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Toy model for the mean-field theory of hard-sphere liquids

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We investigate a toy model of liquid, based on simplified hypernetted chain equations in very large spatial dimension D. The model does not exhibit a phase transition, but several regimes of behavior when $D\rightarrow\infty$ can be observed in different intervals of the density.

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I. INTRODUCTION

The theory of classical liquids [1,2] recently received an important stimulus from the theory of structural glasses [3–11]. In the pioneering series of papers by Kirkpatrick and Thirumalai [12,13] the possible connection of the structural-glass transition with the spin-glass transition in p-spin models was put forward. The analogy was then developed, e.g., in the problem of minimally correlated sequences, which were shown to possess a glassy behavior without quenched randomness [14,15]. Other examples of systems without disorder that nevertheless exhibit glassy behavior were also found [16–19].

However, it would be desirable to take the analogy with true structural glasses further. One of the difficulties occurring in structural glasses, when compared to spin glasses, comes from the absence of any kind of analytically solvable mean-field model involving particles interacting through a two-particle potential. In the case of a spin glass, the role is played by the fully connected Ising model, which is solvable very easily. The disordered version is the well-known Sherrington-Kirkpatrick model [20], of which the understanding is now very close to complete [21].

There are many mean-field results concerning the *dynamic* glass transition, mainly using mode-coupling equations for the p-spin model, which offer exact results [12,13,22]. For spin models, an approach was developed to connect the dynamic and static properties of the glassy phase of spin Hamiltonians [23,24]. As for the general picture that arises from the one-step replica breaking scheme, it is believed that these spin glasses behave in the same way as structural glasses.

Indeed, the approximations for *static* glass transitions in structural glasses [3–11] confirm this conjecture. The statics of a structural glass is investigated essentially as follows. As a starting point, a variational formulation for the liquid is found and the replica trick is used in order to anticipate the possible multiplicity of pure states. This leads to a formulation in terms of a liquid composed effectively of m-particle bound states, where m is the number of replicas. In the variational formulation, m is an additional parameter to be optimized. The optimization involves finding first the two-particle correlation function for the centers of mass of the m-particle complexes and second the entropy of a single particle moving in the field of the others.

The variational formulation is provided by the hypernetted chain (HNC) approximation, which leads naturally to an effective free energy functional. That is why we also focus on the HNC approach in this paper. The two-particle correlation function is found by solving the HNC equations (appropriately modified in the replica treatment). Unfortunately, this step must be done numerically, because no analytic result is available for the HNC equations.

It would be desirable to obtain an analytical solution for the static properties of a ''mean-field'' liquid. Then the need for numerical solution of the HNC equations would be avoided. However, no results for a mean-field, static, structural glass are known, as far as we know. It even sounds not very reasonable to speak about a mean-field liquid, because the relevant high-density phase is characterized by strong short-range correlations, which can hardly be replaced by an effective medium. So the meaning of the mean field should be better specified. In our investigation, we will understand by ''mean field'' the situation that occurs in very high dimension, $D\rightarrow\infty$. The purpose of the present work is to introduce a simple model of a liquid that is analytically solvable in the limit of infinite dimension, at least in a certain well-defined range of densities.

We do not pretend to be able to fully solve the glass properties of the hard-sphere liquid. We present here a partial step only, consisting in providing an analytical solution for the two-particle correlation function. To complete the picture, it would be necessary to find the entropy of a single hard sphere in the effective m-component liquid. This is a quite different task, requiring other methods. We will not cover the latter problem here.

II. SIMPLIFIED HNC EQUATIONS

We consider a liquid composed of hard spheres with the diameter 1. There is only one independent state variable, which is the spatial density of particles ρ.

The configuration of the liquid is described by the radial pair distribution function $g(r)=h(r)+1$. In the hypernetted chain approximation [25] we have a closed set of equations for the correlation function $h(r)$,

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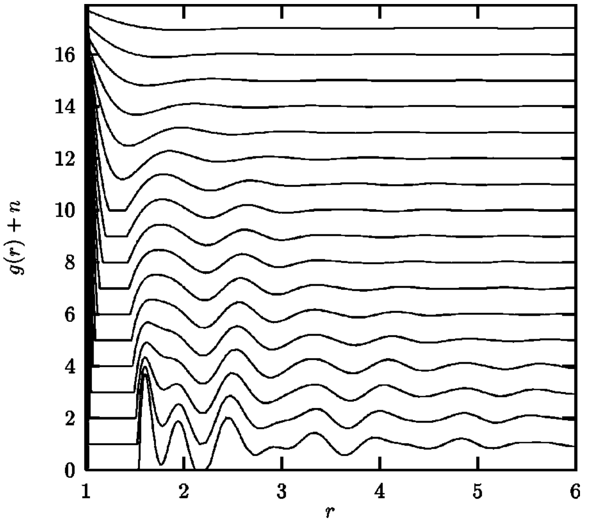

FIG. 1. Pair distribution function $g(r)=h(r)+1$ of the three-dimensional model liquid, for densities (from top to bottom) $\rho=0.6$, 0.7, 0.8, 0.9, 1.00, 1.1, 1.2, 1.23, 1.26, 1.29, 1.32, 1.35, 1.38, 1.41, 1.44, 1.47, 1.5. The *n*th curve from the bottom is shifted upward by *n*.

$$h(r)+1=\exp[W(r)-\beta U(r)], \tag{1}$$

$$\hat{W}(p)=\frac{\rho\hat{h}^2(p)}{1+\rho\hat{h}(p)}.$$

The potential is $U(r)=0$ for $r>1$ and $U(r)=\infty$ for $r<1$. These equations can be interpreted as conditions for minimization of the free energy functional [3]

$$\mathcal{F}[h]=\rho^2\int dr\, r^{D-1}([h(r)+1]\{\ln[h(r)+1]-1+U(r)\}+1)+\frac{1}{(2\pi)^D}\int dp\, p^{D-1}L_3(\rho\hat{h}(p)) \tag{2}$$

with $L_3(x)=-\ln(1+x)+x-x^2/2$. The function $L_3(x)$ has the following behavior: $L_3(x)\to\infty$ for $x\to-1$ and $L_3(x)\simeq-x^3/3$ for $x\ll 1$.

Our main approximation will consist in replacing the function $L_3(x)$ by $L_\infty(x)$, where $L_\infty=\infty$ for $x<-1$ and $L_\infty=0$ otherwise. The motivation for this approximation is that we suppose that the main effect of $L_3(x)$ is to forbid the region where $-\rho\hat{h}(p)>1$. Then minimization of the free energy functional amounts to satisfying the conditions

$$\rho\hat{h}(p)\geqslant-1,$$

$$h(r)\geqslant-1, \tag{3}$$

$$h(r)=-1 \text{ for } r<1,$$

which are in fact the minimum physical requirements for any correlation function $h(r)$. In this sense we are building a ''minimum'' model of a liquid. In addition to the constraints (3) we require that the function $h(r)$ depends continuously on the density. The absence of a solution that is continuous in density would be a signal of a phase transition. This is not found in the present calculations, however.

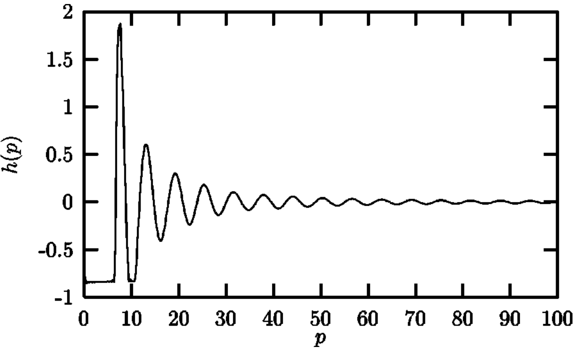

FIG. 2. Fourier transform of the correlation function for a three-dimensional liquid, at the density $\rho=1.2$.

In three dimensions (3D) we can compute the function $h(r)$ numerically by increasing slowly the density ρ and adjusting iteratively the function $h(r)$ so that the conditions (3) are satisfied. The resulting pair distribution function $g(r)=h(r)+1$ is shown in Fig. 1. The Fourier transform $\hat{h}(p)$ for $\rho=1.2$ is shown in Fig. 2.

We can see that for densities up to about $\rho=1$ the pair distribution function agrees qualitatively with the well-known results of the HNC approximation or numerical simulations (see [1]). However, at about $\rho=1.2$ the behavior changes. A gap opens between the principal peak at $r=1$ and the secondary peak at $r\simeq 2$. The gap broadens with increased density and at about $\rho\simeq 1.5$ a second gap occurs around $r\simeq 2.2$. We observed, that further compression leads to the occurrence of a third gap separating the peaks at $r\simeq 1.6$ and $r\simeq 2$. We expect that continued increase of the density will result in an increased number of gaps.

The presence of the gaps is an artifact of the approximation. In reality the values of $g(r)$ will not be strictly zero, but small.

From the value of the radial distribution function at $r=1$ the pressure can be computed [1] and the resulting equation of state is shown in Fig. 3, together with the results obtained by solving the HNC equations (1) and the formula computed in the Percus-Yevick (PY) approximation [1]. We can see that our model behaves qualitatively in the same way as the other approximations, even though quantitative agreement is poor. On the other hand, the equation of state of our

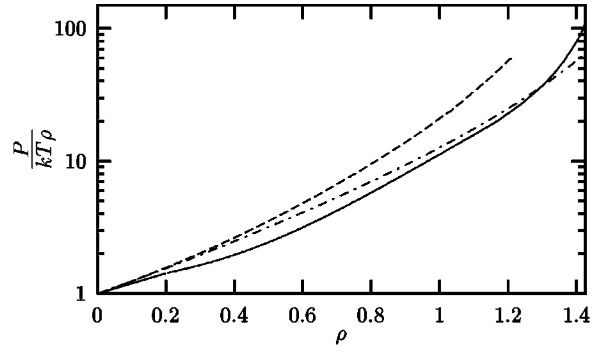

FIG. 3. Equation of state for a three-dimensional liquid. Our model: full line. HNC approximation: dashed line. Percus-Yevick approximation: dash-dotted line.

model does not differ from either the HNC or PY approximation more than these two approximations differ from one another.

We can see from these results that the present approach in 3D gives at least qualitatively sensible results. However, our aim is to provide not a new approximation for real three-dimensional liquids, but a model that describes reasonably well the qualitative features of a liquid and is soluble in the limit of infinite spatial dimension. This will be done in the next section.

III. SOLUTION OF THE MODEL IN HIGH DIMENSION

In this section we will investigate a D-dimensional version of the model, with $D=2N+3$ and $N\to\infty$. While no analytical treatment is available for the HNC approximation, we will see that our scheme yields an analytic result in high dimension.

The main quantity of interest is again the correlation function $h(r)=g(r)-1$. The hard-sphere potential $V(r)=\infty$ for $r<1$ and $V=0$ for $r>1$ implies that $h(r)=-1$ for $r<1$, irrespective of the density. Therefore, we can decompose the correlation function in the form $h(r)=h_0(r)+\overline{h}(r)$ where $h_0(r)=-\theta(1-r)$ and $\overline{h}(r)=0$ for $r<1$.

The pressure is directly related to the value of $h(r)$ at $r=1$, more precisely to $\lim_{r\to 1^+}h(r)=\overline{h}(1^+)$. The formula for pressure in arbitrary dimension reads (see [1])

$$\frac{1}{kT}P=\rho+\frac{1}{2}V_D\rho^2[1+\overline{h}(1^+)]. \tag{4}$$

In the course of the calculations we find that pressure and density occur in combination with the volume of the D-dimensional unit sphere V_D. This leads to the introduction of the rescaled quantity $\overline{\rho}=\rho V_D$ for the density, while for the pressure we use $\overline{P}=V_D P/kT$.

The conditions (3) involve both the function $h(r)$ and its Fourier transform. To find the behavior of $h(r)$ in high dimension D we investigated first the properties of the Fourier transform in the limit $D\to\infty$. A detailed account can be found in Appendix A. The most important formula used throughout this paper is the Fourier transform of the radially symmetric function $f(r)=\theta(1-r)/V_D$. Denoting $N=(D-3)/2$ and rescaling the momentum as $\hat{p}=p/N$ we find that the Fourier transform is $\hat{f}(\hat{p})=\Psi(\hat{p})$, $\Psi(\hat{p})=\Psi_0(\hat{p})=e^{-N\phi_0(\hat{p})}$ for $\hat{p}<1$ and $\hat{f}(\hat{p})=\Psi_1(\hat{p})=e^{-N\phi_1(\hat{p})}\cos N\phi_2(\hat{p})$ for $\hat{p}>1$. Note that $|\Psi(\hat{p})|\leqslant\Psi(0)=1$. The functions ϕ_0, ϕ_1, and ϕ_2 do not depend on N. They are listed explicitly in Appendix A [Eqs. (A9) to (A11)].

In the zeroth approximation we take into account only the hard-sphere potential and not the correlations between particles. Then $h(r)=h_0(r)$ and $\hat{h}(\hat{p})=-V_D\Psi(\hat{p})$, which obeys Eq. (3) as long as $\overline{\rho}<1$. Therefore, for $\overline{\rho}<1$ we have $\overline{h}(r)=0$ and, using Eq. (4), the pressure is given by the first virial correction,

$$\overline{P}=\overline{\rho}+\frac{1}{2}\overline{\rho}^2. \tag{5}$$

For $\overline{\rho}>1$ we should use the decomposition $h(r)=h_0(r)+\overline{h}(r)$. However, there is a nuisance consisting in the discontinuity of $\overline{h}(r)$ at $r=1$. So we modify the decomposition to

$$h(r)=h_0^*(r)+\overline{h}^*(r), \tag{6}$$

where still $\overline{h}^*=\overline{h}(r)$ for $r>1$, but $\overline{h}^*(r)$ is continuous for all r. Hence, for $r>1$ we have $h_0^*(r)=h_0(r)=0$.

To find the Fourier transform of h we proceed first with Fourier-transforming the function h_0^*. At this moment we use an important property of the Fourier transform in very high dimension (see again Appendix A): if a function is zero outside a specific interval and approaches linearly to the upper edge of the interval, then its Fourier transform depends only on the behavior near the upper edge. That is, if the function approaches a nonzero limit at the edge, the Fourier transform depends only on that value. If, on the contrary, the limit is zero, the Fourier transform is determined by the first derivative at the edge. The former case applies to the present situation.

Indeed, we have $h_0^*(r)=0$ for $r>1$ and $h^*(1^-)=-1-A$, where $A=\overline{h}(1^+)=\overline{h}^*(1)$. Then

$$\widehat{h_0^*}(\hat{p})=-(1+A)\,V_D\,\Psi_0(\hat{p}). \tag{7}$$

We will derive an equation determining the value of A later on.

When going from the decomposition $h(r)=h_0(r)+\overline{h}(r)$ to $h(r)=h_0^*(r)+\overline{h}^*(r)$, we did not fix the function $h_0^*(r)$ uniquely: the only thing we required up to now was the continuity of $\overline{h}^*(r)$. Another restriction comes now from the conditions (3), namely, from the inequality $\hat{h}(\hat{p})\geqslant 1/\rho$. This inequality will surely be satisfied, if we set

$$\widehat{\overline{h}^*}(\hat{p})=\theta_1\left((A+1)V_D\,\Psi_0(\hat{p})-\frac{1}{\rho}\right). \tag{8}$$

[We denote $\theta_1(x)=x$ for $x>0$, $\theta_1(x)=0$ for $x\leqslant 0$.] This means that $\widehat{\overline{h}^*}(\hat{p})=0$ for $\hat{p}>\hat{p}_c$, where the value of $\hat{p}_c$ can be obtained by solving the equation

$$\overline{\rho}\,(A+1)\,\Psi_0(\hat{p}_c)=1. \tag{9}$$

Clearly, $\hat{p}_c=0$ for $\overline{\rho}<1$. For $\overline{\rho}>1$ we found it useful to introduce the quantity

$$\rho_1=\frac{\ln\overline{\rho}}{N}. \tag{10}$$

Indeed, one particle occupies space $2^{-D}V_D$, so an absolute upper bound for the density is $\rho_1<\ln 4$.

Let us suppose that $\hat{p}_c<1$. This condition restricts the range of densities investigated to a certain interval, which will be found in what follows. The reason for this restriction consists in the observation that only in the interval $\hat{p}_c<1$ can we ensure, the solution of Eq. (9).

For $\hat{p}<1$ the function $\Psi_0(\hat{p})=\exp[-N\phi_0(\hat{p})]$ is monotonically decreasing and we have the following equation for $\hat{p}_c$:

$$\phi_0(\hat{p}_c)=\rho_1-\frac{\ln(A+1)}{N}. \qquad (11)$$

As we explained above, when computing the inverse Fourier transform of $\widehat{h^*}(\hat{p})$ we need only the behavior close to the point $\hat{p}_c$, which is

$$\widehat{h^*}(\hat{p})\simeq -V_D\,\Psi_0'(\hat{p}_c)\,\hat{p}_c\left(1-\frac{\hat{p}}{\hat{p}_c}\right) \qquad (12)$$

and gives, using Eq. (A15),

$$\hat{h}_1(r)=\left(\frac{N}{2\pi}\right)\frac{V_D^2\,\hat{p}_c^{D+1}[-\Psi_0'(\hat{p}_c)](A+1)}{D+1}\Psi_0(\hat{p}_c r). \qquad (13)$$

Now we can close the equation for the still unknown quantity A,

$$\frac{A}{A+1}=\left(\frac{N}{2\pi}\right)^D\frac{N}{D+1}V_D^2\,\hat{p}_c^{D+1}\phi_0'(\hat{p}_c)\,\Psi_0^2(\hat{p}_c). \qquad (14)$$

The coupled pair of equations (11) and (14) constitute the basis of our approach. Moreover, we will show that for $\hat{p}_c<1$ we can neglect A in the limit $N\to\infty$. Then only a single equation for $\hat{p}_c$ is necessary. A more precise analysis shows that $A\ll 1$ if $p_c<1-O(1/N)$, so if we are closer than a value of order $O(1/N)$ to the point $\hat{p}_c=1$ both Eqs. (11) and (14) should be solved in parallel. We will omit the investigation of this extremely narrow interval here. We should only bear in mind that by writing, for example, $\hat{p}_c<1$ we mean in fact $\hat{p}_c<1-O(1/N)$.

In the interval $\hat{p}_c<1$ we have

$$\phi_0'(\hat{p}_c)=\frac{\hat{p}_c}{1+\sqrt{1-\hat{p}_c^2}}<\hat{p}_c. \qquad (15)$$

Hence, if we suppose that a solution such that $A<1$ exists, we have

$$A\leqslant\left(\frac{N}{2\pi}\right)^D V_D^2\hat{p}_c^{D+2}\Psi_0^2(\hat{p}_c)\simeq\exp[-2NK(\hat{p}_c)], \qquad (16)$$

where

$$K(\hat{p})=\ln(1+\sqrt{1-\hat{p}^2})-\sqrt{1-\hat{p}^2}-\ln\hat{p}. \qquad (17)$$

We have $K(1)=0$ and $K'(\hat{p})=-\sqrt{1-\hat{p}^2}\;/\hat{p}<0$, so $K(\hat{p})>0$ for $\hat{p}<1$. For fixed $\hat{p}_c<1$ and $N\to\infty$ we have $A\ll 1$ and therefore we can neglect A in Eqs. (11) and (14).

The condition $\hat{p}_c<1$ is equivalent to working in the range of densities $\rho_1<\rho_{1c}=\phi_0(1)=1-\ln(2)=0.3068\ldots$. In this region the following equation for $\hat{p}_c$ holds:

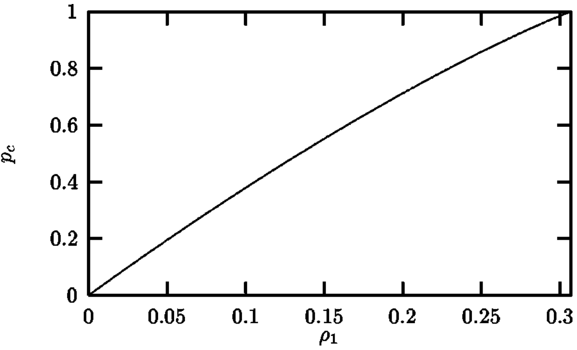

FIG. 4. Dependence of the momentum $\hat{p}_c$ on the rescaled density in the regime $\hat{p}_c<1$.

$$\rho_1=\ln(1+\sqrt{1-\hat{p}_c^2})-\sqrt{1-\hat{p}_c^2}+1-\ln 2. \qquad (18)$$

The solution of this equation can be easily obtained in the form of a power series. We show here only the first several terms (the expansion up to order 16 is given in Appendix B and the graph is shown in Fig. 4):

$$\hat{p}_c^2=4\,\rho_1-2\,\rho_1^2-\frac{2}{3}\rho_1^3-\frac{5}{6}\rho_1^4-O(\rho_1^5). \qquad (19)$$

From the solution of Eq. (18) we can compute the pressure. We write $\overline{P}=\overline{\rho}+\frac{1}{2}\overline{\rho}^2+P_c$ and rescale the correction as $P_c=\exp(NP_1)$. We obtain

$$P_1=2-2\ln 2+\ln\hat{p}_c^2. \qquad (20)$$

We can see that the density $\rho_{1t}=\phi_0(2/\mathrm{e})=0.146\,76\ldots$ separates two regimes. For $\rho_1<\rho_{1t}$ the correction P_c to the lowest virial becomes negligible for large N, while for $\rho_1>\rho_{1t}$ the correction diverges for $N\to\infty$. The graph of the function $P_1(\rho_1)$ is shown in Fig. 5.

For the correlation function in the interval $r<1/\hat{p}_c$ we have $h(r)=\exp[Nh_1(r)]$, where

$$h_1(r)=1-2\ln 2+\ln\hat{p}_c^2-\rho_1+\sqrt{1-\hat{p}_c^2r^2}$$
$$-\ln(1+\sqrt{1-\hat{p}_c^2r^2}). \qquad (21)$$

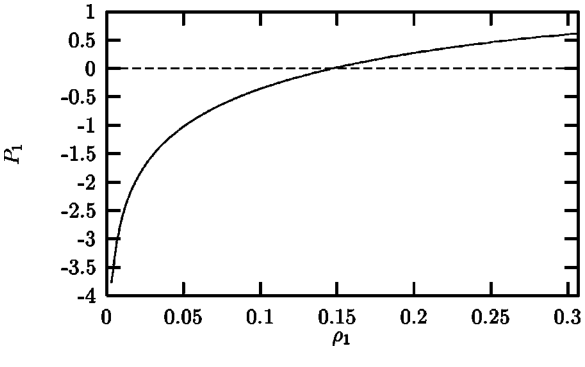

FIG. 5. Equation of state for our model in the limit of infinite dimension, in the range of densities where $\hat{p}_c<1$.

For $r>1/\hat{p}_c$ we can use the following scaling $\hat{h}(r)=\exp[Nh_1(r)]\cos[Nh_2(r)]$ where, using the expressions (A10) and (A11), we obtain

$$h_1(r)=1-2\ln 2+\ln\hat{p}_c-\rho_1-\ln r, \tag{22}$$

$$h_2(r)=\sqrt{\hat{p}_c^2r^2-1}-\arctan\sqrt{\hat{p}_c^2r^2-1}. \tag{23}$$

We can also see that $|h_1(r)|\ll 1$ for $\rho_1<\rho_{1c}$, so that $g(r)>0$ for $r>1$ and the gaps in $g(r)$, discussed in the last section, do not occur. However, when ρ_1 approaches ρ_{1c}, the absolute value of $h_1(r)$ can be of order $O(1)$ and a gap can appear at the density ρ_{1c}. The detailed investigation of this process and the behavior of the model for $\rho_1>\rho_{1c}$ remains an open question.

IV. CONCLUSIONS

We investigated a simple model for a hard-sphere liquid. By numerical solution in three dimensions, we found a qualitatively realistic behavior. The results for the equation of state are compatible with the hypernetted chain and Percus-Yevick approximations. While in three dimensions the difference of the present approach from the HNC and PY approximations is comparable to the difference between HNC and PY themselves, and therefore our approach does not do any better than previous schemes, we consider it clearly superior in high dimension. Indeed, it provides an analytical result, while none is known for the HNC. The PY approximation, solvable exactly in 3D, could perhaps yield an exact result in arbitrary dimension, but, in view of future application in the static glass transition of hard spheres, the PY approach is inconvenient, because it lacks a suitable variational formulation.

We solved the model analytically in the limit of large spatial dimension. We found that two scales of density and pressure appear, which correspond to two regimes of density. For $\overline{\rho}<1$ the equation of state is given by the first virial correction (5), while for $\overline{\rho}>1$ the quantity relevant to further virial corrections is $\rho_1=\ln\overline{\rho}/N$ and the pressure correction itself scales as $P_1=\ln P_c/N$ [Eq .(20)]. We have found the solution in the interval $0<0\rho_1<\rho_{1c}=0.3068\ldots$. Two regimes are present within this interval. For $\rho_1<\rho_{1t}=0.146\,76\ldots$ the correction P_c vanishes for large N, while for $\rho_1<\rho_{1t}$ it diverges for large N. It is expected that the presence of gaps in $g(r)$ will lead to qualitatively different behavior for densities higher than ρ_{1c}.

In order that the present result be useful to the investigation of the static glassy transition, it needs to be accompanied by the analysis of the entropy of a hard sphere surrounded by other hard spheres, distributed according to the correlation function obtained in this work. This second task differs completely in methods used, so we considered it reasonable to treat the two problems separately.

Summarizing, even though we have not completed the analysis of the glass transition in a hard-sphere system, we have achieved a partial step toward the solution.

ACKNOWLEDGMENTS

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APPENDIX A

Here we derive the formula for the Fourier transform in high dimension. The Fourier transform in $D=2N+3$ dimensions is (x and k are D-dimensional vectors)

$$\hat{f}_D(k)=\int d^Dx\,e^{ixk}f_D(x), \tag{A1}$$

$$f_D(x)=(2\pi)^{-D}\int d^Dk\,e^{-ixk}\hat{f}_D(k). \tag{A2}$$

We suppose that the functions depend only on the radial coordinate, $f(r)=f_D(x)$ for $r=|x|$ and $\hat{f}(p)=\hat{f}_D(k)$ for $p=|k|$. After rescaling $\hat{p}=p/N$ we finally have

$$\hat{f}(\hat{p})=C_N\int_0^\infty dr\int_{-1}^1 dz[r^{2(1+1/N)}(1-z^2)e^{i\hat{p}rz}]^N f(r), \tag{A3}$$

where the constant C_N is fixed by the condition that for $f(r)=\theta(1-r)$ we have $\hat{f}(0)=V_D$ with V_D the volume of the D-dimensional sphere,

$$V_D=\frac{2\pi^{D/2}}{D\Gamma(D/2)}\simeq\left(\frac{e\pi}{N}\right)^N. \tag{A4}$$

Similarly, for the inverse Fourier transform we have

$$f(r)=\hat{C}_N\int_0^\infty d\hat{p}\int_{-1}^1 dz[\hat{p}^{2(1+1/N)}(1-z^2)e^{i\hat{p}rz}]^N\hat{f}(\hat{p}) \tag{A5}$$

with coefficient

$$\hat{C}_N=C_N\left(\frac{N}{2\pi}\right)^D. \tag{A6}$$

The calculation of the Fourier transform can be performed by the saddle-point method. The essential result is the Fourier transform of the surface of a unit sphere $f(r)=\delta(r-1)$. We obtain $\hat{f}(\hat{p})\propto\Psi(\hat{p})$ where

$$\Psi(\hat{p})=\Psi_0(\hat{p})=\exp[-N\phi_0(\hat{p})] \tag{A7}$$

for $\hat{p}<1$ and

$$\Psi(\hat{p})=\Psi_1(\hat{p})=\exp[-N\phi_1(\hat{p})]\cos[N\phi_2(\hat{p})] \tag{A8}$$

for $\hat{p}>1$.

The explicit form of the functions ϕ_0,ϕ_1,ϕ_2 is

$$\phi_0(\hat{p})=1-\ln 2+\ln(1+\sqrt{1-\hat{p}^2})-\sqrt{1-\hat{p}^2}, \tag{A9}$$

$$\phi_1(\hat{p})=1-\ln 2+\ln\hat{p}, \tag{A10}$$

$$\phi_2(\hat{p})=\sqrt{\hat{p}^2-1}-\arctan\sqrt{\hat{p}^2-1}. \tag{A11}$$

Note that $\Psi(0)=1$.

From here we can deduce the following Fourier transforms [$\theta(x)=1$ for $x>0$ and $\theta(x)=0$ for $x<0$]. For $f(r)=A\,\theta(r_0-r)$,

$$\hat{f}(\hat{p})=AV_D\,r_0^D\,\Psi(\hat{p}r_0). \tag{A12}$$

For $f(r)=A\,(1-r/r_0)\,\theta(r_0-r)$,

$$\hat{f}(\hat{p})=\frac{AV_D\,r_0^D}{D+1}\Psi_0(\hat{p}r_0). \tag{A13}$$

Because the inverse Fourier transform has the same form and differs only in the factor $\hat{C}_N$ instead of C_N, we can also immediately write for $\hat{f}(\hat{p})=A\,\theta(\hat{p}_c-\hat{p})$

$$f(r)=\left(\frac{N}{2\pi}\right)^D AV_D\,\hat{p}_c^D\,\Psi(\hat{p}_c r) \tag{A14}$$

and for $\hat{f}(\hat{p})=A(1-\hat{p}/\hat{p}_c)\,\theta(\hat{p}_c-\hat{p})$

$$f(r)=\left(\frac{N}{2\pi}\right)^D \frac{AV_D\,\hat{p}_c^D}{D+1}\Psi(\hat{p}_c r). \tag{A15}$$

APPENDIX B

Using *MAPLE V* we get the following expansion for the solution of Eq. (18):

$$\begin{aligned}\hat{p}_c^2={}&4\,\rho_1-2\,\rho_1^2-2/3\,\rho_1^3-5/6\,\rho_1^4-\frac{41}{30}\rho_1^5-\frac{469}{180}\rho_1^6-\frac{6889}{1260}\rho_1^7\\&-\frac{24\,721}{2016}\rho_1^8-\frac{2\,620\,169}{90\,720}\rho_1^9-\frac{64\,074\,901}{907\,200}\rho_1{}^{10}\\&-\frac{1\,775\,623\,081}{9\,979\,200}\rho_1{}^{11}-\frac{1\,571\,135\,527}{3\,421\,440}\rho_1{}^{12}\\&-\frac{1\,882\,140\,936\,521}{1\,556\,755\,200}\rho_1{}^{13}-\frac{70\,552\,399\,533\,589}{21\,794\,572\,800}\rho_1{}^{14}\\&-\frac{2\,874\,543\,652\,787\,689}{326\,918\,592\,000}\rho_1{}^{15}\\&-\frac{25\,296\,960\,472\,510\,609}{1\,046\,139\,494\,400}\rho_1{}^{16}.\end{aligned} \tag{B1}$$

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