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Particle correlations in the strongly coupled two-dimensional one-component plasma

P. Bakshi
Department of Physics and Center for Energy Research, Boston College, Chestnut Hill, Massachusetts 02167

R. Calinon
Départment de Physique, École Polytechnique Fédérale de Lausanne, CH-1007 Lausanne, Switzerland

K. I. Golden
Department of Electrical Engineering, Northeastern University, Boston, Massachusetts 02115

G. Kalman
Department of Physics and Center for Energy Research, Boston College, Chestnut Hill, Massachusetts 02167

D. Merlini
Department of Physics, University of California, San Diego, La Jolla, California 92037
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The equilibrium pair-correlation function and static dielectric response function are calculated for the one-component two-dimensional plasma in the convolution (Totsuji-Ichimaru) approximation. The long-wavelength ($k \rightarrow 0$) compressibility sum rule is exactly satisfied for arbitrary values of the plasma parameter γ. For $\gamma < 2$ the approximation scheme accurately describes the short-range ($r \rightarrow 0$) behavior of the pair-correlation function $g(r)$ while for $\gamma \geq 2$, it does not. As $\gamma \rightarrow 4$ the isothermal compressibility tends to zero as it should. The correlation energy is also calculated for this model and compared with the results for other approximation schemes and the Monte Carlo results.

I. INTRODUCTION

By now a considerable amount of progress has been made on the theoretical side in describing the static ($\omega = 0$) and dynamical ($\omega \neq 0$) behavior of the strongly coupled classical one-component plasma (ocp). Essentially two different approaches, both nonperturbative in the plasma parameter γ, have been followed. One of these which contemplates the introduction of a weak perturbing electric field into the equilibrium ocp, has as its most general objective the calculation of the frequency- and wave-vector-dependent dielectric response functions from the first Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) *kinetic* equation and fluctuation-dissipation theorems.[1,2] Evidently, this approach can lead not only to a static description of the plasma (its equilibrium pair-correlation function and equation of state), but to a dynamical description (high frequency conductivity and collective mode behavior) as well. The second approach—more modest in its scope—is the one which we follow in this paper. It has as its goal the calculation of the equilibrium pair-correlation function $g(r)$ from the second BBGKY *static* equation. Note that recently, and following this latter approach, it has been possible to obtain an analytical solution for $g(k)$ in the Singwi-Tosi-Land-Sjölander (STLS) approximation[3,4] for any coupling strength γ. Here we will consider the more complicated convolution approximation (Totsuji and Ichimaru scheme)[5] for the two-dimensional ocp, where closure for the equation for $g(k)$ is achieved by the introduction of a decomposition of the triplet correlation function into clusters of the pair-correlation functions.

In their treatment of the strongly coupled three-dimensional (3D) classical ocp, Totsuji and Ichimaru[5(b)] found that its isothermal compressibility tends to zero as γ tends to a certain critical value γ_c. They argue that if the ocp constraint on the background particles is removed, their ensuing long-wavelength fluctuations will be greatly enhanced at $\gamma = \gamma_c$. Beyond this, they conjecture that there is a second critical value $\gamma_s > \gamma_c$ at which crystallization occurs. The onset of crystallization has long since been confirmed by 3D classical ocp computer experiment.[6]

The study of the 2D model has been motivated to some extent by the interest in the ideal guiding center plasma whose equation of state is that of the plasma in a strictly two-dimensional world. Moreover, the 2D configuration is of interest in itself and a knowledge of its thermodynamic properties certainly sheds additional light on the 3D configuration. Besides the considerable progress that has occurred over the years in the study of 3D systems, the investigation of the 2D classical ocp is also well developed now through our knowledge of its *exact* equation of state[7-10] and long-

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wavelength compressibility sum rules,[11] and the exact detailed solution for the equilibrium pair-correlation and dielectric response functions, for all coupling strengths, in a particular approximation scheme.[3,4] Our goal in this paper is to analytically and numerically calculate these objects in the Totsuji-Ichimaru approximation for values of γ up through (and somewhat beyond) γ_c. Here we remind the reader that in the two-dimensional world, the relevant plasma parameter $\gamma = \beta e^2$ (e is the charge and β^{-1} the temperature in energy units) is independent of density.

The plan of the paper can now be sketched as follows: In Sec. II, we formulate the approximation scheme in terms of the pair-correlation function and structure factor. In Sec. III, we analyze the long-wavelength behavior of the structure factor and compare it with a recently established compressibility sum rule. An analysis of the short-range properties of the pair-correlation function is presented in Sec. IV. In Sec. V, we present and discuss the numerical solutions. Correspondence is made with the analyses presented in the preceeding two sections, and the effective potential surrounding a test particle is numerically evaluated over the entire range of k values. Section VI deals with the calculation of correlation energy in this approximation scheme, and a comparison with results from other schemes and Monte Carlo results. We draw our conclusions in Sec. VII.

II. FORMULATION OF THE APPROXIMATION SCHEME

In this section, we define quantities of interest and select an approximation scheme which will provide a description of the static behavior of the classical ocp in a strictly 2D configuration. In such a configuration, the Coulombic interaction energy between two particles i and j is logarithmic, i.e., $\phi_{ij} = -e^2 \ln r_{ij}$ where $r_{ij} = |\vec{x}_i - \vec{x}_j|$. The equilibrium pair- and triplet-correlation functions, $g(r_{12})$ and $h(r_{12}, r_{13})$—objects of primary importance in statistical mechanics—provide such a description. They are defined through the following relations involving the one-, two-, and three-particle distribution functions:

$$G(x_1, v_1; x_2, v_2) = F(v_1)F(v_2)[1 + g(r_{12})] ,$$

$$H(x_1 v_1; x_2, v_2; x_3, v_2) = F(v_1)F(v_2)F(v_3)[1 + g(r_{12}) + g(r_{13}) + g(r_{23}) + h(r_{12}, r_{13})] .$$

In this notation, $F(v)$ is the Maxwellian distribution function normalized to N, the total number of particles, in the 2D volume V, i.e., $\int F(1)d1 \equiv \int\int F(v_1)dv_1)dx_1 = N$. Similarly,

$$\iint G(12)d1\, d2 = N(N-1), \quad \iiint H(123) d1\, d2\, d3 = N(N-1)(N-2) .$$

Finally, we note the relation

$$S(k) = 1 + ng(k), \quad n = N/V , \tag{1}$$

between the Fourier transformed pair correlation function and the static structure factor.

For the calculation of $g(k)$ in the 2D ocp, we adopt the approximation scheme used by Totsuji and Ichimaru[5] in their treatment of the 3D ocp. In this scheme, one starts from the second BBGKY static equation

$$\begin{aligned} ng(k) &= -\frac{\kappa^2}{k^2 + \kappa^2}\left(1 + \frac{1}{V}\sum_{\vec{p}} \frac{\vec{k}\cdot\vec{p}}{p^2}\,[g(|\vec{k}-\vec{p}|) + nh(\vec{k}-\vec{p}, \vec{p})]\right) , \\ \kappa^2 &= 2\pi\beta e^2 n , \end{aligned} \tag{2}$$

connecting $g(k)$ to the Fourier-transformed triplet-correlation function, $h(\vec{k}-\vec{p}, \vec{p})$. In the convolution approximation, h is approximated in terms of g clusters as follows:

$$\begin{aligned} h(\vec{k}-\vec{p}, \vec{p}) = g(|\vec{k}-\vec{p}|)g(p) + g(|\vec{k}-\vec{p}|)g(k) \\ + g(k)g(p) + ng(k)g(p)g(|\vec{k}-\vec{p}|) . \end{aligned} \tag{3}$$

Upon combining Eqs. (2) and (3), one obtains

$$ng(k) = \frac{-\kappa^2[1 + u(k)]}{k^2 + \kappa^2[1 + u(k)]} , \tag{4}$$

$$\begin{aligned} u(k) &= \frac{1}{V}\sum_{\vec{p}} \frac{\vec{k}\cdot\vec{p}}{p^2}\,[1 + ng(p)]g(|\vec{k}-\vec{p}|) \\ &= \frac{1}{(2\pi)^2}\int d^2p\, \frac{\vec{k}\cdot\vec{p}}{p^2}\,[1 + ng(p)]g(|\vec{k}-\vec{p}|) . \end{aligned} \tag{5}$$

Note that in the STLS scheme investigated recently[3,4] u is as above without ng in the parenthesis. Equivalently, in terms of the structure factor, we have

$$S(x) = x^2[x^2 + 1 + u(x)]^{-1} , \tag{6}$$

$$u(x)=\frac{\gamma x}{2\pi}\int_0^\infty dy\int_0^{2\pi} d\theta\cos\theta S(y)S(|\vec{x}-\vec{y}|)\,, \tag{7}$$

where $x=k/\kappa$, $y=p/\kappa$, and θ is the angle between $\vec{k}$ and $\vec{p}$. Equations (6) and (7) [or (4) and (5)] form a nonlinear integral equation which has to be solved numerically. Before doing this, however, we shall first analyze S and g in certain asymptotic limits.

III. LONG-WAVELENGTH LIMIT

In the long-wavelength limit $(x\rightarrow 0)$,

$$S(|\vec{x}-\vec{y}|)\approx S(y)-x\cos\theta\frac{dS(y)}{dy}+(x^2/2)\left(\cos^2\theta\frac{d^2S(y)}{dy^2}+\frac{\sin^2\theta}{y}\frac{dS(y)}{dy}\right)$$
$$-(x^3\cos^3\theta/6)\left(\frac{d^3S(y)}{dy^3}+3\tan^2\theta\frac{d}{dy}\frac{1}{y}\frac{dS(y)}{dy}\right)+\cdots\,,$$

so that from Eq. (7),

$$u(x\rightarrow 0)\approx -(\gamma/4)x^2+\left[(\gamma/16)\int_0^\infty\frac{dy}{y}\left(\frac{dS(y)}{dy}\right)^2\right]x^4+\cdots\,. \tag{8}$$

Thus from Eq. (6), one readily obtains

$$\lim_{x\rightarrow 0}\frac{[x^2-S(x)]}{x^2S(x)}=1-(\gamma/4)+O(x^2)\,, \tag{9}$$

a result that is evidently valid for arbitrary values of γ. The 2D ocp compressibility rule[11]

$$\lim_{x\rightarrow 0}x^2[\epsilon(x,0)-1]=[1-(\gamma/4)]^{-1}\quad(\gamma\text{ arbitrary})\,, \tag{10}$$

for the static long-wavelength dielectric response function $\epsilon(x,0)$ is then readily recovered by application of the linear fluctuation-dissipation theorem

$$S(x)=x^2\left(1-\frac{1}{\epsilon(x,0)}\right) \tag{11}$$

to (9). It is therefore clear that the Totsuji-Ichimaru approximation scheme, when applied to the 2D ocp, exactly satisfies its compressibility sum rule for *arbitrary values of the plasma parameter*, in the sense of Eqs. (9), (10), and (11). Clearly, the isothermal sound speed tends to zero as $\gamma\rightarrow 4$. This is related to the fact that what appears in the calculation is the exact thermal pressure given, by $\beta P=n(1-\gamma/4)$, which for ocp plasmas is, in general, different from the kinetic or virial pressure, which is always nonnegative; this point is discussed in the Appendix.

As to the long-wavelength expression for the structure factor when higher-order (in x^2) terms are retained, one again finds from Eqs. (6) and (8) that

$$S(x\rightarrow 0)\approx x^2-[1-(\gamma/4)]x^4+\left[[1-(\gamma/4)]^2-\frac{\gamma}{16}\int_0^\infty\frac{dy}{y}\left(\frac{dS}{dy}\right)^2\right]x^6+\cdots\,. \tag{12}$$

Then to calculate the structure factor in the weakly coupled limit $(\gamma\ll 1)$, one simply replaces S in the integral in Eq. (12) by its Debye-Huckel value $S_0(y)=y^2/(1+y^2)$. The resulting long-wavelength formula

$$S(x\rightarrow 0)\,|\approx x^2-[1-(\gamma/4)]x^4+[1-(13\gamma/24)]x^6+\cdots\,,\quad\gamma\ll 1 \tag{13}$$

is in agreement with the results obtained for the exact formal expression of the BBGKY hierarchy, as given for the 3D situation by O'Neil and Rostoker.[12]

IV. SHORT-RANGE BEHAVIOR

A way of assessing the short-range behavior of $g(r)$ in various ocp approximation schemes, based on an analysis of the configuration space equations, has been proposed[13(a),13(b),13(c)] and may be applied to Eqs. (4) and (5). The starting point is the well-known Ornstein-Zernike relation

$$g(r)=c(r)+\iint d^2r'c(\vec{r}')g(|\vec{r}-\vec{r}'|)\,, \tag{14}$$

which connects the direct correlation function $c(r)$ to $g(r)$. Using the equivalent k-space relation between c and g, one can rewrite Eqs. (4) and (5) in a simpler form, which, upon transformation to the configuration space, leads to the differential equation

$$\nabla^2c(r)=\gamma\vec{\nabla}\psi(r)\cdot\vec{\nabla}g(r)+\kappa^2g^2(r)\,, \tag{15}$$

where for the 2D ocp,

$$\psi(r)=\ln r+\iint d^2r'\ln r' ng(|\vec{r}-\vec{r}'|)\,. \tag{16}$$

Upon combining Eqs. (14) to (16), one obtains the following integrodifferential equation for the pair-correlation function:

$$g''(r)+\{1-\gamma[1+U(r)]\}\frac{1}{r}g'(r)-\kappa^2 g^2(r)$$
$$=\gamma\iint d^2r'\,[1+U(r')]ng(|\vec{r}-\vec{r}'|)\frac{1}{r'}g'(r')$$
$$+\kappa^2\iint d^2r'\,ng(|\vec{r}-\vec{r}'|)g^2(r'), \tag{17}$$

where

$$U(r)\equiv\iint d^2\vec{r}'\frac{\vec{r}\cdot\vec{r}'}{r'^2}ng(|\vec{r}-\vec{r}'|)=\frac{n}{2\pi}\int_0^r dr'r'g(r'), \tag{18}$$

which latter relationship follows by exploiting the similarity of structure between $U(r)$ and u_k in Refs. 3 and 4. Now in the small-r limit, Eq. (17) simplifies to

$$r^{\gamma-1}\frac{d}{dr}r^{1-\gamma}\frac{dg(r)}{dr}\approx\frac{B}{2}, \tag{19}$$

where B is a constant, given by

$$B\equiv\kappa^2\left(1+4\pi\int_0^\infty dr\,rng^3(r)+\int_0^\infty dr\,U(r)\frac{dg^2(r)}{dr}\right)$$
$$=\kappa^2\left(1+\int d^2r\,ng^3(r)\right)$$
$$=-\kappa^2\int d^2r\,ng(r)[1-g^2(r)]. \tag{20}$$

The complete solution of (19) is readily found to be.

$$g(r\to 0)\approx\begin{cases}(A/\gamma)r^\gamma-1+\dfrac{Br^2}{4(2-\gamma)}, & \gamma\neq 2 \quad (21)\\[2ex](A/2)r^2-1+\dfrac{Br^2}{4}(\ln r-\tfrac{1}{2}), & \gamma=2.\end{cases} \tag{22}$$

We note that the small-r approximations in Eqs. (19) to (22) require

$$\kappa^2r^2<2\pi nr^2\ll 1,\quad \gamma<1$$
$$2\pi nr^2<\kappa^2r^2\ll 1,\quad \gamma>1.$$

Concerning the sign of B, it is definitely positive for small and moderate values of γ. A sign change in B can occur only if $|\int d^2r\,ng^3(r)|$ exceeds unity. This is impossible as long as $g(r)$ remains a monotonically increasing function, from $g(0)=-1$ to $g(\infty)=0$, as is the case for small and moderate γ (see the numerical results in the Sec. V). Increasing γ leads to $g<-1$ for some range of r near the origin and oscillations around $g=0$ for large r, causing a reduction in the magnitude of B with increasing γ. A sign reversal can occur only if one or both of these factors become significant over a large range of r.

The constant $A\equiv\gamma C(\gamma)$ is associated with the homogeneous solution

$$g_H(r\to 0)=Cr^\gamma-1 \tag{23}$$

of the complete solution. The homogeneous part is, in fact, the correct expression for $g(r\to 0)$; it follows from the fact that the two-particle potential is $\phi(r)=-e^2\ln r$ and thus the pair-correlation function in the binary approximation $g(r\to 0)=e^{-\beta\phi(r)}-1$ yields the above expression (23). Equations (21) and (22) reveal, however, that for $\gamma<2$, Eq. (21) yields the correct dominant r^γ term, while for $\gamma\geq 2$ it does not, a situation analogous to what happens in the STLS scheme.[4,13]

V. NUMERICAL SOLUTIONS AND COMPARISONS

Equation (4) [or equivalently, Eq. (6)] has been solved numerically by an iterative procedure. The solutions, displayed in Figs. 1 and 2, curves of $ng(k)$ versus (k/κ), and versus ka [where $a=(n\pi)^{-1/2}$ is the ion circle radius], are obtained for values of γ ranging from 0–6. We have carried out a comparison of the numerical data with the long-wavelength structure factor in the weak coupling limit (WCL) as calculated from Eq. (13), and we find a nearly perfect agreement between the two for $k/\kappa\leq 0.1$.

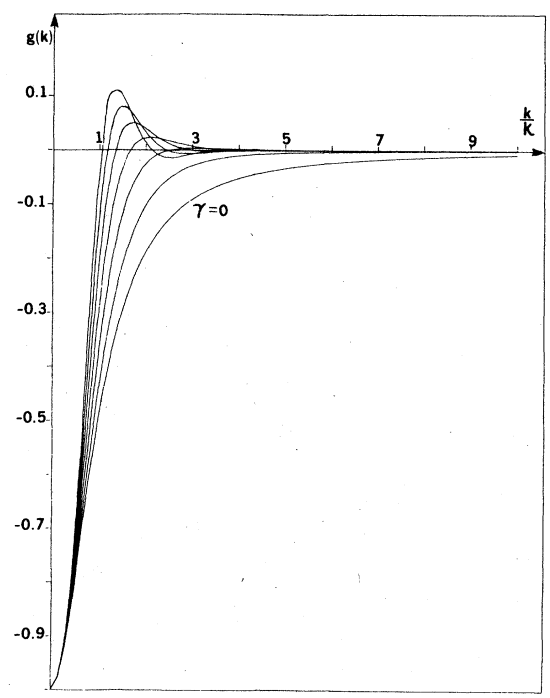

FIG. 1. Correlation function $ng(k)$ versus (k/κ), for coupling strengths $\gamma=0, 1, 2, 3, 4, 5, 6$.

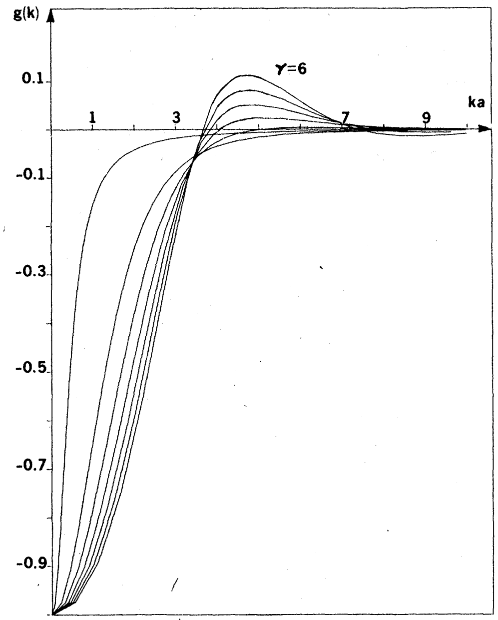

FIG. 2. Correlation function $ng(k)$ versus ka, for coupling strengths $\gamma=0$, 1, 2, 3, 4, 5, 6,.

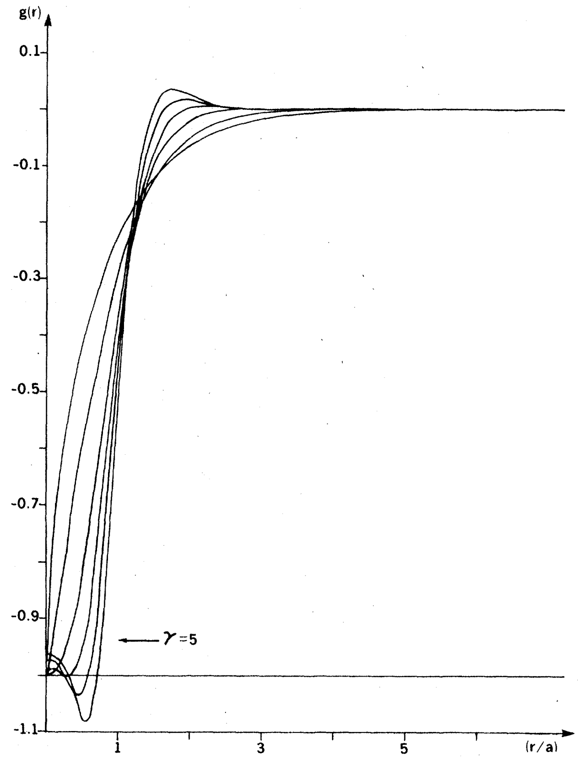

FIG. 3. Correlation function $g(r)$ versus (r/a), for coupling strengths $\gamma=0.5$, 1, 2, 3, 4, 5.

Figure 1 also reveals that for values up to $\gamma \simeq 2$, $ng(k)$ is always negative within the domain of k considered and increases from its value of -1 at $k=0$ to zero as $k\rightarrow\infty$. For higher values of γ, $ng(k)$ exhibits a positively valued peak accompanied by extremely faint oscillations; these become more pronounced as γ increases, and also the oscillatory region shifts towards smaller values of k.

We have also computed the configuration space correlation function $g(r)$ by taking a Fourier transform of $g(k)$, for values of γ ranging from 0.5 to 5. These results, displayed in Fig. 3, indicate that for $\gamma>2$, $g(r)$ becomes less than (-1) over a range of r values near the origin. This leads to a negative probability (in that range) for finding a particle at a distance r from a test particle, since $1+g(r)<0$. This situation is analogous to the three-dimensional version of the Totsuji and Ichimaru scheme, which also leads to negative probability at short distances.[13] This seems to be a general problem for the TI scheme, unlike the STLS scheme in either two[4,13] or three[13] dimensions, which provides a positive probability throughout. The other defect of the TI scheme for short-range behavior for $\gamma \geq 2$ is the dominance of the r^2 term over the physically expected r^γ term in the total solution: The latter can be expected to arise on physical grounds as $\exp(-\beta\phi) = r^\gamma$, where ϕ is the Coulomb potential $\phi(r) = -e^2 \log r$. This problem is analogous to the corresponding shortcoming of the STLS scheme[4,13] or of the 2D classical ocp version of the Vashishta-Singwi[1(b)] scheme where $B=\kappa^2$. The γ-dependence of this criterion is a special feature of the two-dimensional Coulomb plasma; in three dimensions, both the TI and STLS schemes lead[13] to the anomalous dominance of the r^3 term over the physically expected $\exp(-\Gamma a/r)$ for all Γ, where $\Gamma=\beta e^2/a$ is the three-dimensional strong-coupling parameter and a is the ion sphere radius.

We should point out here that our numerical results for $g(r)$ for very small r, $r/a<0.2$, developed spurious fluctuations. These are probably due to the importance of $g(k)$ for large k. The computed results for $g(r)$ for small r were smoothed out, and then they did provide the expected smooth r^2 behavior for $r\rightarrow 0$ for $\gamma \geq 2$. The sign of the coefficients was also in agreement with the analytical prediction. In spite of the smoothing out, however, the computed value $g(0)$ differed slightly from -1, and the computed coefficients of the r^2 terms differed slightly in magnitude from the analytically predicted values. We ascribe these minor discrepancies to the difficulty in achieving sufficient precision in the computation of $g(k)$ for large k. The curves displayed in Fig.

3 are the smoothed out computed curves.

We next consider the effective potential around a test particle Φ_k given by

$$\Phi_k=\frac{\phi_k}{\epsilon(k,0)}=\frac{1}{\beta n x^2\epsilon(x,0)}\ , \tag{24}$$

$$\phi_k=\frac{2\pi e^2}{k^2}=\frac{1}{\beta n x^2}\ ,$$

where $\epsilon(k,\omega)$ is the dielectric function of the system. Upon combining (24) and the fluctuation-dissipation theorem (11), one can express the effective potential as

$$\beta n\Phi(x)=\frac{1}{x^2}\left(1-\frac{S(x)}{x^2}\right). \tag{25}$$

The combination of Eqs. (12) and (25) then gives in the long-wavelength limit

$$n\beta\Phi(x\to 0)=\lim_{x\to 0}\left\{[1-(\gamma/4)]-\left[[1-(\gamma/4)]^2-\left(\frac{\gamma}{16}\right)\int_0^\infty\frac{dy}{y}\left(\frac{dS}{dy}\right)^2\right]x^2\right\}, \tag{26}$$

so that for $\gamma=4$,

$$n\beta\Phi(x\to 0)=\lim_{x\to 0}\tfrac{1}{4}x^2\int_0^\infty\frac{dy}{y}\left(\frac{dS}{dy}\right)^2=0\,. \tag{27}$$

The effective potential has been numerically calculated from Eq. (25) and the results are displayed in Fig. 4.

For $\gamma=0$ one deals with the screened Debye potential and $\beta n\Phi(x=0)=1$, indicating that $\int dr\,\Phi(r)$ is finite (while the same integral for the bare potential $\int dr\,\phi(r)=-e^2\int dr\ln r$ is infinite) and positive, i.e., has the same sign as the bare potential. This is, of course, the manifestation of the screened character of the effective potential. We see, however, that for $\gamma=4$ the situation changes. For $\gamma>4$, $\int dr\,\Phi(r)<0$, even though $\Phi(r=0)>0$ still holds. This is possible only if $\Phi(r)$, rather than being screened assumes an oscillatory character and develops negative domains. A similar behavior has already been observed for the STLS model,[4] where however, the critical value of γ was 2.

From the exact two-dimensional ocp equation of state,

$$\frac{\beta P}{n}=1-\frac{\gamma}{4}\ , \tag{28}$$

we observe that the $\gamma=4$ is the critical value of γ where the isothermal sound speed

$$C_T=\left(1-\frac{\gamma}{4}\right)^{1/2}(\beta m)^{-1/2}$$

tends to zero. The fact that now the effective potential $\Phi(x=0)=0$ at this value of γ, is a consequence of the TI scheme exactly satisfying the compressibility sum rule. As γ increases beyond 4, we observe in Fig. 5 that the smallest-k peaks

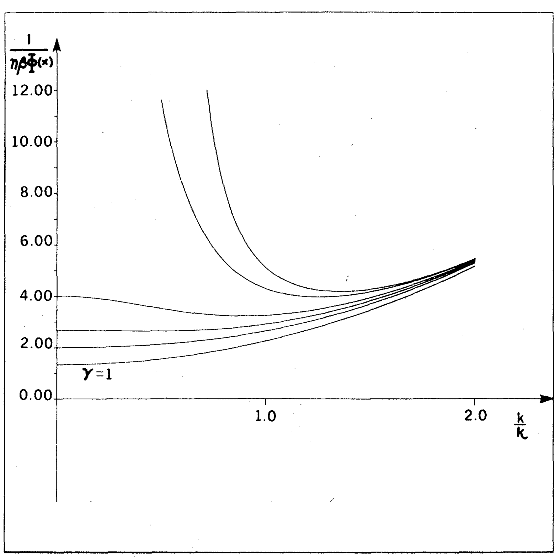

FIG. 4. Inverse of the effective potential $[n\beta\Phi(x)]^{-1}$ versus $x=k/\kappa$, for coupling strengths $\gamma=1,\ 2,\ 2.5,\ 3,\ 4,\ 4.5$.

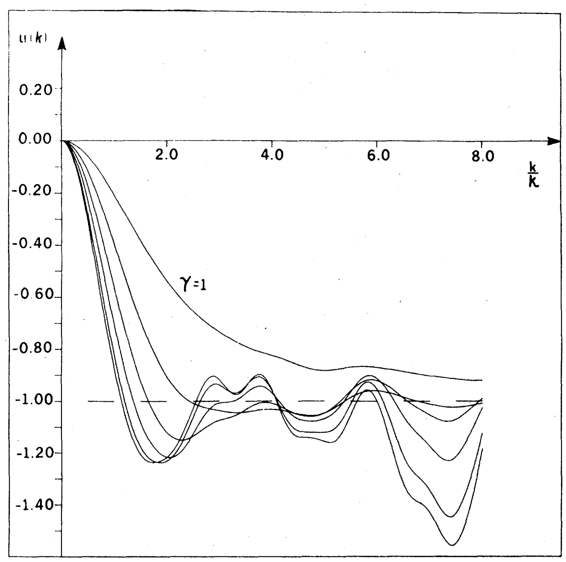

FIG. 5. Screening function $u(k)$ versus k/κ, for coupling strengths $\gamma=1,\ 2,\ 3,\ 4,\ 5,\ 5.5$.

in the screening function $u(k)$ shift to the left and become more and more negative apparently converging to a value of -1.23. In view of this, one can perhaps speculate that there exists a critical value γ_s of γ such that the condition

$$k^2+\kappa^2[1+u(k)]=0 \tag{29}$$

is satisfied at the peak position k_s of k. This would correspond to $S(k_s)\to\infty$ and consequently to the onset of a nonhomogeneous state for the 2D ocp liquid. To estimate γ_s, we assume that k_s is sufficiently small so that one can approximate $u(k_s)$ by its compressibility sum rule value [cf. Eq. (8)]:

$$u(k_s)\approx-(\gamma/4)k_s^2/\kappa^2=k_s^2/8\pi n\,. \tag{30}$$

Taking $u(k_s)\approx-1.23$ with the understanding that this assumed value is speculative, one finds from (29) and (30) that

$$\gamma_s\approx 21.4\,.$$

VI. CORRELATION ENERGY AND EQUATION OF STATE

For the two-dimensional ocp, the correlation energy is given by

$$\beta E_C=-\tfrac{1}{2}\gamma n\int d^2r\,g(r)\log r\,. \tag{31}$$

After Fourier transformation to k space we obtain

$$\beta E_C=-\gamma\left[\frac{C}{2}+\tfrac{1}{4}\log\left(\frac{\gamma}{2}\right)+\tfrac{1}{4}\log(\pi n)-\tfrac{1}{2}Q(\gamma)\right], \tag{32}$$

where

$$Q=\int_0^\infty\frac{dx}{x}\left(G(x)+\frac{1}{1+x^2}\right) \tag{33}$$

with $C=0.5772\ldots$ being the Euler constant. In our earlier work[3] we have analytically evaluated the integral Q in the STLS truncation scheme

$$Q=\tfrac{1}{2}\log(1+\gamma/2)\,, \tag{34}$$

leading to

$$\beta E_C=\gamma\left[a+b\log\left(\frac{\gamma}{\gamma+c}\right)-\tfrac{1}{4}\log(\pi n)\right] \tag{35a}$$

with

$$a=-\frac{C}{2},\quad b=-\tfrac{1}{4},\quad c=2\ \ (\text{STLS})\,. \tag{35b}$$

Recently a unified description of the approximation schemes STLS, TI, and HNC has been given[14] and it is shown that TI scheme gives a more accurate description of ocp than STLS, and HNC than TI. Using our numerical solution for $g(k)$ in the TI scheme [obtained by solving Eqs. (4) and (5) or (6) and (7)], we have evaluated the correlation energy as a function of γ. Then using the expression (35a) we find that a reasonably accurate description of βE_C as a function of γ is obtained if we adopt (35a) as a functional form for representing E_C and choose

$$a=-0.374,\quad b=-0.245\,,\quad c=3.02\,,\ \ (\text{TI})\,. \tag{35c}$$

This result may be compared with results obtained in the STLS and HNC[15] schemes, and Monte Carlo simulation[16] as shown in Fig. 6.

The total heat capacity per particle at constant volume can be easily derived to be

$$C_V=k_B\left(a+\frac{|b|c\gamma}{\gamma+c}\right). \tag{36}$$

C_V increases monotically with γ starting from the perfect gas of 1 and reaching the maximum value of 1.73. This latter limit is to be compared with the STLS value of 1.5 and with the 2D harmonic crystal value of 2.

Similar to the STLS scheme, the 2D ocp equation of state may be obtained for the TI scheme also if we adopt the form (35a). We first calculate the correlational free energy per particle, $F_c=F-F_0$,

$$\frac{\beta F_c}{N}=\frac{\beta}{\gamma}\int_0^\gamma d\gamma' E_c(\gamma')$$
$$=\beta E_c-bc\log\left(\frac{\gamma+c}{c}\right), \tag{37}$$

and then the expression for the thermal pressure $P=-(\partial F/\partial V)_T$ immediately leads to the well-known equation of state

$$\frac{\beta P}{n}=1-\frac{\gamma}{4}\,. \tag{38}$$

Exact values for the correlational free energy F_c

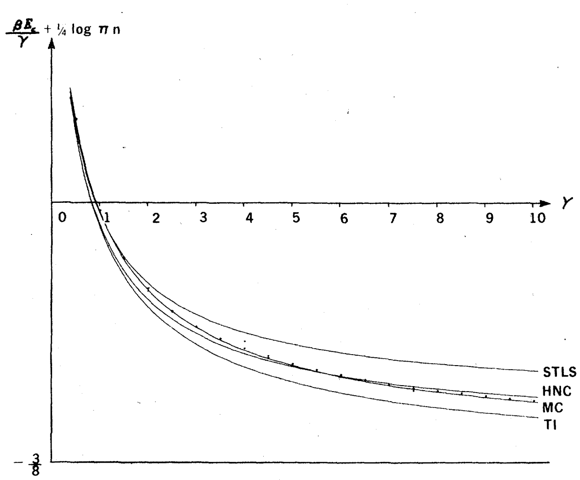

FIG. 6. Correlation energy versus γ; plotted in the form $\beta E_c/\gamma=\frac{1}{4}\log(\pi n)$ versus coupling strength γ.

have recently been obtained by Alastuey and Jancovici[17] for $\gamma \to \infty$ (where it agrees with E_c) and for $\gamma = 2$. It is instructive to compare the STLS, TI, and exact values for $(\beta F_c/N\gamma)$, apart from the $\log(\pi n)$ term, at these points

	$\gamma = 2$	$\gamma \to \infty$
STLS	0.0580	−0.289
TI	0.0395	−0.374
Exact	0.0405	−0.374 38.

Apparently, and not surprisingly, the TI values are closer to the exact figures. A word of caution, however, is in order. As we have noted, the justification for adopting (35a) as a generally valid formula stems from the good numerical fit it provided. Nevertheless, it should be observed that for $\gamma \to 0$ it gives

$$\beta E_c = \gamma [a - b \log c - \tfrac{1}{4} \log(\pi n) + b \log\gamma] .$$

From a comparison of this expression with the Debye correlation energy[3] one can infer the constraints

$$\begin{aligned} &b = -\tfrac{1}{4} , \\ &a - b \log c = -C/2 + \tfrac{1}{4} \log 2 , \end{aligned} \tag{39}$$

which are violated by the TI parameters as given by (35c). Thus, while (35a) is a reasonable formula for intermediate values of γ, it is not so good an approximation for $\gamma \to 0$. Since the correlational free energy $F_c(\gamma)$ is obtained through an integral involving $E_c(\gamma')$ covering the entire γ' domain extending from $\gamma' = 0$ to $\gamma' = \gamma$, the accuracy of the free energy obtained through (35c) is probably much poorer than otherwise warranted by the approximation.

VII. CONCLUSIONS

The equilibrium pair-correlation and static dielectric response functions have been calculated for the strongly coupled 2D classical ocp in the Totsuji-Ichimaru approximation. The long-wavelength ($k \to 0$) and short-range ($r \to 0$) behavior of the correlation function are assessed by use of precise analytical techniques. In particular, a correspondence is established between our numerical results for $g(r)$ and its analytically predicted short-range behavior. We cite the following key results of our study:

(i) The long-wavelength ($k \to 0$) dielectric response function $\epsilon(k, \omega = 0)$ exactly satisfies the compressibility sum rule for arbitrary values of the plasma parameter γ.

(ii) For $0 < \gamma < 2$, the approximation scheme correctly describes the short-range ($r \to 0$) behavior of $g(r)$, while for $\gamma \geq 2$, it does not.

(iii) As $\gamma \to 4$, the isothermal compressibility tends to zero, and changes sign for $\gamma > 4$.

(iv) The effective potential changes character (from screened to oscillatory) at $\gamma = 4$.

(v) Using the numerically obtained $g(k)$, the correlation energy has been calculated for the TI scheme and is compared with the results obtained for other schemes (STLS and HNC), and with Monte Carlo data. It is found that there is an improvement over the STLS results, but that the HNC result comes closer to the Monte Carlo data.

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APPENDIX

The expression for thermal pressure (Sec. III),

$$\beta p = n\left(1 - \frac{\gamma}{4}\right)$$

will assume negative values for $\gamma > 4$. It should be recognized, however, that there are various definitions of "pressure", e.g., the *thermal* pressure and the *kinetic* (or *virial*) pressure. The discrepancy between these two definitions of pressure in a ν-dimensional ocp has been investigated recently by Choquard, Favre, and Gruber[18] and by Navet, Jamin, and Feix.[19] The total force acting on a particle i is given by

$$\vec{F}_i = \vec{F}_{iB} + \vec{F}_{iW} + \sum_j \vec{F}_{ij} .$$

where the three terms refer to forces due to the background, the wall, and other particles. Each term is associated with the corresponding virial

$$V = -\left\langle \sum_i \vec{F}_i \cdot \vec{x}_i \right\rangle .$$

It can be shown by simple arguments that

$$V_B = -\left\langle \sum_i \vec{F}_{iB} \cdot \vec{x}_i \right\rangle = n\pi e^2 \sum_i \langle X_i^2 \rangle = n\pi e^2 N \int f(x) x^2 dx ,$$

$$V_W = -\left\langle \sum_i \vec{F}_{iW} \cdot \vec{x}_i \right\rangle = 2AP_k ,$$

$$V_p = -\left\langle \sum_i \sum_j \vec{F}_{ij} \cdot \vec{x}_i \right\rangle = -\frac{e^2}{2} N(N-1) ,$$

where N is the total number of particles, A the area, P_k the kinetic pressure, and $f(x)$ is the one-particle distribution function.

According to the virial theorem, the kinetic energy

$$K=\tfrac{1}{2}V;$$

on the other hand,

$$K=\nu\frac{NkT}{2}=NkT \quad (\nu=2).$$

Thus,

$$2NkT=-\frac{e^2}{2}N(N-1)+2AP_k+e^2\pi nN\int f(x)x^2dx$$

or

$$\beta P_k=n\left(1-\frac{\gamma}{4}\right)-n\gamma\left(\frac{\pi n}{2}\langle x^2\rangle-\tfrac{1}{4}N\right),$$

where $\gamma=\beta e^2$, $n=N/A$, and $\beta=(kT)^{-1}$. The first term on the right is just the *thermal* pressure (which we will designate as P_T), as obtained from the equation of state and thus the two pressures differ by the expression

$$\beta P_k-\beta P_T=\frac{\gamma nN}{4}\left(1-2\frac{\langle x^2\rangle}{R^2}\right), \tag{A1}$$

where $A=\pi R^2$.

If the system is assumed to be homogeneous,

$$\langle x^2\rangle=\frac{1}{A}\int x^2dx=\tfrac{1}{2}R^2$$

and

$$P_k=P_T. \tag{A2}$$

The assumption of homogeneity must break down, however, when P_T becomes negative, since the kinetic pressure P_k can be shown to be nonnegative in general as follows. In terms of a Hamiltonian

$$H=H_B+H_0,$$

the forces due to the background and the particles are given, respectively, by

$$\vec{F}_{iB}=-\frac{\partial H_B}{\partial\vec{x}_i},\quad \sum_j\vec{F}_{ij}=-\frac{\partial H_0}{\partial\vec{x}_i}.$$

On the other hand, the one-particle distribution function is given by

$$f(\vec{x}_1)=\frac{1}{Z}\int e^{-\beta H}d\vec{p}_N\cdots d\vec{p}_1d\vec{x}_n\cdots d\vec{x}_2.$$

Then

$$\frac{\partial f}{\partial\vec{x}_1}=\frac{1}{Z}\int(-\beta)\frac{\partial H}{\partial\vec{x}_1}e^{-\beta H}d\vec{p}_N\cdots d\vec{x}_2.$$

From the virial,

$$2NkT=2AP_k-\left\langle\sum_i\vec{F}_{iB}\cdot\vec{x}_i\right\rangle-\left\langle\sum_{ij}{}'\vec{F}_{ij}\cdot\vec{x}_i\right\rangle$$

and then

$$\begin{aligned}\beta P_k&=n-\frac{\beta N}{2AZ}\int\frac{\partial H}{\partial\vec{x}_1}\cdot\vec{x}_1e^{-\beta H}d\vec{p}_N\cdots d\vec{x}_2d\vec{x}_1\\&=n+\frac{n}{2}\int\frac{\partial f}{\partial\vec{x}_1}\cdot\vec{x}_1d\vec{x}_1\\&=n\int dx\left(f(x)+\frac{1}{2}\frac{\partial f}{\partial\vec{x}}\cdot\vec{x}\right)=\frac{n}{2}\int dx\vec{\nabla}\cdot[xf(x)]\\&=\frac{n}{2}\oint dl\,Rf(R)=f(R)n\pi R^2\equiv n(R)\geq 0,\end{aligned}$$

where $n(R)$ is just the density at the wall, an obviously nonnegative quantity.

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