Solution of the Percus-Yevick equation for hard disks

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The authors solve the Percus-Yevick equation in two dimensions by reducing it to a set of simple integral equations. They numerically obtain both the pair correlation function and the equation of state for a hard disk fluid and find good agreement with available Monte Carlo results. The present method of resolution may be generalized to any even dimension. © *2008 American Institute of Physics*. [DOI: 10.1063/1.2919123]

I. INTRODUCTION

The description of hard-core fluids by approximate theories has attracted a lot of attention throughout the years.[1] The reason for this interest is twofold: first, a solution of the full problem was, and still is, extremely difficult. Second, approximate methods have allowed for very good predictions in the low density phase. Among the most widely used approximations is the Percus-Yevick (PY) equation for d-dimensional hard spheres.[2]

Baxter developed a powerful method for solving the PY equation that works in odd dimensions.[3] Leutheusser used this method to reduce the nonlinear integral PY equation to a set of nonlinear algebraic equations[4] of order $2^{(d-3)/2}$ (for $d>3$).[5] However, this set of equations can only be solved analytically for odd $d\leq 7$. In general, even the numerical solution of Leutheusser's equations is difficult to obtain[5] for higher dimensions because a general solution to nonlinear algebraic equations of order larger than four is not available. Analytical results have been found for one,[6] three,[7,8] five,[4] and, most recently, seven dimensions.[9]

In two dimensions a numerical solution of the PY equation was found by Lado.[10] Leutheusser[11] was able to fit many of Lado's results using an ansatz for the direct correlation function. Rosenfeld[12] generalized Leutheusser's ansatz to higher dimensions and compared the results with the analytical results in three and five dimensions. All other results available in the literature are based on molecular dynamics (MD) or Monte Carlo (MC) methods.[13–18]

In this paper, we solve the PY equation for hard disks ($d=2$). We develop a method that reduces the problem to a set of integral equations that are solved numerically without major difficulties. The originality of the present method is based on techniques borrowed from the resolution of crack problems[19] and uses some results from Baxter's classical method.[1,3] The main difference from the hard sphere case (and any odd dimension in general) is that the problems of finding the indirect correlation function and the direct correlation function are coupled. This means that the present analysis necessarily yields both correlation functions and therefore provides the equation of state. The advantage of the current method over previous approaches is that it provides all the quantities of interest as power-series in the density. Thus, the calculation is done once for all densities, with no need to recalculate the correlation function and the pressure for each density separately as in Lado's approach.[10] Consequently, it allows for an estimation of the critical density at which the pressure diverges via convergence tests on the series—a question that has not been addressed previously. Finally, one may improve the precision at will by calculating higher terms in the series.

II. THE PY APPROXIMATION

The pair correlation function $g(\mathbf{r})$ is related to the direct correlation function $c(\mathbf{r})$ through the Ornstein-Zernike equation by[1,20]

$$h(\mathbf{r}) = c(\mathbf{r}) + \rho\int_0^\infty h(\mathbf{r}')c(|\mathbf{r}-\mathbf{r}'|)dr', \tag{1}$$

where ρ is the particle number density and

$$h(\mathbf{r}) = g(\mathbf{r}) - 1 \tag{2}$$

is the indirect correlation function. The PY approximation is a closure relation of Eq. (1). For a hard-core pair interaction potential, this approximation reads[1]

$$g(r) = h(r) + 1 = 0, \quad r<1, \tag{3}$$

$$c(r) = 0, \quad r>1 \ . \tag{4}$$

Here and elsewhere, we use the radius of the sphere as the unit of length. Thus in two dimensions, we have $\rho=4\eta/\pi$ where η is the packing fraction, and the space filling density corresponds to $\eta=1$. We define the two-dimensional Fourier transform

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$$\widetilde{F}(q)=2\pi\int_0^{\infty} rJ_0(qr)F(r)dr, \tag{5}$$

where J_0 is the zeroth order Bessel function. The inverse Fourier transform is then given by

$$F(r)=(2\pi)^{-1}\int_0^{\infty} qJ_0(qr)\widetilde{F}(q)dq. \tag{6}$$

In Fourier space Eq. (1) reads

$$[1-\rho\tilde{c}(q)][1+\rho\tilde{h}(q)]=1. \tag{7}$$

Finally, the static structure factor $s(q)$ of wave number $\mathbf{q}$ is related to the pair correlation function through

$$s(q)=1+\rho\tilde{h}(q)\equiv\frac{1}{1-\rho\tilde{c}(q)}. \tag{8}$$

III. RESOLUTION

Condition (4) together with Eq. (6) imposes that $\tilde{c}(q)$ can be written as[19]

$$\tilde{c}(q)=\frac{1}{q}\int_0^1 \phi(t)\sin qt\, dt, \tag{9}$$

where $\phi(t)$ is a real function. Thus, using Eq. (6), $c(r)$ is expressed as[21]

$$c(r)=\int_r^1 \frac{\phi(t)}{\sqrt{t^2-r^2}}\frac{dt}{2\pi}. \tag{10}$$

The function $c(r)$ does not diverge at $r=1^-$, thus the function $\phi(t)$ satisfies

$$\phi(t)\simeq\frac{4c(1^-)t}{\sqrt{1-t^2}} \quad \text{as} \quad t\to 1^-. \tag{11}$$

Define

$$A(q)\equiv\frac{1}{s(q)}=1-\rho\tilde{c}(q)=1-\frac{\rho}{q}\int_0^1 \phi(t)\sin qt\, dt. \tag{12}$$

The function $A(q)$ has the same properties as the corresponding function defined in the odd dimensional case:[1] it has neither zeros nor poles on the real axis, since by definition $s(q)$ has neither zeros nor poles for all q's, $A(q)=A(-q)$, and $A(q)\to 1$ as $q\to\infty$. Therefore, in order to determine $\phi(t)$, we can use the formulation of Baxter,[3] which was developed to solve the PY equation in odd dimensions. We use the Wiener-Hopf method by defining[1,3]

$$A(q)=\widetilde{Q}(q)\widetilde{Q}(-q), \tag{13}$$

where $\widetilde{Q}(q)$ is an analytic function for $\Im(q)>0$. Following the same steps as in Refs. 1 and 3, it may be shown that $\widetilde{Q}(q)$ can be written as

$$\widetilde{Q}(q)=1-\rho\int_0^1 Q(t)e^{iqt}\, dt. \tag{14}$$

Substituting Eqs. (13) and (14) into Eq. (12) gives

$$\frac{1}{q}\int_0^1 \phi(s)\sin qs\, ds=\int_0^1 Q(s)e^{iqs}ds+\int_0^1 Q(s)e^{-iqs}ds - \rho\int_0^1 ds\int_0^1 ds' Q(s)Q(s')e^{iq(s-s')}. \tag{15}$$

Multiplying Eq. (15) by $\exp(-iqt)$, with $t>0$, and integrating with respect to q from $-\infty$ to ∞ gives

$$\int_t^1 \phi(s)ds=2Q(t)-2\rho\int_t^1 Q(s)Q(s-t)ds. \tag{16}$$

By setting $t=1$ in Eq. (16) we see that

$$Q(1)=0. \tag{17}$$

Moreover, Eq. (16) can be simplified further by differentiating with respect to t to give

$$\phi(t)=-2Q'(t)+2\rho\int_t^1 Q'(s)Q(s-t)ds, \quad 0\le t\le 1. \tag{18}$$

Therefore, once the function $Q(t)$ is determined, the functions $\phi(t)$ and $c(r)$ may be determined from Eqs. (18) and (10), respectively.

Now let us work on the function $h(r)$. Since $\tilde{h}(q)=\tilde{h}(-q)$, one can write without loss of generality

$$q\tilde{h}(q)=\int_0^{\infty}\psi(t)\sin qt\, dt, \tag{19}$$

where $\psi(t)$ is a real function and $h(r)$ is given in terms of $\psi(t)$ by

$$h(r)=\int_r^{\infty}\frac{\psi(t)}{\sqrt{t^2-r^2}}\frac{dt}{2\pi}. \tag{20}$$

Substituting this form for $h(r)$ in condition (3) yields

$$\int_r^1 \frac{\psi(t)}{\sqrt{t^2-r^2}}\frac{dt}{2\pi}=-1-\int_1^{\infty}\frac{\psi(t)}{\sqrt{t^2-r^2}}\frac{dt}{2\pi}, \quad 0<r<1. \tag{21}$$

Equation (21) is an Abel integral equation which can be inverted. It is easily shown that the inversion of the equation

$$\int_0^{\zeta_0}\frac{\sigma(\zeta)}{\sqrt{\zeta_0-\zeta}}d\zeta=\tau(\zeta_0), \quad \zeta_0>0, \tag{22}$$

yields

$$\sigma(\zeta)=\frac{d}{d\zeta}\left[\int_0^{\zeta}\frac{\tau(\zeta_0)}{\sqrt{\zeta-\zeta_0}}\frac{d\zeta_0}{\pi}\right]. \tag{23}$$

Therefore, using the change of variables $\zeta=1-t^2$ and $\zeta_0=1-r^2$, the inversion of Eq. (21) gives

$$\psi(t) = \frac{-4t}{\sqrt{1-t^2}}\left[1 + \int_1^\infty \frac{\sqrt{s^2-1}}{s^2-t^2}\psi(s)\frac{ds}{2\pi}\right], \quad 0 < t < 1. \tag{24}$$

Equation (24) is an integral equation fixing $\psi(t)$ for $0<t<1$ as function of $\psi(t)$ for $t>1$.

Now, let us determine the relationship between $Q(t)$ and $\psi(t)$. Putting together the results of Eqs. (12)–(14) and (19) in Eq. (7) gives

$$\left[1-\rho\int_0^1 Q(s)e^{iqs}\,ds\right]\left[1+\frac{\rho}{q}\int_0^\infty \psi(s)\sin qs\,ds\right] = \frac{1}{\tilde{Q}(-q)}. \tag{25}$$

Multiplying Eq. (25) by $\exp(-iqt)$ with $t>0$ and integrating with respect to q from $-\infty$ to ∞ gives[1,3]

$$4Q(t) = \int_0^\infty ds\,\psi(s)(\epsilon(s+t)+\epsilon(s-t)) - \rho\int_0^1 ds Q(s)\int_0^\infty ds'\,\psi(s')(\epsilon(s'+t-s) + \epsilon(s'-t+s)), \tag{26}$$

where $\epsilon(x)=\mathrm{sign}(x)$. Using $\epsilon(x)=-1+2\Theta(x)$, with $\Theta(x)$ the Heaviside function, and differentiating Eq. (26) with respect to t gives

$$2Q'(t) + \psi(t) = \rho\int_0^1 Q(s)[\psi(t-s)-\psi(s-t)]ds, \quad t>0. \tag{27}$$

Recalling that $\psi(t)$ is defined for $t>0$ and that $Q(t)$ is defined for $0<t<1$, Eq. (27) can be split into two integral equations as follows:

$$2Q'(t) + \psi(t) = \rho\int_0^t Q(s)\psi(t-s)ds - \rho\int_t^1 Q(s)\psi(s-t)ds \quad \text{for} \quad 0<t<1, \tag{28}$$

$$\psi(t) = \rho\int_0^1 Q(s)\psi(t-s)ds \quad \text{for} \quad t>1. \tag{29}$$

Our approach has reduced the PY problem for hard disks to the solution of the integro-differential equations (24), (28), and (29) with the additional boundary condition (17). We note that unlike the odd dimensional case,[4] here one cannot separate the problem of finding the direct correlation function $c(r)$ from that of finding the pair correlation function $g(r)$. This is because the behavior of $\psi(t)$ for $0<t<1$ is related to the behavior of $\psi(t)$ for $t>1$ through Eq. (24). Although we were unable to find an analytical solution valid for all ρ, the numerical solution of these equations can be easily implemented. Before dealing with the numerical analysis, let us first consider the equation of state in the present formulation of the problem.

There are two methods used to calculate the equation of state when the radial distribution function, $g(r)$, is known. Without the assumptions made in deriving the PY equation, these two methods would yield the same equation of state. The difference in the equations of state calculated using these two methods therefore provides an estimation of the error made by using the PY approximation. The first equation of state is derived from the virial theorem and is given by[1]

$$\beta P^{(v)} = \rho + \frac{\pi}{2}\rho^2 g(1^+), \tag{30}$$

where β is the inverse temperature $1/k_BT$. Using $g(1^+)=-c(1^-)^1$ and Eqs. (11) and (18), this "virial" equation of state becomes

$$\beta P^{(v)} = \rho + \frac{\pi}{4}\rho^2 \lim_{t\to 1^-}\sqrt{1-t^2}Q'(t). \tag{31}$$

The second method uses the isothermal compressibility κ_T, which is given by[1]

$$\rho\beta^{-1}\kappa_T = \beta^{-1}\left(\frac{\partial\rho}{\partial P^{(c)}}\right)_T = s(q=0). \tag{32}$$

Using Eq. (12) and replacing $\phi(t)$ with $Q(t)$ by using Eq. (18), one has

$$\frac{1}{s(0)} = 1 + 2\rho\int_0^1\left[\rho\int_t^1 Q(s)Q(s-t)ds - Q(t)\right]dt. \tag{33}$$

Integrating Eq. (32) and substituting for $s(0)^{-1}$ from Eq. (33) we find the "compressibility" equation of state:

$$\beta P^{(c)} = \rho + \int_0^\rho 2\rho'\left\{\int_0^1\left[\rho'\int_t^1 Q(s)Q(s-t)ds - Q(t)\right]dt\right\}d\rho'. \tag{34}$$

IV. NUMERICAL PROCEDURE

We found it simplest to implement an iterative procedure for solving the set of integral Eqs. (24), (28), and (29). First, note that for $\rho=0$, the exact solution is given by

$$\psi(t) = \frac{-4t}{\sqrt{1-t^2}}\Theta(1-t), \tag{35}$$

$$Q(t) = -2\sqrt{1-t^2}\Theta(1-t), \tag{36}$$

and that for any ρ, one can write the functions $Q(t)$ and $\psi(t)$ as power series in ρ,

$$\psi(t) = \frac{-4t\Theta(1-t)}{\sqrt{1-t^2}}\sum_{i=0}^\infty \rho^i\Psi^{(i)}(t) + \sum_{i=1}^\infty \rho^i\psi^{(i)}(t)\Theta(t-1)\Theta(i+1-t), \tag{37}$$

TABLE I. Numerical values of the first 20 virial coefficients. The $B_i^{(MC)}$ are the results from Monte Carlo calculations presented in Ref. 18. $B_i^{(v)}$ and $B_i^{(c)}$ are the values found from the solution to the PY equation using Eqs. (54) and (34), respectively.

i	$B_i^{(v)}$	$B_i^{(c)}$	$B_i^{(MC)}$
3	1.930	1.930	1.930
4	1.941	2.084	2.063
5	1.795	2.090	2.031
6	1.594	1.999	1.902
7	1.381	1.852	1.726
8	1.177	1.677	1.534
9	0.922	1.492	1.342
10	0.829	1.309	1.162
11	0.688	1.136	–
12	0.567	0.977	–
13	0.466	0.834	–
14	0.382	0.707	–
15	0.311	0.596	–
16	0.253	0.50(1)	–
17	0.20(5)	0.41(8)	–
18	0.16(6)	0.34(9)	–
19	0.13(5)	0.28(9)	–
20	0.10(9)	0.23(9)	–

$$Q(t) = -2\sqrt{1-t^2}\sum_{i=0}^{\infty} \rho^i q^{(i)}(t), \tag{38}$$

with the definition

$$\Psi^{(0)}(t) = q^{(0)}(t) = 1, \tag{39}$$

$$\psi^{(0)}(t) = 0. \tag{40}$$

Using this power series representation, Eq. (24) yields

$$\Psi^{(i)}(t) = \int_1^{i+1} \frac{\sqrt{s^2-1}}{s^2-t^2}\psi^{(i)}(s)\frac{ds}{2\pi}, \quad i \geq 1, \tag{41}$$

and Eq. (28) becomes

$$(1-t^2)q'^{(i+1)}(t) - tq^{(i+1)}(t) + t\Psi^{(i+1)}(t) = -2\sqrt{1-t^2}\int_0^1 \frac{(t-s)\sqrt{1-s^2}}{\sqrt{1-(t-s)^2}} \times \sum_{k=0}^{i} q^{(k)}(s)\Psi^{(i-k)}(|t-s|)ds, \quad i \geq 0. \tag{42}$$

The boundary condition $q^{(i)}(1)=\Psi^{(i)}(1)$ for $\forall i \geq 0$ is necessary to avoid a singularity in $q^{(i)}(t)$ as $t \to 1$. Finally, Eq. (29) gives

$$\psi^{(i+1)}(t) = \sum_{k=0}^{i}\left[8\int_{t-1}^{1}\frac{s\sqrt{1-(t-s)^2}}{\sqrt{1-s^2}}q^{(k)}(t-s)\Psi^{(i-k)}(s)ds - 2\int_1^t \sqrt{1-(t-s)^2}q^{(k)}(t-s)\psi^{(i-k)}(s)ds\right], \tag{43}$$

$1 \leq t \leq 2,$

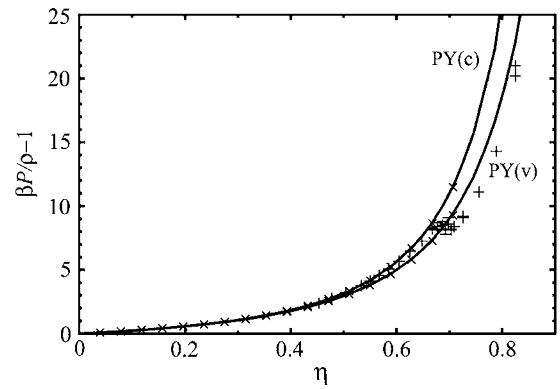

FIG. 1. Reduced pressure $\beta P/\rho - 1$ as a function of the disk packing fraction, η. The results of molecular dynamics simulations reported previously (Refs. 13 and 15) are shown as + along with the results obtained from an earlier solution of the PY equation (Ref. 10), shown as $\times$. The two solid curves show the results of our calculations using the first 20 virial coefficients, with the labels corresponding to the equation of state used to calculate them.

$$\psi^{(i+1)}(t) = -2\sum_{k=0}^{i}\int_{t-1}^{t}\sqrt{1-(t-s)^2}q^{(k)}(t-s) \times \psi^{(i-k)}(s)ds, \quad t > 2. \tag{44}$$

In devising a successful numerical scheme for this problem, it is important to note that several of the integrands have mild singularities, for example at $s=1$ in Eq. (43) and at $s=1$, $t=1$ in Eq. (41). The singularity in Eq. (43) may be dealt with simply by subtraction. To deal with the singularity in Eq. (41), we note that we may integrate Eq. (41) once by parts and write

$$\Psi^{(i)}(t) = \sqrt{1-t^2}\int_1^{i+1} \arctan\sqrt{\frac{s^2-1}{1-t^2}}\frac{d}{ds}\left(\frac{\psi^{(i)}(s)}{s}\right)\frac{ds}{2\pi} - \int_1^{i+1}\sqrt{s^2-1}\frac{d}{ds}\left(\frac{\psi^{(i)}(s)}{s}\right)\frac{ds}{2\pi}. \tag{45}$$

This obviates the need to subtract the singularity and also suggests that we may write

$$\Psi^{(i)}(t) = \alpha^{(i)} + \delta^{(i)}\sqrt{1-t^2} + g^{(i)}(t), \tag{46}$$

with $g^{(i)}(1)=0$, and

$$\alpha^{(i)} = -\int_1^{i+1}\sqrt{s^2-1}\frac{d}{ds}\left(\frac{\psi^{(i)}(s)}{s}\right)\frac{ds}{2\pi} = \Psi^{(i)}(1), \tag{47}$$

$$\delta^{(i)} = \lim_{t\to 1}\int_1^{i+1}\arctan\sqrt{\frac{s^2-1}{1-t^2}}\frac{d}{ds}\left(\frac{\psi^{(i)}(s)}{s}\right)\frac{ds}{2\pi} = -\frac{1}{4}\psi^{(i)}(1). \tag{48}$$

Examining the equation for $q^{(i+1)}(t)$, Eq. (42), we see that the form assumed for Eq. (46) suggests that

$$q^{(i)}(t) = \alpha^{(i)} + \gamma^{(i)}\sqrt{1-t^2} + f^{(i)}(t). \tag{49}$$

Here, the function $f^{(i)}(t)$ satisfies $f^{(i)}(1)=0$ and

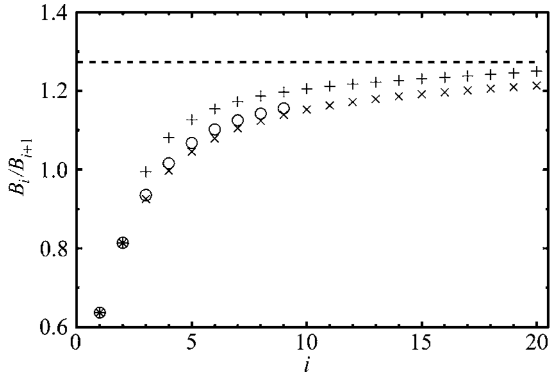

FIG. 2. The ratio between successive virial coefficients B_i/B_{i+1} as a function of i. The ratios determined from the solution to the PY equation are denoted by + (βP^v) and × (βP^c). These results sandwich the virial coefficients determined from Monte Carlo calculations given in Ref. 18, which are represented by ○. The dashed line represents $B_i=4B_{i+1}/\pi$, which appears to be the asymptote as $i\rightarrow\infty$.

$$(1-t^2)f'^{(i+1)}(t)+t[g^{(i+1)}(t)-f^{(i+1)}(t)] = 2\sqrt{1-t^2}[tA^{(i+1)}(1)-A^{(i+1)}(t)], \tag{50}$$

where

$$A^{(i+1)}(t)\equiv\sum_{k=0}^{i}\int_0^1\frac{(t-s)\sqrt{1-s^2}}{\sqrt{1-(t-s)^2}}q^{(k)}(s)\Psi^{(i-k)}(|t-s|)ds. \tag{51}$$

The constant $\gamma^{(i)}$ may be determined by considering the limit $t\rightarrow 1$, which gives

$$\gamma^{(i)}=\frac{1}{2}\delta^{(i)}+A^{(i)}(1). \tag{52}$$

We solve the system of equations by discretizing in space using steps of size Δ. Integrals are evaluated using the trapezoidal rule and derivatives are calculated using forward-differencing, both of which are first-order accurate in space. Iterations proceed from $i=0$ using the values $\Psi^{(0)}$ and $q^{(0)}$, given in Eq. (40), to determine $\psi^{(1)}(t)$. Using $\psi^{(1)}(t)$ in the discretized versions of Eqs. (47) and (48) allows us to determine $\Psi^{(1)}(t)$. Substituting these into the discretized Eq. (50), $q^{(1)}(t)$ may be determined. The whole process is then iterated N times, corresponding to determining the first N terms in the series for the variables $\Psi(t)$, $q(t)$, and $\psi(t)$. The results presented here typically have $N=20$.

V. NUMERICAL RESULTS

Let us begin by presenting our results for the virial coefficients and the equation of state. The virial coefficients, B_i, are defined by

$$\beta P=\sum_{i=1}^{\infty}B_i\rho^i. \tag{53}$$

It is well-known that $B_1=1$ and $B_2=\pi/2$ are exact and are recovered within the PY approximation. The higher order virial coefficients can be calculated from the solution of the PY equation using the expressions in Eqs. (31) and (34). For example, using Eqs. (38) and (31) yields

$$B_i^{(v)}=\frac{\pi}{2}q^{(i-2)}(1),\quad i\geq 2. \tag{54}$$

Thanks to the iterative procedure presented above, these coefficients as well as the $B_i^{(c)}$, which are derived from the isothermal compressibility Eq. (34), are directly given by the numerical resolution of the problem.

Our numerical solution of the PY equation and calculation of the virial coefficients are only first order accurate in space and so we expect to accumulate errors at $O(\Delta)$. To counter this, we calculated each of the virial coefficients for several values of Δ and then extrapolated linearly its value at $\Delta=0$. For each virial coefficient the correlation coefficient was calculated to be <-0.999, confirming that the expected linear dependence of B_i on Δ is indeed observed. The computed values of the first 20 coefficients for the series corresponding to βP^v and βP^c are presented in Table I. The values of the first ten virial coefficients for hard disks were determined recently using a "hit or miss" Monte Carlo integration algorithm in Ref. 18 and are reproduced in Table I for comparison.

As is clear from the definition (53), the virial coefficients are important for determining the equation of state. The value of the pressure, βP, is therefore of considerable interest. Figure 1 shows the dependence of βP on the packing

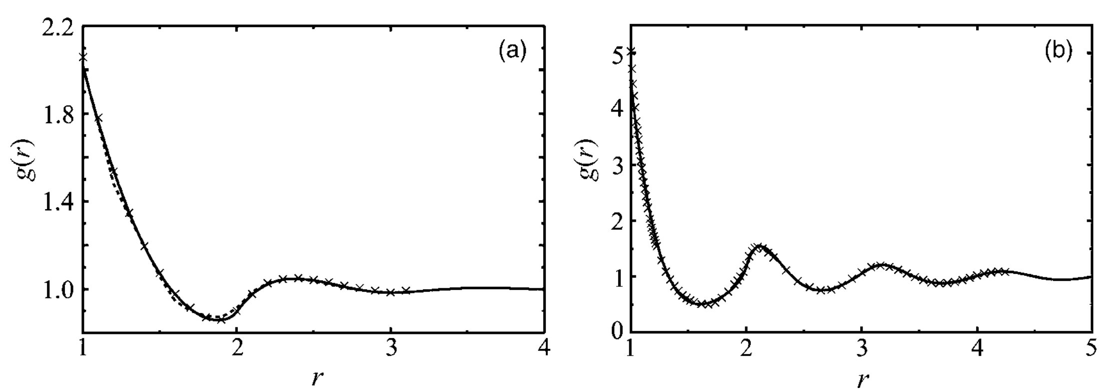

FIG. 3. The correlation function $g(r)$ computed from the PY equation (curves) and from different Monte Carlo simulations (crosses). (a) $\rho=0.462$: Our solution of the PY equation (solid curve) compared to the MC results of Chae *et al.* (Ref. 14) (crosses) and their solution of the PY equation (dashed curve). (b) $\rho=0.794$: Our solution of the PY equation (solid curve) compared to the MC results of Wood (Ref. 16) (crosses). Solid curves were calculated using the first 50 terms of the series with $\Delta=0.001\,25$.

fraction of the disks, η. This shows that there is good agreement between our results and previous ones using a direct approximate numerical resolution of the PY equation.[10] Furthermore, this agreement is within the 2% error estimate given in Ref. 10.

It is clear from Fig. 1 that there is a divergence in βP for relatively large η. The question of interest here is: at what density does this divergence occur? We are thus interested in determining the radius of convergence of the series for βP. To this end, we plot in Fig. 2 the ratio between successive virial coefficients given in Table I. In particular, we observe that as $i \to \infty$

$$\frac{B_i}{B_{i+1}} \to \frac{4}{\pi}. \tag{55}$$

Using d'Alembert's ratio test, this observation suggests that the series for βP will converge absolutely provided that $\rho < 4/\pi$ or, equivalently, $\eta < \eta_c = 1$, the space filling density. This result shows that, similarly to the case of hard spheres ($d=3$), the PY equation for hard disks predicts no phase transition at intermediate density and thus fails at high densities.

Finally, the correlation function $g(r)$ may be calculated numerically from the values of $\psi^{(i)}$. Some typical results are shown in Fig. 3 and compared with the available Monte Carlo results.[14,16] As can be seen, the overall agreement is very good, except in the vicinity of $r=1$. Also note that our solution of the PY equation in Fig. 3(a) agrees better with the Monte Carlo results than a previous numerical solution of the PY equation presented in Ref. 14.

VI. DISCUSSION

In this paper we developed a semi-analytic method to solve the PY equation for hard disks. At the heart of this approach is a reduction of the PY equation to a set of integral equations for two auxiliary functions $Q(s)$ and $\psi(s)$ as given by Eqs. (24), (28), and (29). The correlation functions and the equation of state can be determined easily from these auxiliary functions. We suggest an efficient iterative numerical method to solve these equations and determine the auxiliary functions. Using this method we are able to determine the values of the virial coefficients within the PY approximation and compare with the available 10 virial terms of the full problem.[18] We also obtain results for the pair correlation function, which compare well with the available MC calculations.

The principal advantage of this approach is that it provides directly the virial series, and so it yields the equation of state for all values of ρ at the same time, unlike other approaches where every value of ρ requires a separate calculation. An important consequence is that we can study the convergence of the series, which yields the critical density at which the pressure diverges. We show for the first time that the PY theory for hard disks predicts no phase transition at intermediate densities and diverges at $\eta_c=1$, just like in odd dimensions. As explained above, this method allows, in principle, calculations to arbitrary precision, and it could be interesting to obtain more virial coefficients by so doing. It could also be interesting to generalize this approach to polydisperse mixtures[22] and to higher even dimensions.

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