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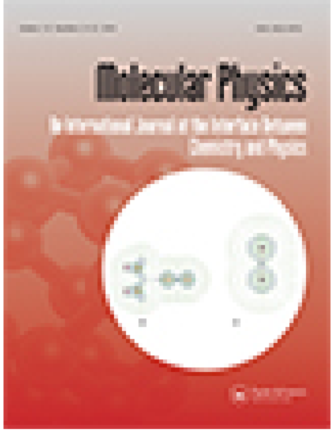

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Liquid pair correlations in four spatial dimensions: theory versus simulation

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SPECIAL ISSUE IN HONOUR OF THOMAS BOUBLIK

Liquid pair correlations in four spatial dimensions: theory versus simulation

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Using liquid integral equation theory, we calculate the pair correlations of particles that interact via a smooth repulsive pair potential in $d = 4$ spatial dimensions. We discuss the performance of different closures for the Ornstein–Zernike equation, by comparing the results to computer simulation data. Our results are of relevance to understand crystal and glass formation in high-dimensional systems.

Keywords: liquid integral equations; molecular dynamics simulations; spatial dimension; pair correlations; equations of state

1. Introduction

Particle-resolved structure in a classical homogeneous bulk liquid is typically measured in terms of pair-correlation functions. In real space, the pair correlations provide the conditional probability density to find a particle at a distance r from another particle. The associated Fourier transform correlates density waves of wavenumber k [1]. While the latter is a typical outcome of a scattering experiment [2], the former can be obtained from the real-space coordinates of the individual particles such as colloids [3,4] or dusty plasmas [5]. Computer simulations of classical many-body systems with a prescribed particle pair-interaction potential are a suitable and well-established route to calculate pair correlations [6]. There are, however, situations that require a (semi-)analytical statistical mechanical approach as an alternative to computer simulations. In such cases, there is a choice of various liquid integral equations that are based on the Ornstein–Zernike equation, and that have often been proven to predict pair correlations accurately and efficiently [1,2,7–13]. The large body of complementary experiments, simulations, and analytical theory have resulted in a good understanding of pair correlations in the fluid or liquid state by now.

Most of the studies so far have focused on the physically most relevant situation of three spatial dimensions ($d = 3$), but liquids can also exist in lower spatial dimensions when they are confined [14,15], e.g., to two-dimensional interfaces [16] or between plates [17] ($d = 2$) or inside narrow cylindrical tubes ($d = 1$) [18]. Though they do not possess an immediate physical realisation, higher spatial dimensions ($d > 3$) have been another focus of recent research. The motivation to consider dimensions higher than three derives from the ambition to understand the salient necessary ingredients for freezing and the glass transition. As the number of dimensions is increased the number of nearest neighbours around a tagged particle also increases, and one can therefore expect mean-field like descriptions to become increasingly accurate. In addition, phase transitions occur at smaller densities in higher dimensions, and one should expect triplet and higherorder particle correlations to be less and less influential. Note that in the framework of the mode coupling theory (MCT) of the glass transition, Biroli and Bouchaud [19] proposed an upper critical dimension $d_c = 6$, that was later corrected to $d_c = 8$ [20]. The MCT of the glass transition of hard hyperspheres in high dimensions [21] suffers from inaccurate structural input for a large but finite number of dimensions d, which can give rise to artefacts in the predicted glass transition lines. Here, liquid integral equations can be used to bridge the gap between low spatial dimensions, $d \lesssim 12$, for which computer simulations are feasible, and very high dimensions, $d \gtrsim 100$, at which limiting infinite-dimensional results apply. The possibility to compute correlation functions in virtually unlimited ranges of particle separation distances and wavenumbers without any statistical noise and in a computationally efficient way, qualifies liquid integral equations as a valuable alternative to computer simulations in every number of spatial dimensions.

In the existing literature on higher dimensional particulate systems, hard hyperspheres have mostly been studied [22–26] while there are less studies for particles with soft pair potentials like, e.g., the Lennard-Jones potential [27,28].

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The computational effort for particle-resolved computer simulations rises quickly as a function of d, which effectively limits computer simulations to dimensions $d \lesssim 12$ [29]. Analytical [30–32] or efficient numerical [11] methods for the calculation of pair correlations in dimensions $d > 3$ are therefore worth aspiring for. In this study, we examine the accuracy of the hypernetted chain (HNC) [33], Percus–Yevick (PY) [34], and Rogers–Young (RY) [35] integral equations, which are compared with numerically accurate computer simulations of particles with soft interactions of the Weeks–Chandler–Andersen (WCA) [36] type, in $d = 4$ spatial dimensions. We find that (just like in $d = 3$ spatial dimensions) the RY scheme predicts paircorrelations in excellent agreement with the computer simulation results, while the PY and HNC scheme show severe over- and under-estimation of the undulations in the static structure factor, respectively.

The remaining parts of this paper are organised as follows: in Section 2, we define the WCA fluid under study. We continue in Section 3 to outline the computer simulations, and in Section 4, the liquid integral equations that we use to compute particle pair correlations. Results for the static structure factor are presented in Section 5, which is followed by our concluding remarks given in Section 6.

2. Weeks–Chandler–Andersen pair potential

We study homogeneous fluids of spherically symmetric, monodisperse particles that interact via a smoothed WCA potential [36], i.e., a Lennard-Jones potential of depth ε, which has been truncated at the minimum position $r = r_c = 2^{1/6}\sigma$, and shifted upwards by ε. Thus, this non-negative (repulsive) pair potential is defined by

$$u(r) = \begin{cases} 0 & \text{for } r > r_c, \\ f(r)\left[4\varepsilon\left(\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right) + \varepsilon\right] & \text{otherwise,} \end{cases} \quad (1)$$

where $f(r) = (r - r_c)^4/[(\sigma/200)^4 + (r - r_c)^4]$ is a smoothing function that decays rapidly from $f(r) \approx 1$ for $r < r_c - \sigma/200$ to $f(r) = 0$ for $r = r_c$. The function $f(r)$ provides continuity of forces at r_c and thus, in a molecular dynamics (MD)simulation, a better numerical stability is achieved when using this smoothing function.

The thermodynamic equilibrium state of the WCA fluid studied here is fully described by two dimensionless parameters: the normalised thermal energy k_BT/ϵ (with Boltzmann constant k_B) and $n\sigma^d$, which is the number of particles in a d-dimensional volume σ^d. Here, $n = N/L^d$ is the number density for N particles in a hypercubic box of edge length L (taken in the thermodynamic limit $N \to \infty$ and $L \to \infty$, where n is held fixed). Note that in the limiting case of vanishing temperature ($T \to 0$ or $\epsilon \to \infty$), the smoothed WCA potential in Equation (1) reduces to the pairpotential of hard spheres with diameter r_c.

3. Computer simulations

We performed MD simulations of a four-dimensional, monodisperse system of 20,000 particles that interact via the WCA potential, as given by Equation (1). Newton's equations of motion were integrated with the velocity form of the Verlet algorithm using a time step of $\delta t = 0.00072$ in units of $\tau = \sqrt{m\sigma^2/\varepsilon}$ (with mass $m = 1.0$). The particles were put into a simulation box with linear dimension $L = 10.511205\,\sigma$, applying periodic boundary conditions in all four spatial directions. Simulations were done at the temperatures $T = 1.66$, 1.7, 1.8, 1.85, 1.9, 2.0, 2.5, 4.0, 7.0 (in units of ε/k_B). At each temperature, the system was fully equilibrated, requiring equilibration runs between 10^5 time steps at $T = 7.0\,\varepsilon/k_B$ and 4×10^7 time steps at $T = 1.66\,\varepsilon/k_B$. The equilibration runs were followed by production runs of double length, from which the structure factor $S(q)$ was computed. During equilibration, temperature was fixed by periodically coupling the system to a stochastic heat bath. The production runs were done in the microcanonical ensemble. Note that none of the runs showed any sign of crystallisation.

4. Liquid integral equations

The Ornstein–Zernike equation for homogeneous and isotropic, d-dimensional fluids reads

$$h(r) = c(r) + n\int d^d r' c(r')h(r - r') \quad (2)$$

in terms of the d-dimensional particle number density and the total and direct correlation functions $h(r)$ and $c(r)$, respectively [1]. To obtain a closed integral equation for a given kind of pairpotential $u(r)$, the Ornstein–Zernike equation must be supplemented by a closure relation. With the exception of very small number densities, exact closure relations are unknown in general and one has to resort to approximate closures. Here, we study three different approximate closures. The first two are the PY closure [34]

$$c(r) = [\gamma(r) + 1] \times \left[e^{-\beta u(r)} - 1\right] \quad (3)$$

and the HNC closure [33]

$$c(r) = -\gamma(r) - 1 + e^{\gamma(r) - \beta u(r)}, \quad (4)$$

both written in terms of the indirect correlation function $\gamma(r) = h(r) - c(r)$ and the inverse thermal energy $\beta = 1/(k_BT)$. Both the PY closure and the HNC closure are thermodynamically inconsistent, in the sense that the predicted normalised inverse isothermal osmotic compressibility computed in the fluctuation route,

$$\frac{1}{\chi_c} = \beta\left(\frac{\partial P_c}{\partial n}\right)_T = 1 - n\int_0^\infty c(r)\,dr, \quad (5)$$

does not match the corresponding expression

$$\frac{1}{\chi_v} = \beta \left(\frac{\partial P_v}{\partial n} \right)_T, \tag{6}$$

from the virial route. Here, P_v is the virial pressure which, for monodisperse particles with WCA pairpotentials as studied here, can be calculated according to

$$\frac{\beta P_v}{n} = \begin{cases} 1 + \dfrac{\beta n \omega_d}{2d} r_c^d g(r_c^+) & \text{for } T = 0, \\ 1 - \dfrac{\beta n \omega_d}{2d} \displaystyle\int_0^\infty dr r^d g(r) \frac{du(r)}{dr} & \text{for } T > 0. \end{cases} \tag{7}$$

In Equation (7), $g(r) = h(r) + 1$ is the radial distribution function, $\omega_d = 2\pi^{d/2}/\Gamma(d/2)$ is the d-dimensional unit hypersphere surface in terms of the Gamma function ($\omega_4 = 2\pi^2$), and $g(r_c^+) = \lim_{r \searrow r_c} g(r)$ is the contact value of the hard-sphere radial distribution function in the special case of $T = 0$.

Thermodynamic inconsistency with respect to the isothermal compressibility can be avoided by using the RY closure [35]

$$c(r) = -\gamma(r) - 1 + e^{-\beta u(r)} \left[1 + \frac{e^{\gamma(r) f(r)} - 1}{f(r)} \right], \tag{8}$$

where $f(r) = 1 - \exp\{\alpha r\}$ is a mixing function that depends on the non-negative inverse length α. The RY closure interpolates between the PY closure (which is recovered in both limits $r \to 0$ and $\alpha \to 0$), and the HNC closure (recovered for $r \to \infty$ or $\alpha \to \infty$). The parameter α is selected such that equal values are obtained for the isothermal osmotic compressibility calculated in the fluctuation route and the virial route. The standard RY scheme, as used in this work, is thermodynamically self-consistent with respect to the isothermal osmotic compressibility only. At the expense of an increased numerical effort, the RY scheme can be further improved by requiring consistency in additional, independent thermodynamic quantities [12]. Note also that the RY scheme usually does not have a solution for non-positive-definite pair potentials. However, for such potentials, different thermodynamically partially self-consistent closure relations have been devised [37,38], similar in spirit to the RY scheme.

The equation of state of four-dimensional WCA fluids at various temperatures is investigated in Figure 1, where we plot the excess part of the normalised pressure, $\beta P/n - 1$, as calculated in the RY scheme.

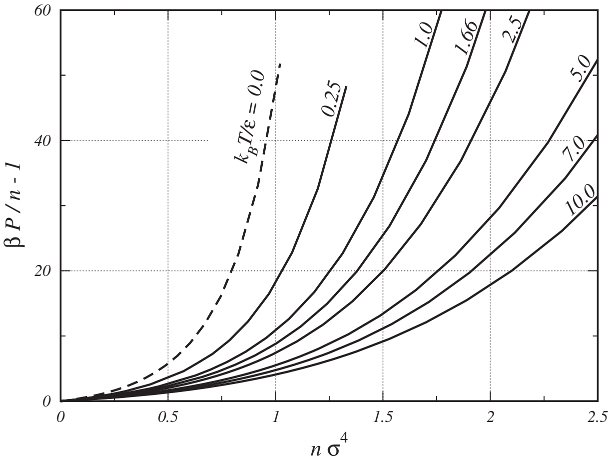

Figure 1. Equations of state for four-dimensional WCA fluids, for eight different reduced temperatures $k_B T/\epsilon = 0.0$, 0.25, 1.0, 1.66, 2.5, 5.0, 7.0, and 10.0, as indicated. The Rogers–Young normalised excess pressure is plotted as a function of the number of particles in a volume σ^4. The dashed curve for $T = 0.0$ is the result for a four-dimensional fluid of hard spheres with diameter $r_c = 2^{1/6}\sigma$.

The (partial) thermodynamic self consistency of the RY scheme usually results in a significantly improved accuracy of the pair-correlation functions including $g(r)$ and the static structure factor $S(q) = 1 + n\mathcal{F}[h(r)](q)$, with $\mathcal{F}$ denoting the d-dimensional Fourier transform of an isotropic function. However, the good accuracy of the RY scheme is essentially an empirical finding that should be tested by comparison to simulation results, for each pairpotential and each number of spatial dimensions.

In the important generic case of hard hyperspheres, the (in this case rather accurate) PY integral equation [34] can in principle be solved analytically for arbitrary odd dimension [30,31], and semi-analytically for arbitrary even dimension [32]. However, these (semi-)analytical solution methods are quite cumbersome, with an analytical effort that rises quickly with increasing number of dimensions d. Moreover, the PY scheme usually over-estimates the undulations in the pair-correlation functions (in particular in the static structure factor), when it is applied to soft repulsive pairpotentials. Another analytically solvable integral equation is obtained in the mean spherical approximation (MSA) $c(r) = -\beta u(r)$ [1], which represents a linear closure for the Ornstein–Zernike equation. The MSA integral equation can be solved analytically in case of hard-sphere systems (for which it reduces to the PY scheme) and for hard spheres with an arbitrary superposition of Yukawa potentials at non-overlap distances (Ref. [39]). Note that the MSA scheme cannot be directly applied to divergent soft-core potentials like the WCA potentials studied here. However, a number of rescaled, semi-analytically solvable versions of the MSA have been proposed in several studies of three-dimensional hard-sphere Yukawa systems [10,40,41], which are all based on the introduction of an effective hard-core radius at small particle separations where the finite pairpotential greatly exceeds the thermal energy $k_B T$. In a similar fashion, the divergent part of a soft-core potential close to $r = 0$ could be replaced by an effective hard-sphere repulsion in a rescaled version of the MSA.

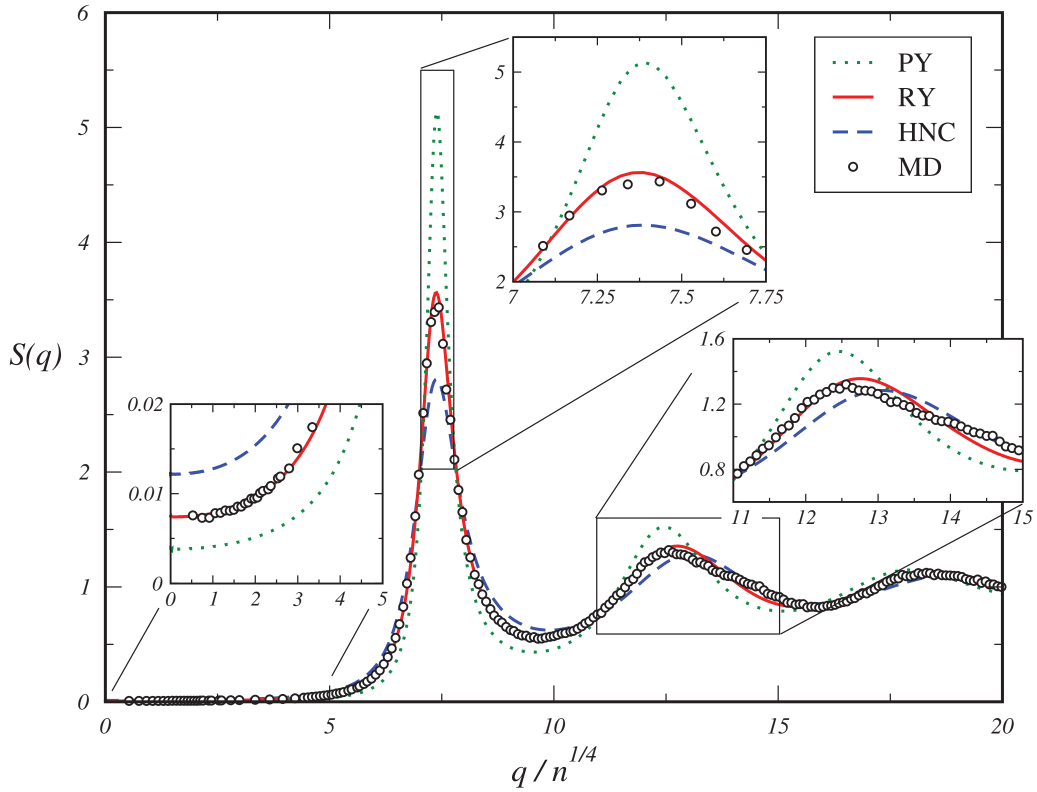

Figure 2. (Colour online) Static structure factor for a four-dimensional fluid of particles interacting via WCA pair potentials [Equation (1)], for particle number density $n = 1.6384\sigma^{-4}$ and for $k_BT = 1.66\varepsilon$. Circles: molecular dynamics simulation results; dotted curve: Percus–Yevick scheme; solid curve: Rogers–Young scheme; and dashed curve: hypernetted chain scheme. The three insets magnify the region of very low wave numbers q, the region around the principal peak, and around the second peak.

A versatile and computationally efficient alternative to the (semi-)analytical solution of arbitrary-dimensional liquid integral equations is the numerical solution by means of a spectral solver. Within this numerical method, employed in this study, it is easy to implement a variety of different closures for the Ornstein–Zernike equation, suitable for a variety of particle pair-interaction potentials. In this work, we employ a numerical method that we have comprehensively outlined in Ref. [11]. This method, based on techniques that were originally published in Refs [42–46], is applicable in all positive spatial dimensions d and is numerically very efficient and robust. Our implementation of the numerical solution algorithm allows to compute solutions for $1 \leq d \lesssim 30$, the upper boundary for d depending on the kind of pairpotentials, the closure relation, and the particle number density.

As a further motivation for studying liquid integral equations in higher dimensions, we note here that MCT has been employed to study the glass transition of hard hyperspheres in very high dimensions [21]. In Ref. [21], the structural input to the MCT equations was generated by approximating $c(r)$ by the Mayer function $\exp\{-\beta u(r)\} - 1$. As outlined in Ref. [21], the latter approximation is exact in the limit of infinite spatial dimension ($d \to \infty$), and remains to be a good approximation of the actual particle pair correlations for dimensions $d \gtrsim 100$. For dimensions d in the range $1 \leq d \lesssim 100$, the approximation $c(r) \approx \exp\{-\beta u(r)\} - 1$ is insufficient unless the particle number density is very low. This leads to unphysical artefacts in the predicted glass transition lines for $d \lesssim 100$ [21]. As an alternative, one can use simulation results for the static pair correlations as input to MCT [47]. However, the computational effort of computer simulations rises quickly as a function d, which limits this approach to dimensions $d \lesssim 12$ [29]. Hence, there is a gap for $12 \lesssim d \lesssim 100$, where neither simulation results nor infinite-dimensional limiting expressions can be used. This gap can be essentially filled in by numerical liquid integral equation solutions as reported in this paper and in Ref. [11].

5. Static structure factors

In Figure 2, we plot the static structure factor, $S(q)$, for a four-dimensional WCA fluid at a rather high number density $n = 1.6384\sigma^{-4}$, and a rather low temperature, $T = 1.66\varepsilon/k_B$. Under these conditions, the fluid exhibits very

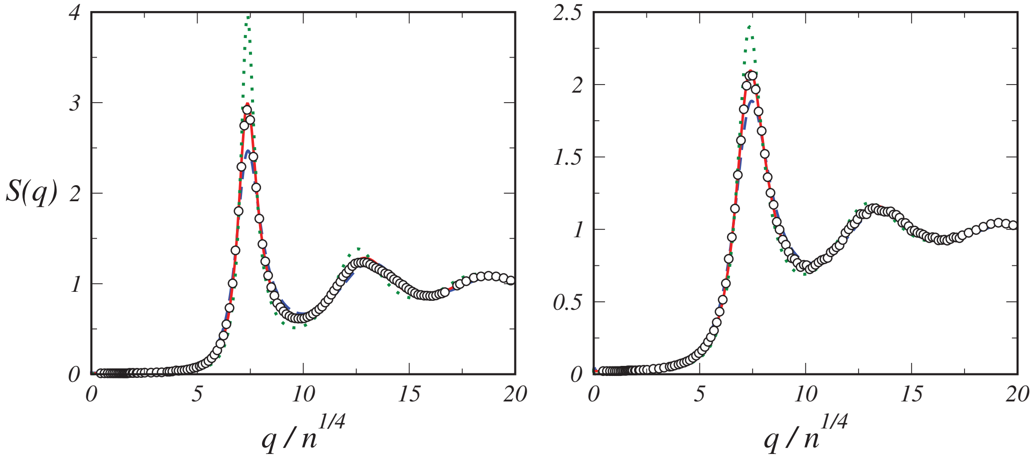

Figure 3. (Colour online) Static structure factors for two four-dimensional fluids of particles interacting via WCA pair potentials [Equation (1)], for dimension $d = 4$, particle number density $n = 1.6384\sigma^{-4}$, and for $k_BT = 2.5\varepsilon$ (left panel) and $k_BT = 7.0\varepsilon$ (right panel). Black circles filled in white: molecular dynamics simulation results; dotted green curves: Percus–Yevick scheme; solid red curves: Rogers–Young scheme; and Blue dashed curves: hypernetted chain scheme.

pronounced pair correlations. Shown are the results from our MD simulation (black circles filled in white), and from the HNC (blue dashed curve), RY (red solid curve), and PY (green dotted curve) integral equations. Three insets magnify the regions of very low wave numbers, $q \gtrsim 0$, the region around the structure factor's principal peak, and the region around the second peak. Note that the HNC scheme predicts a structure factor with considerably underestimated undulations, and that the PY scheme is severely over-estimating these undulations, while the RY scheme is in very good (if not excellent) agreement with the simulation result. Each of these observations is inline with the usual observations that have been made for three-dimensional fluids of purely repulsive particles.

The only obvious difference between the MD structure factor and the RY structure factor (and the PY and HNC results alike) is a failure of the liquid integral equation schemes to predict the shape of the second peak in $S(q)$: the right flank of the second peak in the simulation result exhibits a nearly linear decay of $S(q)$ for values of $q/n^{1/4}$ between 12.5 and 15. This feature is missing in each of the liquid integral equation scheme results, which predict a rounder shape of the second peak. Similar features in the second peak of the structure factor have been discussed as possible freezing precursors, and as signatures of short-ranged order in the liquid phase [48,49] (see also the related Ref. [50]). To the best of our knowledge, the second peak shape feature is not observed in any of the usual liquid integral equation schemes that are formulated on the level of pair-correlation functions. A similar feature (in the radial distribution function, however, and for $d = 3$) has been reported in Ref. [13], where a computationally more sophisticated integral equation scheme was solved that includes non-trivial triplet correlations. The implementation of such a scheme for the four-dimensional fluids under investigation is beyond the scope of the present work.

Note from Figure 3, that the agreement between the MD simulation and RY-scheme structure factors is very good for higher temperatures ($T = 2.5\varepsilon/k_B$ in the left panel of Figure 3, and $T = 7.0\varepsilon/k_B$ in the right panel). For $T = 7.0\varepsilon/k_B$, the flattened second peak feature has practically disappeared in the MD simulation results, and the agreement to the RY scheme is almost perfect.

6. Conclusions

We have demonstrated that the RY integral equation scheme predicts pair correlations in homogeneous four-dimensional fluids of particles with soft repulsive interactions in very good agreement with numerically accurate, but computationally expensive MD simulations. This finding, which is in line with the known excellent performance of the RY scheme for three-dimensional fluids, qualifies the RY scheme as a numerically highly efficient method for calculating the structure input that is needed for theories of dynamics, phase behaviour and vitrification in higher dimensions [21]. Despite its overall very good accuracy, the RY scheme (as well as the PY and HNC schemes) fails to predict the correct shape of the second peak in the static structure factor when the particle repulsion becomes very strong. We expect that inclusion of non-trivial triplet correlations into a (thermodynamically partially self-consistent) liquid integral equation scheme [13] for arbitrary spatial dimensions could result in an improved ability of the theory to reproduce the static structure factor, particularly around its second peak.

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