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Integrals over the triplet distribution function without the triplet distribution function

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While the triplet distribution function of disordered systems appears in a wide variety of problems in statistical mechanics, it does so always under an integral sign. In this paper, we propose a new method of evaluating such integrals that involves only pair functions throughout and avoids altogether the need for any explicit representation of the little-known triplet function. The procedure is based on an extension of integral equation theory of classical fluids. Numerical illustrations of the method are given for integrals that arise in the calculation of moments of a local field distribution.

1. Introduction

The need to evaluate integrals of the form

$$\int d\mathbf{r}_3 \psi(\mathbf{r}_{13})g^{(3)}(\mathbf{r}_{12}, \mathbf{r}_{13}), \quad (1)$$

where $g^{(3)}(\mathbf{r}_{12}, \mathbf{r}_{13})$ is the equilibrium triplet distribution function of a disordered system and $\psi(\mathbf{r})$ is arbitrary, arises in a wide range of applications in statistical mechanics. There is still no reliable way of computing the triplet function for dense systems, thus the evaluation of such integrals has been carried out by approximating $g^{(3)}$, with unpredictable effects on accuracy, using most often the Kirkwood superposition approximation or else the Feenberg convolution approximation [1]. In this paper, we present a new method that involves only pair functions throughout and avoids altogether the need for any explicit representation of the triplet distribution function.

The problem is first set up as a generalization of the Kirkwood integral equation [2]. Consider a fluid of N molecules in a volume V subject to a temperature T , and let $\varphi(r)$ be the intermolecular potential. We adopt the usual definition of the n th-order distribution function [2],

$$g^{(n)}(\mathbf{r}_1, \dots, \mathbf{r}_n) = \frac{N!}{\rho^n Z_N (N-n)!} \int d\mathbf{r}_{n+1} \dots d\mathbf{r}_N \exp(-\beta U_N), \quad (2)$$

where

$$Z_N = \int d\mathbf{r}_1 \dots d\mathbf{r}_N \exp(-\beta U_N) \quad (3)$$

is the canonical partition function,

$$U_N = \sum_{1 \leq i < j \leq N} \varphi(r_{ij}) \quad (4)$$

the internal energy, and $\rho = N/V$, $\beta = (k_B T)^{-1}$. Now single out, say, molecule 1 and assign to it an *additional* interaction potential $\psi(\mathbf{r}_{1,j})/\beta$ with molecules $j = 2, \dots, N$, at coupling strength ξ ; that is, the new internal energy is

$$U_N(\xi) = U_N + \xi \sum_{j=2}^N \psi(\mathbf{r}_{1,j})/\beta. \quad (5)$$

The obvious generalization of (2) is then

$$g^{(n)}(\mathbf{r}_1, \dots, \mathbf{r}_n | \xi) = \frac{N!}{\rho^n Z_N(\xi)(N-n)!} \int d\mathbf{r}_{n+1} \dots d\mathbf{r}_N \exp(-\beta U_N(\xi)), \quad (6)$$

with

$$Z_N(\xi) = \int d\mathbf{r}_1 \dots d\mathbf{r}_N \exp(-\beta U_N(\xi)). \quad (7)$$

Setting $\xi = 0$ of course reduces the generalized functions (6) to the usual versions, (2).

We now proceed as for the Kirkwood integral equation [2], differentiating $g^{(2)}(\mathbf{r}_1, \mathbf{r}_2 | \xi)$ with respect to ξ to obtain

$$\begin{aligned} \frac{dg^{(2)}(\mathbf{r}_1, \mathbf{r}_2 | \xi)}{d\xi} &= -\psi(\mathbf{r}_{12})g^{(2)}(\mathbf{r}_1, \mathbf{r}_2 | \xi) - \rho \int d\mathbf{r}_3 \psi(\mathbf{r}_{13}) [g^{(3)}(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3 | \xi) \\ &\quad - g^{(2)}(\mathbf{r}_1, \mathbf{r}_2 | \xi)g^{(2)}(\mathbf{r}_1, \mathbf{r}_3 | \xi)]. \end{aligned} \quad (8)$$

For a homogeneous system, the distribution functions will depend only on separation vectors $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$; in addition, for spherically symmetric potential $\varphi(r)$ the description of the ordinary fluid depends on just the magnitudes r_{ij} . Then, dropping the superscript for the pair distribution function (PDF) and setting $\xi = 0$, we obtain from (8)

$$\begin{aligned} g'(\mathbf{r}_{12} | 0) &\equiv \left. \frac{dg(\mathbf{r}_{12} | \xi)}{d\xi} \right|_{\xi=0} \\ &= -\psi(r_{12})g(r_{12}) - \rho \int d\mathbf{r}_3 \psi(r_{13}) [g^{(3)}(\mathbf{r}_{12}, \mathbf{r}_{13}) - g(r_{12})g(r_{13})]. \end{aligned} \quad (9)$$

With this equation, an integral of the form (1) can evidently be determined from a knowledge of the usual PDF $g(r)$ and of the new pair function $g'(\mathbf{r} | 0)$ defined in (9).

Successful theories are available to determine $g(r)$ from the pair potential $\varphi(r)$ [3–8]. We shall be concerned here with obtaining the new function $g'(\mathbf{r} | 0)$ to complete the recipe and so bypass the need to know $g^{(3)}$. In the sequel, we shall further assume for simplicity that $\psi(r)$ too is spherically symmetric, though the more general case of orientation-dependent $\psi(\mathbf{r})$ can also be accommodated.

2. Calculation of $g'(\mathbf{r} | 0)$

Equation (6) describes a two-component system, in which molecule 1 interacts with the others though the total potential $\varphi(r) + \xi\psi(r)/\beta$ while the remaining $N - 1$ molecules interact among themselves through $\varphi(r)$ alone. The Ornstein–Zernike equations [8] for a two-component mixture in which one component is at infinite dilution are

$$h(r) \equiv g(r) - 1 = C(r) + \rho \int d\mathbf{r}' h(r')C(|\mathbf{r} - \mathbf{r}'|), \quad (10)$$

$$h(r|\xi) \equiv g(r|\xi) - 1 = C(r|\xi) + \rho \int d\mathbf{r}' h(r'|\xi) C(|\mathbf{r} - \mathbf{r}'|). \quad (11)$$

Here $C(r)$ is the usual direct correlation function (DCF) for the solvent fluid with intermolecular potential $\varphi(r)$ and $C(r|\xi)$ is the corresponding DCF for the solute molecule. These equations for h and C are complemented with the so-called closure relations [8]

$$g(r) = \exp[-\beta\varphi(r) + h(r) - C(r) + B(r)], \quad (12)$$

$$g(r|\xi) = \exp[-\beta\varphi(r) - \xi\psi(r) + h(r|\xi) - C(r|\xi) + B(r|\xi)], \quad (13)$$

which introduce the solvent and solute bridge functions, $B(r)$ and $B(r|\xi)$, respectively. Though formally defined by infinite series, these functions in practice must be approximated; the different closures in use today [3–8] stem from different approximations to the bridge function.

Equations (10) and (12), with some expression for $B(r)$, are the standard fare of liquid state theory. We shall focus here on (11) and (13) in seeking $g'(r|0)$. We first rewrite these equations by eliminating h in favour of the series function $S = h - C$ and deconvoluting (11) using Fourier transforms. The result is

$$C(r|\xi) = \exp[-\beta\varphi(r) - \xi\psi(r) + S(r|\xi) + B(r|\xi)] - 1 - S(r|\xi), \quad (14)$$

$$\tilde{S}(k|\xi) = \rho\tilde{h}(k)\tilde{C}(k|\xi), \quad (15)$$

where the tilde denotes Fourier transform. Now differentiate with respect to ξ and set $\xi = 0$ to obtain

$$C'(r|0) = g(r)[- \psi(r) + S'(r|0) + B'(r|0)] - S'(r|0), \quad (16)$$

$$\tilde{S}'(k|0) = \rho\tilde{h}(k)\tilde{C}'(k|0). \quad (17)$$

Once $B'(r|0)$ is modelled in some appropriate way (see below), these coupled equations can be solved for $S'(r|0)$ and $C'(r|0)$, yielding finally the desired

$$g'(r|0) = g(r)[- \psi(r) + S'(r|0) + B'(r|0)]. \quad (18)$$

This supplies the final ingredient needed in (9) to compute an integral over $g^{(3)}$ using only pair functions.

The final point to be addressed is the modelling of $B'(r|0)$ in (16) and (18). This question has a natural answer in the context of the optimized reference hypernetted chain (RHNC) equation [9–11], in which $B(r|\xi)$ is modelled by the bridge function of a hard sphere fluid,

$$B(r|\xi) = B_{\text{HS}}(r; \sigma(\xi)), \quad (19)$$

where the hard sphere diameter $\sigma(\xi)$ is varied to minimize the free energy. Since σ is the variable that changes with ξ , we obtain within the same approximation

$$B'(r|0) = \sigma \frac{dB_{\text{HS}}(r; \sigma)}{d\sigma} \left(\frac{d \ln \sigma(\xi)}{d\xi} \right)_{\xi=0}. \quad (20)$$

The slope of $\ln \sigma(\xi)$ is obtained numerically by further solving (14) and (15), within the same framework of the optimized RHNC equation, at small values of ξ , including $\xi = 0$, the neat fluid.

Equations (16) and (17), which are *exact*, along with the modelled $B'(r|0)$ of (20), which follows from the successful RHNC closure, constitute the algorithm that

replaces approximations to $g^{(3)}$ for purposes of integrals such as (1). In the next section we illustrate the application of this algorithm for two cases.

3. Moments of a distribution

A common instance in which integrals over $g^{(3)}$ (as well as higher distributions) make an appearance is the calculation of moments. These include frequency moments (also called sum rules) for time correlation functions [12, 13], microstructural moments in two-phase random media [14–16], potential energy moments for thermodynamic derivatives [17], and moments of a local field distribution [18, 19]. In the first two cases, the resulting function $\psi(r)$ is orientation dependent, requiring a generalization of the simple algorithm described in §2 along the lines of the electric microfield calculation [20], and will not be dealt with here. The case of thermodynamic derivatives falls within the scope of §2 but limits $\psi(r)$ to just the intermolecular potential. For present purposes of illustration, we shall cast the discussion in the language of the local field distribution, which affords more variety in $\psi(r)$.

A local field arises at a test particle, say molecule 1, when the particle is subject to a scalar field $\psi(r_{1j})$ from each of the remaining $j = 2, 3, \dots, N$ molecules of a fluid. The field function $\psi(r)$ is essentially arbitrary and does not affect the fluid configurations. The net field strength Ψ experienced by the test particle is a random variable of fluid configuration whose distribution is defined by

$$P(\Psi) = \left\langle \delta \left[\Psi - \sum_{j=2}^N \psi(r_{1j}) \right] \right\rangle, \quad (21)$$

where the angle brackets denote an equilibrium average with the Boltzmann factor of (2) to (4).

The calculational awkwardness of the Dirac delta function in (21) is avoided by dealing rather with the Fourier transform of $P(\Psi)$; writing the delta function in Fourier representation, we obtain

$$P(\Psi) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dK \exp(iK\Psi) \tilde{P}(K), \quad (22)$$

where then

$$\tilde{P}(K) = \left\langle \exp \left(-iK \sum_{j=2}^N \psi(r_{1j}) \right) \right\rangle. \quad (23)$$

The moments of the distribution,

$$m_n = \int_{-\infty}^{\infty} d\Psi \Psi^n P(\Psi), \quad (24)$$

are then generated by the expansion of the exponential in (23),

$$\tilde{P}(K) = 1 - im_1 K - \frac{1}{2!} m_2 K^2 + \frac{i}{3!} m_3 K^3 + \dots, \quad (25)$$

where

$$m_n = \left\langle \left(\sum_{j=2}^N \psi(r_{1j}) \right)^n \right\rangle. \quad (26)$$

Explicitly, the first and second moments are

$$m_1 = \rho \int d\mathbf{r} \psi(r) g(r), \quad (27)$$

$$m_2 = \rho \int d\mathbf{r} \psi^2(r)g(r) + \rho^2 \int d\mathbf{r}_2 d\mathbf{r}_3 \psi(r_{12})\psi(r_{13})g^{(3)}(\mathbf{r}_{12}, \mathbf{r}_{13}), \quad (28)$$

where we have used (2). From these, the second central moment is given by

$$\begin{aligned} c_2 &= m_2 - m_1^2 \\ &= \rho \int d\mathbf{r} \psi^2(r)g(r) \\ &\quad + \rho^2 \int d\mathbf{r}_2 d\mathbf{r}_3 \psi(r_{12})\psi(r_{13})[g^{(3)}(\mathbf{r}_{12}, \mathbf{r}_{13}) - g(r_{12})g(r_{13})]. \end{aligned} \quad (29)$$

The computation of the first and second moments is of particular importance when it is known that $P(\Psi)$ is approximately Gaussian.

Direct evaluation of (29) obviously requires an approximation to $g^{(3)}$. From (9), we see that c_2 may also be written as

$$c_2 = -\rho \int d\mathbf{r} \psi(r)g'(r|0), \quad (30)$$

avoiding the need for the triplet correlation function when the pair function $g'(r|0)$ is computed instead. The reduction from a three-particle integration in (29) to a simple pair expression in (30) is in itself of computational consequence, quite aside from the accuracy of possible approximations to $g^{(3)}$.

We note in passing that (30) can be generalized to all cumulants c_n , defined by

$$c_n = (-1)^n \left. \frac{d^n \ln Z(\xi)}{d\xi^n} \right|_{\xi=0}, \quad (31)$$

so that, e.g., $c_3 = m_3 - 3m_1m_2 + 2m_1^3$; the calculation of c_3 requires knowledge of the two-, three-, and four-particle correlation functions. From (7), however, we have

$$\frac{d \ln Z(\xi)}{d\xi} = -\rho \int d\mathbf{r} \psi(r)g(r|\xi), \quad (32)$$

so that

$$c_n = \rho \int d\mathbf{r} \psi(r)(-1)^{n-1} \left. \frac{d^{n-1} g(r|\xi)}{d\xi^{n-1}} \right|_{\xi=0}, \quad (33)$$

which involves only pair functions. It may, however, prove impractical to extend the technique of §2 for $g'(r|0)$ to higher derivatives of $g(r|\xi)$. No attempt has been made in this direction.

A common expedient for dealing with $g^{(3)}$ in the direct evaluation of (29) or (9) is to invoke the Kirkwood superposition approximation [2],

$$g^{(3)}(\mathbf{r}_{12}, \mathbf{r}_{13}) \approx g(r_{12})g(r_{13})g(r_{23}), \quad (34)$$

which leads to

$$g'_{\text{SA}}(r_{12}|0) = -g(r_{12}) \left(\psi(r_{12}) + \rho \int d\mathbf{r}_3 \psi(r_{13})g(r_{13})h(r_{32}) \right). \quad (35)$$

The convolution integral in (35) can easily be evaluated using Fourier transforms.

Our purpose now is to compute $g'(r|0)$, and from it c_2 , using the extended RHNC technique of §2, as well as the superposition approximation for comparison, for two local field distributions: (a) a Lennard-Jones (LJ) field,

$$\psi(r) = 4[(\sigma/r)^{12} - (\sigma/r)^6], \quad (36)$$

Figure 1. The pair function $g'(r|0)$ of (9) for a Lennard-Jones $\psi(r)$ at a hard sphere test particle in a hard sphere fluid at density $\rho\sigma^3 = 0.4$. Integral equation and superposition approximation results are not clearly distinguishable on this scale.

in a *hard sphere* fluid [18], where the hard sphere diameter is also σ so the test sphere experiences only the attractive part of $\psi(r)$; and (b) a Coulomb field

$$\psi(r) = \frac{e^2}{\epsilon r} \quad (37)$$

in a one-component plasma (OCP). Both fields are written as dimensionless quantities; in (37), $\epsilon = e^2/a$ is the unit of energy, where $a = (3/4\pi\rho)^{1/3}$ is the ion sphere radius.

3.1. The Lennard-Jones field

The pure liquid in this model is the hard sphere system, for which we use the Verlet-Weis [21] and Henderson-Grundke [22] fits to generate $g(r; \sigma)$, $B(r; \sigma)$, and $\sigma dB(r; \sigma)/d\sigma$. These are used in obtaining $g'(r|0)$ from (16) and (17) for the LJ field of (36). The results for reduced densities $\rho\sigma^3 = 0.4$ and 0.8 are shown in figures 1 and 2, respectively. At the lower density, $g'_{SA}(r|0)$ from (35) largely coincides with the curve in figure 1 and is not plotted. Differences between the two results become more apparent at reduced density 0.8 , seen in figure 2. Nevertheless, the two curves are still in relatively good agreement overall.

The calculation then yields by simple quadrature, (30), the second central moment $c_2 = m_2 - m_1^2$ for the LJ local field carried by hard spheres, tabulated in the table for reduced densities 0.2 , 0.4 , and 0.8 . We list also in this table the first moment m_1 from (27), which of course depends only on the hard sphere $g(r)$. These results yield Gaussian shapes that are in good agreement with the local field distributions $P(\Psi)$ for this model obtained by Monte Carlo simulation by Simon, Dobrasavljević, and Stratt [18]. Unfortunately, no conclusions about the relative merits of the two calculations for c_2 can be drawn from this qualitative comparison.

Figure 2. The pair function $g'(r|0)$ of (9) for a Lennard-Jones $\psi(r)$ at a hard sphere test particle in a hard sphere fluid at density $\rho\sigma^3 = 0.8$: (—) integral equation; (---) superposition approximation.

3.2. The Coulomb field

The bridge function and its derivative for the Coulomb system were again obtained from the same parametrizations as above [3]. The long-range nature of the Coulomb potential means that some care must be taken in the numerical calculations of its correlation functions. We have followed the prescription of Ng [23] in dealing analytically with the long range parts of $S(r|\xi)$ and $C(r|\xi)$, leaving only a well behaved short-range residue for the numerical resolution of (16) and (17). Figure 3 displays $g'(r|0)$ obtained from the RHNC algorithm of § 2 and in superposition approximation, (35), at a plasma interaction strength of $\Gamma = \beta e^2/a = 10$. We see here a much greater discrepancy between the two calculations compared to the Lennard-Jones/hard sphere results in figures 1 and 2. This disagreement carries over to the computed moments; the curves in figure 3 yield $c_2 = 0.114$ for the integral equation method and $c_2 = 0.361$ using the superposition approximation. There are no simulation data for comparison, but internal consistency checks [19] strongly favour the integral equation results, suggesting that the superposition approximation is not reliable here.

First moment and second central moment of a Lennard-Jones local field at a hard sphere test particle immersed in a hard sphere fluid, from the present integral equation method (IE) and the superposition approximation (SA).

$\rho\sigma^3$	m_1	$m_2 - m_1^2$	
		SA	IE
0.2	-2.446	0.767	0.754
0.4	-5.261	1.051	1.017
0.8	-11.201	1.072	0.937

Figure 3. The pair function $g'(r|0)$ of (9) for a Coulomb $\psi(r)$ at an ion in a one-component plasma at $\Gamma = 10$: (—) integral equation; (---) superposition approximation.

A comment about the Verlet–Weiss parametrization of $g_{\text{HS}}(r; \sigma)$ is appropriate. It has already been noted in other publications [3, 24] that the modelled bridge function obtained from this fit displays a sharp irregularity around $r = 2\sigma$, leading in turn to a notable spike in $\sigma dB_{\text{HS}}(r; \sigma)/d\sigma$ in the same region. The numerical effect of this is likely to be small but used in, say, (18), the result is a decidedly unphysical bump in $g'(r|0)$ around 2σ . This irregularity was part of the motivation for the ‘crossover’ closure of Foiles, Ashcroft, and Reatto [24]. Here we have taken the simple expedient of numerically smoothing out the irregularity in the fitted series function $S_{\text{HS}}(r)$, which eliminates most of the anomalous effect, but of course does not allow for adaption to the known variation with changing potential [25] in the weak, longer-ranged part of $B(r)$.

We remark further that other parametrizations [26, 27] of the hard sphere correlation functions, while yielding excellent fits to $B_{\text{HS}}(r; \sigma)$, also show, for different reasons, similar irregularities in its derivative with respect to σ . This is much less true for the analytic solution of Waisman [28], but because of the highly non-linear equations for its parameters it is harder to use.

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