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Retraction

Circularly inhomogeneous fluids. Percus–Yevick hard disks: osmotic coefficients and triplet correlations

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It has come to the attention of IOP Publishing that this article should not have been submitted for publication because it plagiarises the text of an earlier paper (P Attard 1989 Spherically inhomogeneous fluids. I. Percus-Yevick hard spheres: osmotic coefficients and triplet correlations *J. Chem. Phys.* **91** 3072 (1989)) although the results are different. Therefore, this article has been retracted by IOP Publishing.

Circularly inhomogeneous fluids. Percus–Yevick hard disks. osmotic coefficients and triplet correlations

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Abstract

For fluids in a circularly symmetric external field, it is shown that the two-dimensional Ornstein–Zernike (OZ) convolution integral becomes a simple algebraic equation using the rotationally invariant basis in two dimensions. Applying the usual closure relations, the full inhomogeneous pair correlation functions become available. The method is here applied to a bulk uniform fluid of hard disks, using the Percus–Yevick (PY) closure, but at the triplet level in the hierarchy of distribution functions. Consequently, the obtained pair distribution function and the osmotic coefficient are better than the previous results.

1. Introduction

The properties of bulk fluids are well understood at the two-particle level. A popular and routine procedure is based on the Ornstein–Zernike (OZ) integral equation (in two or three dimensions), closed with some approximate relation between the correlation functions. Only recently have inhomogeneous fluids in planar geometry been described at a similar level [1–8].

The direct correlation function (DCF) plays an important role in describing the thermodynamical properties and the structure of simple and multi-component fluids in two and three dimensions [9–13]. This function, together with the pair correlation function, constructs the OZ equation [14]. This integral equation [15] can be solved using an appropriate approximation to obtain the DCF of many kinds of fluids [16–18]. The method of OZ convolution integral factors, in three or two dimensions, makes the bulk systems easier to study.

The properties of a fluid in the vicinity of an isolated circularly symmetric external field can hence be described fairly accurately. The Hamiltonian which specifies the system needs only to depend on the positions of pairs of fluid particles via the two radial coordinates and the mutual angle. The inhomogeneous (anisotropic, translationally variant) pair correlations can be calculated explicitly. The results obtained by this method are at the two-particle level, and should be distinguished from the essentially single approaches which use integral equations

for a bulk mixture, even though the components are highly asymmetric in size, charge, or concentration.

A particularly interesting possibility is to consider the circular inhomogeneity to be itself a particle of the fluid (which must be specified by a circularly symmetric pair potential). The consequent inhomogeneous density profile corresponds to the pair distribution function of the bulk fluid.

This paper is divided into two parts. In the following section the circularly inhomogeneous fluid problem is formulated. It is shown that the two-dimensional OZ equation is transformed to an algebraic equation in the rotationally invariant basis in two dimensions. These render feasible the computations in the general case. Examples of closures for the inhomogeneous correlation functions and equations to determine the density profile are given in circular geometry. The second part deals specifically with hard disks and the Percus–Yevick (PY) closure. The Kreizer–Zwanzig (TZ) equation for the profile is applied to this fluid with a hard-disk inhomogeneity. Finally, the results are discussed.

2. Circular inhomogeneous system

2.1. Factorization of the OZ equation

Consider a classical fluid in which the Hamiltonian consists only of one- and two-body terms. A circularly inhomogeneous system is one in which the external potential $V(r)$ depends only on the distance from the origin $r = |\mathbf{r}|$, and the pair potential $u(r_1, r_2, \theta_{12})$ depends on the particles' radial coordinates and mutual angle. This contains circularly symmetric pair potentials such as a hard disk. The inhomogeneous one- and two-particle distribution functions exhibit the same symmetries as the Hamiltonian.

The OZ equation in two dimensions is

$$h(r_1, r_2, \theta_{12}) = c(r_1, r_2, \theta_{12}) + \int r_3 dr_3 d\theta_{13} \rho(r_3) h(r_3, r_2, \theta_{32}), \quad (1)$$

where $h \equiv g - 1$ is the total correlation function, g is the radial distribution function, c is the DCF, and ρ is the singlet density profile. The space element in polar coordinates is $d\mathbf{r} = r dr d\theta$.

Now use the rotationally invariant basis in two dimensions [11]

$$f(r_1, r_2, \theta_{12}) = f(1, 2) = \sum_{m,n=-\infty}^{\infty} f^{mn}(r_1, r_2) \Psi^{mn}(\theta_{12}) \quad (2)$$

where f is an arbitrary function and the invariants $\Psi^{mn}(\theta_{12})$ are given by

$$\Psi^{mn}(\theta_1, \theta_2) = e^{i(m\theta_1 + n\theta_2)}. \quad (3)$$

These invariants are orthogonal and the projections (or the expansion coefficients) f^{mn} can be written as

$$f^{mn}(r_1, r_2) = \frac{1}{4\pi^2} \int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 f(r_1, r_2, \theta_{12}) \Psi^{mn}(\theta_1, \theta_2). \quad (4)$$

We expand the correlation functions in equation (1) and use the orthogonality of invariants to achieve the desired factorization:

$$\begin{aligned} y^{mn}(r_1, r_2) &= h^{mn}(r_1, r_2) - c^{mn}(r_1, r_2) \\ &= 2\pi \sum_{m'=-\infty}^{\infty} \int_0^{\infty} r_3 dr_3 \rho(r_3) c^{m,-m'}(r_1, r_3) h^{m',n}(r_3, r_2), \end{aligned} \quad (5)$$

where $y \equiv h - c$ is an auxiliary function. Since the correlation functions, and thereby the integrand, decay rapidly to zero, the upper limit of the integral can be made finite. In equation (6) we use $m' = -5$ to 5 in our calculations.

2.2. Closure and profile relations

The OZ equation contains three unknown functions—the density, the inhomogeneous direct and total correlation functions. Thus, two more equations are required. There are several approximate closures for the correlation functions which do not depend on translational invariance and can hence be applied directly to the inhomogeneous problem. Two common examples are

$$c(r_1, r_2, \theta_{12}) = c(r_1, r_2, \theta_{12})\{1 - \exp[\beta u(r_1, r_2, \theta_{12})]\}, \quad (6)$$

and the hypernetted-chain

$$h(r_1, r_2, \theta_{12}) = c(r_1, r_2, \theta_{12}) - c(r_1, r_2, \theta_{12}) - \beta u(r_1, r_2, \theta_{12}) - 1. \quad (7)$$

Here $\beta = \frac{1}{k_B T}$ is the inverse temperature and u is the pair potential.

Several exact equations relate the density profile to the external field V [22–27]. One of these popular equations involves the total correlation function [22, 23]:

$$\nabla \rho(\mathbf{r}_1) = -\beta \rho(\mathbf{r}_1) \nabla V(\mathbf{r}_1) - \beta \rho(\mathbf{r}_1) \int d\mathbf{r}_2 h(\mathbf{r}_1, \mathbf{r}_2) \nabla V(\mathbf{r}_2). \quad (8)$$

For circularly inhomogeneous systems, this reads

$$\begin{aligned} \rho'(r_1) &= -\beta \rho(r_1) V'(r_1) - \beta \rho(r_1) \int_0^\infty \int_0^{2\pi} dr_2 d\theta_{12} h(r_1, r_2, \theta_{12}) \cos \theta_{12} V'(r_2) \\ &= -\beta \rho(r_1) V'(r_1) - \pi \beta \rho(r_1) \int_0^\infty r_2 dr_2 [h^{1-1}(r_1, r_2) \\ &\quad + h^{-11}(r_1, r_2)] V'(r_2), \end{aligned} \quad (9)$$

where the prime denotes differentiation with respect to argument. The boundary condition is that the profile should equal the bulk density at large r .

Note that the closures constitute an approximation, as in the bulk case, whereas the OZ and TZ equations are exact. However, the closure is not only approximately produced (besides those necessary for the numerical solution of the problem) and applied to the inhomogeneous problem can be solved with an accuracy comparable to that usually achieved in bulk. In fact, for the case when the circular inhomogeneity is a particle in the fluid, the closure is applied at the triplet level, one step higher in the hierarchy of distribution functions. Hence one expects better results for this problem than the usual bulk formulation.

3. Percus–Yevick hard disk

3.1. Hamiltonian, profile and closure

The method derived above will now be illustrated by application to a hard-disk fluid. This fluid is a suitable test case in two dimensions. The results give some information on the accuracy of the procedure, and hopefully provide new perspectives on the behavior of the correlation functions. The actual data obtained may be applied to other fluids in two dimensions using the hard-disk fluid as a reference.

Atoms of a hard-disk fluid interact via a pair potential

$$u(r_1, r_2, \theta_{12}) = \begin{cases} \infty, & r_{12} < d \\ 0, & r_{12} > d, \end{cases} \quad (10)$$

where r_{12} is the distance between the particles and d is the hard-disk diameter. Now consider a hard-disk particle of diameter D and fixed at the origin. This causes an external potential

$$V(r) = \begin{cases} \infty, & r < S \\ 0, & r > S, \end{cases} \quad (11)$$

where $S = (d + D)/2$. At this time in the analysis, take $D \neq d$. However, when $D = d$, the fixed particle is just one of the particles of the fluid.

First, denote the contact density function

$$\rho_c(r) \equiv \rho_c(S) e^{\beta V(r)} \quad (12)$$

and note that

$$\beta V'(r) = -\beta V(r) \frac{d}{dr} (1 - e^{-\beta V(r)}) = -\delta(r - S), \quad (13)$$

where $\delta(r)$ is the Dirac delta function. Then, for the present problem, equation (9) becomes

$$\rho'(r) = \rho_c(r - S) + \pi \rho_c(S) \rho_c(S) S [h^{1-1}(r, S) + h^{-11}(r, S)]. \quad (14)$$

This may be integrated to yield ($r > S$)

$$\rho(r) = \rho(R) + \pi \rho_c(S) S \int_R^r dr' \rho(r') [h^{1-1}(r', S) + h^{-11}(r', S)], \quad (15)$$

where $\rho_c(S) = \rho(S^+)$ is the contact density and R is some large radius (several hard-disk diameters) after which bulk properties are assumed.

For a hard-disk fluid the PY closure (equation (6)) becomes

$$c(r_1, r_2, \theta_{12}) = 0, \quad r_{12} > d, \quad (16)$$

which is supplemented with the exact result

$$g(r_1, r_2, \theta_{12}) = 0, \quad r_{12} < d. \quad (17)$$

This is closure to be used for the present problem since it works well for a bulk hard-disk fluid where the results exist [28–33].

3.2. Osmotic coefficient and compressibility

Results will now be presented for a bulk two-dimensional uniform fluid of hard-disks, i.e. $D = S = d$. Since, in this case, the method corresponds to using the closure at the triplet level, we shall designate our results ‘PY3’ to distinguish them from the analytic solution of the PY closure for the bulk pair correlation (‘PY2’).

The osmotic coefficient is related to the pressure by

$$\phi = \frac{p}{\rho k_B T}, \quad (18)$$

where ρ denotes the bulk density. For hard disks in two dimensions the equation of state is

$$\phi_v = 1 + 2\eta g(d^+), \quad (19)$$

where the packing fraction

$$\eta \equiv (\pi/4) \rho d^2 \quad (20)$$

Table 1. Osmotic coefficients: virial (ϕ_v), and compressibility (ϕ_c , in parenthesis).

ρd^2	MC	PY3	PY2	CS
0.10		1.184	1.179	1.178
		(1.184)	(1.184)	
0.20	1.682	1.537	1.412	1.408
		(1.538)	(1.540)	
0.30	1.920	1.737	1.716	1.712
		(1.730)	(1.851)	
0.40	2.141	1.922	2.131	2.127
		(2.311)	(2.321)	
0.50	2.938	2.854	2.713	2.713
		(2.691)	(2.702)	
0.60	3.641	3.546	3.546	3.579
		(3.701)	(3.852)	
0.70	4.971	4.872	4.795	4.938
		(4.902)	(4.902)	
0.80	7.001	6.851	6.795	7.248
		(7.002)	(7.002)	

is the only parameter required to specify the hard-disk fluid nontrivially. In the circular system when the inhomogeneity is an atom of the fluid, the one-particle distribution (the density profile) corresponds to the pair distribution function of the bulk. Hence, the value of the bulk radial distribution function at contact is here

$$g(d^+) = \rho_0(d^+)/\rho, \tag{21}$$

where the subscript indicates that the density profile is about an atom fixed at the origin.

One can also calculate the osmotic coefficient via the compressibility relation

$$\phi_c = \frac{1}{\rho} \int_0^\rho \frac{d\rho'}{\rho' k_B T \kappa_T}, \tag{22}$$

where the isothermal compressibility κ_T is given by

$$\rho k_B T \kappa_T = [1 + \rho \tilde{h}(0)] \equiv 1 + \rho \int dr h(r). \tag{23}$$

The Carnahan–Starling (CS) equation of state for the hard-disk fluid is

$$\phi^{CS} = \frac{1}{(1 - \eta)^2}. \tag{24}$$

Table 1 compares the osmotic coefficient calculated by two different thermodynamic routes: compressibility and virial, with Monte Carlo (MC) results. It is manifest that the PY3 virial performs better than the PY2, being in closer agreement with the simulations. The PY3 virial and compressibility results are also more consistent than the PY2.

The compressibility osmotic coefficient is less reliable at high densities. The radial distribution function decays more slowly at higher couplings, and it becomes exceedingly difficult to calculate the isothermal compressibility with numerical accuracy. This is evident from the data in table 2, and is the reason that values for κ_T are not usually available in numerical schemes.

The fundamental reason why PY3 performs better than PY2 is because the approximate closure is used at a higher level in the hierarchy of distribution functions. The difference between the triplet and pair levels is the exact profile relationship. The computations are more demanding than the usual bulk numerical procedures (in general).

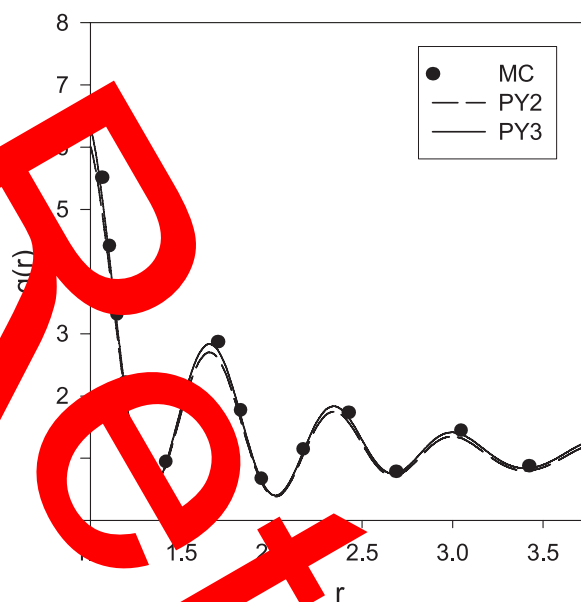


Figure 1. Radial distribution function $g(r)$ as given by PY3 (solid line) and PY2 (dashed line) at $\rho d^2 = 0.794$. The dots are MC data.

Table 2. Isothermal compressibility, $\rho k_B T \kappa_T$.

ρd^2	PY3	PY2
0.10	0.7305	0.7308
0.20	0.6594	0.6592
0.30	0.3649	0.3623
0.40	0.2813	0.2740
0.50	0.1375	0.1279
0.60	0.0952	0.0934
0.65	0.0873	0.0854
0.70	0.0588	0.0670
0.75	0.0340	0.0427

3.3. Pair and triplet distribution functions

We use equations (5), (6) and (15) simultaneously to obtain the results as the expansion coefficients of the correlation functions and the density profile.

Figure 1 displays a comparison of the bulk radial distribution function given by the MC, PY2, and PY3 approximations. In the latter approach, $g(r) \equiv \rho_0(r)/\rho$ and the data follow the pronounced oscillations of the function quite accurately (and somewhat better than PY2). Lengths here and below are in units of the hard-disk diameter d . Values of $g(r)$ are tabulated in table 3 on a coarse grid in the x - y plane. A direct comparison between PY3 and PY2 is possible from the values below and above the diagonal respectively.

The inhomogeneous pair correlation function calculated in the PY3 scheme, $g(r_1, r_2)$, gives, when multiplied by ρ , the probability of finding an atom at \mathbf{r}_2 , given atom fixed at \mathbf{r}_1 and the origin. Hence, it is simply related to the bulk triplet correlation function by

$$g(0, \mathbf{r}_1, \mathbf{r}_2) \equiv g(r_1)g(r_2)g_0(\mathbf{r}_1, \mathbf{r}_2). \quad (2)$$

Table 3. Radial distribution function $g(r)\mathbf{r} = x\mathbf{i} + y\mathbf{j}$: PY3 (on and below) and PY2 (above) the diagonal $x = y$, for $\rho d^2 = 0.794$.

	0	0.25	0.50	0.75	1.00	1.25	1.5	1.75	2.00	2.25	2.50
0	0.000	0.000	0.000	0.000	4.261	1.662	0.630	0.759	1.385	1.352	0.832
0.25	0.000	0.000	0.000	0.000	3.991	1.011	0.541	0.633	1.481	0.812	0.722
0.50	0.000	0.000	0.000	0.000	3.061	0.732	0.550	0.769	1.455	0.846	0.735
0.75	0.000	0.000	0.000	0.000	1.012	0.653	0.550	0.891	1.501	0.875	0.672
1.00	4.231	4.231	3.031	1.328	0.743	0.650	0.859	1.475	1.225	0.901	0.792
1.25	1.642	1.642	0.751	0.593	0.662	0.509	1.490	1.469	0.875	0.751	0.779
1.50	0.630	0.630	0.555	0.540	0.882	1.493	1.235	1.040	0.971	0.943	1.003
1.75	0.753	0.655	0.779	0.853	1.481	1.473	1.041	0.951	0.972	0.987	1.025
2.00	1.398	1.501	1.495	1.515	1.311	0.885	1.012	0.969	0.959	0.984	1.025
2.25	1.352	1.352	0.864	0.881	0.988	0.961	0.955	0.981	1.029	1.028	1.005
2.50	0.832	0.765	0.753	0.680	0.801	0.887	1.005	1.021	1.023	1.002	0.988
2.75	0.722	0.694	0.702	0.816	1.007	1.024	1.025	1.015	0.995	0.985	0.990
3.00	1.025	1.023	1.022	1.029	1.027	1.017	1.003	0.991	0.986	0.991	1.001
3.25	1.142	1.026	1.081	1.004	1.000	0.995	0.986	0.988	0.996	1.004	1.007
3.50	0.988	0.992	0.986	0.990	0.990	0.995	1.002	1.007	1.007	1.007	1.002
3.75	0.992	0.992	0.992	0.992	0.997	1.004	1.002	1.002	1.001	1.005	0.997
4.00	1.004	1.004	1.003	1.003	1.005	1.006	1.003	1.000	0.997	0.996	0.997
4.25	1.001	1.001	1.003	1.001	1.002	0.995	0.997	0.995	0.997	0.997	0.996
4.50	0.990	0.991	0.999	0.999	0.985	0.995	0.998	0.996	0.995	0.999	0.998
4.75	0.995	0.998	0.998	0.998	1.007	1.001	1.002	1.003	1.002	1.001	1.001
5.00	1.001	0.998	1.001	1.001	1.001	1.002	1.001	1.001	1.001	1.000	1.002

The triplet distribution function approaches unity only when all of the trio are far apart.

The Kirkwood superposition approximation [11] consists of approximating the inhomogeneous pair correlation everywhere by the bulk form,

$$g_0(\mathbf{r}_1, \mathbf{r}_2) \approx g(r_{12}). \tag{26}$$

This approximation is exact asymptotically when any one of the three atoms is far separated from the others.

A direct and extensive test of the superposition approximation can be made from the data in tables 4 and 5. These contain $g_0(\mathbf{r}_1, \mathbf{r}_2)$ on the same mesh as $g(r)$ in table 3.

Figure 2 gives the PY3 radial distribution function $g(r)$ at the density $\rho d^2 = 0.730$. These are compared to the triplet correlation function $g(0, \mathbf{r}_1, \mathbf{r}_2)$ for isosceles angle configurations, ($r_1 = r_2 = s, r_{12} = r$), divided by $g(s)^2$. This ratio (which is just $g_0(\mathbf{r}_1, \mathbf{r}_2)$) approaches $g(r)$ for large s or large r , as is to be expected from the asymptotic nature of the superposition approximation.

4. Conclusion

In this paper a method has been given for treating circularly inhomogeneous systems, in two dimensions, with integral equation theories. The full inhomogeneous pair correlation functions are available from the procedure. That the approach is practical was demonstrated by the results obtained for a hard-disk fluid. Those data were more accurate than when the pair closure is used in the usual bulk formulation of the problem, evidently because the approximation is being applied at a higher level in the hierarchy of distribution functions. The formalism introduced in this paper allows application of this principle to more general fluids, in two dimensions, and arbitrary closures, and at a further level (the triplet level) in the hierarchy.

Table 4. Inhomogeneous pair correlation function $g_0(\mathbf{r}_1, \mathbf{r}_2)$, as a function of $\mathbf{r}_2 = (x, y)$, with one disk fixed at the origin $(0, 0)$ and the second at $\mathbf{r}_1 = (0, 1)$, and $\rho d^2 = 0.794$.

	0.00	0.25	0.50	0.75	1.00	1.25	1.5	1.75	2.00	2.25	2.50
0.00	2.198	1.190	0.684	0.998	1.366	1.259	0.833
0.25	2.488	0.678	0.547	0.696	1.495	0.761	0.722
0.50	2.742	0.762	0.582	0.702	1.425	0.856	0.746
0.75	0.000	2.122	1.142	0.600	0.703	1.444	0.951	0.692
1.00	0.000	0.000	0.000	0.000	2.890	1.412	0.838	1.170	1.209	1.030	0.805
1.25	0.000	0.000	0.000	0.000	2.996	1.144	1.254	1.158	0.959	0.896	0.761
1.50	0.000	0.000	0.000	0.000	2.446	1.581	0.829	0.869	1.157	1.054	1.067
1.75	0.000	0.000	0.000	2.391	1.663	1.127	0.761	0.966	1.183	1.015	0.934
2.00	3.012	2.845	2.138	1.543	1.062	0.633	0.931	1.146	1.084	0.926	0.946
2.25	1.527	1.477	0.816	0.711	0.813	0.886	1.020	1.143	1.014	0.939	0.975
2.50	0.657	0.623	0.571	0.767	0.975	1.146	1.024	0.942	0.952	1.010	1.010
2.75	0.670	0.582	0.629	0.818	1.110	1.112	1.014	0.947	0.945	0.992	1.032
3.00	1.082	1.089	1.005	1.104	1.056	0.990	0.948	0.952	0.992	1.028	1.025
3.25	1.068	1.056	1.099	0.992	0.967	0.957	0.966	0.999	1.029	1.025	0.998
3.50	0.970	0.961	0.961	0.969	0.969	0.991	1.019	1.034	1.020	0.997	0.985
3.75	0.974	0.976	0.976	1.002	1.006	1.023	1.019	1.005	0.990	0.990	0.991
4.00	1.016	1.014	1.018	1.018	1.011	0.998	0.989	0.987	0.994	1.004	1.005
4.25	1.010	1.009	1.002	0.998	0.991	0.988	0.994	0.999	1.004	1.005	1.005
4.50	0.986	0.993	0.993	0.990	0.991	0.998	1.002	1.005	1.006	1.001	1.001
4.75	0.992	0.992	0.996	1.001	1.001	1.003	1.005	1.005	1.001	0.998	0.995
5.00	1.002	1.002	1.004	1.004	1.004	1.003	1.002	0.999	0.998	0.997	0.998

Table 5. Same as table 4, but with $\mathbf{r}_1 = (1, 0)$.

	0.00	0.25	0.50	0.75	1.00	1.25	1.5	1.75	2.00	2.25	2.50
0.00	0.69	0.658	0.813	0.935	1.258	1.266	0.882
0.25	2.198	0.822	0.768	0.816	1.350	0.736	0.765
0.50	2.488	0.667	0.791	0.913	1.314	0.810	0.780
0.75	0.000	2.742	0.644	0.740	0.920	1.372	0.897	0.735
1.00	0.960	1.010	1.122	1.168	0.89	0.873	0.973	1.318	1.115	0.959	0.868
1.25	0.805	0.840	0.880	0.950	0.967	0.807	1.40	1.299	0.809	0.882	0.838
1.50	0.781	0.775	0.771	0.772	0.777	1.484	1.2	1.043	0.968	0.943	1.131
1.75	1.302	1.254	1.045	0.660	1.044	1.180	1.113	1.113	1.038	0.948	0.976
2.00	3.118	3.010	2.372	1.748	1.17	0.643	0.932	0.932	1.060	0.936	0.959
2.25	0.000	0.000	0.000	2.326	1.401	0.766	0.766	1.136	1.015	0.954	0.954
2.50	0.000	0.000	0.000	0.000	1.923	0.992	0.87	1.106	1.052	0.988	0.988
2.75	0.000	0.000	0.000	0.000	2.676	1.33	0.812	0.838	1.068	1.074	0.964
3.00	0.000	0.000	0.000	0.000	3.000	1.33	0.831	0.831	0.963	1.079	0.967
3.25	0.000	0.000	0.000	0.000	2.700	1.33	0.824	0.824	1.089	1.073	0.960
3.50	0.000	0.000	0.000	0.000	3.007	1.087	0.978	0.978	1.108	1.051	0.953
3.75	0.000	0.000	0.000	2.452	1.387	0.880	0.795	0.98	1.056	0.956	0.956
4.00	2.828	2.629	2.025	1.355	0.919	0.781	0.891	1.120	1.054	0.953	0.953
4.25	1.319	1.250	1.049	1.148	0.785	0.850	1.027	1.085	1.092	0.953	0.977
4.50	0.805	0.815	0.777	0.793	0.875	1.025	1.125	1.045	0.959	0.966	1.004
4.75	0.825	0.834	0.875	0.974	1.095	1.122	1.044	0.965	0.951	0.88	1.023
5.00	1.105	1.112	1.133	1.135	1.086	1.012	0.955	0.950	0.950	1.020	1.021

Treating the inhomogeneous fluid at the two-particle level is equivalent to describing three-body interaction, the fixed particle being the third member of the trio. As we know

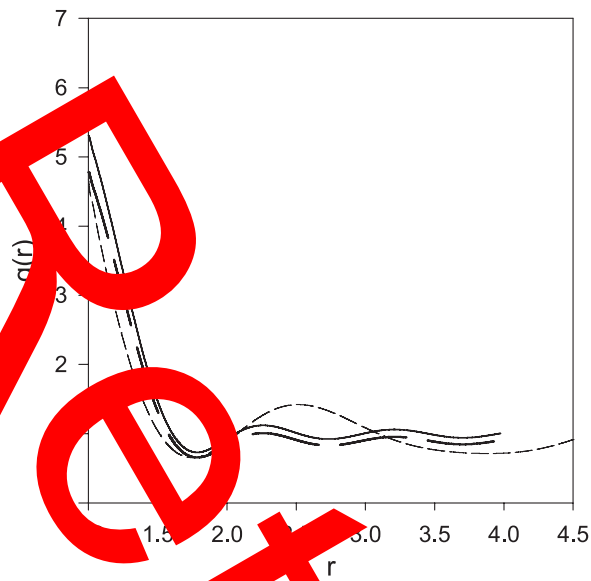


Figure 2. The homogeneous pair correlation function $g_0(\mathbf{r}_1, \mathbf{r}_2)$ for $\mathbf{r}_1 = \mathbf{r}_2 = s$ as a function of $r_{12} = r$, compared to the PY3 distribution function $g(r)$ (solid line). The long dashes and short dashes correspond to $\rho d^2 = 0.730$ and $\rho d^2 = 0.730$, respectively. The density is $\rho d^2 = 0.730$.

correlations reach to the bulk, one away from the fixed particle and, according to the accuracy used in this paper, the two-level correlation is enough to achieve the results and the triplet level is not required.

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