Bridge function and other structural properties of core-softened model fluids from molecular dynamics simulations

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(Received 28 March 2002; revised manuscript received 10 May 2002; published 28 August 2002)

Molecular dynamics (MD) simulations in three dimensions have been performed for a fluid with particles interacting with a continuous version of the Stell-Hemmer core-softened potential that in two dimensions has been known to reproduce most of the static and dynamic anomalies of liquid water. The pair distribution function obtained from the MD simulation is extrapolated with the help of integral equation theory with a suitable closure relation and the bridge function is extracted. A strong dependence of the bridge function on the system size, i.e., the total number of particles (N) used in the simulation box is observed, which leads to spurious values of the structure factor at long wavelengths. A simple self-consistent correction scheme for the finite size effect has been adopted to correct the bridge function and this scheme produces the correct bridge function even for a small system size. The effects of temperature, number density, and potential parameters on the pair distribution functions and extracted bridge functions are extensively studied.

DOI: 10.1103/PhysRevE.66.021206 PACS number(s): 61.20.Ja, 61.20.Gy, 61.20.Ne

I. INTRODUCTION

Water, the most important liquid on earth, is known to possess in its properties not only various static anomalies but dynamic anomalies as well [1–3]. As for example, liquid water exhibits static anomalies such as anomalous density maximum [2] at $T=4\,^{\circ}\mathrm{C}$ and increase in isothermal compressibility upon cooling, and dynamical anomalies such as increase in diffusion coefficient or decrease in viscosity with increase in pressure in certain ranges of temperature [3]. Such anomalies are manifested not only in water, but in some other liquids [4–6] as well. Apart from these anomalies, liquid-liquid phase separation of a monodispersed pure liquid that has recently been experimentally observed [7] in phosphorus is also an interesting phenomenon. Understanding these phenomena from a microscopic viewpoint is a long standing interest in the liquid state physics and various efforts to mimic these phenomena with some spherically symmetric model potentials have already been made [8–12]. The core-softened potential [13] has so far been shown to be the most successful model potential in this regard. In a pioneering work, Stell and Hemmer (SH) have proposed [13] that a second critical point apart from the normal gas-liquid critical point is possible for a core-softened potential that has a region of negative curvature in the repulsive core. Using thermodynamic arguments, Debenedetti, Raghavan, and Borick [14] have noted that a ''softened core'' in potential may be responsible for the density anomaly, one of the anomalies found in liquid water. An analytical solution of the equation of state for a double well SH-type potential in one dimension has been obtained by Cho, Singh, and Robinson [15] and has been shown to yield density anomaly and the correct pressure effects on the temperature dependent density. The computer simulation study of Sadr-Lahijany *et al.* [8] has shown that the discrete as well as continuous versions of a two-dimensional (2D) SH core-softened potential are able to reproduce various liquid state anomalies. A detailed 2D simulation study has also been reported [10] on the same problem. A core-softened potential can be regarded as a first-order approximation to the interaction between water molecules as suggested [16,17] by *ab initio* calculation and inversion of the experimental oxygen-oxygen radial distribution function. Recent experimental results [7] reveal that phosphorus, a single-component system, shows a coexistence between the high-density liquid phase and the low-density liquid phase. Very recently a core-softened potential has successfully been used [12] to explain the mechanism of this liquid-liquid phase separation for a three-dimensional single-component model fluid. A slightly modified form of the SH potential has also been shown to reproduce both the density anomaly [9] and the liquid-liquid phase separation phenomena [11]. Furthermore, a perturbation theory analysis shows a complex phase behavior [18] of a fluid-solid transition for a modified SH potential.

Most of the studies on fluids with particles interacting with the SH potential so far have concentrated on obtaining an equation of state from the computer simulation. However, a much easier and computationally economic way of studying the liquid state is the well-known integral equation theory [19,20]. In this theory, one has to solve the Ornstein-Zernike (OZ) equation [21] with the help of a suitable closure relation. The accuracy of this approach depends on the accuracy of the closure relation, which in turn depends on how successfully one can construct the so-called bridge function that is essentially the sum of diagrams that are free of nodal circles. In principle, if the bridge function is given beforehand, the radial distribution function and the direct correlation function of a model fluid can easily be determined from the integral equation theory. There have been attempts to arrive at a universal [22] bridge function for an arbitrary pair potential through that of an effective hard sphere like reference system. Although this concept has been successful [23,24] in many situations, its applicability has been rather limited [25–27] and several studies [28,29] on

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the bridge function have, in fact, included other contributions, thus making the bridge function dependent on the pair potential in general. One of the important routes to the bridge function for a given pair potential is through computer simulation. As the radial distribution function (RDF) $g(r)$ obtained from the computer simulation is accurate and devoid of any approximation to the many-body problem, it can be inverted to construct the bridge function in the intermediate range accurately. However, the range of RDF obtained from the molecular dynamics (MD) simulation is limited to only half of the box length of the simulation cell, where the box length is related to the number of particles taken in the simulation cell, i.e., the system size. This imposes difficulty in calculating the bridge function due to the truncation error in the Fourier transform of $h(r)[=g(r)-1]$, the total correlation function of the system. Various extrapolation schemes have been used to overcome this difficulty. Long ago, Verlet [30] used an extrapolation scheme to obtain the bridge function of the Lennard-Jones fluid. Recently, the extrapolation scheme due to Verlet is modified and applied [25] to extract the bridge function of the Lennard-Jones as well as empty-core pseudopotential for aluminum in the intermediate range. However, the problem due to finite size in the computer simulation results for various quantities still remains and a correction scheme for obtaining the correct static structure factor, compressibility, and intermediate scattering function has been formulated and applied [31] to a model pair potential for dense fluid krypton. This scheme has further been extended [26] in the coordinate space and applied to the correction of the finite size effect on RDF and bridge function in the intermediate range.

In the present work, we intend to extract the bridge function of a core-softened SH potential from the RDF data obtained from the MD simulation through extrapolation. The MD simulation in microcanonical NVE ensemble is performed to obtain the radial distribution function data for the continuous version of the SH potential in three dimensions. The bridge function in the intermediate range is then calculated through a self-consistent extrapolation procedure [25]. The finite size effect on the bridge function obtained from such extrapolation is corrected through the scheme of Baumketner and Hiwatari [26]. In what follows, in Sec. II we discuss the model potential and the simulation procedure. In Sec. III, we outline the extrapolation scheme along with the correction scheme for the finite size effect. The results for the RDF and the bridge function are gathered in Sec. IV. Finally a few concluding remarks are offered in Sec. V.

II. MODELS AND MOLECULAR DYNAMICS SIMULATION

A. Model potential

The continuous version of the core-softened SH potential $u(r)$ that we study here is obtained by augmenting an inverted Gaussian well with the well-known Lennard-Jones (LJ) potential and is given by

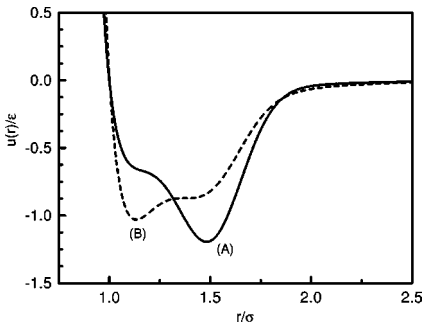

FIG. 1. Plot of core-softened potential $u(r)$ as a function of r/σ. The solid line represents $u(r)$ for system *A* and the dashed line represents that of system *B*.

$$u(r)=4\epsilon\lambda_1\left[\left(\frac{\sigma}{r}\right)^{12}-\left(\frac{\sigma}{r}\right)^{6}\right]-\epsilon\lambda_2\exp\left[-\alpha\left(\frac{r}{\sigma}-\frac{r_0}{\sigma}\right)^2\right] \tag{1}$$

for $r\leqslant r_c$ and vanishes for $r>r_c$. In the above expression, σ is the distance at which $u(r)$ is zero and is related to the size of the particle and ϵ is related to the depth of the potential. In all our studies we use $r_c=4.0\sigma$. Two sets of potential parameters have been used in the present work. In one case, the second or the outer well is deeper which we call as system *A*, while in the other case the inner well is deeper (system *B*) and both the potentials are shown in Fig. 1 as a function of the interparticle distance *r*. The parameters we use are: $\lambda_1=0.5882$, $\lambda_2=1.0$, $\alpha=20.0$ and $r_0=1.5\sigma$ for system *A* and $\lambda_1=1.03$, $\lambda_2=0.714\,285$, $\alpha=20.0$, and $r_0=1.5\sigma$ for system *B*.

B. Simulation

In the present work, molecular dynamics simulations are performed in the NVE ensemble for two different temperatures and number densities. Simulations are started by placing all the particles in a cubic box with fcc lattice configuration. Periodic boundary conditions are employed in all the three directions. The particle numbers (N) in the box are taken to be 864 and 2048. The potential cutoff in all the cases as has already been mentioned is set to be $r_c=4.0\sigma$. The velocity Verlet algorithm along with the velocity scaling to maintain the temperature close to the desired value is employed. The systems are equilibrated for over 3×10^5 time steps whereas the time averages for various quantities are taken over 2×10^5 time steps with the time step $t^*=0.01$, where $t^*=t[\epsilon/(m\sigma^2)]^{1/2}$ with m being the mass of a particle. All the quantities are expressed in dimensionless form, viz. the temperature T is expressed as $T^*=k_BT/\epsilon$, where k_B is the Boltzmann constant, the pressure P as $P^*=P\sigma^3/\epsilon$, and the distance r as $r^*=r/\sigma$, etc.

III. EXTRACTION OF THE BRIDGE FUNCTION

A. Extrapolation scheme without correction for the finite size

In order to obtain the bridge function from the RDF generated by MD simulation, one has to solve the OZ equation, which for an isotropic and homogeneous fluid can be written as

$$h(r_{12}) = c(r_{12}) + \rho \int d\mathbf{r}_3 c(r_{13}) h(r_{32}), \tag{2}$$

where $c(r)$ is the direct correlation function and ρ is the bulk density of the fluid, along with a closure relation involving the $g(r)$ obtained from the computer simulation. It is this closure that defines the bridge function $B(r)$ through the exact relation between $h(r)$, $u(r)$, and the indirect correlation function $\gamma(r)[=h(r)-c(r)]$ as given [19] by

$$h(r_{12}) + 1 = \exp[-\beta u(r_{12}) + \gamma(r_{12}) + B(r_{12})], \tag{3}$$

where $\beta(=1/k_B T)$ is the inverse temperature.

The scheme that we have employed in the present work to extract the bridge function is originally due to Verlet [30] and modified recently by Kambayashi and Chihara [25]. The original extrapolation scheme of Verlet employs an extrapolation technique for the values of RDF for $r > L/2$, L being the length of the simulation box, in which the Percus-Yevick, (PY) approximation for $g(r)$ for $r > L/2$ is combined with the simulated $g(r)$ for $r \leqslant L/2$, viz.,

$$g(r) = g^N_{\mathrm{MD}}(r), \quad r < R, \tag{4}$$

$$g(r) = \exp[-\beta u(r)][1 + \gamma(r)], \quad r \geqslant R, \tag{5}$$

where $g^N_{\mathrm{MD}}(r)$ is the RDF obtained from MD simulation and R is the extrapolating distance that is set as less than or equal to $L/2$. The superscript N on $g_{\mathrm{MD}}(r)$ implies that the RDF is obtained for a closed system with fixed N. It is easy to recast Eqs. (4) and (5) in the form of Eq. (3) and use the resulting equation as closure for the OZ equation that when numerically solved yields simultaneously $g(r)$ and $c(r)$ for the entire range and $B(r)$ for the intermediate range. Verlet in his work [30] performed MD simulation and applied this method to LJ fluid near its triple point. Different schemes for this closure relation are reported [32,27] in which the right hand side of Eq. (5) is replaced by some better approximation, such as hypernetted chain (HNC) or mean spherical approximations.

In the present work, we have used HNC approximation for the closure relation in Eq. (5) in place of PY approximation used by Verlet:

$$\begin{aligned} g(r) &= g^N_{\mathrm{MD}}(r), \quad r < R \\ &= \exp[-\beta u(r) + \gamma(r)], \quad r \geqslant R, \end{aligned} \tag{6}$$

with $R = L/2$, the largest extrapolating distance possible. In order to obtain the bridge function $B_{\mathrm{MD}}(r)$, one has to rewrite the above equation with the help of Eq. (3) as

$$\begin{aligned} B_{\mathrm{MD}}(r) &= \beta u(r) - \gamma(r) + \ln[g^N_{\mathrm{MD}}(r)], \quad r < R \\ &= 0, \quad r \geqslant R. \end{aligned} \tag{7}$$

Solving Eq. (2) numerically with the closure relation given by Eq. (7), one obtains $g(r)$, $c(r)$, and $B(r)$ simultaneously. The closure relation given by Eq. (7) has been employed by Kambayashi and Chihara [25] for calculating the bridge function for LJ as well as a model potential for dense krypton. In the present work, we have employed this approach for the core-softened continuous version of the SH potential in three dimensions and the results for $B(r)$ obtained from this approach show finite size dependence, i.e., dependence on the number of particles N used in the simulation. The finite size dependence of $B(r)$ obtained from computer simulated $g(r)$ and of other quantities such as the static structure factor, intermediate scattering function, etc. has already been reported and a correction scheme for this finite N has been devised [31,26]. In the following section, we briefly outline this correction scheme [31] that we have implemented here.

B. Extrapolation scheme with correction for the finite size

The RDF $g^N_{\mathrm{MD}}(r)$ calculated in a MD simulation in a closed ensemble like NVE, with fixed number of particles N, differs from the same calculated in an open system where N is allowed to fluctuate, i.e., in grand canonical ensemble. Only in the thermodynamic limit $N \to \infty$, these two functions coincide and any difference between these two functions is known as finite size effect in computer simulation. It is to be noted that the closure relation used in the present work [i.e., Eq. (7)] utilizes $g^N_{\mathrm{MD}}(r)$ obtained from the MD simulation with finite N and thus introduces error in the calculation of $B(r)$. This finite system RDF can, however, be corrected following the work of Salacuse *et al.* [31], who have derived an expression relating the finite system RDF $g^N(r)$ to its open system counterpart $g(r)$ as follows: The two-particle density $\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2)$ in the grand canonical ensemble is expressed as [19]

$$\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{N=0}^{\infty} P(N) \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2; N), \tag{8}$$

where $P(N)$ is the probability that the system contains N particles, and $\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2; N)$ is the two-particle density for a system of N particles. Expanding $\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2; N)$ about the average number of particles $\overline{N}[=\Sigma_{N=0}^{\infty} P(N) N]$ in powers of $1/N$, one has

$$\begin{aligned} \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2) = \sum_{N=0}^{\infty} P(N) \Bigg[& \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2; \overline{N}) \\ & + (N - \overline{N}) \frac{\partial}{\partial \overline{N}} \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2; \overline{N}) \\ & + \frac{1}{2} (N - \overline{N})^2 \frac{\partial^2}{\partial \overline{N}^2} \rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2; \overline{N}) + \cdots \Bigg]. \end{aligned} \tag{9}$$

Using the normalization condition for $P(N)$, considering the results $\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2) \to \rho^2 g(r)$ and $\rho^{(2)}(\mathbf{r}_1, \mathbf{r}_2; \overline{N}) \to \rho^2 g^N(r)$ in the uniform limit and relating the coefficients to the compressibility via fluctuation theory, one arrives at the final expression relating $g(r)$ with $g^N(r)$ as

$$g(r)=g^N(r)+\frac{S(0)}{2N}\frac{\partial^2}{\partial\rho^2}[\rho^2 g^N(r)]+O(1/N^2)$$
$$=g^N(r)+\frac{S(0)}{2N}\left[2g^N(r)+4\rho\frac{\partial}{\partial\rho}g^N(r)+\rho^2\frac{\partial^2}{\partial\rho^2}g^N(r)\right], \quad (10)$$

where $S(0)$ is the value of the static structure factor $S(k)$ at $k=0$ and is related to the compressibility. Equation (10) is a standard relation for transformation between ensembles with correction term of order $1/N$. As the correction term above contains density derivatives, a precise solution of Eq. (10) by MD simulation is possible only through performing the simulations at several densities, which is not only an impractical choice but in some cases, even infeasible. Thus, by neglecting the density dependence of $g^N(r)$, Eq. (10) further simplifies to

$$g(r)=g^N(r)+\frac{S(0)}{N}g^N(r). \quad (11)$$

The expression (11) for the correction of $g^N(r)$ for finite size can be utilized to correct the simulation RDF provided $S(0)$ is known. Equation (11) cannot be employed as such since $S(0)$ is not known *a priori*. However, the fact that $S(0)$ is related to the Fourier transform of RDF through the relation

$$S(0)=4\pi\rho\int[g(r)-1]r^2dr \quad (12)$$

makes it possible to construct a self-consistent iterative scheme for calculating the bridge function from the simulated RDF $g^N_{\mathrm{MD}}(r)$. The simulation RDF $g^N_{\mathrm{MD}}(r)$ is first corrected through Eq. (11) and the corrected $g^N_{\mathrm{MD}}(r)$ is then substituted into the closure relation (7) and the OZ equation is solved numerically with this corrected closure. The resulting $g(r)$ is then transformed according to Eq. (12) to calculate the new estimate for $S(0)$ and the whole cycle is iterated until a desired convergence between the $S(0)$'s from two successive iterations is achieved. Finally, we obtain $B(r)$, $S(0)$, $g(r)$, and $c(r)$ for the entire range for a given pair potential. This method when applied [26] to the pair potential modeling liquid sodium has been shown to correct the bridge function for finite size effect. In the present study, we employ this correction scheme to obtain the corrected bridge function for a fluid interacting with the continuous version of the core-softened SH potential by inverting the RDF data obtained from MD simulations.

IV. RESULTS AND DISCUSSION

A. Results for system *A*

The simulation results for $g(r)$ obtained from the MD simulation of $N=2048$ particles for various temperatures and densities are shown in Fig. 2 for the potential parameters corresponding to system *A* (see Sec. II A for the values of potential parameters). The RDF at $T^*=1.5$ for two different number densities ρ^* $(=\rho\sigma^3)=0.8$ and $\rho^*=0.6$ is plotted in the upper panel of Fig. 2. In both the cases, the first two major peaks correspond to the two wells in the potential. In the case of lower density $\rho^*=0.6$, the first peak is reduced as compared to that for $\rho^*=0.8$ but the height of the second peak due to outer well is increased. It indicates that at lower density (pressure), the second well is relatively more populated in comparison to that in case of higher density (pressure). This ''split first peak'' behavior is characteristic of a core-softened potential that generally has two characteristic length scales. Similar behavior is also observed [33] in the case of an overlapping core potential modeling star polymer in good solvent. In order to study the effect of temperature, in the lower panel of Fig. 2, we have shown the results for $g(r)$ at a lower temperature $T^*=1.0$. From a comparison of the two cases, it is clear that with decrease in temperature, the outer well population increases at lower density while it is the inner well population that shows more increase at higher density.

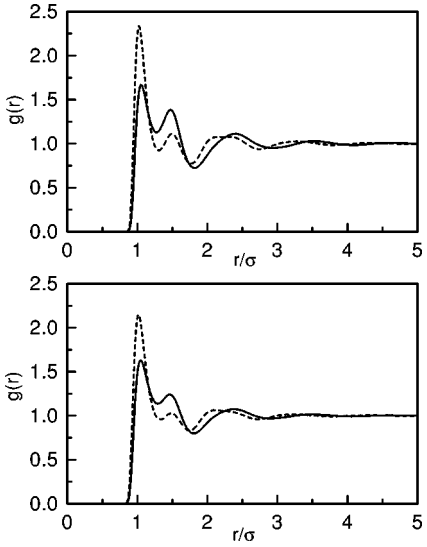

FIG. 2. Plot of the radial distribution function $g(r)$ vs r/σ for system *A* at $T^*=1.5$ (upper panel) and $T^*=1.0$ (lower panel). The solid line represents results for $\rho^*=0.6$ and the dashed line represents those for $\rho^*=0.8$.

By inverting these computer simulated $g(r)$ data, we have extracted the bridge functions using the schemes mentioned in Sec. III and the results are plotted in Fig. 3. The uncorrected $B(r)$ that we denote as $B^u(r)$ as obtained through the scheme depicted in Sec. III A from $g(r)$ of MD simulation corresponding to $N=864$ particles for $T^*=1.5$ and $\rho^*=0.6$ is shown in Fig. 3 along with the same for $N=2048$ particles. It is clear from the figure that there is a considerable difference between these two results, which can be attributed to the N dependence of the bridge function. These $B(r)$ values have been corrected [which we denote as $B^c(r)$] according to the scheme described in Sec. III B and are plotted in the same figure (Fig. 3) for $N=2048$ as well as $N=864$ particles. These two corrected $B^c(r)$'s are very close to each other and also to the uncorrected $B^u(r)$ for $N=2048$ particles. Thus, the correction of the bridge function is most essential when we extract it from the $g(r)$ obtained from a simulation with smaller number of particles. As

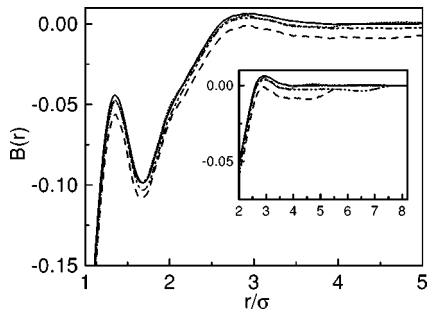

FIG. 3. Plot of corrected and uncorrected bridge functions for system A at $T^*=1.5$ and $\rho^*=0.6$ extracted from the $g(r)$ data obtained from MD simulation with various values of N, the number of particles used in simulation. The dashed line represents $B^u(r)$ for the $N=864$ particle system, the dotted line represents $B^c(r)$ for the $N=864$ particle system, the dash-dot-dot line represents $B^u(r)$ for the $N=2048$ particle system, and the solid line represents $B^c(r)$ for the $N=2048$ particle system. In the inset, the same plots are shown for a larger range.

shown in the inset of Fig. 3, the uncorrected bridge functions have a plateau extending from intermediate r to the extrapolation distance R where it drops down to zero (see inset). This trend is observed even for the case of 2048-particle system where the plateau extends to larger values of r. However, the corrected bridge function for the $N=2048$ particle system does not have this plateau region and smoothly extrapolates to zero. It is to be noted that although the corrected $B^c(r)$ for $N=864$ is very close to that for $N=2048$, it still has a plateau region extending over a small region up to $r=4\sigma$.

Now we discuss the effect of finite size in simulation on the various structural quantities, namely, $g(r)$ and $S(k)$ obtained from the extrapolation of the simulated $g(r)$ data. Although we have not shown here the $g(r)$ obtained from simulation, the same obtained from uncorrected extrapolation method for even $N=864$ particles and the corrected one

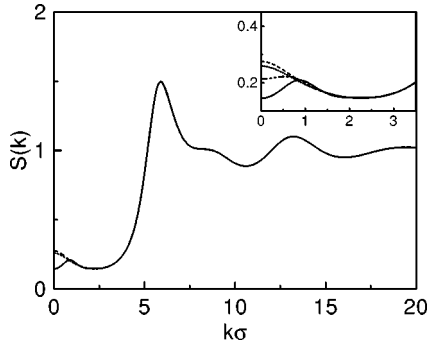

FIG. 4. Plot of static structure factor as a function of $k\sigma$ obtained from the extrapolated $g(r)$ data with and without the finite size correction for $T^*=1.5$ and $\rho^*=0.6$ and various values of N. The solid line represents $S(k)$ for the $N=864$ particle system without correction, the dotted line is for the $N=864$ particle system with correction, the dash-dot-dot line represents $S(k)$ for the $N=2048$ particle system without correction (shown in the inset only), and the dashed line represents the same for the $N=2048$ particle system with correction. In the inset, all four plots are shown for the small $k\sigma$ region.

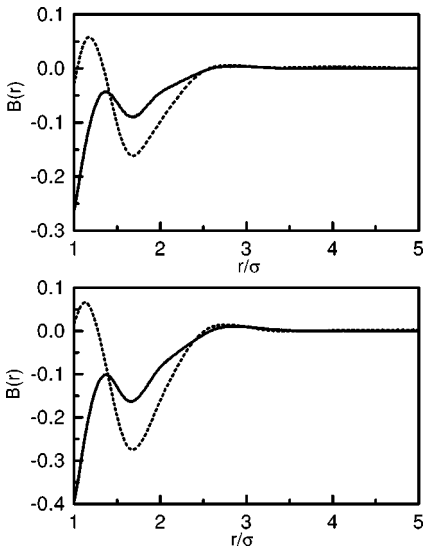

FIG. 5. Plot of the bridge function $B(r)$ vs r/σ for system A at $T^*=1.5$ (upper panel) and at $T^*=1.0$ (lower panel). The dotted line represents results for $\rho^*=0.8$ while the solid line corresponds to the same for $\rho^*=0.6$.

are, in fact, almost indistinguishable. This is understandable also from the correction term $[S(0)/N]g(r)$ that has a value of the order of 10^{-4} at large r, where $g(r)$ assumes the asymptotic value of unity and is thus too small to be visible when $g(r)$'s are plotted. In order to investigate the effect of finite size on the static structure factor $S(k)$ or the sensitivity of $S(k)$ on the details of the bridge function, in Fig. 4, we have shown the calculated static structure factor obtained from the extrapolation of MD RDF data at $T^*=1.5$ and $\rho^*=0.6$ with and without the correction due to the finite size effect. The corrected data for $N=864$ as well as for $N=2048$ almost coincide with each other everywhere including the region of small wave vector ($k\sigma$) values, whereas the uncorrected $S(k)$ data for $N=864$ shows spurious maximum in this long-wavelength region. For clarity, we have not shown in the main figure (but have shown in the inset) the

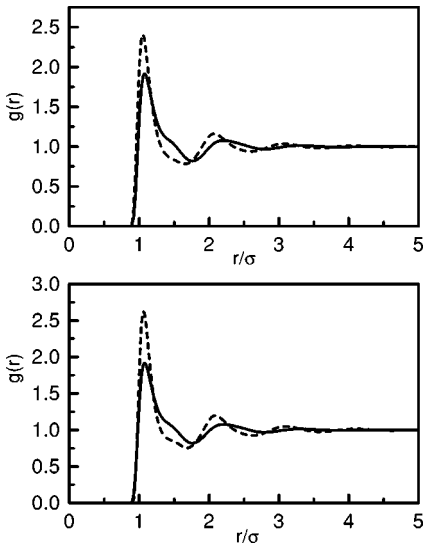

FIG. 6. Same as in Fig. 2 but for system B.

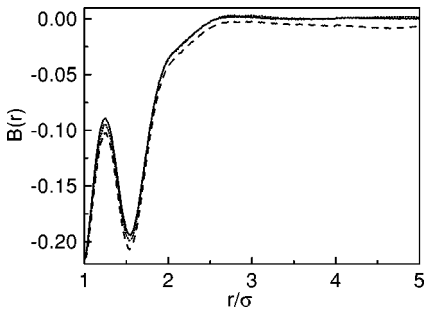

FIG. 7. Same as in Fig. 3 but for system *B* and except that the uncorrected $B^u(r)$ for the $N=2048$ particle system is not shown here.

uncorrected $S(k)$ data for $N=2048$, which coincide with other data except at low $k\sigma$ values where these data also show a slight spurious maximum but with smaller deviation from the corrected value as has been shown in the inset.

In order to study the effect of density and temperature on the bridge function, we have shown in Fig. 5 the corrected bridge function of the $N=2048$ particle system for densities $\rho^*=0.8$ and 0.6 at temperatures $T^*=1.5$ (upper panel of the figure) and $T^*=1.5$ (lower panel of the same figure). At a particular temperature, larger oscillations in $B(r)$ are observed at higher density as compared to lower density and it may be noted that at higher density, $B(r)$ passes through a positive maximum at lower r/σ values. The nature of $B(r)$ is similar at low temperature as well, but the oscillations are more at lower temperature indicating a larger deviation from the standard HNC result.

B. Results for system *B*

Same set of results [except plot for $S(k)$] for the parameters corresponding to system *B* (see Sec. II A for the values of potential parameters) are also shown in Figs. 6–8. The values of $g(r)$ obtained directly from the MD simulation for the $N=2048$ particle system for $T^*=1.5$ and for $\rho^*=0.8$ and 0.6 are shown in the upper panel of Fig. 6, while $g(r)$ for the same two densities but at a lower temperature $T^*=1.0$ are plotted in the lower panel of the same figure. In this case, due to smaller depth of the outer well in the pair potential, the peak due to this well at around $r/\sigma=1.5$, which is distinctly seen in the $g(r)$ of system *A*, is not visible and instead just a shoulder appears around this region. As expected, the oscillations in $g(r)$ are more at higher density due to stronger packing effect.

As in system *A*, the finite size effect on the extracted bridge function is manifested here too as shown in Fig. 7 for $T^*=1.5$ and $\rho^*=0.6$. The values of the corrected $B(r)$ for $N=864$ are very close to the corrected $B(r)$ with $N=2048$. The corrected values of $B(r)$ for the two densities $\rho^*=0.8$ and 0.6 for the $N=2048$ particle system are shown in Fig. 8 for the two temperatures $T^*=1.5$ and 1.0. Here too, the oscillation of $B(r)$ at higher density is higher as compared to that at lower density.

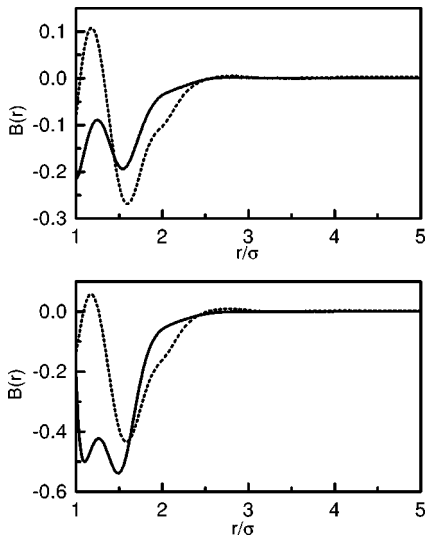

FIG. 8. Same as in Fig. 5 but for system *B*.

V. CONCLUDING REMARKS

We have presented a MD simulation study for the radial distribution function of a fluid with particles interacting with the continuous version of a core-softened SH potential in three dimensions. Extrapolation of these computer generated RDF's of finite range with the help of integral equation theory has been carried out yielding $g(r)$, direct correlation function $c(r)$ for the entire range and the bridge function $B(r)$ has been extracted in this process of extrapolation. The bridge function thus generated is found to depend strongly on the system size. Although the finite size effect has a little effect on the RDF's, the values of the static structure factor $S(k)$ at smaller wave vectors are found to be strongly affected by the finite size of the system. The bridge function extracted for this core-softened potential will be helpful in studying this system through integral equation theory, computationally a much more economic way as compared to the simulation study. Further studies on this system are in progress.

ACKNOWLEDGMENTS

It is a pleasure to thank Dr. T. Mukherjee and Dr. J. P. Mittal for their kind interest and encouragement.

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