divergence at T_c arising from the collapse of N-clusters with $N>2$, in accord with a previous conjecture.[5] Therefore, the equation of state (1.7) may be given a meaning for $k_BT>\frac{1}{2}q^2$. In order to get some ideas about the derivatives of Q^* with respect to T^{-1}, which define the canonical thermodynamic functions, it appears useful to pay some attention to a uniform Q^* lower bound. The integrand in Eq. (2.3) is positive, so that

$$Q^*>\int_{D\times\delta}dz\,d\xi\,(\Delta\bar{\Delta})^{2\gamma},$$

$$z_i=r_ie^{i\theta_j},\quad \xi_j=r_je^{i\theta_j}, \quad (2.9)$$

where δ and Δ denote the integration domains pictured in Fig. 1 with one pair $(+-)$ in D and $(N-1)$ pairs in δ, the positive particles being located at ξ_i and the negative ones at z_i, so that the pair

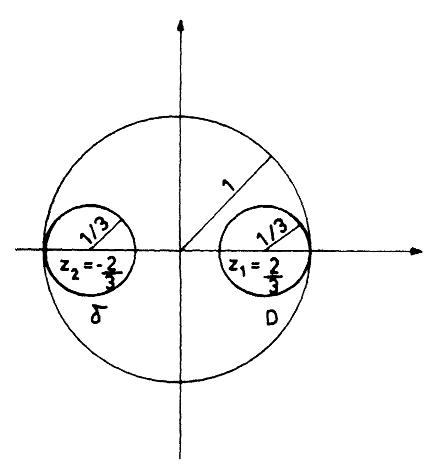

FIG. 1. Integration domain used for the Q^* lower bound.

(z_1, ξ_1) is located in the circle D of radius $\frac{1}{3}$ centered at $z_1 = \frac{2}{3}$ while the remaining $N-1$ pairs are located in the circle δ of radius $\frac{1}{3}$ centered at $z_2 = -\frac{2}{3}$. The integrand of Eq. (2.9) is then split into three parts corresponding to interactions in D, δ and between D and δ, respectively. The inequalities

$$\tfrac{2}{3} < |z_1 - z_i|, \quad |z_1 - \xi_i| < 2,$$
$$\tfrac{2}{3} < |\xi_1 - \xi_i|, \quad |\xi_1 - z_i| < 2$$
$$\text{all } i = 2, \ldots, N$$

are introduced in the last contribution. Therefore the right-hand side of Eq. (2.9) may be given the lower bound $(4\gamma = \beta q^2)$

$$\int_D \frac{dz_1\, d\xi_1}{|z_1 - \xi_1|^{\beta q^2}} \int_\delta \prod_{i=2}^N dz_i\, d\xi_i \times \frac{\prod_{2\le i<j}^N |z_i - z_j|^{\beta q^2} |\xi_i - \xi_j|^{\beta q^2}}{\prod_{i,j=2}^N |z_i - \xi_j|^{\beta q^2}} \left(\frac{1}{3}\right)^{2\beta q^2 (N-1)} \tag{2.10}$$

with the recurrence formula

$$(\tfrac{1}{3})^{4N(1+\gamma)-8\gamma} Q_1^* Q_{N-1}^* < Q^* \tag{2.11}$$

whence the final result $(4\gamma = \beta q^2)$

$$(\tfrac{1}{3})^{2N(N-1)(1+\gamma)-(2N-1)^{4\gamma-4}} (Q_1^*)^N < Q^* < (N!)^{\max(\beta q^2, 1)} (Q_1^*)^N \tag{2.12}$$

with upper and lower bounds remaining finite for N finite. Equation (2.12) renders apparent the importance of the two-body clustering in the vicinity of T_c. This point will be given further attention in Sec. III.

C. Speculations about the thermodynamic limit (two-components gas)

The foregoing Q^* upper bound allows us to question in a natural way the existence of the thermodynamic limit for the two-component gas, i.e., the existence of finite thermodynamic functions per particle in the limit $N \to \infty$, $V \to \infty$ with N/V bounded.

The existence of the thermodynamic limit for a three-dimensional many-component system has been firmly established only very recently through the powerful efforts of Dyson, Lenard, Lieb and Lebowitz.[11] However, the basic features of the corresponding demonstration (i.e., the existence of a regular packing allowing for a long-range screening of the Coulomb potential) are expected to be valid irrespective of the dimension, once that the stability problem (existence of the linear lower bound $\langle \varphi | H_N | \varphi \rangle > -AN$ for the average value of the total N-body Hamiltonian) has been solved. More precisely, the basic question is how much have we to pay in order to get this stability. In one dimension,[8] the classical Coulomb system is stable thanks to the vanishing at the origin of the potential, while in three dimensions the full quantum requirements—Schrödinger N-body and Fermi statistics—at least in one species have to be met. It is our opinion that more powerful weapons than the present ones have to be used to settle the same question in two dimensions. However, the upper bound obtained previously for Q^* may be helpful in a preliminary investigation toward this goal. So, let us consider the two-component partition function $(N = N_+ = N_-)$

$$Q = \left(\frac{V}{N!\Lambda}\right)^N \left(\frac{V^{1/2}}{L}\right)^{\beta q^2 N} Q^* \tag{2.13}$$

with Q^* given by (1.6), the potential energy $-q_i q_j \ln|r_{ij}/L|$ and the De Broglie wavelength $\Lambda = h/(2\pi m k_B T)^{1/2}$. The corresponding free energy $F = -k_B T \ln Q$ is then

$$\beta F = 2N(\ln\rho\Lambda^2 - 1) + \tfrac{1}{2}\beta q^2 N \ln(V/L^2) - \ln Q^*, \quad \rho = 2N/V, \tag{2.14}$$

so that it appears tempting to introduce the estimate[12]

$$\ln Q^* \to \tfrac{1}{2}\beta q^2 \ln 2N \quad (N \to \infty, V \to \infty, N/V \text{ bounded}) \tag{2.15}$$

in Eq. (2.14) to get a finite expression. Actually, Eq. (2.15) provides only a sufficiency condition (perhaps too strong when compared to the true but still unknown answer) for the existence of the thermodynamic limit.[13] More precisely, the corresponding Q could be approximated by

$$Q^* \simeq (2N!)^{\beta q^2/4} Q_1^{*N} \simeq \left(\frac{2N}{e}\right)^{\beta q^2 N/2} Q_1^{*N}, \tag{2.16}$$

while our upper bound

$$Q^* < (N/e)^{\max(1, \beta q^2) N} Q_1^{*N} \tag{2.17}$$

appears too large. Nevertheless, no decisive conclusion can be drawn from this discrepancy. The estimate (2.15) shows simply that the free energy F may be given the lower bound $-\infty$, as expected.

D. Thermodynamic functions

It is well-known that the thermodynamic functions may be obtained as derivatives of Q^* with respect to T^{-1} in the form

$$E = k_B T^2 \left(\frac{\partial \ln Q^*}{\partial T}\right)_{V,N} = -\frac{k_B}{Q^*}\left(\frac{\partial Q^*}{\partial (T^{-1})}\right)_V,$$

$$C_V = \left(\frac{\partial E}{\partial T}\right)_{V,N} = -T^{-2}\left(\frac{\partial E}{\partial (T^{-1})}\right)_V . \qquad (2.18)$$

Therefore it appears worthwhile to extend the foregoing bounds to $dQ^*/d\gamma$ and $d^2Q^*/d\gamma^2$. This is performed in a straightforward way with

$$Q^* = \int |\Delta|^{4\gamma}\, dz_1 \cdots d\xi_N$$

and

$$\left|\frac{dQ^*}{d\gamma}\right| \leq 4\int (\ln|\Delta|)\, |\Delta|^{4\gamma}\, dz_1 \cdots d\xi_N \leq \left(\int (\ln|\Delta|)^k\right)^{k^{-1}} \left(\int |\Delta|^{4\gamma k'}\right)^{(k')^{-1}} \qquad (2.19)$$

where $k^{-1} + (k')^{-1} = 1$. The relation $\int \ln^k x\, dx < +\infty$, for all k, enables us to choose $k' \neq 1$, so that $|dQ^*/d\gamma|$ keeps a clear meaning for $k_B T > \frac{1}{2}q^2$. The same argument may be immediately applied to $d^2Q^*/d\gamma^2$. As a consequence, E and C_V make sense for N finite and $k_B T > \frac{1}{2}q^2$.

III. EQUIVALENT OF $Q_N(T)$ WHEN $T \to T_c^+$

In our upper and lower bounds, the coefficients of $[Q_1(T)]^N$ attain their worst values for $T = T_c$, as can easily be checked. For example, if the temperature is infinite, we have approximately

$$(\tfrac{1}{3})^{2N^2} < [Q_1(T)]^{-N} Q_N(T) < N!,$$

whilst for $T = T_c$

$$(\tfrac{1}{3})^{3N^2} < [Q_1(T)]^{-N} Q_N(T) < (N!)^2.$$

We want then to strengthen these bounds in the vicinity of T_c. More precisely, we want to show

$$\lim_{T \to T_c^+} \{[Q_1(T)]^{-N} Q_N(T)\} = N! .$$

We shall just outline the method, which will be developed in a subsequent paper.

A. Replacement of the system by N weakly interacting pairs

The first step is to rewrite $Q_N(T)$ in the form

$$Q_N(T) = N! \int e^{-\gamma w(z_1, \ldots, \xi_N)} \prod_{i=1}^{N} \frac{dz_i\, d\xi_i}{|z_i - \xi_i|^{\beta q^2}} , \qquad (3.1)$$

where $w(z_1, \ldots, \xi_N)$ is a bounded function.

We can interpret this as the partition function of an associated system composed of N pairs $\Xi_i = (z_i, \xi_i)$, each having the internal Coulomb energy $q^2 \ln|z_i - \xi_i|$, and which interact together by means of the weak nonlocal N-body potential $w(\Xi_1, \ldots, \Xi_n)$, by contrast with the strong local $2N$-body potential we had initially.

To show this, let us first note the inequality

$$\left|\det\left(\frac{1}{z_i - \xi_j}\right)\right|^{\beta q^2} \leq (N!)^{\chi} \sum_P \frac{1}{\prod_{i=1}^N |z_i - \xi_{P_i}|^{4\gamma}} \ \forall (z_1, \ldots, \xi_N), \qquad (3.2)$$

where $\chi = \max(0, \beta q^2 - 1)$ which can be proven by means of the complete Hölders inequality (that is, by using both cases: $0 < k < 1$ and $1 \leq k$). If we denote, respectively, the left and the right-hand sides of (3.2) by $|\Delta_N|^{\beta q^2}$ and $(N!)^{\chi} M_\gamma$, we have $(4\gamma = \beta q^2)$

$$Q_N(T) = \int |\Delta_N|^{\beta q^2} dz\, d\xi = \int \frac{|\Delta_N|^{\beta q^2}}{M_\gamma} (M_\gamma\, dz\, d\xi) = \sum_P \frac{|\Delta_N|^{\beta q^2}}{M_\gamma} \prod_{i=1}^N \frac{dz_i\, d\xi_i}{|z_i - \xi_{P_i}|^{\beta q^2}} = N! \int \frac{|\Delta_N|^{\beta q^2}}{M_\gamma} \prod_{i=1}^N \frac{dz_i\, d\xi_i}{|z_i - \xi_i|^{\beta q^2}} .$$

The last equality is obtained by noticing that the ratio $e^{-\gamma w} = |\Delta_N|^{\beta q^2}/M_\gamma$ is invariant under a permutation of $\xi_1, \ldots, \xi_N$; (3.2) and thus (3.1) is proven.

We finally remark that our new system

$$Q_N(T) = N! \int e^{-\gamma w} \prod_{i=1}^N \frac{dz_i\, d\xi_i}{|z_i - \xi_i|^{\beta q^2}} , \qquad (3.3a)$$

$$e^{-\gamma w} \leq (N!)^{\chi} \leq N! \qquad (3.3b)$$

contains the information of the existence of the upper bound (2.14) because it gives it back trivially.

B. New system of coordinates for pair

The second step consists in using a new system of coordinates where $\rho_i = |z_i - \xi_i|$, that is where we have, say, concentrated the divergence of each term $1/|z_i - \xi_i|^{\beta q^2}$ onto only one real variable.

This we can perform by taking, for each positive particle z_i, polar coordinates centered at the origin, and for each negative particle ξ_i, polar coordinates centered at its associated ion z_i.

Equation (3.3) is then transformed into

$$Q_N(T) = N! \int_{D_0} e^{-\gamma w} \prod_{i=1}^N \rho_i^{1-\beta q^2}, \qquad (3.4a)$$

the integration over each pair being

$$\int_0^{2\pi} d\theta_i \int_0^1 R_i\, dR_i \int_0^{2\pi} d\varphi_i \int_0^{l_i(R_i, \varphi_i)} d\rho_i , \qquad (3.4b)$$

where we have set (see Fig. 2)

$$R_i = |z_i|, \quad \rho_i = |z_i - \xi_i|,$$
$$l_i(R_i, \varphi_i) = |Z_i - z_i| = R_i \cos\varphi_i + (1 + R_i^2 \sin^2\varphi_i)^{1/2} \qquad (3.4c)$$

and where D_0 stands for the whole domain of variation of all the variables.

In this system of coordinates, we have also

$$Q_1(T) = \int \rho^{1-\beta q^2}$$

and thus

$$[Q_1(T)]^N = \int_{D_0} \prod_{i=1}^{N} \rho_i^{1-\beta q^2}. \tag{3.5}$$

C. Extraction of a large subdomain with negligible interactions

1. *Loose statement of the method*

We have seen that, if we neglect w, the potential of interaction between pairs, the $Q_N(T)$ becomes simply $N![Q_1(T)]^N$.

We are then led to the problem: can we actually approximate w by 0 everywhere in D_0? The answer is trivially no, because w becomes infinite when two particles of the same sign come close together.

Nevertheless, though the problem is hopeless in whole D_0, we'll show that, provided the temperature is sufficiently close to T_c, we can extract a subdomain where the potential of interaction can be neglected, and such that its complementary part contributes negligibly to $Q_N(T)$ and $[Q_1(T)]^N$. This implies that, even in this complementary part, the interacting system can be approximated by the noninteracting one, because this approximation consists only in interchanging two negligible quantities.

2. *Preliminary definitions*

In order to give a more precise meaning to our statement, we have to explain what we mean by a negligible quantity, and what is the chosen subdomain.

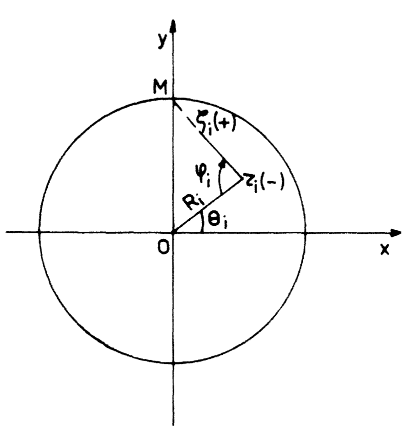

FIG. 2. Coordinate system used in the evaluation of Eq. (3.1).

To define the first point, let us introduce an arbitrarily small constant ϵ: we shall say that the contribution of a subdomain is negligible if its contribution to $[Q_1(T)]^N$ is less than ϵ times the lower bound. It is then obvious, that its contribution to $Q_N(T)$ will be negligible too, with the constant ϵ': $(N!)^2$ because of (3.3).

To define the second point, let us introduce another arbitrarily small quantity η and let us say that the pair (z_i, ξ_i) forms an atom if $|z_i - \xi_i| \leq \eta$. Our subdomain will then be defined in the following way: (i) We have exactly N atoms formed: $|z_i - \xi_i| \leq \eta$ for any i. (ii) No positive particle is too close to the boundary: $|z_i| \leq 1 - \eta$ for any i. (iii) All the atoms are far from each other: $|z_i - \xi_j| < \eta^{1/2}$ $\forall i, j \neq i$.

3. *Why do we choose such a subdomain?*

So far, we have introduced the main steps of our method, and shown how the subdomain is chosen. Let us now explain why we choose it so.

Conditions (i) originates in the equivalence

$$\int_0^\eta \rho^{1-\beta q^2} d\rho \sim \int_0^1 \rho^{1-\beta q^2} d\rho,$$

which is valid even if η is very small, provided T is sufficiently close to T_c (that is, $1 - \beta q^2 \sim -1$). Thus, because the integral, in the vicinity of T_c, is insensitive to a change in the upper limit of integration, we should like to replace $\int_0^{l(R,\varphi)}$ by $\int_0^\eta$ in order to simplify (3.4).

But we see immediately that this last equivalence is valid only if $l(R, \varphi) \neq 0$. This drawback leads us then to impose condition (ii) which is just the condition $l(R, \varphi) \neq 0$ disguised in the simpler and more flexible form $R \leq 1 - \eta$ [and stronger too, because $R \leq 1 - \eta \Rightarrow \eta < l(R, \varphi) \Rightarrow l(R, \varphi) \neq 0$].

Finally, we impose condition (iii) in order to have $e^{-\gamma w} \sim 1$ in the whole subdomain. To see this, let us rewrite the two quantities $|\Delta_N|^{\beta q^2}$ and M_γ, whose quotient defines $e^{-\gamma w}$, under the following forms:

$$|\Delta_N|^{\beta q^2} \left(\prod_{i=1}^{N} |z_i - \xi_i|^{\beta q^2} \right) = \left(\prod_{i<j} \frac{|z_i - \xi_j|^{\beta q^2}}{|z_i - \xi_j|^{\beta q^2}} \right) \left(\prod_{i<j} \frac{|\xi_i - \xi_j|^{\beta q^2}}{|\xi_i - z_j|^{\beta q^2}} \right), \tag{3.6}$$

$$M_\gamma \left(\prod_{i=1}^{N} |z_i - \xi_i|^{\beta q^2} \right) = 1 + \sum_{P \neq Id} \prod_{i=1}^{N} \frac{|z_i - \xi_i|^{\beta q^2}}{|z_i - \xi_{P_i}|^{\beta q^2}} .$$

Because of condition (i), all the distances $|z_j - \xi_j|$ are very small, and z_j and ξ_j are almost the same. We should like then to replace z_j by ξ_j in (3.6) so as to get $|z_i - z_j| / |z_i - \xi_j| \sim 1$ and $|\xi_i - \xi_j| / |\xi_i - z_j|$

~1. Moreover, we should like to write the right-hand side of (3.7) as 1 plus a sum of negligible terms because $|z_i - \xi_i|$ is very small.

But this can be realized only if the distances $|z_i - \xi_j|$, $i \neq j$, are very large compared to all the $|z_i - \xi_i|$.

D. The proof made rigorous

It is now a technical job to make rigorous the preceding arguments. We shall just state the five lemmas needed for the complete proof.

First, we define the sequence of decreasing subdomains $D_0 \supset D_i \supset D_{i+1}$, $i = 1, 2, 3$, by means of conditions (ii), (i), and (iii):

$$D_1 = \{(z_1, \ldots, \xi_N) \in D_0 \,|\, |z_i| \leq 1 - \eta, \ \forall i = 1 \ldots, N\},$$

$$D_2 = \{(z_1, \ldots, \xi_N) \in D_1 \,|\, |z_i - \xi_i| < \eta, \ \forall i = 1, \ldots, N\},$$

$$D_3 = \{(z_1, \ldots, \xi_N) \in D_2 \,|\, |z_i - \xi_j| > \eta^{1/2}, \ \forall i, j = 1, \ldots, N, \ i \neq j\}$$

we use the equivalence $\int_0^\eta \sim \int_0^1$ in the following.

Lemma 1: Let $\epsilon \in [0, 1]$ and $L \in [0, 2]$ be given. The condition

$$(1-\epsilon)\int_0^1 \rho^{1-\beta q^2}\, d\rho < \int_0^L \rho^{1-\beta q^2}\, d\rho < (1+\epsilon)\int_0^1 \rho^{1-4\gamma}\, d\rho$$

is realized if the condition $T_c < T \leq T_1(\epsilon, L)$ is realized, with $T_1(\epsilon, L) = \inf(T_1'(\epsilon, L), T_1''(\epsilon, L))$ and

$$T_1'(\epsilon, L) = T_c\left(1 - \frac{\ln(1-\epsilon)}{2\ln L}\right)^{-1}, \quad 0 \leq L \leq 1;$$

$$T_1''(\epsilon, L) = T_c\left(1 - \frac{\ln(1+\epsilon)}{2\ln 2}\right)^{-1}, \quad 1 \leq L \leq 2.$$

We now state the negligibility of the disjoint subdomains $D_i \backslash D_{i+1}$ $i = 0, 1, 2$:

Lemma 2:

$$N!\int_{D_0 \backslash D_1} \prod \rho_i^{1-\beta q^2} \leq \epsilon\left(\tfrac{1}{3}\right)^\alpha [Q_1(T)]^N$$

if $\eta < \eta_1 = \dfrac{\epsilon}{4N(N!)^2\, 3^\alpha}$;

Lemma 3:

$$N!\int_{D_1 \backslash D_2} \prod \rho_i^{1-\beta q^2} \leq \tfrac{5}{4}\epsilon\left(\tfrac{1}{3}\right)^\alpha [Q_1(T)]^N$$

if $\eta < \eta_1$ and $T < T_1(\eta_1, \eta_1)$;

Lemma 4:

$$N!\int_{D_2 \backslash D_3} \prod \rho_i^{1-\beta q^2} \leq \epsilon\left(\tfrac{1}{3}\right)^\alpha [Q_1(T)]^N$$

if $\eta < \eta_2 = \dfrac{\epsilon}{32\pi(N!)^2\, 3^\alpha N(N-1)}$.

The negligibility of w in D_3 gives

$$\left| N!\int_{D_3} e^{-\gamma w} \prod \rho_i^{1-\beta q^2} - N!\int_{D_3} \prod \rho_i^{1-4\gamma} \right| < \epsilon\left(\tfrac{1}{3}\right)^\alpha [Q_1(T)]^N$$

provided $T < 2T_c$ and

$$\eta^{1/2} < \eta_3^{1/2} = \frac{\epsilon}{N!\, 3^\alpha \sup[N(N-1) + (N!)^{1/2}, N(N-1)\, 2^{N(N-1)}]}.$$

By combining the five lemmas with

$$D_0 = D_3 \bigcup_{i=0}^{2} (D_i \backslash D_{i+1}),$$

we obtain the definitive result:

$$|Q_N(T) - N![Q_1(T)]^N| < 5\epsilon\left(\tfrac{1}{3}\right)^\alpha [Q_1(T)]^N$$

provided $\eta < \eta_0$ and $T < T_0$, with $\eta_0 = \inf(\eta_1, \eta_2, \eta_3)$ and $T_0 = T_1(\eta_0, \eta_0)$ which proves the result.

IV. BEHAVIOR UNDER T_c

The above treatment shows clearly the pre-eminence of the two-body interaction in the canonical partition function near T_c. Therefore, although the canonical expression (1.6) for Q^* does not make sense for $T < T_c$, it appears tempting to extend the binary approximation below T_c. This approach has been initiated by Hauge and Hemmer[4] who considered a system of charged hard disks (diameter d) interacting only in pairs of opposite charges with (no more sealing here!)

$$Q \underset{T<T_c}{\simeq} N!\,V^N\left(\int_{r<d} d^2r\, e^{-\beta q^2}\ln r\right)^N = N!\,V^N\left(\frac{2\pi}{(\beta q^2 - 2)\, d^{\beta q^2 - 2}}\right)^N, \quad (4.1)$$

where $N!$ is a counting factor and V^N, the configuration integral over the pair's center of gravity. The corresponding free energy is

$$F = -k_B T \ln d^{\beta q^2 - 2}, \quad d \geq 0 \quad (4.2)$$

and it diverges when $d \to 0$. However, its partial derivatives

$$\frac{P}{k_B T} = \lim_{d\to 0} \frac{\partial \ln Q}{\partial V} = \frac{N}{V}, \quad (4.3)$$

$$\frac{C_V}{2Nk_B} = 1 + \frac{1}{2N}\lim_{d\to 0} \beta^2 \frac{\partial^2}{\partial \beta^2}\ln Q = 1 + \tfrac{1}{2}(1 - T/T_c)^{-2} \quad (4.4)$$

remain meaningful for all d. The equation of state (4.3) intersects the high-temperature expression (1.6) at T_c, so that it could support the picture of a perfect gas of N noninteracting $(+-)$ pairs appearing suddenly at the transition temperature. Although this description looks very appealing, it appears necessary to put it on a firmer ground though a quantum description for the $(+-)$ interaction below T_c. Therefore we shall use the properties of the corresponding Schrödinger equation studied in detail in the following paper[14] to evaluate the required sum-over states.

For the present purpose it appears sufficient to restrict our investigations to semiquantitative information about the spectrum of the given Schrödinger equation. First, general properties of the Sturn-Liouville equation and the monotone increasing behavior of $V(r)$ easily convince us that its spectrum consists only of discrete levels located between $-\infty$ and $+\infty$. Moreover, the number of eigenvalues smaller than an arbitrary λ is given by the asymptotic estimate[15] ($|\lambda| >> 1$)

$$N(\lambda) \sim \frac{1}{2}\int_{V<\lambda}[\lambda - V(r)]\, r\, dr = \tfrac{1}{8}q^2 e^{2\lambda/q^2}, \qquad (4.5)$$

a very fast increasing function of λ, which shows the very interesting property of a lower semiboundedness of the spectrum, i.e.,

$$\int_{-\infty}^{\lambda_a}\frac{dN(\lambda)}{d\lambda}\,d\lambda < 1 \text{ with } \lambda_a < \frac{q^2}{2}\ln\left|\frac{8}{q^2}\right| \qquad (4.6)$$

so that the spectrum is void for $\lambda < \lambda_a$. At this point it must be emphasized that these properties still stand[15] for the solutions of the Schrödinger equation in a compact domain, a point which could also be checked[14] independently through numerical evaluation on a computer.

As a consequence, the restriction of the pair partition function to an infinite volume does not bring in any essential restriction, so we may replace Eq. (1) by

$$Q(V,T) = N!\,V^N \lim_{V\to\infty}[Q_{+-}(V,T)]^N \qquad (4.7)$$

with[16]

$$Q_{+-}(V,T) = \int d^2\vec{r}\sum_\alpha \psi_\alpha(1,2)e^{-\beta H}\psi_\alpha(1,2). \qquad (4.8)$$

$\psi_\alpha(1,2)$ denotes the two-body eigenfunction of $H = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) + V(r_{12})$ written as

$$\psi_\alpha(1,2) = (e^{i\vec{P}\cdot\vec{R}}/\sqrt{V})\,\psi_{m,n} \qquad (4.9)$$

with $\alpha \equiv (\vec{P}, m, n)$, $\vec{P}_2 = \vec{P}_1 + \vec{P}_2$, $\vec{R}_2 = (r_1 + r_2)/2$ and $E_\alpha = \frac{1}{4}P^2 + \lambda_{m,n}$, $\vec{P}$ and $\vec{R}$ are the usual variables attached to the pair center of mass. Equation (4.8) then becomes

$$Q_{+-}(V,T) = \frac{2V}{\Lambda^2}\left(\sum_{n=0}^{n=\infty} e^{-\beta\lambda_{0,n}} + 2\sum_{m=1,n_0=0}^{m=\infty,n=\infty} e^{-\beta\lambda_{m,n}}\right),$$
$$\beta = (k_B T)^{-1} \qquad (4.10)$$

with the eigenvalues labeled by the nodal number n and the magnetic quantum number m. The factor 2 arises from the angular degeneracy in the Schrödinger equation. The large distance between $\lambda_{0,0}$ and the higher $\lambda_{m,n}$ allows us to split Eq. (4.10) as

$$Q_{+-}(V,T) \sim \beta^{-1}\left(\sum_{n=0}^{n_0} e^{-\beta\lambda_{0,n}} + 2\sum_{m=1,n=0}^{m_0,n_0} e^{-\beta\lambda_{m,n}} + 2\int_{\lambda_{m_0,n_0}}^{\infty}\frac{dN(\lambda)}{d\lambda}e^{-\beta\lambda}\,d\lambda\right). \qquad (4.11)$$

Indices m and n run over the sums of Eq. (4.11) till an eigenenergy λ_{m_0,n_0} reaches a value above which the spectrum appears as a quasicontinuum for numerical techniques. Now, it is important to emphasize that expression (4.11) remains finite if

$$\int_{\lambda_{m_0,n_0}}^{\infty} e^{(2/q^2-\beta)\lambda}\,d\lambda < +\infty, \quad k_B T < \tfrac{1}{2}q^2 \qquad (4.12)$$

a condition complementing the one already found for the high-temperature partition function [Eq. (1.8)]

$$\int_0^\infty r^{1-\beta q^2}\,dr < +\infty, \quad k_B T > \tfrac{1}{2}q^2.$$

At low temperature ($\beta >> 1$) it appears possible to put Eq. (4.11) in the simpler form

$$Q_{+-}(V,T) \simeq e^{a\beta+b} + \frac{2}{\beta}\,\frac{e^{(2-\beta)\lambda_{m_0,n_0}}}{\beta-2} \qquad (4.13)$$

with $(m_0, n_0) \simeq (905, 0)$ and

$$\ln\left(\sum_{n=0}^{n_0} e^{-\beta\lambda_{0,n}} + 2\sum_{m=1,n=0}^{m_0,n_0} e^{-\beta\lambda_{m,n}}\right) \underset{\beta>>1}{\sim} a\beta + b, \qquad (4.14)$$

where $q=1$, $2<\beta<12$ with $a = -2.6093$ and $b = -0.5307$. From these results it is possible to deduce in a straightforward way the canonical thermodynamical functions per particle. For instance the free energy

$$F = \tfrac{1}{2}\beta^{-1}\ln Q_{+-} = \frac{1}{2}\left(2.6093 + \frac{0.5307}{\beta} - \frac{0.157\times 10^8 e^{-5.063\beta}}{\beta^2(\beta-2)}\right) \qquad (4.15)$$

and the constant-volume specific heat

$$C_V = \tfrac{1}{2}\beta^2\frac{\partial^2}{\partial\beta^2}\ln Q_{+-} = \frac{0.1575\times 10^8 e^{-5.063\beta}}{\beta(\beta-2)^3} \times [12.817\beta^4 - 41.142\beta^3 - 99.536\beta^2 + 14.252\beta + 4] \qquad (4.16)$$

are defined in the whole range $0 \leq T < T_c$; Eqs. (4.15) and (4.16) are especially accurate ($\beta \gg 1$) near $T=0$, while they diverge at $T_c = q^2/2k_B$ ($\beta = 2$) and thus confirm the preliminary conclusions drawn by Hauge and Hemmer[5] from a hard-disk model.

V. PAIR-CORRELATION FUNCTION IN THE DEBYE APPROXIMATION

As is usual for the case of a Coulomb system, we shall use the well-known Debye-Hückel approximation to derive a high-temperature approximation for the pair-correlation function of a one-component system (negative for instance) in the presence of a neutralizing background with opposite charge. Before going on with the development of the Debye formalism, we feel it useful to emphasize the high-temperature behavior of the canonical partition function [Eq. (1.6)] which has the infinite-temperature limit

$$\lim_{\beta\to 0} Q^* = \lim_{\beta \to 0} \prod_i^N \int_0^1 dr_i\, r_i \int_0^{2\pi} d\theta_i\, (\Delta\bar{\Delta})^{\beta q^2} = \pi^{N_+ + N_-} \tag{5.1}$$

as a result of the uniform bound $|\Delta|^{\beta q^2} < 1 + |\Delta|$ with $0 < \beta q^2 < 1$. The same procedure works for the one-dimensional Coulomb analog but does not in three dimensions.[16a]

A. Graphical expansion and first-order contribution

Now we turn to the standard Debye treatment for the one-component pair-correlation function taken in the usual form[17-19]

$$g_2(r_{12}) = e^{+w_2(r_{12})}, \tag{5.2}$$

where $w_2(r_{12})$ denotes the potential of average force for two particles located at a relative distance r_{12}, such that

$$w_2(r_{12}) = \frac{-u(r_{12})}{k_B T} + \sum_{k=1}^{\infty} \beta_k(r_{12})\rho^k \tag{5.3}$$

in terms of the bare potential $u(r_{12}) = -q^2 \ln r_{12}$, the density $\rho = N_-/V$ and the "simple 12-irreducible" cluster integrals

$$\beta_k(r_{12}) = \frac{1}{k!}\int\cdots\int d^2r_3\cdots d^2r_{k+2} \sum{}^{(k)} f_{ij} \tag{5.4}$$

with $\sum^{(k)}$ denoting the summation over all possible "simple 12-irreducible" cluster diagrams that can be obtained from the root points 1 and 2 and k given field points.

$f_{ij} = e^{-u(r_{ij})/k_BT} - 1$ is the usual Mayer function. Equation (5.4) is defined in the limit $N, V \to \infty$ and for k finite. Let us introduce the high-temperature approximation with the condition

$$(q^2/k_BT)\ln|r_{ij}| \ll 1, \quad r_{ij} \sim \rho^{-1/2}, \tag{5.5}$$

and without any further restriction on the number density ρ. Then we hope to find a small parameter in terms of which the cluster expansion may be constructed with

$$u(r_{ij}) > M \gg 0, \quad r_{ij} < r_M \tag{5.6a}$$

$$u(r_{ij}) \sim \epsilon > 0, \quad r_M < r < \lambda \tag{5.6b}$$

$$u(r_{ij}) \text{ decreases faster than } r^{-2}, \quad r > \lambda \tag{5.6c}$$

and $r_M/\lambda \ll \epsilon < 1$. f_{ij} is then approximately equal to -1 in the region (5.6a), of order ϵ in (5.6b) and negligible in (5.6c) with $\int u(r)\, d^2r \sim \epsilon\lambda^2$.

Now only cases where the range of the potential is long compared to $\rho^{-1/2}$ (i.e., $\rho\lambda^2 > 1$) will be considered. Each cluster integral β_k contains k field points located at $\vec{r}_i$ and l lines. The order of magnitude is given by $\epsilon^l(\rho\lambda^2)^k = \epsilon^{l-k}(\rho\epsilon\lambda^2)^k$. Although ϵ is by definition small, the quantity $\rho\epsilon\lambda^2$ may be large for sufficiently large λ. It is therefore useful to regroup the cluster-expansion terms for $w_2(r_{12})$ according to the value of $l-k$; the summation is over k values for fixed $l-k$. The only dimensionless parameter in the problem being q^2/k_BT, one has to put $\epsilon = \beta q^2$.

In order to meet these requirements we may consider the Coulomb potential in the form $u(r) = K_0(\alpha r)$, with α denoting the usual positive, vanishingly small, quantity and the Fourier transform $u(p) = (p^2+\alpha^2)^{-1}$. So, in the sequel, we should have to evaluate the cluster integrals β_k with this modified $u(r)$, assume that the Tauberian properties are well satisfied, and take the $\alpha \to 0$ limit at the end of the calculation. However, in view of the complexity of the analytical manipulations, we shall restrict ourselves to $\alpha = 0$ from the beginning. The corresponding quadratures remaining finite at infinity. (This short cut is equivalent to taking care of only the diagrams that are convolutions and neglecting bridge diagrams.[20]) Morèover, as explained below, the first- and second-order contributions may be checked through another derivation free of the previous requirements and using the BBGKY hierarchy.

So the first-order ($l-k=1$) contribution to Eq. (5.3) corresponds to the usual Debye chain

$$\delta(r_{12}) = f(r_{12}) + \sum_{n=1}^{\infty} \rho^n \int\cdots\int d^2r_3\cdots d^2r_{n+2} \times f(r_{13})\cdots f(r_{n+2,2}). \tag{5.7}$$

The introduction of $f_{ij} \sim -u(r_{ij})/k_BT$ in Eq. (5.7) leads to the Hauge-Hemmer expression[4]

$$\delta(r_{12}) = (2\pi)^{-1}\int \frac{d^2\vec{p}\,\tilde{V}(p)e^{i\vec{p}\cdot\vec{r}_{12}}}{1-\rho\tilde{V}(p)}$$
$$= -(2\pi)^{-1}\int d^2\vec{p}\,\frac{2q^2\beta e^{i\vec{p}\cdot\vec{r}_{12}}}{p^2+2\pi\rho\beta q^2}$$
$$= -\beta q^2 K_0(r_{12}/\lambda_D),\quad \lambda_D^2 = k_B T/2\pi q^2\rho \qquad (5.8)$$

$-k_B T\tilde{V}(p)$ denotes the Fourier transform of the Coulomb potential equal to q^2/p^2, and $K_0(z)$, the modified Bessel function of second kind. So, we get the first-order result

$$w_2^1(r_{12}) \sim -\epsilon K_0(r_{12}/\lambda_D) \qquad (5.9)$$

satisfying the requirements (5.6a)–(5.6c). Equation (5.9) has also been obtained by Vahala and Montgomery[21] with the use of the Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) hierarchy.

B. Second-order contribution ($l-k=2$)

Once the long-range behavior of the $-q^2\ln r$ potential has been resummed in the Debye chain (5.8), we have to pay attention to the short-range behavior. Fortunately, this task appears much easier in two dimensions than in three dimensions, by virtue of the summability at even order of the watermelon (Meeron) graph[20] (3a) in Fig. 4 with

$$\frac{1}{n!}\int d^2r\, e^{i\vec{p}\cdot\vec{r}}(C_D)^n$$
$$= 2\pi\int_0^\infty dr\, r I_0(pr) K_0^n(r/\lambda_D) < +\infty \quad (\text{all } n) \qquad (5.10)$$

where (C_D) represents the Debye chain, while the three-dimensional analog

$$\frac{4\pi}{n!}\int_0^\infty dr\, r\sin pr\,\frac{e^{-nr}}{r^n} < +\infty,\quad n\leq 2 \qquad (5.11)$$

has no meaning for $n>2$.

This feature allows us to consider the "simple 12-irreducible" cluster diagrams as constructed from Debye chains and nodal field points where three or more Debye chains are converging. This point is a fundamental one, because it makes clear that no further resummation over the most divergent ladder diagrams is needed, as opposed to the familiar three-dimensional situation where the basic bricks of the cluster diagrams are the Debye chains and the resummed chain[19]

$$\int_{-1}^{+1} d(\cos\theta)\int_0^\infty dr\, e^{ipr\cos\theta}\left(e^{-\epsilon e^{-r}/r} - 1 + \frac{\epsilon e^{-r}}{r}\right). \qquad (5.12)$$

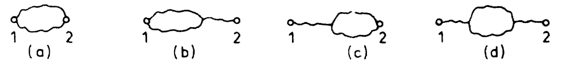

FIG. 3. Second-order diagrams ($l-k=2$) for $w_2(r_{12})$.

As a consequence, we list in Fig. 3, the second-order nodal graphs to be considered in the next higher approximation to $w_2(r_{12})$. The first one is straightforward, it reads as

$$(2a) = \frac{1}{2!}[-K_0(r_{12})]^2 \qquad (5.13)$$

with r_{12} evaluated in terms of λ_D. The next two are equal and are easily explained with the aid of the Fourier transform-convolution techniques[22] for quadratures of the general form ($r_{12} = |\vec{r}_1 - \vec{r}_2|$):

$$I(|\vec{r}_1-\vec{r}_2|) = \int\cdots\int K_0(|\vec{r}_1-\vec{r}_3|)\cdots$$
$$\times K_0(|\vec{r}_n\cdots\vec{r}_2|)\,d\vec{r}_3\cdots d\vec{r}_n \qquad (5.14)$$

so we obtain

$$(2bc) = (2b) = (2c)$$
$$= \frac{1}{2!(2\pi)}\int d\vec{p}\, e^{i\vec{p}\cdot\vec{r}_{12}} G(p) H(p), \qquad (5.15)$$

where

$$G(p) = \frac{1}{2\pi}\int d(\vec{r}''-\vec{r}_2)e^{i(\vec{r}''-\vec{r}_2)\cdot\vec{p}} K_0^2(|\vec{r}''-\vec{r}_2|)$$
$$= \int_0^\infty dx\, x K_0^2(x) J_0(px)$$
$$= \frac{1}{p(4+p^2)^{1/2}}\, Q_0^0((1+4/p^2)^{1/2}), \qquad (5.16)$$

$Q_\nu^\mu(z)$ being the associated Legendre function of the second kind, and

$$H(p) = -\frac{1}{2\pi}\int d(\vec{r}-\vec{r}'')e^{i(\vec{r}-\vec{r}'')\cdot\vec{p}} K_0(|\vec{r}-\vec{r}''|)$$
$$= -\int_0^\infty dx\, x K_0(x) J_0(xp)$$
$$= -(p^2+1)^{-1}. \qquad (5.17)$$

The resulting expression

$$(2bc) = -\frac{1}{2!}\int d\vec{p}\,\frac{e^{i\vec{p}\cdot\vec{r}_{12}} Q_0^0((1+4/p^2)^{1/2})}{p(4+p^2)^{1/2}(p^2+1)} \qquad (5.18)$$

is suitable for numerical evaluation with r_{12} taken as a running parameter. However, it appears too compact to extract in a convenient way the very important $r_{12}\to 0$ and $r_{12}\to\infty$ behaviors. Therefore it appears of interest to reconsider (2bc) under the form

$$(2bc) = -\frac{1}{2!(2\pi)}\int d\vec{p}\,\frac{e^{i\vec{p}\cdot\vec{r}_{12}}}{p^2+1}\int_0^\infty du\, u K_0^2(u) J_0(pu), \qquad (5.19)$$

invert the order of summation, and make use of

$$\int_0^\infty \frac{dp\, p J_0(pr_{12}) J_0(pu)}{p^2+1} = \begin{cases} I_0(u)K_0(r_{12}), & r_{12} \geq u \\ I_0(r_{12})K_0(u), & r_{12} \leq u \end{cases} \tag{5.20}$$

$I_0(z)$ being the modified Bessel function of first kind. Identical methods lead to

$$(2d) = \frac{1}{2!\,2\pi} \int d\vec{p}\, \frac{e^{i\vec{p}\cdot\vec{r}_{12}}}{p(4+p^2)^{1/2}(p^2+1)^2}\, Q_0^0((1+4/p^2)^{1/2})$$
$$= \frac{1}{2!} \int_0^\infty \frac{dp\, p}{(p^2+1)^2}\, I_0(pr_{12}) \int_0^\infty du\, u K_0^2(u) J_0(pu) \tag{5.21}$$

the last expression could also be explained through

$$\int_0^\infty \frac{dp\, p J_0(pr_{12}) J_0(pu)}{(p^2+1)^2} = \begin{cases} \frac{1}{2}[-uI_1(u)K_0(r_{12}) + r_{12}I_0(u)K_1(r_{12})], & r_{12} \geq u \\ \frac{1}{2}[-r_{12}I_1(r_{12})K_0(u) + I_0(r_{12})K_1(u)u], & r_{12} \leq u. \end{cases} \tag{5.22}$$

By collecting together the above expressions, the second-order contribution $w_2^2(r_{12})$ to the potential of average force may be written as

$$w_2^2(r_{12}) = \frac{\epsilon^2}{2!}\Big[K_0^2(r_{12}) - 2\left(\int_0^{r_{12}} du\, uK_0^2(u)I_0(u)\right)K_0(r_{12}) - 2I_0(r_{12})\int_{r_{12}}^\infty du\, uK_0^3(u)$$
$$+ \frac{1}{2}\int_0^{r_{12}} du\, uK_0^2(u)[-uI_1(u)K_0(r_{12}) + I_0(u)r_{12}K_1(r_{12})]$$
$$+ \frac{1}{2}\int_{r_{12}}^\infty du\, uK_0^2(u)[-K_0(u)r_{12}I_1(r_{12}) + uK_1(u)I_0(r_{12})]\Big] \tag{5.23}$$

delivering in a straightforward way the limit behaviors

$$\lim_{r_{12}\to 0} w_2^2(r_{12}) \sim \frac{\epsilon^2}{2!}[\ln(\tfrac{1}{2}\gamma r_{12})]^2, \tag{5.24}$$

$$\lim_{r_{12}\to\infty} w_2^2(r_{12}) \sim \frac{\epsilon^2}{2!}\left(\frac{\pi}{2}\right)^{1/2}\left[\left(\frac{1}{2}\right)^{1/2}\frac{e^{-2r_{12}}}{r_{12}} - 0.6705\,\frac{e^{-r_{12}}}{r_{12}^{1/2}} + 0.1511\, r_{12}^{1/2} e^{-r_{12}}\right] \tag{5.25}$$

where γ is Euler's constant. Equations (5.24) and (5.25) are obtained with the aid of the following quadratures[23]:

$$\int_0^\infty du\, uI_0(u)K_0^2(u) = 0.6046,$$

$$\int_0^\infty du\, u^2K_0^2(u)I_1(u) = 0.2636,$$

$$\int_0^\infty du\, uK_0^2(u)I_0(u) = 0.6046,$$

$$\int_0^\infty du\, uK_0^3(u) = 0.5861,$$

$$\int_0^\infty du\, u^2K_0^2(u)K_1(u) = 0.3907.$$

At this point it must be noticed that Eq. (5.23) may also be derived from the BBGKY hierarchy.[24] However, the present diagram analysis appears more powerful in view of its systematicity and its straightforward extension to third and higher orders, while the same operation appears untractable through the hierarchy. Equation (5.24) shows that the only diverging contribution at the origin arises from the ladder (2a). Equation (5.25) exhibits a slower decrease, reduced by the multiplicative factor r_{12} [recalling $\lim_{z\to\infty} K_0(z) \sim (\pi/2z)^{1/2}e^{-z}$] when compared to the first order result (5.9).

This behavior reproduces the earlier three-dimensionai findings,[18,20] and it could be considered as a general feature of the Debye approximation which is confirmed by the one-dimensional version of $w_2(r_{12})$

$$w_2^I(r_{12}) \simeq -\epsilon' e^{-r_{12}} + \epsilon'^2\{\tfrac{1}{2}e^{-2r_{12}} - \tfrac{4}{3}(2e^{-r_{12}} + e^{-2r_{12}}) + (1/96\pi)[\tfrac{2}{3}e^{-2r_{12}} + e^{-r_{12}}(\tfrac{2}{3} + r_{12})]\} + O(\epsilon'^3), \tag{5.26}$$

where $\epsilon' = q^2\lambda_D/k_BT$, $\lambda_D^2 = k_BT/2q^2\rho$ for the one-dimensional Coulomb potential $\phi_{ij} = -q^2|r_{ij}|$, with $\rho = N/L$.

VI. THIRD-ORDER CONTRIBUTION (l-k=3) TO $w_2(r_{12})$

The motivations for pursuing the Debye analysis up to the third order in ϵ, are not only completeness, although this is not a point to neglect if one remembers that the three-dimensional analog of the third-order calculation cannot make sense for diverging graphs such as (3b) or (3d) [see Eq. (5.11)]. Nevertheless, these motivations are essentially provided by the necessity to confirm the conclusions drawn from the second-order limits (5.24) and (5.25) and also by the possibility to suggest an extrapolation to higher orders of these $r_{12}\to 0$ and $r_{12}\to\infty$ behaviors. More especially, it appears highly desirable to make sure that the most diverging graph amongst those in a given order remains the ladder one. A possible drawback in this program could be afforded by the rapidly increasing number of nodal diagrams with $l-k$, as may be seen in Fig. 2 with the third-order contribution. Fortunately, the previously used Fourier transform-convolution techniques prove to be helpful for nearly all graphs, the exception being the compact topology (3*m*). Less then half of the $l-k=3$ diagrams given in Fig. 2 had already been considered by Salpeter[17] and also Mitchell and Ninham[18] in three dimensions. The first quadratures are straightforward extensions of (2*a*), (2*bc*), and (2*d*) computed in the foregoing section. So, we get

$$(3a)=(1/3!)[-K_0(r_{12})]^3, \tag{6.1}$$

$$(3bc)=(3b)=(3c)=\frac{1}{3!}\left(\int_0^{r_{12}} du\, u\, K_0^3(u) I_0(u)\right) K_0(r_{12}) + I_0(r_{12})\int_{r_{12}}^{\infty} du\, u K_0^4(u) \tag{6.2}$$

with

$$\lim_{r_{12}\to 0}(3bc)=\frac{1.035}{3!},\qquad \lim_{r_{12}\to\infty}(3bc)=\frac{0.6145}{3!}\left(\frac{\pi}{2r_{12}}\right)^{1/2} e^{-r_{12}}, \tag{6.3}$$

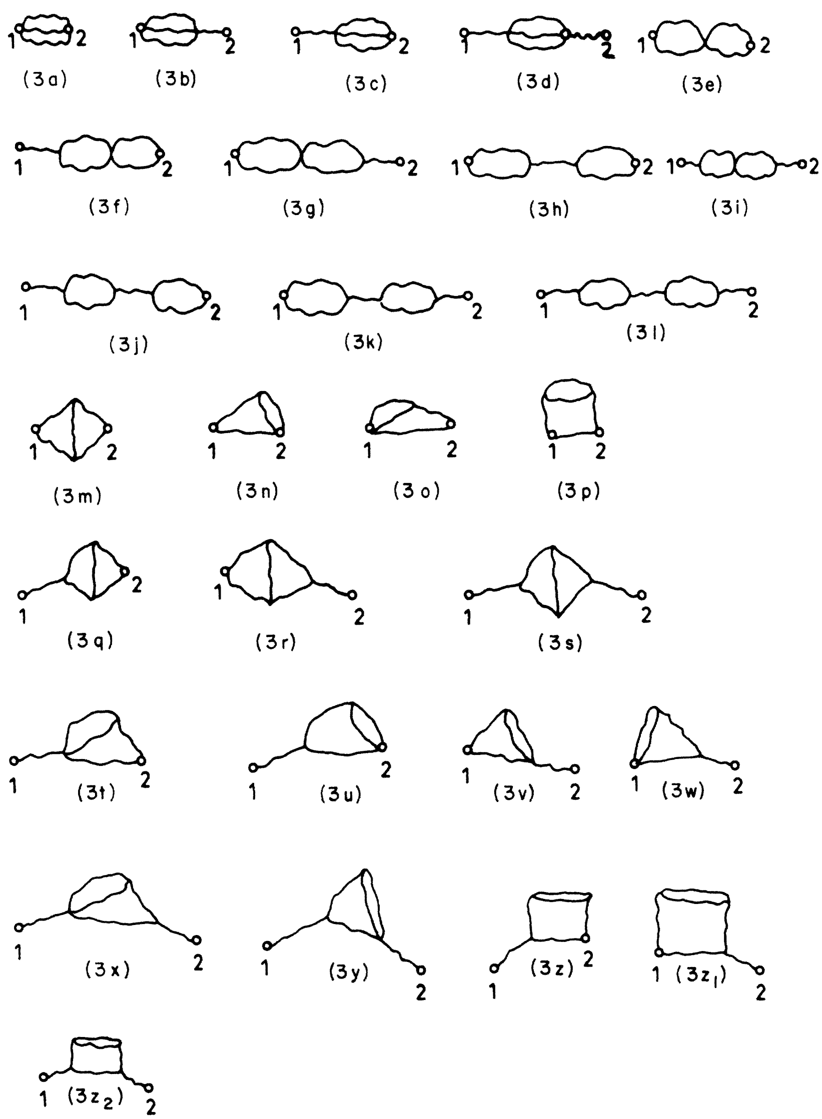

FIG. 4. Third-order diagrams ($l-k=3$) for $w_2(r_{12})$.

$$(3d)=\frac{1}{3!2}\int_0^{r_{12}} du\, uK_0^3(u)[uI_1(u)K_0(r_{12})-I_0(u)r_{12}K_1(r_{12})]$$
$$+\frac{1}{3!2}\int_{r_{12}}^{\infty} du\, uK_0^3(u)[K_0(u)r_{12}I_1(r_{12})-uK_1(u)I_0(r_{12})], \tag{6.4}$$

where

$$\lim_{r_{12}\to 0}(3d)=-\frac{0.2618}{3!},$$
$$\lim_{r_{12}\to\infty}(3d)=\frac{1}{3!}\left(\frac{\pi}{2}\right)^{1/2}\left(\frac{0.03328}{r_{12}^{1/2}}-0.3073r_{12}^{1/2}\right)e^{-r_{12}}. \tag{6.5}$$

The following eight diagrams $(3e)-(3l)$ cannot be analyzed so transparently. Therefore we shall leave them in a more compact form appropriate for numerical evaluation. We then obtain

$$(3e)=\frac{1}{(2!)^2}\int_0^{\infty}\frac{dpJ_0(pr_{12})Q_0^{02}((1+4/p^2)^{1/2})}{p(4+p^2)} \tag{6.6}$$

which makes sense for $p\to 0$, if one pays attention to $Q_0^0(z)\sim z^{-1}$, for $z\gg 1$. The representation $Q_0^0(z)=z^{-1}F(1,\frac{1}{2};\frac{3}{2};1/z^2)$ allows for an easy and accurate computation of Eq. (6.6):

$$(3fgh)=(3f)=(3g)=(3h)$$
$$=-\frac{1}{(2!)^2}\int_0^{\infty}\frac{dpJ_0(pr_{12})Q_0^{02}((1+4/p^2)^{1/2})}{p(4+p^2)(p^2+1)}, \tag{6.7}$$

$$(3ijk)-(3i)=(3j)=(3k)$$
$$=\frac{1}{(2!)^2}\int_0^{\infty}\frac{dp\,J_0(pr_{12})Q_0^{02}((1+4/p^2)^{1/2})}{p(4+p^2)(p^2+1)^2}, \tag{6.8}$$

and

$$(3l)=(3l)=-\frac{1}{(2!)^2}\int_0^{\infty}\frac{dp\,J_0(pr_{12})Q_0^{02}((1+4/p^2)^{1/2})}{p(4+p^2)(p^2+1)^3}. \tag{6.9}$$

The corresponding graphs are given numerically in Table I. At infinity they show the interesting behavior

$$(3f)<(3g)<(3k)<(3l), \tag{6.10}$$

i.e., the longest chain decreases the slowest, a feature already noticed in three dimensions by De Witt and Del Rio.[25] The foregoing inequalities are reversed for $r_{12}\to 0$. Before going on with the calculation of the remaining diagrams, we observe that the chain-structured graphs $(3q-3z_3)$ may be worked out with the same Fourier transform-convolution techniques if we have at our disposal the

TABLE I. Numerically evaluated graphs as a function of reduced distance.

Reduced distance r_{12}	$(2!)^2(3e)$	$(2!)^2(3h)$	$(2!)^2(3j)$	$(2!)^2(3l)$
0.2	0.3375	−0.053 36	0.021 40	−0.012 90
0.4	0.1440	−0.044 78	0.020 46	−0.012 64
0.6	0.062 02	−0.036 42	0.019 13	−0.012 24
0.8	0.032 21	−0.029 50	0.017 59	−0.011 72
1.0	0.021 02	−0.023 99	0.015 97	−0.011 11
1.2	0.015 61	−0.019 59	0.014 35	−0.010 43
1.4	0.011 78	−0.016 02	0.012 78	−0.009 71
1.6	0.008 66	−0.013 08	0.011 31	−0.008 98
1.8	0.006 19	−0.010 66	0.009 94	−0.008 24
2.0	0.004 27	−0.008 66	0.008 68	−0.007 52
2.2	0.002 93	−0.007 02	0.007 55	−0.006 82
2.4	0.001 97	−0.005 68	0.006 53	−0.006 15
2.6	0.001 33	−0.004 58	0.005 63	−0.005 53
2.8	0.000 90	−0.003 69	0.004 84	−0.004 94
3.0	0.0006	−0.002 98	0.004 14	−0.004 40
3.2	0.000 42	−0.002 40	0.003 54	−0.003 90
3.4	0.000 28	−0.001 934	0.003 01	−0.003 45
3.6	0.000 20	−0.001 557	0.002 56	−0.003 04
3.8	0.000 14	−0.001 254	0.002 17	−0.002 67
4.0	0.000 09	−0.001 009	0.001 83	−0.002 34
4.2	0.000 07	−0.000 81	0.001 55	−0.002 04
4.4	0.000 04	−0.000 65	0.001 31	−0.001 78
4.6	0.000 03	−0.000 53	0.001 10	−0.001 55
4.8	0.000 02	−0.000 42	0.000 93	−0.001 34
5.0	0.000 01	−0.000 34	0.000 78	−0.001 16
5.2	0.000 01	−0.000 27	0.000 65	−0.001 00
5.4	0.000 004	−0.000 22	0.000 54	−0.000 86
5.6	0.000 003	−0.000 18	0.000 45	−0.000 75
5.8	0.000 003	−0.000 14	0.000 38	−0.000 64
6.0	0	−0.000 11	0.000 32	−0.000 55

Fourier transforms of the four bubbles $(3m)-(3p)$. The first bubble $(3m)$ is also the most intricate one, and we must confess that we were not able to derive for it a comfortable expression suitable for numerical evaluation. However, taking advantage of its close analogy with a part of the fourth virial coefficient for a gas of hard spheres already considered by Nijboer and Van Hove,[26] we show in Appendix A how $r_{12}\to 0$ and $r_{12}\to\infty$ may be worked out, a result enabling us to reach estimates for the corresponding chains $(3q)$ and $(3s)$. More precisely, we get

$$(3m)=-\frac{1}{2\pi}\int d\vec{p}\,e^{i\vec{p}\cdot\vec{r}_{12}}\frac{|G(\vec{p})|^2}{p^2+1} \tag{6.11}$$

with

$$G(\vec{p})=\int d(\vec{r}_3-(\vec{r}_1-\vec{r}_2)/2)\,e^{i\vec{p}\cdot\vec{r}_3}$$
$$\times K_0(|\vec{r}_1-\vec{r}_3|)K_0(|\vec{r}_3-\vec{r}_2|)$$

and the limit behaviors

$$\lim_{r_{12}\to 0}(3m)=-(2\pi)^2\times 0.0577, \tag{6.12a}$$

$$\lim_{r_{12}\to\infty}(3m) \leqslant \frac{4\pi^5 \ln 2}{2r_{12}^2} e^{-2r_{12}} \equiv A\frac{e^{-2r_{12}}}{r_{12}^2}, \qquad (6.12b)$$

corresponding to a rapid decrease at infinity. Taking into account the continuity of expression (6.11) with respect to r_{12} we may use (6.12a) and (6.12b) in order to get estimates for the corresponding chains (3q), (3r), and (3s). The same procedure may be applied to all the remaining graphs as soon as the bubbles (3n), (3ϕ), and (3p) are explicited. The given procedure is straightforward but leads to cumbersome manipulations detailed in Appendix B.

VII. SHORT-RANGE AND LONG-RANGE BEHAVIOR OF $w_2(r_{12})$

Our final result for $w_2(r_{12})$ is given as

$$w_2(r_{12}) = w_2^1(r_{12}) + w_2^2(r_{12}) + w_2^3(r_{12}) + \cdots \qquad (7.1)$$

with $w_2^1(r_{12})$ and $w_2^2(r_{12})$ shown in Eqs. (4.9) and (4.23), respectively, and

$$w_2^3(r_{12}) = \epsilon^3[(3a)+2(3bc)+(3d)+(3e)+3(3fgh)+3(3ijk)+(3l)+(3m) + 2(3no)+(3p)+2(3qr)+(3s)+4(3tuvw)+2(3xy)+2(3zz_1)+(3z_2)], \qquad (7.2)$$

with the $r_{12}\to\infty$ behavior ($\epsilon=\beta q^2$)

$$\lim_{r_{12}\to\infty} w_2^3(r_{12}) = \epsilon^3\left(\frac{\pi}{2}\right)^{1/2}\left[-\frac{\pi}{2}\,\frac{r_{12}^{-3/2}e^{-3r_{12}}}{3!} + \frac{2A}{r_{12}^2} + \left(\frac{A}{r_{12}^2}+\frac{\pi}{2}(0.7362\,r_{12}^{-1} - 0.03023)\right)e^{-2r_{12}} + \left(\frac{1.26228}{3!} + 2B - \frac{C}{2}\right) r_{12}^{-1/2} e^{-r_{12}} + \left(-\frac{0.3073}{3!}+\frac{D}{2}\right) r_{12}^{1/2} e^{-r_{12}}\right] + \lim_{r_{12}\to\infty}[(3e)+(3h)+(3j)+(3l)], \qquad (7.3)$$

where A, B, C, and D denote finite constants such that

$$B = 2\alpha - 4\alpha' + 2\alpha'', \quad C = \gamma + 2\gamma' + \gamma'', \quad D = \delta + 2\delta' + \delta'' \qquad (7.4)$$

with the Greek constants given in Appendix B. By retaining only the most important terms and taking into account Eq. (6.10), Eq. (7.3) is well-approximated by

$$\lim_{r_{12}\to\infty} w_2^3(r_{12}) \simeq \epsilon^3\left(\frac{\pi}{2}\right)^{1/2}\left[\left(-\frac{0.3073}{3!}+\frac{D}{2}\right) \times r_{12}^{1/2}e^{-r_{12}} + (3l)\right], \qquad (7.3')$$

with

$$\lim_{r_{12}\to\infty}(3l) > r_{12}^{1/2}e^{-r_{12}} \qquad (7.5)$$

thus generalizing the slower decrease at infinity [when compared to the first order $-\epsilon K_0(r_{12})$] already found in the second-order [see Eq. (5.25)]. Although this is an interesting result, we feel that the short-range expression

$$\lim_{r_{12}\to 0} w_2^3(r_{12}) = \epsilon^3\left(-\frac{[\ln(\gamma r_{12}/2)]^3}{3!} + 0.3909\ln(\gamma r_{12}/2)\right) \qquad (7.6)$$

is of a greater importance, because it allows us to approximate the short-range behavior of the potential of average force with

$$\lim_{r_{12}\to 0} w_2(r_{12}) \simeq -\epsilon K_0(r_{12}) + \frac{\epsilon^2}{2!}K_0^2(r_{12}) - \frac{\epsilon^3}{3!}K_0^3(r_{12}) + \cdots = e^{-\epsilon K_0(r_{12})} - 1 \qquad (7.7)$$

so that when $\epsilon \ll 1$, the short-range behavior of the correlation function is given by

$$\lim_{r_{12}\to 0} g_2(r_{12}) \simeq e^{-\epsilon K_0(r_{12}/\lambda_D)} \simeq \left(\frac{r_{12}}{\lambda_D}\right)^{\beta q^2}, \quad \epsilon \ll 1 \qquad (7.8)$$

with the λ_D dependence shown.

The resummation (7.7) is much easier to obtain in two dimensions than in three in view of the order-by-order possibility of evaluating the ϵ^n corrections to $w_2(r_{12})$. This fact allows us to extrapolate to high orders ($n \geqslant 4$) the more diverging behavior of the ladder graph at $r_{12}=0$, when compared to other diagrams with the same $l-k$. At this point it must be mentioned that DeWitt[27] has recently obtained in three dimensions a resummed behavior of $g_2(r_{12})$ similar to Eq. (7.7).

VIII. DEBYE THERMODYNAMIC FUNCTIONS

Owing to the complexity of expressions (5.23) and (7.2) for $w_2^2(r_{12})$ and $w_2^3(r_{12})$, we shall restrict ourselves to a computation of the Debye thermodynamic functions up to ϵ with

$$g_2(r_{12}) \simeq e^{-\epsilon K_0(r_{12})} \simeq 1 - \epsilon K_0(r_{12}). \quad (8.1)$$

The first term on the right-hand side refers to the usual perfect gas contribution, so it will sometimes be omitted in the following. It must be stressed that the direct use of Eq. (8.1) in the various virial expressions keeps a clear meaning because the series expansion of $e^{-\epsilon K_0(r_{12})}$ may be integrated term-by-term with $\int_0^\infty dr\, r K_0^p(r) < +\infty$, all p, while it is a well-known fact that the similar procedure is forbidden in three dimensions, where more sophisticated techniques are needed.[19]

A. Pressure

The right-hand side of Eq. (8.1) introduced in the virial quantity

$$\frac{p}{k_BT} = \rho - \frac{\rho^2}{4k_BT}\int_0^\infty r\frac{d\phi}{dr}[-\epsilon K_0(r)]2\pi r\, dr \quad (8.2)$$

produces easily

$$\frac{p}{k_BT} = \rho - \frac{\rho q^2}{4k_BT}. \quad (8.3)$$

This is nothing else but the canonical exact result valid for one- and two-component systems derived previously. Thus we reach the unexpected conclusion that the first-order Debye pressure does not need any high-order corrections to approximate the complete expression. We have been able to check after a lengthly calculation that $w_2^2(r_{12})$ taken in the first order in Eq. (8.1) gives a vanishing correction to Eq. (7.3). However, this appears to be a very painful way to prove the consistency of (8.3), and it proves much more convincing to rely on a more global argument of the type recently proposed by Hauge and Hemmer,[4] who also obtained the result (8.3) through a diagram expansion of the pressure. Following these authors, the high-order contributions to Eq. (8.3) are all contained in the nodal and vanishing quantities

$$\left(1 - \frac{\rho\partial}{\partial\rho}\right)\left(\rho^n \prod_{i=2}^{n} \int d^2r_i \prod_{k=1}^{n}[-\epsilon K_0(ar_{ik}\rho^{1/2})]\right) \sim \left(1 - \frac{\rho\partial}{\partial\rho}\right)\rho = 0 \quad (8.4)$$

attached to nodal diagrams with n field points, a being a constant. This is a two-dimensional feature neither encountered in three dimensions, nor in one dimension because if one introduces Eq. (5.26) in Eq. (8.2) with $g_2^I(r_{12}) \sim 1 - w_2^I(r_{12})$, one obtains

$$p/k_BT = \rho - \tfrac{1}{2}\rho\epsilon' + w\epsilon'^2 + O(\epsilon'^3), \quad w \sim 0.25. \quad (8.5)$$

B. Free energy

The virial expression for the internal energy per particle is

$$\begin{aligned}\frac{E}{Nk_BT} &= 1 + \frac{\rho}{2k_BT}\int_0^\infty \phi(r)[-\epsilon K_0(r)]2\pi r\, dr \\ &= 1 + \frac{\beta q^2}{2}\int_0^\infty dx\, x[\ln x + \ln(\lambda_D/L)]K_0(x) \\ &= 1 + \tfrac{1}{2}\beta q^2[1 - \gamma + \ln(\lambda_D/2L)]. \quad (8.6)\end{aligned}$$

The last expression is obtained with the aid of

$$K_0(x) = \int_0^\infty du\, e^{-x\,ch u},$$

$$\int_0^\infty \frac{du}{(ch u)^2} = 1,$$

and

$$\int_0^\infty du \frac{\ln(ch u)}{(ch u)^2} = \ln\tfrac{1}{2}. \quad (8.7)$$

In order to appreciate more thoroughly the physical content of Eq. (8.6), it appears desirable to rewrite the Coulomb potential $u(r) = -q^2\ln(r/L)$ as a sum $-q^2\ln(R/L) - q^2\ln(r/R)$, involving the linear dimension of the configuration space, so that the factor $\ln(R/L)$ enters only the factor multiplying the one-component partition function [Eq. (8.15) below] written as $Q^* = e^{-\beta F^*}$. The interacting contribution to the energy may be then given the form $[u(r) = -q^2\ln(r/R)]$

$$\begin{aligned}\frac{\beta E^*}{N} &= \frac{\beta\rho}{2}\int_0^R u(r)g^*(r)2\pi r\, dr \\ &= \frac{\beta\rho}{2}\int_0^R \left(-q^2\ln\frac{r}{R}\right)[-\beta q^2 K_0(r/\lambda_D)]\, 2\pi r\, dr \\ &= \frac{\beta q^2}{2}\left[\ln\left(\frac{\lambda_D}{2R}\right) + 1 - \gamma\right], \quad (8.6')\end{aligned}$$

which is Eq. (8.6) except for R replacing L with

$$\frac{\lambda_D}{R} = \frac{1}{(2\beta q^2 N)^{1/2}}$$

independent of the volume and

$$\beta E^* = -\frac{\beta q^2 N}{4}\ln(\beta q^2 N) + \cdots.$$

Now the total energy reads

$$\begin{aligned}\beta E &= 1 + \frac{\beta q^2}{2}\ln\frac{R}{L} - \frac{\beta q^2}{4}N\ln(\beta q^2 N) \\ &= 1 + \frac{\beta q^2 N}{4}\ln\left(\frac{R^2}{N}\right)\frac{1}{L^2\beta q^2} \\ &= 1 + \frac{\beta q^2 N}{2}\ln\frac{\lambda_D}{L}, \quad (8.6'')\end{aligned}$$

reproducing the content of Eq. (8.6).

The potential free energy is therefore

$$\beta F^{\text{exc}} = \int_0^\beta d\beta' \, E^{\text{exc}}(\beta') = \frac{\epsilon}{2}\left[\frac{3}{2} - \gamma + \ln\left(\frac{\lambda_D}{2L}\right)\right], \tag{8.8}$$

with

$$\lim_{\beta\to 0} F^{\text{exc}} \sim -\tfrac{1}{2}q^2(\ln\beta - 1). \tag{8.9}$$

The corresponding constant-volume specific heat C_V

$$C_V = \left(\frac{\partial E}{\partial T}\right)_N = k_B(1 + \tfrac{1}{4}\epsilon) \tag{8.10}$$

is free from the low-temperature divergence present in the low-temperature expression

$$C_V = k_B\left(1 + \frac{1}{2(T/T_c - 1)^2}\right)$$

considered previously.

The potential entropy per particle is

$$S^{\text{exc}} = \beta^2 \frac{\partial F^{\text{exc}}}{\partial \beta} = -\epsilon. \tag{8.11}$$

As a concluding remark, it is worth noting that the infinite-temperature ($\beta\to 0$) behavior of Eqs. (8.9)–(8.11) coincides with the Mehta exact results[10] for the one-component system of point charges restricted to the unit circumference.

C. Speculations about the thermodynamic limit (one-component gas)

Once again, we try to speculate about the implications of the possible existence of the thermodynamic limit for the one-component gas with neutralizing background. Now our analysis is based upon the Debye approximate expression (8.6) for the internal energy. As in Sec. II C we start with the one-component canonical partition function[4]

$$Q = \int e^{-\beta\phi} \prod_{i=1}^{N} d^2 r_i \tag{8.12}$$

with ($\sigma = qN/V$)

$$\begin{aligned}\phi &= H_{pp} + H_{pb} + H_{bb} \\ &= -q^2 \sum_{1<j}^{N} \ln\left(\frac{r_{ij}}{L}\right) + \sigma q \sum_{i=1}^{N} \int_V d^2 r \ln(|\vec{r}_i - \vec{r}|/L) \\ &\quad - \frac{\sigma^2}{2}\int_V \int_V d^2 r\, d^2 r' \ln(|\vec{r} - \vec{r}'|/L).\end{aligned} \tag{8.13}$$

The scaling trick (1.4) works again. It gives

$$Q \simeq \frac{V^N}{N!\Lambda^{2N}} \left(\frac{V^{1/2}}{L}\right)^{\beta q^2 N/2} Q^* \cdots, \tag{8.14}$$

where

$$Q^* \simeq e^{-\beta\sigma^2\pi^2/8} \prod_{i=1}^{N} \int_C d^2 r_i \times \exp\left(\beta q^2 \sum_{1<j}^{N} \ln|r_{ij}| - \beta\sigma q \frac{\pi}{2}\sum_{i=1}^{N}(r_i^2 - 1)\right), \tag{8.15}$$

with $L = 1$ in the last quantity. As before,[12] Eq. (8.14) may be used to derive a sufficient estimate for the existence[13] of a finite free energy per particle

$$\beta F = -\ln Q = N\left(\ln\frac{N\lambda^2}{V} - 1\right) + \frac{\beta q^2}{4} N \ln\frac{V}{L^2} - \ln Q^*,$$

$$\rho = \frac{N}{V} \tag{8.16}$$

in the form

$$\ln Q^* \xrightarrow[N\to\infty,\, V\to\infty]{} \tfrac{1}{4}\beta q^2 N \ln N, \quad \rho \text{ finite}. \tag{8.17}$$

The latter requirement is equivalent to approximating Q^* by

$$Q^* \simeq (N!)^{\beta q^2/4}[f(\beta q^2)]^N \tag{8.18}$$

with the free energy given as

$$\beta F = N[(\ln\rho\lambda^2 - 1) - \tfrac{1}{4}\beta q^2 \ln\rho L^2 - \ln f(\beta q^2)] \tag{8.19}$$

and the internal energy

$$\beta E = \beta\frac{\partial \beta F}{\partial \beta} = N\left(1 - \frac{\beta q^2}{4}\ln\rho L^2 - \beta\frac{\partial \ln f(\beta q^2)}{\partial\beta}\right). \tag{8.20}$$

The exact result for the pressure

$$\beta P = -\frac{\partial \beta F}{\partial V} = \rho\left(1 - \frac{\beta q^2}{4}\right) \tag{8.21}$$

is recovered once more. It is shown to be independent of whether the thermodynamic exits or not, and it satisfies the required thermodynamic relation

$$-\frac{\partial}{\partial V}(\beta E) = \frac{\partial \beta P}{\partial \beta}.$$

Now let us write the Debye expression (8.6) for the internal energy per particle as $[\lambda_D = (2\pi\beta q^2\rho)^{-1/2}]$

$$\beta E/N = 1 - \tfrac{1}{4}\beta q^2[\ln\rho L^2 + \ln 2\pi\beta q^2 - 2(1 - \gamma - \ln 2)]. \tag{8.22}$$

The important point to notice is that expression (8.22) is in substantial agreement with expression (8.20), so that the first-order Debye approximation for the free energy fulfills the strong and sufficient requirement for the existence of the thermodynamic limit. In order to put this conclusion on a firmer basis, we shall investigate in a future work the higher-order corrections to Eq. (8.6).

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APPENDIX A

The purpose of this appendix is to provide an estimate as accurate as possible for the bubble diagram $(3m)$. We can no longer work with the Fourier-transform–convolution techniques. However, recalling the Nijboer and Van Hove[26] approach to the fourth virial coefficient for a hard-sphere gas, we may write:

$$(3m) = -\int K_0(r_{13})K_0(r_{12})K_0(r_{14}) \times K_0(r_{42})K_0(r_{34})\,d\vec{r}_3\,d\vec{r}_4 \qquad \text{(A1)}$$

$$= -\frac{1}{2\pi}\int F(p)\,|G(\vec{p})|^2\,d\vec{p}, \qquad \text{(A2)}$$

with

$$F(p) = \frac{1}{2\pi}\int d\vec{r}\,e^{i\vec{p}\cdot\vec{r}}K_0(r) = (p^2+1)^{-1}, \qquad \text{(A3)}$$

$$G(p) = \int d\vec{r}_3\,e^{i\vec{p}\cdot\vec{r}\,'_3}K_0(|\vec{r}\,'_1-\vec{r}\,'_3|)K_0(|\vec{r}\,'_3-\vec{r}\,'_2|), \qquad \text{(A4)}$$

and $\vec{r}\,'_i = \vec{r}_i - (\vec{r}_1 - \vec{r}_2)/2$. Equation (A4) is ready for evaluation in the symmetric frame shown in Fig. 5 with

$$G(p) = \int_0^{2\pi} d\theta \int_0^\infty dw\,wK_0((w^2+\tfrac{1}{4}r_{12}^2 - r_{12}w\cos\theta)^{1/2}) \times K_0((w^2+\tfrac{1}{4}r_{12}^2 + r_{12}w\cos\theta)^{1/2})\,e^{ipw\cos\theta} \qquad \text{(A5)}$$

which proved to be too involved for our efforts. Fortunately, we can derive from it efficient upper bounds for (B2). Our techniques are based on the simple observation that (B1) is a continuous function of r_{12}, so that sufficient upper bounds for $r_{12} \to 0$ and $r_{12} \to \infty$ will ensure the existence of the Fourier transform of $(3m)$. Let us first consider

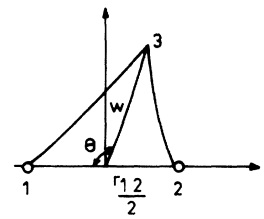

FIG. 5. Coordinate system used for $(3m)$.

the $r_{12} \to 0$ limit with

$$\lim_{r_{12}\to 0} |G(p)| \le 2\pi \int_0^\infty dw\,wK_0^2(w)J_0(pw) = \frac{2\pi}{p(4+p^2)^{1/2}}\,Q_0^0((1+4/p^2)^{1/2}), \qquad \text{(A6)}$$

$$\lim_{r_{12}\to 0} |(3m)| \le \frac{1}{2\pi}\int_0^{2\pi} d\theta \int_0^\infty \frac{dp\,p}{p^2+1} \times \left(\frac{2\pi}{p(4+p^2)^{1/2}}\,Q_0^0((1+4/p^2)^{1/2})\right)^2 = (2\pi)^2 \times 0.05772\,. \qquad \text{(A7)}$$

A convenient upper bound is possible through the McDonald formula:

$$K_0((w^2+\tfrac{1}{4}r_{12}^2 - wr_{12}\cos\theta)^{1/2})\,K_0((w^2+\tfrac{1}{4}r_{12}^2 + wr_{12}\cos\theta)^{1/2}) = \frac{1}{2}\int_0^\infty \frac{dv}{v}\exp\left[-\frac{v}{2} - \left(w^2 + \frac{r_{12}^2}{4}\right)v^{-1}\right] \times K_0([(w^2+\tfrac{1}{4}r_{12}^2)^2 + (wr_{12}\cos\theta)^2/v]^{1/2}), \qquad \text{(A8)}$$

with

$$G(p) \le \pi \int_0^\infty \frac{dv}{v}\exp\left(-\frac{v}{2} - \frac{r_{12}^2}{4v}\right)\int_0^\infty dw\,wJ_0(pw) \times e^{-w^2/4}K_0((w^2+\tfrac{1}{4}r_{12}^2)v^{-1}) < \frac{\pi}{2}\int_0^\infty dv\,\exp\left[-\frac{v}{2}\left(1+\frac{p^2}{2}\right)\right]K_0\left(\frac{r_{12}^2}{4v}\right)e^{-r_{12}^2/4v} \qquad \text{(A9)}$$

and

$$\lim_{r_{12}\to\infty} K_0\left(\frac{r_{12}^2}{4v}\right) \sim \frac{(2\pi v)^{1/2}}{r_{12}}\,e^{-r_{12}^2/4v}, \qquad \text{(A10)}$$

so that

$$G(p) < \frac{\pi}{2}\,\frac{(2\pi)^{1/2}}{r_{12}}\int_0^\infty dv\,v^{1/2}\,e^{-v(1+p^2/2)/2}\,e^{-r_{12}^2/2v} = \frac{\pi^{3/2}2^{1/4}}{r_{12}^{1/2}}\,\frac{1}{(\frac{1}{2}+\frac{1}{4}p^2)^{1/4}}\,K_{1/2}(r_{12}(1+\tfrac{1}{2}p^2)^{1/2}) \qquad \text{(A11)}$$

and finally

$$(3m) < \frac{2^{3/2}\pi^4}{r_{12}} \int_0^\infty \frac{dp\, p K_1^2(r_{12}(1+\frac{1}{2}p^2)^{1/2})}{(p^2+1)(\frac{1}{2}+\frac{1}{4}p^2)^{1/2}} \simeq \frac{\pi^5}{r_{12}^2} \int_0^\infty \frac{dp\, p \exp[-2r_{12}(1+\frac{1}{2}p^2)^{1/2}]}{(p^2+1)(\frac{1}{2}+\frac{1}{4}p^2)}$$

$$= \frac{\pi^5}{2r_{12}^2} \int_0^\infty \frac{dx \exp[-2r_{12}(1+x/2)^{1/2}]}{(1+x)(\frac{1}{2}+\frac{1}{4}x)} < \frac{\pi^5 e^{-2r_{12}}}{2r_{12}^2} \int_0^\infty \frac{dx}{(1+x)(\frac{1}{2}+\frac{1}{4}x)} = \frac{4\pi^5 \ln 2}{r_{12}^2} e^{-2r_{12}}. \tag{A12}$$

The upper bounds (A7) and (A12) are introduced in Eqs. (6.12a) and (6.12b) in the main text.

APPENDIX B

Here we detail the evaluation of the remaining third-order graphs ($3n$) to ($3z_2$). First, the results (6.12a) and (612b) are used to estimate the chains ($3q$), ($3r$) and ($3s$). Then, the bubbles ($3n$), ($3o$) and ($3p$) are easily explicited and introduced in the remaining chain diagrams. So, we first obtain

$$(3qr) = (3q) = (3r) = -\int_0^{r_{12}} du\, u I_0(u)(3m)(u) K_0(r_{12}) + \left(\int_{r_{12}}^\infty du\, u K_0(u)(3m)(u)\right) I_0(r_{12}) \tag{B1}$$

with

$$\left| \int_0^\infty du\, u I_0(u)(3m)(u) \right| = \alpha < +\infty,$$

$$\left| \int_0^\infty du\, u K_0(u)(3m)(u) \right| = \beta < +\infty$$

and

$$\lim_{r_{12}\to 0} (3qr) = \beta,$$
$$\lim_{r_{12}\to\infty} (3qr) = \alpha\left(\frac{\pi}{2r_{12}}\right)^{1/2} e^{-r_{12}}, \tag{B2}$$

$$(3s) = \frac{1}{2}\int_0^{r_{12}} du\, u(3m)(u)[-uI_1(u)K_0(r_{12}) + I_0(u) r_{12} K_1(r_{12})] + \frac{1}{2}\int_{r_{12}}^\infty du\, u(3m)(u)[uK_1(u)I_0(r_{12}) - K_0(u) r_{12} I_1(r_{12})], \tag{B3}$$

where

$$\lim_{r_{12}\to 0} (3s) = \left(\int_0^\infty du\, u^2 K_1(u)(3m)(u)\right) = \xi, \quad |\xi| < +\infty \tag{B4a}$$

$$\lim_{r_{12}\to\infty} (3s) = \frac{1}{2}\left(\frac{\pi}{2}\right)^{1/2}\left(-\frac{\gamma}{r_{12}^{1/2}} + \delta r_{12}^{1/2}\right) e^{-r_{12}}, \tag{B4b}$$

and

$$\gamma = \left| \int_0^\infty du\, u^2 I_1(u)(3m)(u) \right| < +\infty,$$

$$\delta = \left| \int_0^{+\infty} du\, u I_0(u)(3m)(u) \right| < +\infty.$$

The bubble ($3m$) has already been considered in three dimensions by Mitchell and Ninham[18] who investigated its $r_{12}\to\infty$ limit. The three following bubbles ($3n$, $3o$, $3p$) are fortunately reducible to previous quadratures:

$$(3no) = -K_0(r_{12})(2bc) \tag{B5}$$

diverges for $r_{12}\to 0$ with

$$\lim_{r_{12}\to 0} (3no) = 0.2931 \ln\left(\frac{\gamma r_{12}}{2}\right). \tag{B6a}$$

At infinity it behaves like

$$\lim_{r_{12}\to\infty} (3no) = 0.1511 \frac{\pi}{r_{12}} e^{-2r_{12}}. \tag{B6b}$$

The corresponding chains are

$$(3tuvw) = (3t) = (3u) = (3v) = (3w) = -\left(\int_0^{r_{12}} du\, u I_0(u)(o)(u)\right) K_0(r_{12}) + \left(\int_{r_{12}}^\infty du\, u K_0(u)(o)(u)\right) I_0(r_{12}). \tag{B7}$$

As previously obtained, the relationships (6.18a) and (6.18b) show that the $r_{12}\to 0$ and $r_{12}\to\infty$ limits of the quadratures define finite α' and β', respectively, so we get

$$\lim_{r_{12}\to 0} (3tuvw) = -\beta',$$
$$\lim_{r_{12}\to\infty} (3tuvw) = -\alpha'\left(\frac{\pi}{2r_{12}}\right)^{1/2} e^{-r_{12}}, \tag{B8}$$

while the two-legged extension of ($3no$) is

$$(3xy) = (3x) = (3y) = \frac{1}{2}\int_0^{r_{12}} du\, u(o)(u)[-uI_1(u)K_0(r_{12}) + I_0(u) r_{12} K_1(r_{12})] + \frac{1}{2}\int_{r_{12}}^\infty du\, u(o)(u)[uK_1(u)I_0(r_{12}) - K_0(u) r_{12} I_1(r_{12})], \tag{B9}$$

with

$$\lim_{r_{12}\to 0}(3xy)=\frac{1}{2}\int_0^\infty du\, u^2(o)(u)K_1(u)<+\infty, \quad \text{(B10a)}$$

$$\lim_{r_{12}\to\infty}(3xy)=-\frac{1}{2}\left(\int_0^\infty du\, u^2(o)(u)I_1(u)\right)\left(\frac{\pi}{2r_{12}}\right)^{1/2}e^{-r_{12}}+\frac{1}{2}\left(\int_0^\infty du\, u(o)(u)I_0(u)\right)\left(\frac{\pi r_{12}}{2}\right)^{1/2}e^{-r_{12}}=\frac{1}{2}\left(\frac{\pi}{2}\right)^{1/2}\left(-\frac{\gamma'}{r_{12}^{1/2}}+\delta' r_{12}^{1/2}\right)e^{-r_{12}}. \quad \text{(B10b)}$$

In the same way, the last bubble $(3p)$ is

$$(3p)=-K_0(r_{12})\times(2d) \quad \text{(B11)}$$

with

$$\lim_{r_{12}\to 0}(3p)=-\ln\left(\frac{\gamma r_{12}}{2}\right)0.1953, \quad \text{(B12a)}$$

$$\lim_{r_{12}\to\infty}(3p)=\frac{\pi}{2}\left(\frac{0.1318}{r_{12}}-0.03023\right)e^{-2r_{12}}. \quad \text{(B12b)}$$

The corresponding chains are

$$(3zz_1)=(3z)=(3z_1)$$

with an expression analogous to (5.19) and $(3no)$ replaced by $(3p)$, with

$$\lim_{r_{12}\to 0}(3zz_1)=\int_0^\infty du\, uK_0(u)(3p)(u)<+\infty, \quad \text{(B13a)}$$

$$\lim_{r_{12}\to\infty}(3zz_1)=\left(\int_0^\infty du\, uI_0(u)(3p)(u)\right)\left(\frac{\pi}{2r_{12}}\right)^{1/2}e^{-r_{12}}=\alpha''\left(\frac{\pi}{2r_{12}}\right)^{1/2}e^{-r_{12}}, \quad |\alpha''|<+\infty. \quad \text{(B13b)}$$

$(3z_2)$ is given by an expression similar to (B9) satisfying

$$\lim_{r_{12}\to 0}(3z_2)=\frac{1}{2}\int_0^\infty du\, u^2(3p)(u)K_1(u)=\xi', \quad |\xi'|<+\infty \quad \text{(B14a)}$$

$$\lim_{r_{12}\to\infty}(3z_2)=\frac{1}{2}\left(\frac{\pi}{2}\right)^{1/2}\left(-\frac{\gamma''}{r_{12}^{1/2}}+\delta'' r_{12}^{1/2}\right)e^{-r_{12}}, \quad \text{(B14b)}$$

γ'' and δ'' being finite quadratures analogous to γ' and δ' in Eq. (B10).

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