# From Monotonic to Oscillatory Decay of Correlations: Analytical Approximation for the Two-Dimensional, One-Component Plasma 

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#### Abstract

An approximate evaluation of the pair distribution and the structure factor is performed analytically for the two-dimensional, one-component plasma at any value of the coupling constant $\Gamma$. The approximate distribution remains positive and satisfies three sum rules, including the compressibility one. When $\Gamma \rightarrow 0$ or $\Gamma \rightarrow 2$, exact results are found. At $\Gamma=2$ the transition from monotonic ( $\Gamma<2$ ) to oscillatory ( $\Gamma>2$ ) decay of correlations takes place. Comparison with the Monte Carlo simulations shows good agreement for $0<\Gamma<4$.


KEY WORDS: One-component plasma; correlation functions.

## 1. INTRODUCTION

We study the two-dimensional, one-component plasma at equilibrium. We thus consider identical particles of charge $e$ interacting via the logarithmic Coulomb potential

$$
\begin{equation*}
e^{2} v(r)=-e^{2} \ln (r / L) \tag{1.1}
\end{equation*}
$$

and embedded in a uniform neutralizing background of opposite charge ( $L$ is a length scale, $r$ the distance between the particles).

A remarkable fact about this two-dimensional plasma is that in addition to the high-temperature limit, where the Debye-Hückel theory applies, its equilibrium distribution functions can be also exactly evaluated at the finite temperature $T_{0}=e^{2} / 2 k_{\mathrm{B}}$ ( $k_{\mathrm{B}}$ is Boltzmann's constant). ${ }^{(1)}$ Our

[^0]object here is to use the knowledge of the reduced distributions at $T_{0}$ to find an approximate equation for the pair distribution at an arbitrary temperature $T$. To this end, we consider the BGY hierarchy equation relating the two- and three-particle number densities $\rho_{2}$ and $\rho_{3}$ :
\[

$$
\begin{align*}
{\left[\frac{\partial}{\partial \mathbf{r}_{1}}\right.} & \left.+\Gamma \frac{\partial v\left(\mathbf{r}_{12}\right)}{\partial \mathbf{r}_{12}}\right] \rho_{2}\left(\mathbf{r}_{1}, \mathbf{r}_{2} \mid \Gamma\right) \\
& =-\Gamma \int d \mathbf{r}_{3} \frac{\partial v\left(\Gamma_{13}\right)}{\partial \mathbf{r}_{13}}\left[\rho_{3}\left(\mathbf{r}_{1}, \mathbf{r}_{2}, \mathbf{r}_{3} \mid \Gamma\right)-\rho_{2}\left(\mathbf{r}_{1}, \mathbf{r}_{2} \mid \Gamma\right)\right] \tag{1.2}
\end{align*}
$$
\]

Here $\Gamma=e^{2} / k_{\mathrm{B}} T$ is the dimensionless coupling constant, whose value at $T=T_{0}$ equals 2 . The translational invariance of the equilibrium state enables us to write the cluster decomposition of the densities $\rho_{2}$ and $\rho_{3}$ in the form

$$
\begin{align*}
\rho_{2}\left(\mathbf{r}_{1}, \mathbf{r}_{2} \mid \Gamma\right)= & \rho^{2}\left[1+h_{2}\left(r_{12} \mid \Gamma\right)\right]  \tag{1.3}\\
\rho_{3}\left(\mathbf{r}_{1}, \mathbf{r}_{2}, \mathbf{r}_{3} \mid \Gamma\right)= & \rho^{3}\left[h_{2}\left(r_{12} \mid \Gamma\right)+h_{2}\left(r_{13} \mid \Gamma\right)+h_{2}\left(r_{23} \mid \Gamma\right)\right. \\
& \left.+h_{3}\left(\mathbf{r}_{12}, \mathbf{r}_{13} \mid \Gamma\right)\right] \tag{1.4}
\end{align*}
$$

where $\rho$ is the constant one-particle density, $\mathbf{r}_{i j}=\mathbf{r}_{i}-\mathbf{r}_{j}$, and $r_{i j}=\left|\mathbf{r}_{i j}\right|, i, j=$ $1,2, \ldots$ From Eq. (1.2) we find that the dimensionless correlation functions $h_{2}$ and $h_{3}$ are related to each other by equation

$$
\begin{align*}
{\left[\frac{\partial}{\partial \mathbf{r}_{1}}\right.} & \left.+\Gamma \frac{\partial v\left(r_{12}\right)}{\partial \mathbf{r}_{12}}\right] h_{2}\left(r_{12} \mid \Gamma\right) \\
& =-\Gamma \int d \mathbf{r}_{3} \frac{\partial v\left(r_{13}\right)}{\partial \mathbf{r}_{13}}\left[\rho h_{2}\left(r_{23} \mid \Gamma\right)+\delta\left(\mathbf{r}_{23}\right)+\rho h_{3}\left(\mathbf{r}_{12}, \mathbf{r}_{13} \mid \Gamma\right)\right] \tag{1.5}
\end{align*}
$$

The Coulomb potential satisfies the Poisson equation

$$
\begin{equation*}
\Delta v(r)=-2 \pi \delta(\mathbf{r}) \tag{1.6}
\end{equation*}
$$

Combining this with the perfect screening relation

$$
\begin{equation*}
\int d \mathbf{r}\left[\rho h_{2}(r \mid \Gamma)+\delta(\mathbf{r})\right]=0 \tag{1.7}
\end{equation*}
$$

one finds

$$
\begin{align*}
\int d \mathbf{r}_{3} & \frac{\partial v\left(r_{13}\right)}{\partial \mathbf{r}_{13}}\left[\rho h_{2}\left(r_{23} \mid \Gamma\right)+\delta\left(\mathbf{r}_{23}\right)\right] \\
\quad & =-2 \pi \rho \Gamma \frac{\partial v\left(r_{12}\right)}{\partial \mathbf{r}_{12}} \int_{r_{12}}^{\infty} d r r h_{2}(r \mid \Gamma) \tag{1.8}
\end{align*}
$$

Equation (1.5) can be thus rewritten in the form

$$
\begin{align*}
\left(\frac{\partial}{\partial \mathbf{r}_{1}}\right. & \left.-\Gamma \frac{\mathbf{r}_{12}}{r_{12}^{2}}\right) h_{2}\left(r_{12} \mid \Gamma\right)+2 \pi \rho \Gamma \frac{\mathbf{r}_{12}}{r_{12}^{2}} \int_{r_{12}}^{\infty} d r r h_{2}(r \mid \Gamma) \\
& =\rho \Gamma \int d \mathbf{r}_{3} \frac{\mathbf{r}_{13}}{r_{13}^{2}} h_{3}\left(\mathbf{r}_{12}, \mathbf{r}_{13} \mid \Gamma\right) \tag{1.9}
\end{align*}
$$

where the explicit form of $v(r)$ has been used.

## 2. APPROXIMATION AND ITS ANALYTICAL SOLUTION

At $\Gamma=2$, the two-particle correlation function reads

$$
\begin{equation*}
h_{2}\left(r_{12} \mid 2\right)=-\exp \left(-\pi \rho r_{12}^{2}\right) \tag{2.1}
\end{equation*}
$$

Equation (1.9) implies that

$$
\begin{equation*}
\rho \int d \mathbf{r}_{3} \frac{\mathbf{r}_{13}}{r_{13}^{2}} h_{3}\left(\mathbf{r}_{12}, \mathbf{r}_{13} \mid 2\right)=\frac{1}{2} \frac{\partial}{\partial \mathbf{r}_{12}} h_{2}\left(r_{12} \mid 2\right) \tag{2.2}
\end{equation*}
$$

The three-particle correlation function

$$
\begin{align*}
h_{3}\left(\mathbf{r}_{12}, \mathbf{r}_{13} \mid 2\right) & =2 \operatorname{Re}\left\{\exp \left[-\pi \rho\left(r_{12}^{2}+r_{13}^{2}-r_{12} r_{13} e^{i \theta}\right)\right]\right\}  \tag{2.3}\\
\cos \theta & =\left(\mathbf{r}_{12} \cdot \mathbf{r}_{13}\right) / r_{12} r_{13}
\end{align*}
$$

found by a direct calculation from the canonical distribution, can be shown to satisfy Eq. (2.2). We shall now make an important step by postulating the validity of Eq. (2.2) for all temperatures,

$$
\begin{equation*}
\rho \int d \mathbf{r}_{3} \frac{\mathbf{r}_{13}}{r_{13}^{2}} h_{3}\left(\mathbf{r}_{12}, \mathbf{r}_{13} \mid \Gamma\right)=\frac{1}{2} \frac{\partial}{\partial \mathbf{r}_{12}} h_{2}\left(r_{12} \mid \Gamma\right) \tag{2.4}
\end{equation*}
$$

Equation (1.9), when combined with Eq. (2.4), yields a closed equation for $h_{2}$ :

$$
\begin{equation*}
\left[\left(1-\frac{\Gamma}{2}\right) \frac{d}{d r}-\frac{\Gamma}{r}\right] h_{2}(r \mid \Gamma)+\frac{2 \pi \rho \Gamma}{r} \int_{r}^{\infty} d x x h_{2}(x \mid \Gamma)=0 \tag{2.5}
\end{equation*}
$$

The closure relation (2.4) has the obvious advantage of being exact at $\Gamma=2$. Moreover, it is consistent with the three sum rules satisfied by the exact two-particle correlations at any value of $\Gamma^{(2)}$ :

1. Perfect screening:

$$
\begin{equation*}
\rho \int d \mathbf{r} h_{2}(r \mid \Gamma)=-1 \tag{2.6a}
\end{equation*}
$$

2. Stillinger-Lovett rule:

$$
\begin{equation*}
\rho \int d \mathbf{r} r^{2} h_{2}(r \mid \Gamma)=-2 / \pi \rho \Gamma \tag{2.6b}
\end{equation*}
$$

3. Compressibility sum rule:

$$
\begin{equation*}
\rho \int d \mathbf{r} r^{4} h_{2}(r \mid \Gamma)=-16\left(1-\frac{1}{4} \Gamma\right) /(\pi \rho \Gamma)^{2} \tag{2.6c}
\end{equation*}
$$

Indeed, multiplying Eq. (2.5) by $r^{n}$ and integrating over the position space, one finds

$$
\begin{equation*}
\int d \mathbf{r} r^{n} h_{2}(r \mid \Gamma)=\frac{2 \pi \rho \Gamma}{(n+2)(n+2-n \Gamma / 2)} \int d \mathbf{r} r^{n+2} h_{2}(r \mid \Gamma) \tag{2.7}
\end{equation*}
$$

provided the moments under study exist. For $n=0$ and 2, Eq. (2.7) reproduces correctly the relations between the moments of $h_{2}$ in full accordance with Eq. (2.6), which is quite encouraging. In fact, the compressibility sum rule usually causes difficulties in approximation schemes. For instance, it is violated by the HNC approximation. ${ }^{(3)}$

The great advantage of Eq. (2.5) is that it can be solved, yielding a closed analytical formula for $h_{2}(r \mid \Gamma)$ for any $\Gamma$. It is convenient to multiply it by $r$ and differentiate once with respect to this variable. A second-order differential equation is obtained in this way, which, when written in terms of the dimensionless distance

$$
\begin{equation*}
z=r(\pi \rho)^{1 / 2} \tag{2.8}
\end{equation*}
$$

takes the form

$$
\begin{equation*}
\left[z \frac{d^{2}}{d z^{2}}+(1-2 \mu) \frac{d}{d z}-4 \mu\right] h_{2}(z \mid \Gamma)=0 \tag{2.9}
\end{equation*}
$$

where

$$
\begin{equation*}
\mu=\Gamma /(2-\Gamma) \tag{2.10}
\end{equation*}
$$

Equation (2.9) is known to lead to the Bessel functions. Requiring that

$$
\begin{equation*}
h_{2}(0 \mid \mu)=-1 \tag{2.11}
\end{equation*}
$$

and $h_{2}(z \mid \mu) \rightarrow 0$, for $z \rightarrow \infty$, selects the desired solution. One has to distinguish between two cases.

### 2.1. The Case 「<2

In this region $(\mu>0)$ the pair correlation function reads

$$
\begin{equation*}
h_{2}(z \mid \mu)=-\frac{2}{\Gamma(\mu)}(z \sqrt{\mu})^{\mu} K_{\mu}(2 z \sqrt{\mu}) \tag{2.12}
\end{equation*}
$$

where the standard notation for the gamma and Bessel functions has been used.

The inequality

$$
\begin{equation*}
\frac{d}{d x}\left[x^{\mu} K_{\mu}(x)\right]=x^{\mu} K_{\mu-1}(x)>0 \quad(x>0) \tag{2.13}
\end{equation*}
$$

shows that the pair distribution

$$
\begin{equation*}
g_{2}=1+h_{2} \tag{2.14}
\end{equation*}
$$

attains its minimum at $z=0$. In view of Eq. (2.11), we thus conclude that

$$
\begin{equation*}
g_{2}(z \mid \Gamma)>0 \quad \text { for } \quad z>0 \tag{2.15}
\end{equation*}
$$

which is quite satisfactory. This shows in particular that in the hightemperature limit $\Gamma \rightarrow 0$, the solution (2.12) approaches the Debye-Hückel pair distribution

$$
\begin{equation*}
g_{2}^{\mathrm{DH}}(z)=1-\Gamma K_{0}(z \sqrt{2} \Gamma) \tag{2.16}
\end{equation*}
$$

in a nonuniform way. Indeed, when $x \rightarrow 0, K_{0}(x)$ diverges logarithmically to $+\infty$, so that $g_{2}^{\mathrm{DH}}$ becomes negative for short distances. As we have shown, the approximation (2.12) guarantees the positivity of $g_{2}$ at arbitrarily high temperatures. For $z \rightarrow \infty, g_{2}(z \mid \Gamma)$ tends monotonically to 1 , in accordance with the formula

$$
\begin{equation*}
g_{2}(z \mid \Gamma)_{z} \simeq 1-\frac{\sqrt{\pi}}{\Gamma(\mu)}(z \sqrt{\mu})^{\mu-1 / 2} \exp (-z \sqrt{\mu}) \tag{2.17}
\end{equation*}
$$

It can be checked that $h_{2}$ given by Eq. (2.12) satisfies the sum rules (2.6).

Let us finally evaluate the corresponding static structure factor

$$
\begin{equation*}
S(q \mid \Gamma)=1+\hat{h}_{2}(q \mid \Gamma) \tag{2.18}
\end{equation*}
$$

where

$$
\begin{equation*}
\hat{h}_{2}(q \mid \Gamma)=2 \int_{0}^{\infty} d z z h_{2}(z \mid \Gamma) J_{0}(q z) \tag{2.19}
\end{equation*}
$$

is the Fourier transform of $h_{2}(z \mid \Gamma)$. Using Eq. (2.12), we find

$$
\begin{equation*}
S(q \mid \Gamma)=1-{ }_{2} F_{1}\left(\frac{2}{2-\Gamma}, 1,1,-\frac{q^{2}}{4}\left(\frac{2-\Gamma}{\Gamma}\right)\right) \quad(\Gamma<2) \tag{2.20}
\end{equation*}
$$

where ${ }_{2} F_{1}$ is the Gauss hypergeometric function. In accordance with the Stillinger-Lovett rule, the small- $q$ expansion of $S(q \mid \Gamma)$ reads

$$
\begin{equation*}
S(q \mid \Gamma)=\frac{q^{2}}{2 \Gamma}-\left(1-\frac{\Gamma}{4}\right)\left(\frac{q^{2}}{2 \Gamma}\right)^{2}+\cdots \tag{2.21}
\end{equation*}
$$

In order to understand how the case $\Gamma=2$,

$$
\begin{equation*}
S(q \mid 2)=1-\exp \left(-q^{2} / 4\right) \tag{2.22}
\end{equation*}
$$

is approached, it is convenient to consider the sequence

$$
\begin{equation*}
\Gamma_{N}=2-2 / N, \quad N=2,3, \ldots \tag{2.23}
\end{equation*}
$$

Equation (2.19) then simplifies to

$$
\begin{equation*}
S\left(q \mid \Gamma_{N}\right)=1-\left[1+q^{2} / 4(N-1)\right]^{-N} \tag{2.24}
\end{equation*}
$$

In the complex $q$ plane the singularities of $S\left(q \mid \Gamma_{N}\right)$ lie on the imaginary axis at points

$$
\begin{equation*}
q_{+,-}^{N}= \pm 2 i(N-1)^{1 / 2} \tag{2.25}
\end{equation*}
$$

when $N \rightarrow \infty, q_{+,-}^{N}$ run away to infinity, and the structure factor acquires the Gaussian form (2.22). One can expect that a qualitative change in the behavior of $S(q \mid \Gamma)$, and thus also of $g(z \mid \Gamma)$, will occur when the point $\Gamma=2$ is crossed.

### 2.2. The Case $\Gamma>2$

For negative values of $\mu$

$$
\begin{equation*}
-\mu=\Gamma /(\Gamma-2)=v>1 \tag{2.26}
\end{equation*}
$$

the physically relevant solution of Eq. (2.9) reads

$$
\begin{equation*}
h_{2}(z \mid v)=-\Gamma(1+v)(z v)^{-v} J_{v}(2 z \sqrt{v}) \tag{2.27}
\end{equation*}
$$

Let us begin the discussion of this result by proving the positivity of the corresponding pair distribution $g_{2}=1+h_{2}$. Using the integral representation of the Bessel function

$$
\begin{equation*}
J_{\nu}(x)=2 \frac{(x / 2)^{v}}{\Gamma(v+1 / 2) \Gamma(1 / 2)} \int_{0}^{\pi / 2} d \theta \sin ^{2 v} \theta \cos (x \cos \theta) \tag{2.28}
\end{equation*}
$$

one readily finds the required inequality

$$
\begin{equation*}
\left|h_{2}\right| \leqslant \frac{2 \Gamma(1+v)}{\Gamma(v+1 / 2) \Gamma(1 / 2)} \int_{0}^{\pi / 2} d \theta \sin ^{2 v} \theta=1 \tag{2,29}
\end{equation*}
$$

Hence $g_{2}(z \mid \Gamma)>0$ for $z>0$. The approximation studied here preserves thus the positivity of the pair distribution for any value of $\Gamma$. This should be stressed, as this property is easily lost in approximate theories.

The Bessel functions $J_{v}$ are known to show oscillatory behavior. In particular, when $z \rightarrow \infty$, we find the asymptotic formula

$$
\begin{equation*}
h_{2}(z \mid v)_{z \rightarrow \infty}^{\simeq}-\frac{\Gamma(1+v)}{\sqrt{\pi}}(z \sqrt{v})^{-v-1 / 2} \cos \left[2 z \sqrt{v}-\frac{\pi}{2}\left(v+\frac{1}{2}\right)\right] \tag{2.30}
\end{equation*}
$$

Within the approximation studied here the temperature $T_{0}=e^{2} / 2 k_{\mathrm{B}}$ thus occurs as the transition point between the region of monotonically vanishing correlations $(\Gamma<2)$ and oscillating correlations with powerlike falloff ( $\Gamma>2$ ). In order to analyze the underlying mechanism, let us study $S(q \mid \Gamma)$ for $\Gamma>2$. The evaluation of the Fourier transform (2.19) yields

$$
S(q \mid \Gamma)= \begin{cases}1-\left[1-\frac{1}{4}(\Gamma-2) q^{2} / \Gamma\right]^{2 /(\Gamma-2)}, & \frac{1}{4} q^{2}<\Gamma /(\Gamma-2)  \tag{2.31}\\ 1, & \frac{1}{4} q^{2}>\Gamma /(\Gamma-2)\end{cases}
$$

The singularities of the structure factor now lie on the real axis, at points

$$
\begin{equation*}
q_{+,-}^{\Gamma}= \pm 2\left(\frac{\Gamma}{\Gamma-2}\right)^{1 / 2} \tag{2.32}
\end{equation*}
$$

at which $S(q \mid \Gamma)$ attains its asymptotic value

$$
S(\infty \mid \Gamma)=1
$$

Hence, when the temperature is lowered, they move first along the imaginary axis, escaping to $\pm i \infty$ for $\Gamma \rightarrow 2-0$, and, once the temperature $T_{0}=e^{2} / 2 k_{\mathrm{B}}$ is crossed, they reappear on the real axis, approaching, for $\Gamma \rightarrow \infty$, the limiting positions $\pm 2$. Such a picture is quite different from the one usually proposed. ${ }^{(4)}$ It is, of course, an open question whether the transition mechanism corresponding to the audaciously adopted closure relation (2.4) is a correct one, but it is certainly a possible one. Clearly, when $\Gamma \rightarrow 2+0$, formula (2.31) reproduces the Gaussian form (2.22). One can also check that the sum rules (2.6) are satisfied by $h_{2}$ given by Eq. (2.27). The small- $q$ expansion of the structure factor (2.31) is thus also given by Eq. (2.21).

When $\Gamma \rightarrow \infty, v \rightarrow 1$, and we find

$$
\begin{equation*}
g_{2}(z, \infty)=1-(1 / z) J_{1}(2 z) \tag{2.33}
\end{equation*}
$$

It seems to be a curious coincidence that the same formula has been found within a quite different approximation scheme, where, however, oscillations are found already at $\Gamma=2$. ${ }^{(5)}$

Before closing this section, let us examine the internal energy density $u$, related to the correlation function $h_{2}$ by

$$
\begin{equation*}
u=-k_{\mathrm{B}} T \Gamma \int_{0}^{\infty} d z z h_{2}(z \mid \Gamma) \ln \frac{z}{L(\pi \rho)^{1 / 2}} \tag{2.34}
\end{equation*}
$$

The evaluation of the integral occurring in Eq. (2.34) yields the following result:

$$
\begin{equation*}
\frac{u}{k_{B} T}=\frac{\Gamma}{4}\left[-C-\ln \left(\pi \rho L^{2}\right)+\psi\left(\frac{\Gamma}{|2-\Gamma|}\right)-\ln \left(\frac{\Gamma}{|2-\Gamma|}\right)+\frac{2-\Gamma}{\Gamma} \theta(2-\Gamma)\right. \tag{2.35}
\end{equation*}
$$

where $C=0.577215 \ldots$ is Euler's constant, $\psi(x)$ is the Euler psi function and

$$
\theta(2-\Gamma)=\left\{\begin{array}{lll}
0 & \text { for } & \Gamma>2 \\
1 & \text { for } & \Gamma<2
\end{array}\right.
$$

When $\Gamma \rightarrow 0$ we find

$$
\begin{equation*}
u / k_{\mathrm{B}} T=\frac{1}{4} \Gamma\left[\ln \left(\pi \rho L^{2}\right)+2 C+\ln (\Gamma)-\ln (2)\right] \tag{2.36}
\end{equation*}
$$

as predicted by the Debye-Hückel theory. At $\Gamma=2$, all the derivatives of the energy density $u$ with respect to $\Gamma$ exist and are continuous. The asymptotic expansion around $\Gamma=2$ has the form

$$
\begin{align*}
u= & \frac{e^{2}}{4}\left[-C-\ln \left(\pi \rho L^{2}\right)+\left(\frac{1}{\Gamma}-\frac{1}{2}\right)\right. \\
& \left.-\sum_{k=1}^{n} \frac{B_{2 k}}{2 k}\left(\frac{2-\Gamma}{\Gamma}\right)^{2(k-1)}+\cdots\right] \tag{2.37}
\end{align*}
$$

$B_{2 k}$ are the Bernoulli numbers. The series (2.37) is divergent, showing that at $T=T_{0}(\Gamma=2)$ the energy density $u$ is not analytic. From the expansion (2.37) we readily find the specific heat at $\Gamma=2$ :

$$
\begin{equation*}
c=\left.\frac{d \mu}{d T}\right|_{T=T_{0}}=\frac{k_{\mathrm{B}}}{4} \tag{2.38}
\end{equation*}
$$

This should be compared with the exact result ${ }^{(1)}$

$$
\begin{equation*}
c=k_{\mathrm{B}}\left(\ln 2-\pi^{2} / 24\right)=0.28131 k_{\mathrm{B}} \tag{2.39}
\end{equation*}
$$

The discrepancy between (2.39) and (2.38) shows that the neighborhood of the point $\Gamma=2$ is not quite accurately represented by our approximate equation (2.5). This is even more clearly seen when one compares the expansions around $\Gamma=2$ for the correlation function. Equation (2.5) leads to the asymptotoc series

$$
\begin{equation*}
h_{2}(z \mid \Gamma)=-e^{-z^{2}}\left[1+\frac{1}{2}\left(\frac{z^{4}}{2}-z^{2}\right)(2-\Gamma)+\cdots\right] \tag{2.40}
\end{equation*}
$$

The exact expansion begins as

$$
\begin{align*}
h_{2}(z \mid \Gamma)= & -e^{-z^{2}}\left\{1+\left[\ln \left(z^{2}\right)+C-\operatorname{Ei}\left(-z^{2}\right) e^{z^{2}}\right.\right. \\
& \left.\left.+\frac{1}{2} \operatorname{Ei}\left(-\frac{1}{2} z^{2}\right) e^{z^{2}}-\frac{1}{2} \operatorname{Ei}\left(\frac{1}{2} z^{2}\right)\right](\Gamma-2)+\cdots\right\} \tag{2.41}
\end{align*}
$$

where Ei is the exponential integral function. In Eq. (2.40) the dominant correction has the structure of a polynomial multiplying the Gaussian $\exp \left(-z^{2}\right)$, whereas in Eq. (2.41) the analogous term decays at large distances as $\exp \left(-z^{2} / 2\right)$. In order to further elucidate the consequences of the simple closure relation (2.4), we compare in the next section the approximate formulas for $g_{2}(z \mid \Gamma)$ and $S(q \mid \Gamma)$ derived here with the results obtained by the Monte Carlo simulation of the system.

## 3. COMPARISON WITH SIMULATION RESULTS: CONCLUSIONS

This section is devoted to establishing the domain of validity of the method described in the preceding section. This is done by comparins the two-body correlation functions calculated from Eq. (2.9) and from Monte Carlo (MC) simulations. The MC simulations were carried out for systems of 256 particles confined on the surface of a three-dimensional sphere, following the procedure described in Ref. 6. The numbers of configurations generated in the MC runs were, respectively, $5 \times 10^{5}$ at $\Gamma=0.5,1.5,2.8$, and $10 / 3 ; 2 \times 10^{5}$ at $\Gamma=2$; and $1 \times 10^{6}$ at $\Gamma=6$. These values of the MC samplings were sufficient to achieve a precision of $\sim 1-2 \%$ on the two-body distribution function $g_{2}(r)$ and on the internal energy. From the MC data for $g_{2}(r)$, the static structure factor $S(k)$ can be evaluated by a Fourier transform (cf. Ref. 6). In Figs. 1 and 2 we have plotted $g_{2}(r)$ and $S(k)$, respectively, obtained from (2.9), by MC simulations and by the HNC approximations. ${ }^{(3)}$ These figures clearly show the domain of validity of the


Fig. 1. Distribution function $g_{2}(r)$ versus $r / a=z\left[a=(\pi \rho)^{-1 / 2}\right]$ at $\Gamma=(\mathrm{a}) 0.5$, (b) 1.5 , (c) 2.8, (d) 6. (-) Present theory; (-) HNC approximation; (+) MC data.

(c)

(d)

Fig. 1 (continued)


Fig. 2. Static structure factor $S(k)$ versus $k a=q$ for $\Gamma=(a) 0.5$, (b) 1.5 , (c) 2.8, (d) 6 . Symbols have the same meaning as in Fig. 1.

(c)

(d)

Fig. 2 (continued)
approximation presented in this article. From the discussion of Section 2 we know that this approximation gives exact values of $g_{2}(r)$ for $\Gamma=2$ and in the limit $\Gamma \rightarrow 0$. From Figs. 1a, 1b, 2a, and $2 b$ and from Table I we see that also gives accurate $g_{2}(r)$ and $S(k)$ and a good estimation of $u$ for the values of $\Gamma$ between 0 and 2 . The analytical solutions of (2.9) are in agreement with the MC data at the same degree of accuracy as the numerical solutions of the HNC equation. For $2<\Gamma<4$, (see Figs. 1c and 2c) the solutions of (2.9) stay in quantitative agreement with the MC results, in spite of the fact that they lead to $S(k)$ functions constant (equal to 1 ) for $k>[4 \Gamma \pi \rho /(\Gamma-2)]^{1 / 2}$. The disagreement of the results of the two approximate theories [HNC equation and Eq. (2.9)] with the MC data is obvious for $\Gamma=6$ (see Figs. 1d and 2 d ). Clearly, the figures show that the inadequacy of the approximation discussed here is due to the bad description of the correlations at small distances for all values of $\Gamma$ for which the comparison is done. The HNC approximation gives a better estimation of $g_{2}(r)$ for $z<0.5$. But, because the $g_{2}(r)$ functions calculated from (2.9) satisfy the three exact sum rules (2.6), the low- $k$ values of $S(k)$ functions are in an excellent agreement with the MC data. The fact that the sum rule (2.6) is satisfied ensures that the compressibility is exactly determined by the present theory.

In conclusion, the approximate theory developed in this article has roughly the same domain of validity as other methods proposed in the literature ${ }^{(5,7,8)}$ and it has the obvious advantage of giving an analytical representation of $g_{2}(r)$ and $S(k)$ of the 2D-OCP system that satisfy three exact sum rules and becomes exact both for $\Gamma \rightarrow 0$ and $\Gamma=2$. The analytical behavior of the solution of (2.9) around $\Gamma=2$ gives a possible description of the transition between two regimes of the decay of

Table 1. Internal Energy per Particle ${ }^{a}$

|  | $u / k_{\mathrm{B}} T$ |  |  |  |  |
| :--- | :---: | :---: | :---: | :---: | :---: |
| $\Gamma$ | MC data | Eq. $(2.35)$ | HNC approximation |  |  |
| 0.5 | $+0.049 \pm 0.001$ | 0.04867 | 0.0518 |  |  |
| 1.0 | $-0.034 \pm 0.001$ | -0.0386 | -0.0302 |  |  |
| 1.5 | $-0.153 \pm 0.001$ | -0.1574 | -0.1459 |  |  |
| 2 | $-0.290 \pm 0.002$ | -0.2886 | -0.278 |  |  |
| 2.8 | $-0.528 \pm 0.001$ | -0.5088 | -0.5083 |  |  |
| 3.33333 | $-0.696 \pm 0.001$ | -0.6586 | -0.6699 |  |  |
| 6 | $-1.582 \pm 0.0005$ | -1.4192 | -1.526 |  |  |

[^1]correlations: a monotonic exponential decay ( $\Gamma<2$ ) and an oscillatory algebraic decay $(\Gamma>2)$. The two decay laws have been shown to be compatible with the exact hierarchy equations satisfied by the reduced distribution functions. ${ }^{(9)}$

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[^1]:    ${ }^{a}$ The values of $u / k_{\mathrm{B}} T$ are calculated with the choice $L=a=(\pi \rho)^{-1 / 2}$.

