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Uniqueness for the BBGKY Hierarchy for Hard Spheres in One Dimension

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We prove that the stationary BBGKY hierarchy for an infinite system of hard spheres in one dimension has a unique solution for all densities, within a symmetry class that pertains to either a fluid array or to a perfect crystalline array. The solution is shown to correspond to the uniform fluid, which is the only equilibrium state of the infinite system. The proof is subject to the recursion relation for the correlation functions found by Salsburg, Zwanzig, and Kirkwood, which we show exactly reduces the infinite hierarchy to a pair of coupled equations. A brief discussion is given of the existence of multiple solutions of an approximate BBGKY equation.

KEY WORDS: Solution of BBGKY hierarchy; one-dimensional hard spheres; correlation functions; uniqueness.

1. INTRODUCTION

We consider a classical hard-sphere system of N identical particles on an interval of length L, in the limit $N \to \infty$, $L \to \infty$, with $N/L = \rho$, the number density, fixed. The potential energy U_n for a subset of n particles at the positions $x_1, ..., x_n$ is given by

$$U_n(x_1, ..., x_n) = \sum_{1 \le i < j \le n} \sum u(|x_{ij}|) \tag{1a}$$

with

$$x_i - x_j = x_{ij} \tag{1b}$$

and

$$\begin{aligned} u(|x_{ij}|) &= \infty, \qquad |x_{ij}| < d \\ &= 0, \qquad |x_{ij}| \geqslant d \end{aligned} \tag{1c}$$

where d is the length of a particle.

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If $\rho_n(x_1,\ldots, x_n)$ denotes the probability density for finding particles simultaneously at $x_1,\ldots, x_n$, independent of the positions of all other particles in the system, then correlation functions $G_n(x_1,\ldots, x_n)$ can be defined by

$$\rho_n(x_1,\ldots, x_n)/\rho^n = G_n(x_1,\ldots, x_n) \tag{2}$$

For the hard-sphere potential, it is convenient to deal with the functions $G_n{}^*$, which are defined so that they are continuous at $|x_{ij}| = d$, for any i, j in the subset,

$$G_n{}^*(x_1,\ldots, x_n) = \left\{\exp\left[\beta \sum_{1\leq i<j\leq n}\sum u(|x_{ij}|)\right]\right\} G_n(x_1,\ldots, x_n) \tag{3}$$

with $\beta = 1/k_BT$, where T is the absolute temperature and k_B is Boltzmann's constant. The functions $G_1{}^*$ and G_1 are identical since the interaction contains no terms that depend on the position of just a single particle, and if all $|x_{ij}| \geqslant d$, $G_n{}^* \equiv G_n$.

In terms of these functions, the BBGKY hierarchy of equations is

$$\begin{aligned}\nabla_{x_i} \ln G_n{}^*(x_1,\ldots, x_n)\\ = -\rho\beta \int dx_{n+1} \exp\left[-\beta \sum_{j=1}^{n} u(|x_j - x_{n+1}|)\right] \frac{G^*_{n+1}(x_1,\ldots, x_{n+1})}{G_n{}^*(x_1,\ldots, x_n)}\\ \otimes \nabla_{x_i} u(|x_i - x_{n+1}|), \qquad n = 1, 2, 3,\ldots\end{aligned} \tag{4}$$

where x_i is any one of the positions, and the integration is over the entire line, $-\infty < x_{n+1} < \infty$.

In this paper we investigate the solutions of (4). We note that the hierarchy of equations does not form a closed set, that is, one needs the function G^*_{n+1} in order to obtain an equation for $G_n{}^*$. An exact recursion relation for the correlation functions in the one-dimensional hard-sphere system has been computed by Salsburg, Zwanzig, and Kirkwood[1] (SZK). The recursion relation was obtained[1] by directly integrating the classical phase space probability density, using the method of residues. One can choose, for convenience, a particular ordering of the particle positions and, because (1c), the arbitrarily chosen ordering will remain unchanged for all interparticle separations in the one-dimensional system. Furthermore, because the range of the potential energy is just the point d, the only terms in (1) that contribute in the ordered array are nearest neighbors.

Using these properties, SZK were able to show that for the ordered array $x_1 < x_2 < \cdots < x_n$, there is an exact recursion relation

$$\frac{G_{n+1}(x_1,\ldots, x_{n+1})}{G_n(x_1,\ldots, x_n)} = \frac{G_2(x_n, x_{n+1})}{G_1(x_n)} \tag{5}$$

and by applying (1c) and (3) one finds that this recursion relation applies to the functions $G_m{}^*$.

The purpose of this paper is to study the solution of the hierarchy (4) subject to the SZK recursion relation (5). We will show, in Section 2, that (5) is an exact truncation of the hierarchy; that is, for all $n > 2$, the recursion relation yields the same equation as is obtained at $n = 2$. Therefore with (5), the infinite hierarchy is reduced to coupled equations for the pair (G_1, G_2). Then, in Section 3, we study this pair and we ask whether its solution is unique. We prove that, within a certain symmetry class, which includes correlation functions for both uniform and crystalline arrays, the solution is in fact unique for all densities. We show that the solution corresponds to the uniform fluid, which is known to be the only equilibrium state of the infinite system.

The discussion is given in Section 4. We briefly consider the uniqueness result in terms of recent investigations of a molecular theory of crystallization based on the BBGKY equations.[2,3] The result of the theory for the one-dimensional hard-sphere system[2,3] is, in fact, the motivation of this investigation.

2. THE SZK RECURSION RELATION

The hard-sphere interaction is such that in one dimension,

$$\nabla_{x_i} \exp[-\beta u(|x_{ij}|)] = \operatorname{Sign}(x_{ij})\, \delta(|x_{ij}| - d) \tag{6}$$

Applying this and (5) to (4) with $n = 2$ gives, for $x_1 < x_2$,

$$\begin{aligned} &\frac{\partial}{\partial x_1} \ln G_2^*(x_1, x_2) \\ &\quad = \rho \exp[-\beta u(|x_{21} + d|)] \frac{G_2^*(x_1 - d, x_1)}{G_1(x_1)} \\ &\qquad - \rho \exp[-\beta u(|x_{21} - d|)] \frac{G_2^*(x_1 + d, x_2) G_2^*(x_1, x_1 + d)}{G_1(x_1 + d) G_2^*(x_1, x_2)} \end{aligned} \tag{7}$$

In this section we show that with (5), the form of the BBGKY hierarchy for $n \geqslant 2$ does not depend on n. That is, we show that for $n > 2$, all equations generated by the hierarchy are identical to (7).

With (6) and (4) we have that for $n \geqslant 2$, the BBGKY hierarchy is

$$\begin{aligned} &\frac{\partial}{\partial x_1} \ln G_n^*(x_1,..., x_n) \\ &\quad = \rho \exp\left[-\beta \sum_{j=2}^{n} u(|x_j - x_1 + d|)\right] \frac{G_{n+1}^*(x_1,..., x_n, x_1 - d)}{G_n^*(x_1,..., x_n)} \\ &\qquad - \rho \exp\left[-\beta \sum_{j=2}^{n} u(|x_j - x_1 - d|)\right] \frac{G_{n+1}^*(x_1,..., x_n, x_1 + d)}{G_n^*(x_1,..., x_n)} \end{aligned} \tag{8}$$

and this pertains to all orderings. We suppose that the particles have the particular ordering $x_1 < x_2 < \cdots < x_n$, and use the fact that since the correlation functions determine probability densities,

$$G_{n+1}^*(x_1, \ldots, x_n, y) = G_{n+1}^*(y, x_1, \ldots, x_n).$$

As we have already mentioned, any chosen ordering will remain unchanged for all interparticle separations because of (1c). By repeated application of (5) we find

$$G_n^*(x_1, \ldots, x_n) = \frac{G_2^*(x_{n-1}, x_n)}{G_1(x_{n-1})} \frac{G_2^*(x_{n-2}, x_{n-1})}{G_1(x_{n-2})} \cdots \frac{G_2^*(x_2, x_3)}{G_1(x_2)} G_2^*(x_1, x_2) \tag{9a}$$

$$\begin{aligned} \frac{G_{n+1}^*(x_1 - d, x_1, \ldots, x_n)}{G_n^*(x_1, \ldots, x_n)} &= \frac{G_2^*(x_{n-1}, x_n)}{G_1(x_{n-1})} \frac{G_n^*(x_1 - d, x_1, \ldots, x_{n-1})}{G_n^*(x_1, \ldots, x_n)} \\ &= \frac{G_2^*(x_1 - d, x_1)}{G_1(x_1)} \end{aligned} \tag{9b}$$

and

$$\begin{aligned} \frac{G_{n+1}^*(x_1, x_1 + d, x_2, \ldots, x_n)}{G_n^*(x_1, \ldots, x_n)} &= \frac{G_2^*(x_{n-1}, x_n)}{G_1(x_{n-1})} \frac{G_n^*(x_1, x_1 + d, x_2, \ldots, x_{n-1})}{G_n^*(x_1, \ldots, x_n)} \\ &= \frac{G_2^*(x_1 + d, x_2) G_2^*(x_1, x_1 + d)}{G_2^*(x_1, x_2) G_1(x_1 + d)} \end{aligned} \tag{9c}$$

Using these and the fact that for the ordered array all the exponential factors in (8) are unity except those involving $|x_{21} \pm d|$, we obtain the result that with the SZK recursion relation, (8) and (7) are identical.

Therefore with (5) the infinite hierarchy reduces to

$$\nabla_{x_1} \ln G_1(x_1) = \rho \int dx_2 \frac{G_2^*(x_1, x_2)}{G_1(x_1)} \nabla_{x_1} \exp[-\beta u(x_{12})] \tag{10a}$$

and

$$\begin{aligned} &\nabla_{x_1} \ln G_2^*(x_1, x_2) \\ &\quad = \rho \int dx_3 \exp[-\beta u(x_{23})] \frac{G_3^*(x_1, x_2, x_3)}{G_2^*(x_1, x_2)} \nabla_{x_1} \exp[-\beta u(x_{13})] \end{aligned} \tag{10b}$$

These coupled equations are the subject of our investigation.

Since we wish to study the solution of the pair for all of one-dimensional space, we must consider configurations where $x_1 > x_2$ and also where $x_2 > x_1$. By considering both cases we will, with the SZK relation, have considered all orderings of the infinite one-dimensional system. Applying (6) to (10a) gives

$$\frac{d \ln G_1(x_1)}{dx_1} = \frac{\rho G_2^*(x_1, x_1 - d)}{G_1(x_1)} - \frac{\rho G_2^*(x_1, x_1 + d)}{G_1(x_1)} \tag{11}$$

Using the SZK recursion relation in (10b) yields the following equations depending on whether $x_{12} > 0$ or $x_{21} > 0$:

$$\frac{\partial \ln G_2^*(x_1, x_2)}{\partial x_1} = \frac{\rho G_2^*(x_1 - d, x_1) G_2^*(x_2, x_1 - d)}{G_2^*(x_1, x_2) G_1(x_1 - d)} - \frac{\rho G_2^*(x_1, x_1 + d)}{G_1(x_1)}, \qquad x_{12} \geqslant 2d \tag{12a}$$

$$\frac{\partial \ln G_2^*(x_1, x_2)}{\partial x_1} = -\frac{\rho G_2^*(x_1, x_1 + d)}{G_1(x_1)}, \qquad 0 \leqslant x_{12} < 2d \tag{12b}$$

$$\frac{\partial \ln G_2^*(x_1, x_2)}{\partial x_1} = \frac{\rho G_2^*(x_1 - d, x_1)}{G_1(x_1)} - \frac{\rho G_2^*(x_1 + d, x_2) G_2^*(x_1, x_1 + d)}{G_1(x_1 + d) G_2^*(x_1, x_2)}, \qquad x_{21} \geqslant 2d \tag{12c}$$

and

$$\frac{\partial \ln G_2^*(x_1, x_2)}{\partial x_1} = \frac{\rho G_2^*(x_1 - d, x_2)}{G_1(x_1)}, \qquad 0 \leqslant x_{21} < 2d \tag{12d}$$

We must now investigate whether the set (11) and (12), that is, the exact BBGKY hierarchy for the pair (G_1, G_2), has a unique solution.

3. UNIQUENESS

We will, at first, consider the set (11), (12b), and (12d); that is, we consider the coupled set of equations for those configurations where two particles are separated by distances that are less than twice their length. We show that the solution is unique in this interval and then, by using (12a) and (12c), we show that there is a unique extension of the solution to all of one-dimensional space.

From (12b) and (12d) we have that

$$\ln G_2^*(x_1, x_2) = e(x_1) + f(x_2), \qquad 0 \leqslant x_{12} < 2d \tag{13a}$$

and

$$\ln G_2^*(x_1, x_2) = k(x_1) + l(x_2), \qquad 0 \leqslant x_{21} < 2d \tag{13b}$$

Since the probability density determined from G_2^* must be invariant under the exchange of the positions of identical particles,

$$G_2^*(x_1, x_2) = G_2^*(x_2, x_1) \tag{14}$$

and from (13),

$$\ln G_2^*(x_1, x_2) = k(x_1) + l(x_2), \qquad 0 \leqslant x_{21} < 2d \tag{15a}$$

and

$$\ln G_2^*(x_1, x_2) = l(x_1) + k(x_2), \qquad 0 \leqslant x_{12} < 2d \tag{15b}$$

Since, for a uniform fluid or perfect crystalline structure, the probability density determined from G_2^* must also remain unchanged if the position vectors are reflected through the origin,

$$G_2^*(x_1, x_2) = G_2^*(-x_1, -x_2) \tag{16}$$

We emphasize that it is assumed from the outset that both G_1 and $G_2^*(x_1, x_2)$ are compatible with either a crystalline array or a uniform fluid. Hence we can always choose the origin of the coordinate system so that the condition (16) is fulfilled. For a uniform fluid we can put the origin anywhere; for a perfect crystalline array we put the origin at a lattice site. This, together with (15), requires

$$l(-x) = k(x) + \kappa \tag{17}$$

where κ is a constant. Therefore we are led to

$$\ln G_2^*(x_1, x_2) = k(x_1) + k(-x_2) + \kappa, \qquad 0 \leqslant x_{21} < 2d \tag{18a}$$

and

$$\ln G_2^*(x_1, x_2) = k(-x_1) + k(x_2) + \kappa, \qquad 0 \leqslant x_{12} < 2d \tag{18b}$$

Using (11), (12b), (12d), and (15), we find that

$$\frac{d \ln G_1(x_1)}{dx_1} = \frac{dk(x_1)}{dx_1} + \frac{dl(x_1)}{dx_1} \tag{19}$$

which upon integration and application of (17) leads to

$$k(-x) = \ln G_1(x) - k(x) - \lambda - \kappa \tag{20}$$

where λ is a constant of integration. With this and (18) we obtain

$$G_2(x_1 - d, x_1) = G_1(x_1) \exp[-\lambda - k(x_1) + k(x_1 - d)] \tag{21a}$$

and

$$G_2(x_1 + d, x_1) = G_1(x_1 + d) \exp[-\lambda + k(x_1) - k(x_1 + d)] \tag{21b}$$

Using (19), (21), (12b), and (12d), we obtain

$$\frac{dG_1(x_1)}{dx_1} = \rho\Big\{\exp[-\lambda - k(x_1) + k(x_1 - d)] - \frac{G_1(x_1 + d)}{G_1(x_1)} \exp[-\lambda + k(x_1) - k(x_1 + d)]\Big\} \tag{22}$$

and

$$dk(x_1)/dx_1 = \rho \exp[-\lambda - k(x_1) + k(x_1 - d)] \tag{23}$$

But with (15b), (17), and (21), this can be simplified to

$$\frac{d \ln G_1(x_1)}{dx_1} = \rho\{\exp[-\lambda - k(x_1) + k(x_1 - d)] - \exp[-\lambda - k(-x_1) + k(-x_1 - d)]\} \tag{24}$$

Since the right side of (24) involves just $k(x)$, we need only solve (23) to obtain a solution of the BBGKY hierarchy over the interval $|x_{12}| < 2d$. Therefore, with the SZK recursion relation, we have reduced the hierarchy to the solution of one functional differential equation. In general, this equation may possess more than one solution. We will now show that for the problem in question, a simple physical criterion is sufficient to guarantee that the solution is unique.

It is advantageous to further simplify (23); we multiply it by

$$r(x) = \exp[k(x)] \tag{25}$$

to obtain the linear equation

$$dr(x)/dx = \rho e^{-\lambda} r(x - d) \tag{26}$$

Since $G_2{}^*(x_1, x_2)$ must be positive because it determines the pair probability density, $k(x)$ must be a real-valued function and hence,

$$r(x) > 0 \tag{27}$$

In addition to the invariance of $G_2{}^*(x_1, x_2)$ under the exchange of the particle positions and their reflection through the origin, we also require that

$$G_2{}^*(x_1, x_2) = G_2{}^*(x_1 + a, x_2 + a) \tag{28}$$

We note that this is satisfied for both a translationally invariant function, that is, a function corresponding to a uniform fluid, and also for a crystal with periodicity a. From (18), (25), and (28) we find

$$r(x)/r(x + a) = e^{\mu} \tag{29}$$

where μ is a real constant. Defining the function $t(x)$ by

$$r(x) = t(x) \exp(-\mu x/a) \tag{30}$$

we obtain the result that $t(x)$ must be periodic,

$$t(x) = t(x + a) \tag{31}$$

and because of (27),

$$t(x) > 0 \tag{32}$$

Putting (30) in (26) gives

$$dt(x)/dx = (\mu/a)t(x) + \rho[\exp(-\lambda + \mu d/a)]t(x - d) \tag{33}$$

Considering (31), we write $t(x)$ as the Fourier series,

$$t(x) = \sum_m A(m) \exp(i2\pi mx/a) \tag{34}$$

and this together with (33) requires

$$A(m)[(i2\pi m/a) - (\mu/a) - \rho \exp(-\lambda + \mu d/a) \exp(-i2\pi md/a)] = 0 \tag{35}$$

for all m. From (32) we note that the integral of $t(x)$ over one period cannot vanish and therefore

$$A(0) \neq 0$$

which, when applied to (35) yields

$$-\mu/a = \rho \exp(-\lambda + \mu d/a) \tag{36}$$

For $A(m) \neq 0$, the real and imaginary parts of (35) demand that

$$2\pi m/a = (\mu/a) \sin(2\pi md/a) \tag{37a}$$

and

$$1 = \cos(2\pi md/a) \tag{37b}$$

The only solution of (37) is

$$m = 0$$

and therefore

$$t(x) = e^{\nu} \tag{38}$$

where ν is a real constant. Using this, (25), and (30), we find

$$k(x) = -(\mu x/a) + \nu \tag{39}$$

and from (20),

$$\ln G_1(x) = 2\nu + \lambda + \kappa \tag{40}$$

but since the normalization of $G_1(x)$ is

$$\lim_{L \to \infty} (1/L) \int_L dx\, G_1(x) = 1$$

the constants in (40) must be such that

$$2\nu + \lambda + \kappa = 0 \tag{41}$$

Applying (39) and (41) to (18) we arrive at the pair correlation function,

$$G_2(x_1, x_2) = \exp[-\lambda + (\mu/a)x_{21}], \qquad 0 \leqslant x_{21} < 2d \tag{42a}$$

and

$$G_2(x_1, x_2) = \exp[-\lambda + (\mu/a)x_{12}], \qquad 0 \leqslant x_{12} < 2d \tag{42b}$$

The constants in (42) can be related to physical quantities; with (36) we obtain

$$\exp(-\lambda) = G_2(d)\exp(-\mu d/a) \tag{43a}$$

and

$$\mu/a = -\rho G_2(d) \tag{43b}$$

where $G_2(d)$ denotes the value of G_2 when the particles at x_1 and x_2 are in contact. It is a physically significant quantity because it determines, through application of the virial theorem, the pressure P of the system in the limit of a uniform fluid,

$$\beta P/\rho = 1 + \rho G_2(d)$$

With (43), the pair correlation function simplifies to

$$G_2{}^*(x_1, x_2) = G_2(d)\exp[-\rho G_2(d)(x_{21} - d)], \qquad 0 \leqslant x_{21} < 2d \tag{44a}$$

and

$$G_2{}^*(x_1, x_2) = G_2(d)\exp[-\rho G_2(d)(x_{12} - d)], \qquad 0 \leqslant x_{12} < 2d \tag{44b}$$

Since the particle positions are ordered, we can replace x_{21} (and x_{12}) by its modulus. With (40)–(42) we obtain the solution of the BBGKY hierarchy for all densities over the interval $|x_{12}| < 2d$,

$$G_1(x_1) = 1 \tag{45a}$$

and

$$G_2{}^*(x_1, x_2) = G_2(d)\exp[-\rho G_2(d)(|x_{12} - d|)], \qquad |x_{12}| < 2d \tag{45b}$$

This pair of functions is invariant under all translations and therefore it corresponds to the uniform fluid.

The extension of the solution at (45) to all of one-dimensional space goes as follows. Consider, for example, the case where $x_1 > x_2$ and suppose $3d > x_1 - x_2 > 2d$. Use the fact that $G_1(x) = 1$ for all x, and (44b) together with (12a). These yield

$$\begin{aligned}\frac{\partial}{\partial x_1} G_2{}^*(x_1, x_2) = {}& \rho[G_2(d)]^2 \exp[-\rho G_2(d)(x_{12} - 2d)] \\ & - \rho G_2(d) G_2{}^*(x_1, x_2)\end{aligned} \tag{46a}$$

which upon integration gives

$$\begin{aligned}G_2{}^*(x_1, x_2) = {}& \rho[G_2(d)]^2 x_1 \exp[-\rho G_2(d)(x_{12} - 2d)] \\ & + \exp[-\rho G_2(d) x_1] F(x_2)\end{aligned} \tag{46b}$$

Now we can determine the arbitrary function $F(x_2)$ from (44b) by letting $x_1 = x_2 + 2d$, since $G_2{}^*$ is continuous. This and (46b) lead to

$$G_2{}^*(x_1, x_2) = \rho[G_2(d)]^2(x_{12} - 2d)\exp[-\rho G_2(d)(x_{12} - 2d)] + G_2(d)\exp[-\rho G_2(d)(x_{12} - 2d)] \quad (47)$$

Therefore, $G_2{}^*(x_1, x_2)$ is determined in the interval $x_2 + 3d > x_1 > x_2 + 2d$ and, as in (45), it depends only on $|x_{12}|$ in this region. Continuing in this way, the value of $G_2{}^*(x_1, x_2)$ can be obtained for all values of x_1 and x_2. The resulting formula for $G_2{}^*(x_1, x_2)$ is the same as that found by SZK. It should be noted that whereas $G_2{}^*(x_1, x_2)$ is continuous for $|x_{12}| > d$, the nth derivative has a simple jump discontinuity at $|x_{12}| = nd$.

4. DISCUSSION

We have shown that the SZK recursion relation (5) exactly reduces the infinite BBGKY hierarchy to a pair of coupled equations for the correlation functions G_1 and G_2. We have proven that the pair of equations has a unique solution for all densities within the symmetry class defined by (28). This symmetry pertains to either a uniform fluid or to a perfect crystal. Since we have shown that the solution is such that $G_1(x_1) = 1$ and $G_2(x_1, x_2) = G_2(|x_1 - x_2|)$ for all positions x_1 and x_2, we conclude that the infinite BBGKY hierarchy, together with the SZK relation, gives the uniform fluid as the unique state of the one-dimensional hard-sphere system.

The uniqueness expresses, in terms of correlation functions, the earlier result of Gursey[4] and van Hove[5] that there can be no phase transition for a one-dimensional system with finite-range forces. The extent to which the SZK recursion relation forced this result is not, at present, known to the authors. We recall that the SZK recursion relation is an exact result,[1] independent of the BBGKY equations.

We conclude with a brief discussion of the uniqueness result in terms of solutions of an approximate BBGKY equation developed in a molecular theory of crystallization.[2,3] In that theory we consider the BBGKY hierarchy truncated at the first equation, namely the equation for G_1 in terms of G_2. By writing

$$G_2(\mathbf{x}_1, \mathbf{x}_2) = G_1(\mathbf{x}_1)G_1(\mathbf{x}_2)g_2(\mathbf{x}_1, \mathbf{x}_2) \quad (48)$$

where $\mathbf{x}_1$ and $\mathbf{x}_2$ may denote multidimensional vectors, and by imposing the constraint that

$$g_2(\mathbf{x}_1, \mathbf{x}_2) = g_2(|\mathbf{x}_1 - \mathbf{x}_2|) \quad (49)$$

where $g_2(|\mathbf{x}_1 - \mathbf{x}_2|)$ is taken to be the known pair correlation function of the uniform fluid, we obtain a closed nonlinear equation. The theory is applied to the hard-sphere system in one, two, and three dimensions, and the existence of solutions for $G_1(\mathbf{x}_1)$ with all the symmetries required of perfect crystals is sought. We prove that the BBGKY equation does in fact have solutions for $G_1(\mathbf{x})$ with long-range order and that these bifurcate from the fluid phase solution, $G_1(\mathbf{x}) = 1$. We show that bifurcation is associated with metastable states and that it does not occur at the equilibrium phase transition. The predicted bifurcation points in two and three dimensions[(2)] are quite consistent with the results of computer simulations. Since the bifurcation occurs in the metastable region, its existence in the one-dimensional hard-sphere system does not necessarily contradict the result that there can be no phase transition. However, the uniqueness result in this paper explicitly shows, in the one-dimensional case at least, that the existence of bifurcation depends on how the BBGKY hierarchy is closed. The validity of truncating the hierarchy for a crystalline phase with (49) has been investigated further[(6)]; using the solutions for G_1, thermodynamic properties have been calculated away from the bifurcation point. These have been compared to computer simulation results for the two- and three-dimensional hard-sphere system and to the exact results for the one-dimensional system.

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