Lower bounds for thermodynamic quantities of d-dimensional classical one-component plasmas with d-dimensional Coulomb interactions ($d = 1$, 2, and 3)

Hiroo Totsuji
Department of Electronics, Okayama University, Tsushimanaka, Okayama 700, Japan
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An exact lower bound for the correlation energy of a three-dimensional classical one-component plasma (OCP), based on Mermin's inequality for the structure factor and a trivial inequality for the pair correlation function, is generalized to the cases of d-dimensional OCP's with d-dimensional Coulomb interaction where $d = 1$, 2, and 3. For $d = 1$ and $d = 3$, this lower bound gives values close to the known exact values and the results of numerical experiments, respectively. In the case of $d = 2$, where the interaction potential is logarithmic, this lower bound improves upon the known one in the domain $e^2/T < 25.0$, e and T being the charge and the temperature in energy units.

I. INTRODUCTION

The system of charged particles in the uniform background of opposite charges, the one-component plasma (OCP), has been studied not only as a model system of real plasmas, but also as one of the simplest systems having the long-range interaction. It is sometimes useful to investigate similar systems with different dimensionalities d from a unified point of view. As systems of charged particles in the uniform background there are two classes of d-dimensional OCP's, d-dimensional OCP's with three-dimensional $(1/r)$ Coulomb interaction and d-dimensional OCP's with d-dimensional Coulomb interaction. To the first class belong usual three-dimensional OCP's and two-dimensional OCP's which have recently become available on the surface of liquid helium or in the metal-oxide-semiconductor (MOS) inversion layer. To the second class belong three-dimensional OCP's and systems of charged rods[1,2] and of charged sheets[3-5] where interaction potentials are logarithmic and linear functions of the distance, respectively. The system of charged rods has been investigated also in relation to the dislocation theory of two-dimensional melting.[6]

I have recently given exact lower bounds[7] for thermodynamic quantities of three- and two-dimensional OCP's with three-dimensional Coulomb interaction based on a method which is independent of dimensionality. I have also obtained a much improved lower bound[7] by making use of the inequality for the structure factor suggested by Mermin,[8] which is valid for three-dimensional classical OCP's with three-dimensional Coulomb interaction.

In this paper I generalize the latter lower bound to the cases of d-dimensional OCP's with d-dimensional Coulomb interaction where $d=1$, 2, and 3. Unified approaches to some properties of this class of d-dimensional OCP's have been given by Deutsch[9] and by Sari and Merlini.[10] I will give, when possible, expressions for general values of the dimensionality d, including noninteger values. Lower bounds will be given for the correlation energy, from which other thermodynamic quantities are easily derived.

II. COULOMB POTENTIAL IN d DIMENSIONS

The Coulomb potential $\phi(r)$ in d dimensions may be defined as the solution of the Poisson equation

$$\Delta\phi(r) = -2\pi^{d/2}\Gamma(\tfrac{1}{2}d)^{-1}\delta(\vec{r}), \tag{2.1}$$

where $\delta(\vec{r})$ denotes the d-dimensional δ function. When we take the zero level of the potential $\phi(r)$ as

$$\phi(r=l) = 0, \tag{2.2}$$

$\phi(r)$ is given by

$$\phi(r) = (2\pi)^{-d}\int d\vec{k}\,\phi(k)(e^{i\vec{k}\cdot\vec{r}} - e^{i\vec{k}\cdot\vec{l}}), \tag{2.3}$$

where $\vec{l}$ is a vector of length l,

$$\phi(k) = 2\pi^{d/2}\Gamma(\tfrac{1}{2}d)^{-1}k^{-2}, \tag{2.4}$$

and $d\vec{k}$ denotes the d-dimensional volume integral in the Fourier space. Performing the integral, we have

$$\begin{aligned}\phi(r) &= 2^{1-d}\pi^{-(d+1)/2}\Gamma[\tfrac{1}{2}(d-1)]^{-1} \\ &\quad\times\int_0^\infty dk\,k^{d-1}\phi(k)\int_0^\pi d\theta\,\sin^{d-2}\theta(e^{ikr\cos\theta} - e^{ikl\cos\theta}) \\ &= 2^{1-d/2}\Gamma(\tfrac{1}{2}d)^{-1} \\ &\quad\times\int_0^\infty dk\,k^{d/2-2}[r^{1-d/2}J_{d/2-1}(kr) - l^{1-d/2}J_{d/2-1}(kl)] \\ &= \begin{cases}(d-2)^{-1}[r^{2-d} - l^{2-d}] & (0<d<5,\ d\neq 2) \\ -\ln(r/l) & (d=2),\end{cases}\end{aligned} \tag{2.5}$$

where $J_\nu(x)$ is the Bessel function. Taking $l=\infty$ for $d>2$ and $l=0$ for $d<2$, we obtain

$$\phi(r)=(2\pi)^{-d}\int d\vec{k}\,\phi(k)\left(e^{i\vec{k}\cdot\vec{r}}-\begin{cases}\Theta(2-d)\\ e^{i\vec{k}\cdot\vec{l}}\end{cases}\right)$$
$$=\begin{cases}(d-2)^{-1}r^{2-d} & (0<d<5,\ d\neq 2)\\ -\ln(r/l) & (d=2),\end{cases} \tag{2.6}$$

where $\Theta(x)$ is the unit step function. It is to be noted that we have to retain the second term in the integrand for $d\leq 2$.

In what follows, I do not make use of the integral of the inverse-Fourier-transform type for $\phi(r)$,

$$\Phi(k)=\int d\vec{r}\,\phi(r)\exp(-i\vec{k}\cdot\vec{r}), \tag{2.7}$$

which is meaningful only as the result of some limiting procedure.[11]

III. CORRELATION ENERGY

The total potential energy Ne_c of a system composed of N particles with the charge e and neutralizing uniform background of opposite charges, interacting via the Coulomb potential $\phi(r)$, is given by

$$Ne_c=\frac{e^2}{2}\int d\vec{r}\int d\vec{r}'\left\langle\left(\sum_i\delta(\vec{r}-\vec{r}_i)-n\right)\left(\sum_j\delta(\vec{r}'-\vec{r}_j)-n\right)-\delta(\vec{r}-\vec{r}')\sum_i\delta(\vec{r}-\vec{r}_i)\right\rangle\phi(|\vec{r}-\vec{r}'|)$$
$$=\frac{n^2e^2}{2}\int d(\vec{r}-\vec{r}')\int d\vec{r}'[f_2(\vec{r}-\vec{r}',\vec{r}')-1]\phi(|\vec{r}-\vec{r}'|), \tag{3.1}$$

where n denotes the number density, $\langle\ \rangle$ the statistical average, and

$$n^2f_2(\vec{r},\vec{r}')=\left\langle\sum_{i\neq j}\delta(\vec{r}+\vec{r}'-\vec{r}_i)\delta(\vec{r}'-\vec{r}_j)\right\rangle. \tag{3.2}$$

Introducing the pair correlation function $h(\vec{r})$ by

$$h(\vec{r})=\left(\int d\vec{r}'f_2(\vec{r},\vec{r}')\Big/\int d\vec{r}'\right)-1, \tag{3.3}$$

we have

$$e_c=\frac{ne^2}{2}\int d\vec{r}\,h(\vec{r})\phi(r). \tag{3.4}$$

The structure factor $S(\vec{k})$ defined by

$$S(\vec{k})=\langle|\rho_{\vec{k}}|^2\rangle/N, \tag{3.5}$$

$$\rho_{\vec{k}}=\sum_i\exp(-i\vec{k}\cdot\vec{r}_i), \tag{3.6}$$

is related to the pair-correlation function $h(\vec{r})$ by

$$nh(\vec{r})=(2\pi)^{-d}\int d\vec{k}[S(\vec{k})-1]e^{i\vec{k}\cdot\vec{r}}. \tag{3.7}$$

Fundamental relations (3.4) and (3.7) are also valid when system is in the crystalline state, as in the case of $d=1$ with the free- (impenetrable-wall) boundary condition.[5]

Substituting (2.6) into (3.4) and using (3.7) and the relation

$$n\int d\vec{r}\,h(\vec{r})=-1, \tag{3.8}$$

we can rewrite Eq. (3.4) as

$$e_c=\frac{e^2}{2}(2\pi)^{-d}\times\int d\vec{k}\,\phi(k)\left(S(\vec{k})-1+\begin{cases}\Theta(2-d) & (d\neq 2)\\ e^{i\vec{k}\cdot\vec{l}} & (d=2)\end{cases}\right). \tag{3.9}$$

Note the difference in the integrand for $d>2$, $d=2$, and $d<2$.

IV. GENERALIZATION OF MERMIN'S LOWER BOUND FOR THE STRUCTURE FACTOR

For three-dimensional classical OCP's, Mermin[8] has shown an exact inequality for the structure factor:

$$S(\vec{k})\geq S_{\mathrm{RPA}}(k)=k^2/(k^2+k_D^2), \tag{4.1}$$

where the right-hand side is the random-phase-approximation (RPA) value of the structure factor, and the Debye wave number k_D is defined by

$$k_D^2=4\pi ne^2/T,$$

where T denotes the temperature in energy units. It is easy to generalize the proof to the cases of d-dimensional OCP's with d-dimensional Coulomb interaction where $d=1$, 2, and 3. We finally obtain Eq. (4.1), where the Debye wave number is defined by

$$k_D^2=2\pi^{d/2}\Gamma(\tfrac{1}{2}d)^{-1}ne^2/T. \tag{4.2}$$

Substituting Eq. (4.1) into Eq. (3.9), we have an exact lower bound

$$e_c/T \geq e_c^{\mathrm{RPA}}/T$$
$$= -2^{1-d}\Gamma(\tfrac{1}{2}d)^{-2}\epsilon \int_0^\infty dx\, x^{d-3}[(x^2+1)^{-1} - 2^{d/2-1}\Gamma(\tfrac{1}{2}d)(k_D l x)^{1-d/2} J_{d/2-1}(k_D l x)]$$
$$= \begin{cases} \tfrac{1}{2}\epsilon & (d=1) \\ -\tfrac{1}{4}\epsilon[2\gamma + \ln(\tfrac{1}{2}\epsilon) + \ln(\pi n l^2)] & (d=2) \\ -\tfrac{1}{2}\epsilon & (d=3)\,. \end{cases} \tag{4.3}$$

Here ϵ denotes the plasma parameter defined by

$$\epsilon = e^2 k_D^{d-2}/T = \begin{cases} e(2nT)^{-1/2} & (d=1) \\ e^2 T^{-1} & (d=2) \\ (4\pi n)^{1/2} e^3 T^{-3/2} & (d=3)\,, \end{cases} \tag{4.4}$$

and γ the Euler's constant $\gamma = 0.577\,21\ldots$.

V. LOWER BOUNDS FOR THE CORRELATION ENERGY

Rewriting $\phi(k)$ in Eq. (3.9) as

$$\phi(k) = \int_0^\infty dt\, f(k,t) = \left(\int_0^G + \int_G^\infty\right) dt\, f(k,t)\,, \tag{5.1}$$

with an arbitrary parameter $G > 0$, we have

$$e_c = \frac{e^2}{2}(2\pi)^{-d}\int d\vec{k}\int_0^G dt\, f(k,t)\left(S(\vec{k}) - \frac{k^2}{k^2+k_D^2}\right) + \frac{ne^2}{2}\int d\vec{r}\int_G^\infty dt\, f(r,t)[h(\vec{r})+1] + B_1[f,G]\,, \tag{5.2}$$

where $f(r,t)$ is the Fourier transform of $f(k,t)$ and

$$B_1[f,G] = -\frac{e^2}{2}(2\pi)^{-d}\int d\vec{k}\left(\int_0^G dt\, f(k,t)\frac{k_D^2}{k^2+k_D^2} - \phi(k)\begin{Bmatrix}\Theta(2-d) \\ e^{i\vec{k}\cdot\vec{l}}\end{Bmatrix}\right) - \frac{ne^2}{2}\int_G^\infty dt\, f(k=0,t) \quad \begin{matrix}(d\neq 2) \\ (d=2)\,.\end{matrix} \tag{5.3}$$

Noting the inequalities (4.1) and

$$h(\vec{r}) \geq -1\,, \tag{5.4}$$

and assuming

$$f(k,t) \geq 0 \text{ and } f(r,t) \geq 0\,, \tag{5.5}$$

we have an exact lower bound for the correlation energy

$$e_c \geq B_1[f,G]\,. \tag{5.6}$$

The best lower bound within our method is given by the maximum of the right-hand side at $G = G_0$. When $G = \infty$, this lower bound reduces to the RPA value given by Eq. (4.3).

The lower bound $B_1[f, G_0]$ depends on the function $f(k,t)$. In the case of $d=3$, we have found that the lower bound given by the function[7]

$$f_0(k,t) = 2\pi^{d/2}\Gamma(\tfrac{1}{2}d)^{-1} e^{-k^2/4t^2}/2t^3 \tag{5.7}$$

is effective among ones given by several simple functions[12] which satisfy the conditions (5.5). The lower bound thus obtained nearly reproduces experimental values. This indicates that the RPA approximation in the long-range domain and the approximation $h(\vec{r}) = -1$ in the short-range domain are very useful zeroth approximations when we divide the calculation of the correlation energy into two domains by the function f_0.

For one-dimensional classical OCP's, Baxter[3,4] and Kunz[5] have given exact values of thermodynamic quantities. In order to show the effectiveness of our lower bounds, we compare in Fig. 1 exact values of the correlation energy[13] with our effective lower bounds,[12] Eq. (4.3) for $\epsilon < 1$, and

$$B_1[f_0, G]/T = \tfrac{1}{2}\epsilon + \tfrac{1}{2}\epsilon[2\pi^{-1/2}x - 1 + e^{x^2}\mathrm{erfc}(x)] - \tfrac{1}{2}x^2\,, \tag{5.8}$$

where $x = k_D/2G$ and

$$\mathrm{erfc}(x) = 2\pi^{-1/2}\int_x^\infty dt\, e^{-t^2}$$

for $\epsilon > 1$. When $\epsilon \gg 1$ and $1 \gg \epsilon - 1 > 0$ the latter lower bound is given approximately by

$$B_1[f_0, G_0]/T \cong \epsilon^2/2\pi + \tfrac{1}{2} \quad (\epsilon \gg 1)\,,$$
$$\cong \tfrac{1}{2}\epsilon + \tfrac{1}{24}\pi(\epsilon-1)^3 \quad (1 \gg \epsilon - 1 > 0)\,. \tag{5.9}$$

We also plot the lower bound[10] derived from On-

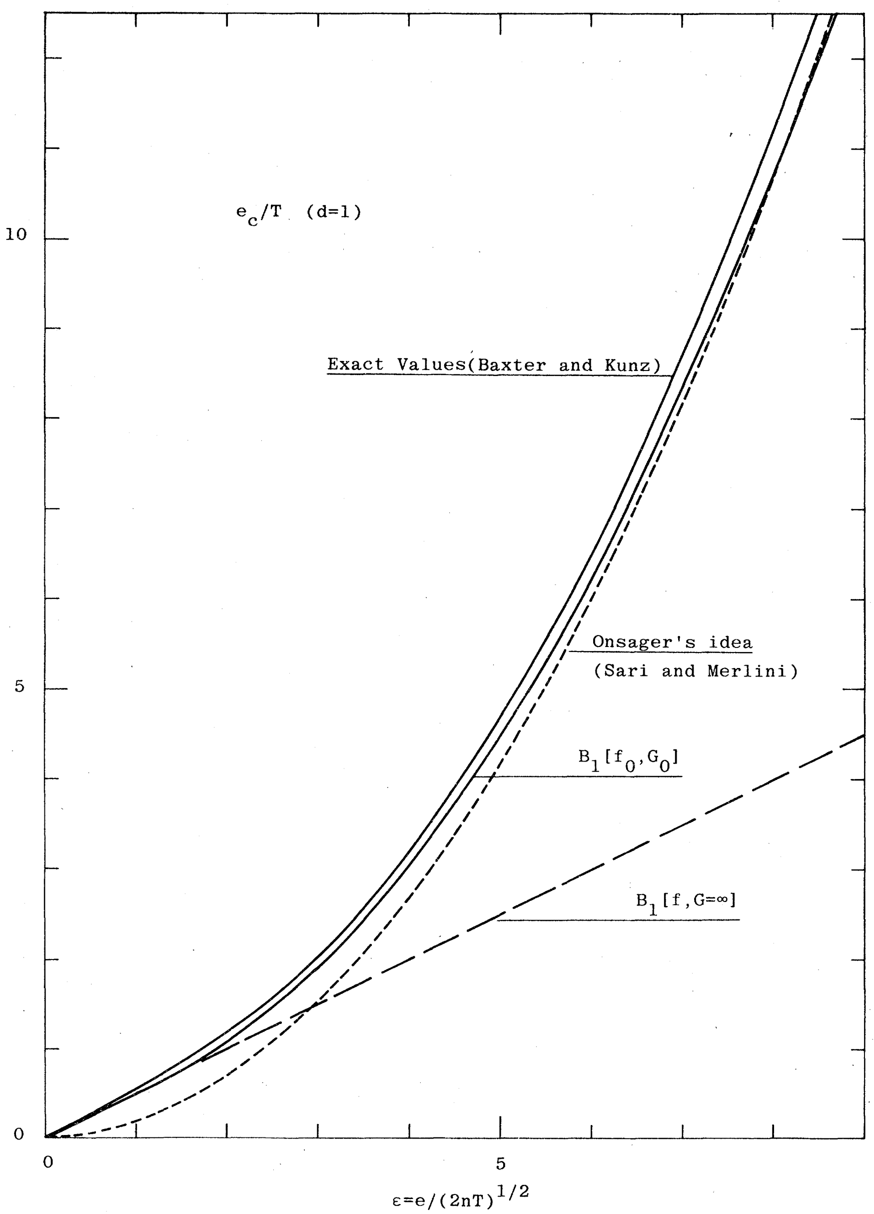

FIG. 1. Correlation energy of the one-dimensional classical one-component plasma. Exact values by Baxter (Refs. 3 and 4) and Kunz (Ref. 5) are represented by the solid line, the lower bounds, Eqs. (4.3) and (5.8), by the solid (or broken when not effective) lines, and that (Ref. 10) due to Onsager's idea (Ref. 14) by the dotted line.

sager's idea,[14]

$$e_c/T \geq \tfrac{1}{6}\epsilon^2 . \qquad (5.10)$$

Our lower bounds, Eqs. (4.3) and (5.8), improve upon the lower bound (5.10) in the domain $\epsilon < 8.11$ and give values closer to exact ones.

In the case of $d=2$, $f_0(k,t)$ gives[12] an effective lower bound,

$$B_1[f_0, G]/T = e_c^{\mathrm{RPA}}/T + \tfrac{1}{4}\epsilon[\gamma + 2\ln x - e^{x^2}\mathrm{Ei}(-x^2)] - \tfrac{1}{2}x^2 , \qquad (5.11)$$

where $x = k_D/2G$ and

$$-\mathrm{Ei}(-x) = \int_x^\infty dt\, \frac{e^{-t}}{t} .$$

In this case the lower bound[10] suggested by Onsager[14] is given as

$$e_c/T \geq -\tfrac{1}{4}\epsilon[\tfrac{3}{2} + \ln(\pi n l^2)]$$
$$= e_c^{\mathrm{RPA}}/T + \tfrac{1}{4}\epsilon[2\gamma - \tfrac{3}{2} + \ln(\tfrac{1}{2}\epsilon)] . \qquad (5.12)$$

I show in Fig. 2 and Table I the lower bounds given by Eqs. (4.3), (5.11), and (5.12). It is shown that my lower bound, Eq. (5.11), greatly improves upon the known lower bound, Eq. (5.12), in the domain $\epsilon < 25.0$.

When $\epsilon \gg 1$ and $\epsilon \ll 1$, the lower bound given by Eq. (5.11) reduces to

$$B_1[f_0, G_0]/T \cong -\tfrac{1}{4}\epsilon[\gamma+1+\ln(\pi n l^2)]+\tfrac{1}{2} = e_c^{\mathrm{RPA}}/T+\tfrac{1}{4}\epsilon[\gamma-1+\ln(\tfrac{1}{2}\epsilon)]+\tfrac{1}{2} \quad (\epsilon \gg 1)\,, \tag{5.13}$$

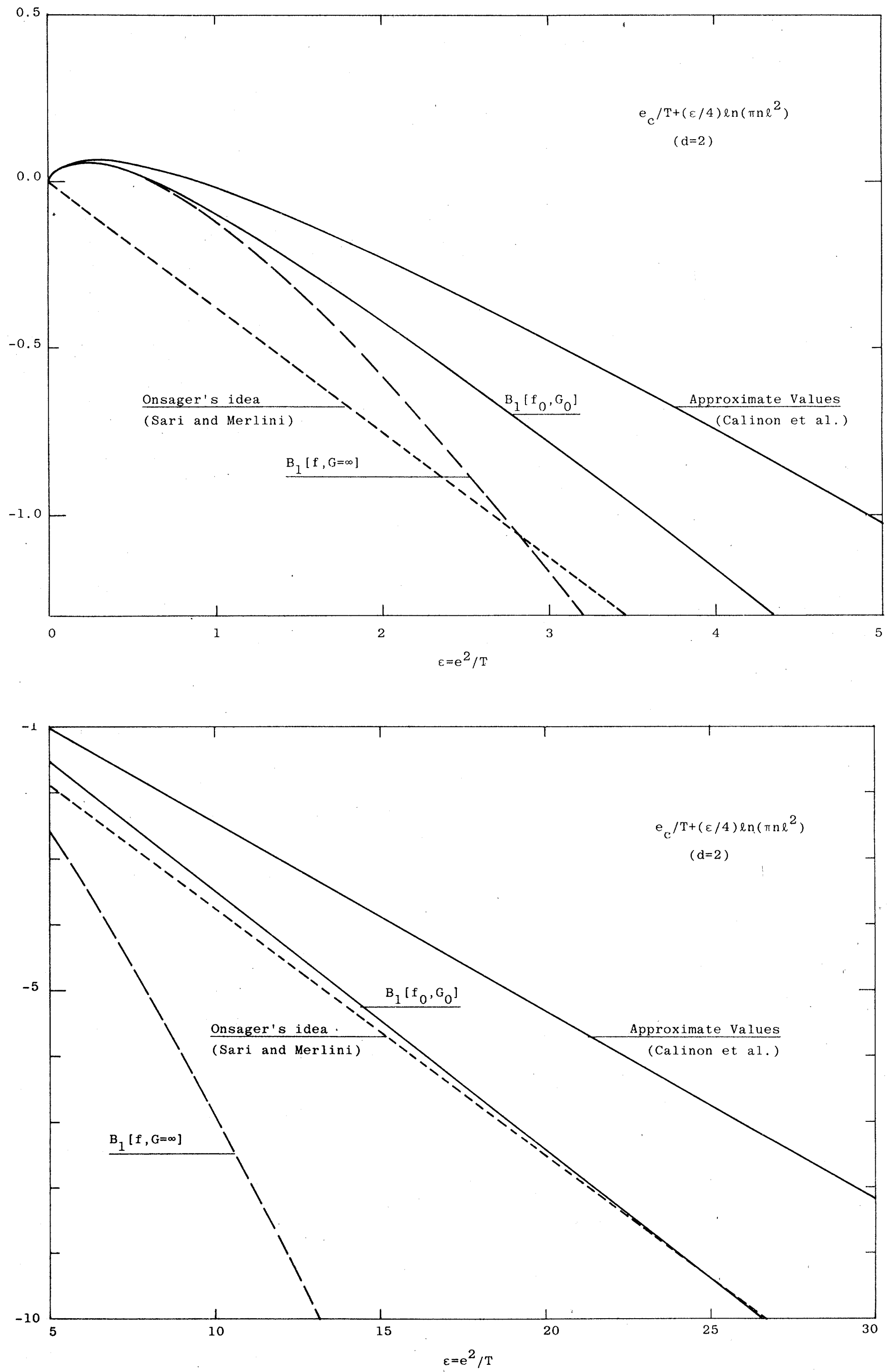

FIG. 2. Correlation energy of the two-dimensional one-component plasma. The lower bounds, Eqs. (4.3) and (5.11), are represented by the solid (or broken when not effective) lines, and the lower bound (Ref. 10) due to Onsager's idea (Ref. 14) by the dotted line, and also approximate values (Ref. 15) by the solid line.

TABLE I. Various exact lower bounds and an approximate value (Ref. 15) for the correlation energy of the two-dimensional classical one-component plasma. Values of $e_c/T + \frac{1}{4}\epsilon \ln(\pi n l^2)$ are given.

Plasma parameter $\epsilon = e^2/T$	Lower bounds: Present paper, Eq. (5.11)	Lower bounds: Present paper, Eq. (4.3)	Lower bounds: Sari and Merlini[a], Eq. (5.12)	Approximate values[b]
0	0	0	0	0
0.1	4.603×10^{-2}	4.603×10^{-2}	-3.75×10^{-2}	4.725×10^{-2}
0.2	5.741×10^{-2}	5.741×10^{-2}	-7.5×10^{-2}	6.217×10^{-2}
0.5	3.031×10^{-2}	2.898×10^{-2}	-1.875×10^{-1}	5.688×10^{-2}
1.0	-9.300×10^{-2}	-1.153×10^{-1}	-3.75×10^{-1}	-1.395×10^{-2}
2.0	-4.224×10^{-1}	-5.772×10^{-1}	-7.5×10^{-1}	-2.306×10^{-1}
5.0	-1.543	-2.588	-1.875	-1.022
10.0	-3.484	-6.910	-3.75	-2.430
20.0	-7.408	-1.729×10	-7.5	-5.296
25.0	-9.376	-2.300×10	-9.375	-6.734
30.0	-1.134×10	-2.897×10	-1.125×10	-8.174

[a]Reference 10.
[b]Reference 15.

$$B_1[f_0 G_0]/T \cong e_c^{\mathrm{RPA}}/T + \tfrac{1}{4}\epsilon^{/\epsilon-\gamma} (\epsilon \ll 1), \tag{5.14}$$

respectively.

Recently, Calinon *et al.*[15] have obtained the solution of the two-dimensional version of the approximate integral equation for the structure factor of strongly coupled three-dimensional OCP's due to Singwi *et al.*[16] Their result for the correlation energy is also plotted in Fig. 2. We see that their solution satisfies both lower bound conditions, Eqs. (5.11) and (5.12).

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[11]One method is to use the relations (Ref. 9) $(0 < d < 5)$

$$\int_0^\infty dk\, J_{d/2-1}(kr) \frac{k^{d/2}}{k^2+\lambda^2} = \lambda^{d/2-1} K_{d/2-1}(\lambda r),$$

$$\int_0^\infty dr\, J_{d/2-1}(kr) K_{d/2-1}(\lambda r) = (k/\lambda)^{d/2-1}\, \Gamma(\tfrac{1}{2}d)/(k^2+\lambda^2),$$

where $K_\nu(x)$ is the modified Bessel function. In this case Eqs. (2.3) and (2.7) become

$$\phi(r) = \lim_{\lambda\to 0} (2\pi)^{-d} \int d\vec{k}\, \Phi(k) \exp(i\vec{k}\cdot\vec{r})$$

$$= \lim_{\lambda\to 0} 2^{1-d/2}\, \Gamma(d/2)^{-1} [(\lambda/r)^{d/2-1} K_{d/2-1}(\lambda r)$$

$$- (\lambda/l)^{d/2-1} K_{d/2-1}(\lambda l)],$$

$$\Phi(k) = \lim_{\lambda\to 0} \int d\vec{r}\, \phi(r) \exp(-i\vec{k}\cdot\vec{r})$$

$$= \lim_{\lambda\to 0} 2\pi^{d/2}\, \Gamma(\tfrac{1}{2}d)^{-1} [(k^2+\lambda^2)^{-1} - (2\pi)^{d/2}$$

$$\times (\lambda/l)^{d/2-1} K_{d/2-1}(\lambda l)\, \delta(\vec{k})].$$

[12]As trial functions I have taken f_0, $ce^{-k/t}t^{-3}$, and $c(k^2t^{-2}+1)^{-\nu}t^{-3}$, with $\nu=\frac{3}{2}$ and 2.

[13]According to our definition of the correlation energy Eq. (3.1), the energy $\frac{1}{6}\epsilon^2 T$ is added to the values given in Ref. 3 in order to adjust the zero level.

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