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Jastrow wave function for condensed phases of Bose particles: Hard-sphere system

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By a Monte Carlo variational calculation, it is shown that the description of the ground-state properties of a hard-sphere Bose system is improved if the Jastrow wave function contains a correlation structure at distances intermediate between the first and the second shell of neighbors. We relate these correlations to the zero-point motion of rotons. We predict that the oscillations of the structure factor $S(k)$ and of the radial distribution function $g(r)$ increase at finite temperatures. Such intermediate-distance correlations improve the description of the solid phase by a Jastrow wave function, but the description is still not satisfactory compared to localized wave functions. Backflow associated with rotons induces explicit three-particle correlations in the wave function, and a new form for such correlations is proposed for variational calculation for ^{4}He.

I. INTRODUCTION

In recent years our knowledge of the ground-state properties of Bose particles at high density has greatly improved. The most successful approach at high density is based on Monte Carlo simulations of a large but finite number of particles. The ground-state properties of liquid ^{4}He have been rather successfully explained[1] on the basis of variational calculations based on Jastrow trial wave functions:

$$\psi_J(\vec{r}_1,\ldots,\vec{r}_N)=\prod_{i<j}^{1\cdots N}\exp[-\tfrac{1}{2}u(\vec{r}_i-\vec{r}_j)]. \qquad (1)$$

Here $\vec{r}_i$ indicates the coordinate of the ith particle and $u(r)$ is a real function. More recently an algorithm has been invented[2,3] which permits the exact calculation of some properties of more than 100 particles in their ground state by a numerical solution of the Schrödinger equation. The ground-state energy and microscopic correlations, such as the radial distribution function and the one-particle density matrix, have been calculated using both methods for Lennard-Jones particles[2,4,5] and for hard spheres.[3,6] The solid phase of such systems has been similarly studied,[3,6,7] the variational calculation being based on a Hartree-Jastrow (HJ) trial wave function[8]

$$\psi_{\mathrm{HJ}}(\vec{r}_1,\ldots,\vec{r}_N)=\prod_{i=1}^{N}\phi(\vec{r}_i-\vec{R}_i)\times\prod_{i<j}^{1\cdots N}\exp[-\tfrac{1}{2}u(\vec{r}_i-\vec{r}_j)], \qquad (2)$$

where $\phi(r)$ is a localization factor, e.g., $\phi(r)=e^{-Ar^2/2}$, at the prescribed sites $\vec{R}_i$ of the equilibrium lattice.

The possibility of performing exact calculations for a many-body Bose system does not reduce the interest in having a variational wave function as good as possible. Different reasons can be adduced. The structure of the wave function, which is not given by the exact calculation, is of interest in itself and in particular one would like to know how different aspects of the system manifest themselves in ψ_0. The exact calculation requires as a starting point an approximate wave function not too far from the exact one, in particular for calculation of quantities other than the energy. The exact calculation requires a quite elaborate algorithm and rather long computing time so that the simpler variational method is in practice irreplaceable, at least in a first stage, in the study of different problems, for instance the effect of the form of the pair potential on the properties of the system.

On the basis of the previous variational calculations for the Lennard-Jones and the hard-sphere system, three problems, which are most interesting in our view, remain unsettled in the bulk system. The variational results give a less-pronounced short-range order, as shown by the oscillations of the radial distribution function $g(r)$ or of the structure factor $S(q)$, than the one shown experimentally by liquid ^{4}He or by the exact calculation for hard spheres. Secondly ^{4}He at zero pressure forms a bound state at an equilibrium density ρ_{eq}. The variational calculation gives, indeed, a bound state, i.e., the expectation value of the Hamiltonian has a minimum negative value at a certain density. However this density is imposed by suitable boundary conditions and is not obtained as a self-bound-state as in the case of the physical system which forms a drop of liquid if the volume available to the particles is larger than the one corresponding to the density ρ_{eq}. This is because the Jastrow functions which have been used describe a system which fills uniformly any allowed volume, apart from possible surface effects.

The final question concerns the solid phase. This phase has a broken symmetry, the translational invariance of the Hamiltonian. A wave function such as (2) describes explicitly such a broken symmetry by the appearance in ψ_{HJ} of the assumed equilibrium position $\vec{R}_i$ and therefore there is a fixed center of mass. Also the Jastrow wave function (1) can describe a solid phase[4,9] but in this case there is no fixed center of mass and ψ_J describes a floating solid.[10] However, the corresponding energy was found by previous calculations[4,7] to be very much higher than the one corresponding to ψ_{HJ}. The interesting question, also in connection with the possibility of Bose-Einstein condensation in a solid,[9] is if the broken symmetry must appear explicitly in the wave function or if the failure of nonlocalized wave functions to describe the solid phase is due to the fact that the search has been performed on a too-restricted family of Jastrow wave functions. In fact at helium density the only computations that do not rely on uncontrolled approximations are, so far, the ones based on Monte Carlo computation of the configurational integrals[4] or those based on the method of molecular dynamics.[5] These methods are taken from the field of classical liquids because in the Jastrow approximation the averages one has to compute with ψ_J^2 are identical to the ensemble averages of a *classical* fluid at temperature T^* and interacting by a pair potential $U^*(r)$ such that $U^*(r)/k_B T^* = u(r)$. With these numerical methods one needs to parametrize the pseudopotential $u(r)$ and, therefore, one can explore a very restricted family of all possible Jastrow wave functions. Therefore an open question is if the limitations of the Jastrow wave functions described above are due to this restriction or if they are due to the fact that the true wave function has a structure very much different from the one of (1) or from the straightforward generalization obtained by including three- or four-particle correlations in addition to the two-particle term of (1).

There is a method for systematically improving on a given Jastrow wave function: the paired-phonon analysis.[1] We have chosen not to follow this route for a practical reason, because that method involves the computation of matrix elements on the Feynman phonon states and this computation is difficult to perform reliably because three- and four-particle correlations are involved and some uncontrolled approximations have to be introduced. In the second place the paired-phonon analysis gives the best Jastrow wave function in the space spanned by Feynman phonon states, i.e., $\psi_k = \rho_k \psi_0 / \sqrt{\mathfrak{N}_k}$, where ρ_k is the Fourier component of the microscopic density and $\mathfrak{N}_k$ is the normalization constant, and these states form by no means a complete set of functions for particles with hard core so that ψ_0 is either zero or exponentially small when there is core overlap.

We have undertaken a study of the merits of Jastrow wave functions both for hard spheres and for Lennard-Jones particles by Monte Carlo computation for a wider class of ψ_J than previously considered. In previous calculations the pseudopotential $u(r)$ has been chosen as smooth as possible and incorporating at very small distance the behavior of the two-body problem. As a consequence $u(r)$ has been essentially constrained to be a non-negative and monotonically decreasing function of r. Our extension involves the introduction of a negative term in $u(r)$ so that $f(r) = e^{-u(r)/2}$ can overshoot the unity and, moreover, of a repulsive structure centered at an intermediate distance between the first and the second shell of neighbors of a particle. The first term allows the existence of a self-bound-state so that it is considered only for the Lennard-Jones system. The second one is related to the zero-point motion of rotons as discussed in Sec. III and it is considered both for the Lennard-Jones system and for hard spheres.

A different approach[11,12] has also been developed in the variational calculation based on ψ_J. The pseudopotential $u(r)$ is eliminated in favor of the radial distribution function $g(r)$ by means of a closure relation as the Bogoliubov-Born-Green-Kirkwood-Yvon one, as introduced in the theory of classical liquids.[13] In this case $g(r)$ is considered as a variational function and minimization of the energy determines also the pseudopotential. Such calculation[11,12] for liquid ^{4}He produced some structure in $u(r)$ but the reliability of this result remained untested because of the known breakdown in the high-density regime of the closure relation which has been used. In fact the discrepancy between $u(r)$ thus obtained and the smooth one used in numerical calculation[4,5] was presented[12] more as an effect of uncertainty of the theory than as a real difference.

In this paper we study the hard-sphere system. In Sec. II we discuss the numerical method, in Sec. III we present the results for the fluid phase and the solid phase is discussed in Sec. IV. Section V contains a discussion of our results and of some extensions of our work. In a separate paper we present the results for the Lennard-Jones system. Short communications of some of these results have been presented previously.[14-16]

II. COMPUTATIONAL ASPECTS

The expectation value of the Hamiltonian

$$H=-\frac{\hbar^2}{2m}\sum_i \nabla_i^2+\frac{1}{2}\sum_{i\neq j} v(\vec{r}_i-\vec{r}_j) \qquad (3)$$

taken with the Jastrow wave function (1) can be written in terms of the radial distribution function $g(r)$ and the energy per particle reads

$$E_J \equiv \frac{\langle H\rangle}{N}=\frac{\rho}{2}\int d\vec{r}\left(v(r)+\frac{\hbar^2}{4m}\nabla^2 u(r)\right)g(r)\,. \qquad (4)$$

ρ is the average density and $g(r)$ is

$$g(\vec{r}_1-\vec{r}_2)=V^2\left(1-\frac{1}{N}\right)\int d\vec{r}_3\cdots d\vec{r}_N\,\psi_J^2(\vec{r}_1,\ldots,\vec{r}_N)\Big/\int d\vec{r}_1\cdots d\vec{r}_N\,\psi_J^2\,. \qquad (5)$$

For hard spheres of diameter a,

$$v(r)=\begin{cases}\infty\,, & r<a\\ 0\,, & r>a\end{cases} \qquad (6)$$

the interaction term is not present in (4) so that

$$E_J=\frac{\rho\hbar^2}{8m}\int dr\,[\nabla^2 u(r)]g(r)\,. \qquad (7)$$

The computation of the multidimensional integrals in (5) is performed by the usual Metropolis Monte Carlo method.[13,4] We have considered systems of 64 and of 108 particles in a cubic box with the nearest image convention. Averages have been computed with Markovian chains of length from 10^5 to 4×10^5 configurations; after that the first 60 moves per particles starting from the initial configuration have been eliminated from the average. To speed up convergence, we have introduced a limitation on density fluctuations[17]: the box is partitioned in l parts and the moves of the particles are restricted by the condition that the number of particles N_i in each sub-box does not differ by more than Δ from the average value N/l. For 64 particles the typical values we have used are $l=4$ and $\Delta=6$. The value of Δ is chosen so that it is larger than the mean fluctuation expected for a macroscopic system.[17] This eliminates some unlikely configurations (we find that about one configuration out of 10^4 is rejected because of this limitation on density fluctuation) but the expected error is well inside the statistical error and, more important, it does not affect the comparison between similar wave functions. For computational convenience we have discretized all distances on the basis of a grid of about $\frac{1}{200}$ of the repulsive diameter. Typically, the reported result for a given $u(r)$ is the average of different runs, one started from an ordered configuration and others from an aged configuration.

Our computation produces a spherically averaged $g(r)$ for $r<\frac{1}{2}L$, where L is the box side. We have extended[18] $g(r)$ at larger distances by use of the Ornstein-Zernicke relation and of the Percus-Yevick relation $c(r)=-g(r)(e^{u(r)}-1)$ for $r>\frac{1}{2}L$; $c(r)$ is the direct correlation function.[13] The extended $g(r)$ is used to compute the structure factor

$$S(q)=1+\rho\int d\vec{r}\,[g(r)-1]\,e^{i\vec{q}\cdot\vec{r}} \qquad (8)$$

and the tail correction to the energy (4), i.e., the contribution to the integral (4) from distances $r>\frac{1}{2}L$.

In the case of hard spheres the direct evaluation of the contribution to the energy (7) from the region near the hard-sphere diameter a cannot be performed directly because the variance of $g(r)\nabla^2 u(r)$ is not bound at $r=a$. On the other hand the ratio of $g(r)$ and of the two-particle factor $e^{-u(r)}$ is expected[19] to be a smooth function of r. Thus in the interval $a<r<a(1+\delta)$ in the Monte Carlo calculation we compute only $g(r)$ and from $A(r)\equiv g(r)\,e^{u(r)}$ a smoothed A_{sm} is produced. This gives a smoothed radial distribution function $g_{\text{sm}}(r)=A_{\text{sm}}(r)\,e^{-u(r)}$ that is used to compute analytically the contribution to the energy. We use $\delta\simeq 10^{-2}$ and the contribution to the energy from this interval is about 3% of the total.

III. FLUID PHASE

For hard spheres a variational calculation has been performed previously with the Jastrow factor[6]

$$f_0(r)\equiv e^{-u_0(r)/2}=\tanh\left(\frac{(r/a)^m-1}{b^m}\right),\quad r>a$$
$$=0\,,\quad r<a \qquad (9)$$

m and b being variational parameters. We have considered a pseudopotential which, in addition to this short-range term, has a repulsive Gaussian

$$u(r) = u_0(r) + Ae^{-(r-\lambda)^2/\Lambda^2}\,, \tag{10}$$

where A, λ, and Λ are new variational parameters with $\lambda \simeq 2a$: the Gaussian is centered around the position of the first minimum of $g(r)$ (see Fig. 3).

The initial evidence for the presence of this structure in high-density Bose systems has been obtained in our search[14] of a self-bound wave function for Lennard-Jones particles. By this structure we tried to simulate by a two-body term the effect of a Jastrow three-body term $w(\vec{r}_i, \vec{r}_j, \vec{r}_l)$ which had been hypothetized to the present in ψ_0 in order to explain some features of the fluid-solid phase transition[7] and of the behavior of $g(r)$ in the fluid phase.[20] Afterwards we have found[15] a direct physical motivation for the presence of the repulsive peak in (10) as an effect of the zero-point motion of rotons.

Phonons and rotons are elementary excitations of helium and the ground-state wave function ψ_0 is the vacuum of these excitations. This requirement on ψ_0, as far as phonons are concerned, has been considered some time ago[21] and, as a consequence, it was shown that $u(r)$ must contain a long-range term. With rotons one finds two difficulties. The first derives from the fact that we do not have yet a good description[22] of these excitations. If we content ourselves with a qualitative effect we may use the simplest description,[1] i.e., Feynman's description of a roton as a density fluctuation so that the one roton state is

$$\psi_{\vec{k}} = \rho_{\vec{k}}\,\psi_0/[NS(k)]^{1/2}\,,$$

where

$$\rho_{\vec{k}} = \sum_i e^{i\vec{k}\cdot\vec{r}_i} \tag{11}$$

and $S(k)$ is the structure factor (8). The second difficulty derives from the fact that, k^{-1} being of the order of the interparticle distance, the correspondence principle is no more of avail in identifying the position operator $\vec{r}$ with the coordinate in the wave function.[1] In any case if we assume this identification, then the previous calculation[21] for phonons is directly extended with the provision that the phonon energy $\hbar ck$ must be substituted either by the true spectrum $\epsilon(k)$ or by Feynman's expression $\hbar^2k^2/2mS(k)$ for $\epsilon(k)$. The ground state has the Jastrow form (1) and the pseudopotential, which we now call $\nu_0(r)$, is

$$\nu_0(r) = \frac{1}{N}\sum_{\vec{k}}\left(\frac{1}{S(k)} - 1\right)e^{i\vec{k}\cdot\vec{r}} \tag{12}$$

if we use Feynman's expression for $\epsilon(k)$, and

$$\bar{\nu}_0(r) = \frac{1}{N}\sum_{\vec{k}}\left(\frac{2m\epsilon(k)}{\hbar^2k^2} - 1\right)e^{i\vec{k}\cdot\vec{r}} \tag{13}$$

if we choose the use of $\epsilon(k)$. Such a wave function is formally identical[23] to the one of a weak coupling system if $\epsilon(k)$ is the appropriate excitation spectrum.

We have computed these functions using the experimental[24] $S(k)$ and $\epsilon(k)$: ν_0 and $\bar{\nu}_0$ have a similar shape and in Fig. 1 ν_0 is plotted. Equation (12) contains both the effect of zero-point motion of phonons and of rotons. In order to put in evidence the contribution due to rotons we have also plotted

$$\chi(r) = \frac{mc}{\pi^2\rho\hbar}\,\frac{1}{r^2 + k_c^{-2}}\,, \tag{14}$$

the contribution of phonons (m is helium mass, c is the sound velocity). We have used $k_c = 0.5$ Å^{-1} for the phonon cutoff for the purpose of exemplification. The rapid rise of $\nu_0(r)$ at $r \sim \sigma$ is roughly similar to the behavior of the pseudopotential which has been used previously for the Lennard-Jones system. The other feature of $\nu_0(r)$ is a repulsive peak at $r \sim 5.4$ Å $= 2.1\sigma$ ($\sigma = 2.556$ Å is the Lennard-Jones parameter we use) which is due to rotons and this position corresponds to the position of the first minimum of $g(r)$. This calculation concerns liquid helium but roton excitations are expected to be present in any high-density Bose fluid when appreciable short-range order is present as in the case of hard spheres. Due to the approximate character of the Feynman wave function of a roton we cannot take the shape of $\nu_0(r)$ too seriously and we have chosen in (10) a Gaussian to represent the roton structure.

We have performed extensive calculations for hard spheres with the pseudopotential [Eqs. (9) and (10)] at the reduced density $\rho a^3 = 0.200$ which in some sense is near[3] to the equilibrium density of liquid ^{4}He and at the density $\rho a^3 = 0.270$ where the fluid phase is metastable with respect to the

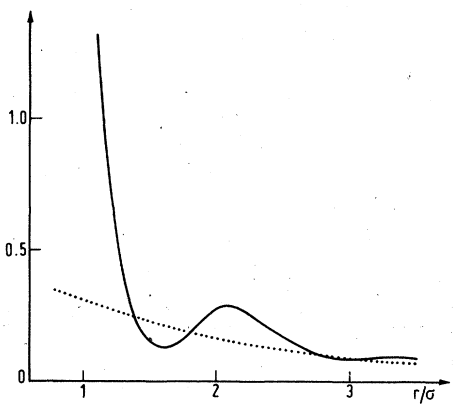

FIG. 1. Jastrow function for phonon-roton model. Full line: $\nu_0(r)$ [Eq. (12)]. Dotted line: $\chi(r)$ [Eq. (14)].

TABLE I. Monte Carlo results at density $\rho a^3 = 0.20$ for 64 particles. Energies in units of $\hbar^2/ma^2$; errors are standard deviations of the averages. $g_{\max}$ and $g_{\min}$ are the values of $g(r)$ at the first maximum and at the first minimum, respectively. $\bar{g}$ is the average of $g(r)$ over the range $a < r < 1.3a$. $S_{\max}$ is the value of $S(k)$ at the first maximum, n is the number of configurations per particle of Monte Carlo run.

A	λ/a	Λ/a	E_J	$g_{\max}$	$g_{\min}$	$\bar{g}$	$S_{\max}$	n
0			6.06 ± 0.03	1.29	0.93	0.351	1.25	6.000
0.05	2.44	0.73	5.92 ± 0.04	1.30	0.93	0.346	1.26	3.000
0.10	2.44	0.73	5.92 ± 0.04	1.30	0.92	0.340	1.28	3.000
0.15	2.44	0.73	6.01 ± 0.03	1.31	0.91	0.341	1.29	6.000
0.20	2.44	0.73	6.08 ± 0.07	1.33	0.91	0.335	1.30	1.500
0.25	2.44	0.73	6.12 ± 0.05	1.32	0.90	0.342	1.31	3.000
0.35	2.44	0.73	6.17 ± 0.03	1.34	0.88	0.337	1.34	4.500
0.15	2.32	0.73	6.03 ± 0.05	1.30	0.91	0.350	1.28	1.500
0.15	2.44	0.61	6.07 ± 0.05	1.32	0.90	0.339	1.30	1.500

solid phase. In Table I and in Fig. 2 the results at the lower density are shown. All energies are expressed in units of $\hbar^2/ma^2$. Errors of E_J are standard deviation of the averages. For the short-range part (9) we have used the values $m = 2$ and $b = 1.2$ determined by Hansen *et al.*[6] With only this short-range part we find good agreement for the energy E_J and for $g(r)$ with the previous result[6] ($E_J = 6.0$). From the position of the first minimum of $g(r)$ we have explored values of λ around $2.45a$ for the repulsive Gaussian (10). We find that E_J is lowered by the presence of the Gaussian (Fig. 2) and the effect is outside the statistical errors. The minimum is obtained for $A \simeq 0.1$ and this intensity roughly corresponds to the one given by rotons (Fig. 1). We have not optimized the choice of λ and Λ but $\lambda = 2.44a$ and $\Lambda = 0.73a$ appear to be close to the optimum. The minimum energy ($E_J = 5.92$) that we find should be compared with the exact value[3] $E_0 = 5.80$ so we conclude that the roton structure is responsible for half of the discrepancy between exact and variational results.

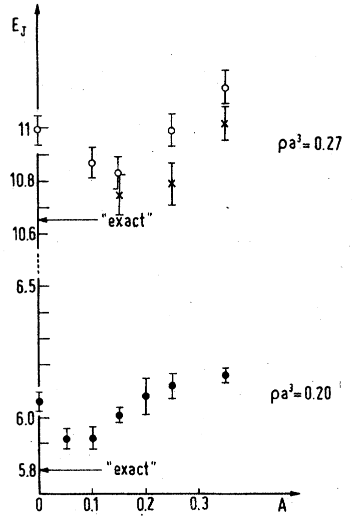

FIG. 2. Variational energy as function of the strength parameter A at density $\rho a^3 = 0.2$ with $\lambda/a = 2.44$ and $\Lambda/a = 0.73$ (••). Results at density $\rho a^3 = 0.27$ with $\lambda/a = 2.21$ and $\Lambda/a = 0.55$ (○○) and with $\lambda/a = 2.38$ and $\Lambda/a = 0.55$ (××). The arrow marked "exact" gives the energy of the exact calculation (Ref. 3).

Let us discuss the origin of the decrease of the energy in presence of the roton structure. If it were not for the presence of $g(r)$ in the expression (4) for E_J the introduction of the Gaussian would not cost any energy since the space integral of $\nabla^2 u(r)$ is zero when $u(r)$ is a regular function everywhere. But the presence in (4) of $g(r)$ makes this contribution positive because the Gaussian enhances the structure of $g(r)$ and $g(r)$ is depressed where $\nabla^2 u(r)$ is negative and vice versa $\nabla^2 u(r)$ is positive where $g(r)$ increases. However the presence of the Gaussian not only enhances the oscillations of $g(r)$ but depresses $g(r)$ near the core $r \sim a$ since the first peak of $g(r)$ becomes sharper. This effect is shown in Table I where we give in addition to the value of $g(r)$ at the first maximum and at the first minimum also the average of $g(r)$ over the range $a < r < 1.3a$. The resulting reduction of the contribution of $u_0(r)$ to the kinetic energy from the region $r \sim a$, where $\nabla^2 u_0(r)$ is largest, more than compensates the direct contribution from the Gaussian.

The main discrepancy between the previous variational $g(r)$ and the exact $g(r)$ consists of the more-pronounced structure of the exact $g(r)$. The presence of the roton structure improves the variational results at all distances as shown in Fig. 3 where the differences $g(r, A = 0.10) - g(r, A = 0)$ and $g(r, A = 0.15) - g(r, 0)$ are plotted as well as

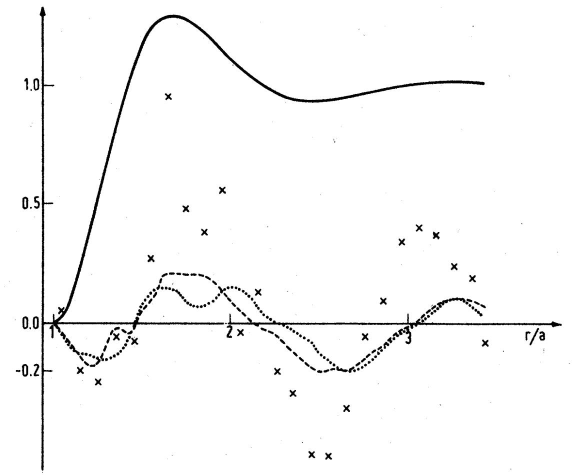

FIG. 3. Radial distribution function of hard spheres at density $\rho a^3 = 0.2$. Full line gives our smoothed variational result for $A = 0$. Dotted and dashed lines give, respectively, $10 \times [g(r, A = 0.1) - g(r, A = 0)]$ and $10 \times [g(r, A = 0.15) - g(r, A = 0)]$. Crosses represent the difference between exact (Ref. 3) and variational (Ref. 3) $g(r)$ multiplied by 10.

the difference between the exact and the previous variational result.[3] For purpose of clarity of the figure our $g(r)$ has been smoothed by a five-point interpolation algorithm. We note that the roton structure enhances also the second maximum of $g(r)$ but does not remove the discrepancy in the position of the third zero of $g(r) - 1$. The reason for this might be due to an inadequacy of the Gaussian to represent the roton structure at large distances and, in fact, $\nu_0(r) - \chi(r)$ is slightly negative (Fig. 1) at distances of order of the second maximum of $g(r)$.

We find similar results at the higher density $\rho a^3 = 0.27$ (Table II and Fig. 2). With the short-range part $u_0(r)$ (with $m = 3$ and $b = 1.2$) we find good agreement with the results of Hansen *et al.*[6] ($E_J = 11.0$). For the repulsive Gaussian we have considered two sets of parameters. The first set,

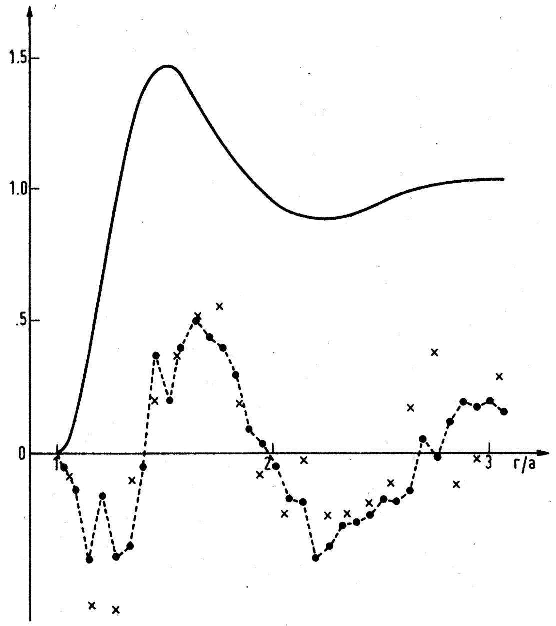

FIG. 4. Radial distribution function at density $\rho a^3 = 0.27$. Full line gives our smoothed variational result for $A = 0$. Dots give $10 \times [g(r, A = 0.15) - g(r, A = 0)]$ with $\lambda/a = 2.21$ and $\Lambda/a = 0.55$. Crosses represent the difference between exact and variational $g(r)$ of the fluid phase (Ref. 3) multiplied by 10.

$\lambda = 2.21$ and $\Lambda = 0.55$, is modeled on $g(r)$ of the liquid metastable phase and the second one, $\lambda = 2.38$ and $\Lambda = 0.55$, on $g(r)$ of the solid phase. Both sets have a minimum at a nonzero value of A with the second set giving a slightly lower minimum. The corresponding $g(r)$ are shown in Fig. 4 together with the results of the exact calculation. The presence of the Gaussian centered at $\lambda = 2.38$ induces fluctuations which make $g(r)$ intermediate between the exact $g(r)$ of the liquid phase and the one of the solid phase.

We conclude that the Jastrow wave function of hard spheres contains a correlation structure at intermediate distances reflecting the zero-point

TABLE II. Monte Carlo results at density $a^3 = 0.27$.

A	λ/a	Λ/a	E_J	$g_{\max}$	$g_{\min}$	$\bar{g}$	$S_{\max}$	n
0			10.99±0.06	1.47	0.89	0.432	1.39	4.000
0.10	2.21	0.55	10.87±0.06	1.49	0.87	0.418	1.43	3.000
0.15	2.21	0.55	10.83±0.06	1.50	0.86	0.408	1.46	3.000
0.25	2.21	0.55	10.99±0.06	1.51	0.84	0.399	1.52	3.000
0.35	2.21	0.55	11.15±0.07	1.53	0.81	0.389	1.56	2.000
0.15	2.13	0.55	10.91±0.08	1.49	0.86	0.424	1.46	1.500
0.15	2.38	0.55	10.75±0.08	1.48	0.86	0.410	1.46	1.500
0.25	2.38	0.55	10.79±0.08	1.50	0.84	0.397	1.50	1.500
0.35	2.38	0.55	11.02±0.07	1.51	0.84	0.389	1.55	2.500

motion of rotons. This structure is density dependent, the strength of the roton feature increasing at higher density.

IV. SOLID PHASE

The solid phase of quantum systems has been generally described by the Hartree-Jastrow wave function (2) containing localization factors, so that the translational broken symmetry is explicitly contained in the wave function. Also a Jastrow wave function ψ_J without localization factors can describe a solid phase.[4] The pseudopotential $u(r)$ is essentially repulsive at short distance, for instance $u(r) = (b/r)^5$ for a Lennard-Jones system, and the fluid-solid transition is similar to that of classical hard spheres.[13] However ψ_J does not give a satisfactory[5] description of the solid phase because the corresponding expectation value of the Hamiltonian is much higher than the value corresponding to ψ_{HJ}. In fact Hansen and Pollock[7] have presented an argument to explain this: in classical systems it is known that the short-range part of the intermolecular potential plays a basic role in freezing but the precise r dependence is not important.[25] For instance, an empirical rule[17] says that a classical fluid freezes when the first maximum of $S(k)$ reaches the value $S_{\max} = 2.85$, the value found at the solidification point of classical hard spheres. On the solid side of the transition melting takes place when the Lindemann ratio f, i.e., the ratio of the rms displacement to the nearest-neighbor distance, is close to the value $f \sim 0.14$. Such rules extended to Jastrow wave functions imply, for instance, that also for quantum systems at the solidification point the maximum of $S(k)$ should have the value 2.85. This is wrong because quantum hard spheres have $S_{\max} \simeq 1.40$ at solidification[3] and ^{4}He has $f \simeq 0.25$ at melting[7] so that some other mechanism for solidification must be present in quantum systems. For this reason it was surmised that the non-Jastrow terms, for instance three-body correlations, must play an important role in Bose systems, at least near solidification.

Our result on the presence of the roton structure in ψ_J makes the simple extension of the freezing rule of classical systems to Jastrow wave functions suspicious because ψ_J contains a structure, absent in classical systems, which is density dependent and directly related to the short-range order present in the system. For this reason we have investigated the transition to the solid phase of quantum hard spheres on the basis of the new Jastrow wave function.

In the first place we must choose the signature of the solid phase of the small system on which we perform the numerical simulation. For classical systems different signatures of the solid phase have been considered but the most precise one, based on comparison of the free energies of the fluid and of the solid phase,[17] cannot be used in the present case. In fact this method would imply the study at different densities of the same Jastrow wave function. If the roton structure directly influences solidification, then we do not necessarily expect that the phase diagram of ψ_J with *fixed* pseudopotential has the simple behavior of the physical systems because a given roton structure helps to stabilize the solid phase only over the small range of densities where the position of the repulsive shoulder (10) corresponds to the position of the minimum of $g(r)$. For this reason we have chosen the simpler but less precise method of determining the phase transition region by looking at the presence of metastability phenomena: with a given Jastrow wave function ψ_J we start two different runs, one from the fcc configuration and the second one from a disordered configuration. If after 3000 moves per particle the two energies have values well outside the average fluctuation we conclude that ψ_J is in the phase transition region.

We have performed calculations at the density $\rho a^3 = 0.27$ which is indicated by the exact calculation[3] to be roughly the melting density of hard spheres. All our calculations are for 108 particles so that the fcc lattice fits in our basic cube. In addition to the pseudopotential (10) we have also considered the more general form

$$u(r) = u_0(r) + A e^{-(r-\lambda)^2/\Lambda^2} - B e^{-(r-\mu)^2/M^2} \qquad (15)$$

with $\mu \sim 3a$ so that $u(r)$ can contain also attractive correlations at a distance of order of the second maximum of $g(r)$. We have performed computations for quite a few choices of the parameters in $u(r)$ and here we present only some typical results.

The short-range order of the system is very sensitive to the presence of the structure in $u(r)$ and with suitable choice of the parameters $g(r)$ can be made almost to coincide with the spherical average of $g(r)$ of the *solid* phase as given by the exact computation. For instance in Fig. 5 the exact solid $g(r)$ is compared with our Jastrow result for the parameters: $m = 3$, $b = 1.2$, $A = 0.55$, $\lambda = 2.38a$, $\Lambda = 0.39a$, and $B = 0$. The corresponding energy is $E_J = 12.1$ which should be compared with the variational results[3] $E_{\mathrm{HJ}} = 10.5$ for the solid wave function (2). Although the short-range order given by this ψ_J is almost identical to the one of the solid phase, this ψ_J describes a fluid because it does not show any evidence of metastability at this or at neighboring densities. Solidification can be obtained only if $u(r)$ contains much stronger

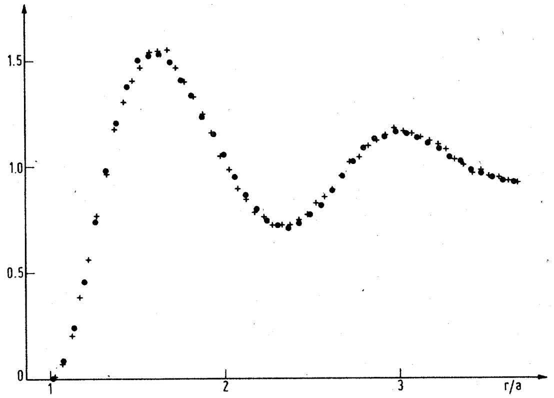

FIG. 5. Exact $g(r)$ at density $\rho a^3=0.27$ for the solid phase (Ref. 3) (+++) and our variational result with $A=0.55$, $\lambda/a=2.38$, and $\lambda/a=0.39$ (···).

structures but in this case the short-range order becomes more pronounced than the exact one and the energy rises too. For instance, metastability is found for the following parameters: $m=3$, $b=1.6$, $A=0.45$, $\lambda=2.1a$, $\Lambda=0.22a$, $B=0.6$, $\mu=3.05a$, and $M=0.22a$. The runs started from a disordered and from the ordered configuration give, respectively, $E_J=47.5$ and $E_J=78.6$. From $g(r)$ of the disordered run we compute the value $S_{\max}=2.0$ of the structure factor at the first maximum, a value intermediate between the values 2.85 mentioned above relative to classical hard spheres and 1.40 of quantum hard spheres at the solidification point.

From such calculations we conclude that the presence of intermediate-distance structures in the pseudopotential improves the description of the solid phase by the Jastrow wave function but ψ_J is still not good enough and we doubt that any modeling of a spherical symmetric pseudopotential $u(r)$ can improve significantly our results. We believe that this is due to the requirement of self-consistency we have put in evidence for the wave function of the fluid phase: the correlations in the wave function depend on the spectrum of elementary excitations of the system but this depends on the short-range order which is present. In a solid the spectrum of excitations, the phonon spectrum, is anisotropic, for instance the maximum of $\epsilon(k)$ in the (100) or equivalent directions in a fcc lattice takes place at a smaller k value than in the (111) direction. In the phase transition region we may think that the solidlike local order induces an anisotropic excitation spectrum and, as a consequence, anisotropic correlations. When the solid phase becomes stable the angular-dependent terms become locked together to the axis of the crystal. Therefore the minimum requirement on a Jastrow wave function for the solid phase is that the pseudopotential $u(\vec r)$ is anisotropic. Since in a fcc lattice the spatial periodicity in the (100) or equivalent directions is larger than in the (111) directions, the basic anisotropy of $u(\vec r)$ should be contained in the parameter λ of the pseudopotential (10) with $\lambda(\vec r)$ increasing in such directions. This wave function displays rotational broken symmetry but it is translational invariant and allows Bose-Einstein condensation. Calculations with such wave functions are feasible because the problem is similar to the one of simulation of a classical fluid composed of anisotropic molecules.

V. CONCLUSION

Our calculations have shown that the wave function of quantum hard spheres in the fluid phase is better described by a Jastrow wave function which has a repulsive structure in the pseudopotential at intermediate distances. This structure has been related to the zero-point motion of rotons. Rotons are expected to exist in any high-density Bose fluid of particles with hard core so that such structure is expected to be present in the wave function of any Bose fluid and, in particular, of ^{4}He; this conclusion has been confirmed by our calculation.[14,26] The roton structure removes roughly half of the discrepancy on the energy and on the radial distribution function $g(r)$ between previous variational calculations and the exact results for hard spheres.

An important consequence[16] of the presence of the roton structure in the ground state is that the short-range order in a Bose fluid should increase as the temperature increases at least as long as rotons can be considered elementary excitations of the system. In fact, one can take into account thermal excitation of rotons by constructing the density matrix.[21] The radial distribution function is determined by the diagonal part of the density matrix which has the Jastrow form (1) with a temperature-dependent $u(r)$. For instance, in place of expression (12) for $\nu_0(r)$ one obtains

$$\nu_T(r)=\frac{1}{N}\sum_{\vec k}\left(\frac{\tanh(\epsilon_k/2K_BT)}{S(k)}-1\right)e^{i\vec k\cdot\vec r}\,. \tag{16}$$

This thermal population factor produces an enhancement of the roton peak of $\nu_T(r)$ and, therefore, the oscillations of $g(r)$ and of $S(k)$ increase. Such behavior has been observed in liquid helium[27] and has been interpreted successfully in this way.[16]

We have interpreted the structure in the pseudopotential as an effect of the zero-point motion of rotons and this has been based on Feynman form of the wave function of the roton excited state. It is well known[1] that this form is quite rough because it does not take into account interparticle correlations, the so-called backflow. These correlations are included, for instance, in the Feynman-Cohen (FC) wave function[28]:

$$\psi_{\vec{k}} = F_{\vec{k}}\psi_0, \tag{17}$$

$$F_{\vec{k}} = \frac{1}{(N\mathfrak{N}_k)^{1/2}}\sum_j e^{i\vec{k}\cdot\vec{r}_j}\left(1 + i\sum_l{}' g_{\vec{k}}(\vec{r}_{jl})\right), \tag{18}$$

where ψ_0 is the ground-state wave function, $\mathfrak{N}_k$ is the normalization constant, the prime in the l summation indicates that $l \neq j$ and $g_{\vec{k}}$ is

$$g_{\vec{k}}(\vec{r}) = A_k \vec{k}\cdot\vec{r}/r^3, \tag{19}$$

A_k being a variational parameter. The Feynman form is recovered when $A_k = 0$. We should ask which is the effect of the backflow on the ground state. If we boldly proceed as in Sec. III with the Feynman form, i.e., we assume that F_k has the role of the coordinate of a normal mode, then the ground state contains the factor

$$\phi = e^{-(1/4)\Sigma_{\vec{k}}|F_{\vec{k}}|^2} \tag{20}$$

which gives rise to two-, three-, and four-particle correlation terms. The terms of second order in the backflow parameter A_k are rather small and for simplicity we do not write them here. Then (20) contains only two- and three- particle terms:

$$\phi = \exp\left(-\frac{1}{2}\sum_{i<j}\nu_{\rm FC}(\vec{r}_i - \vec{r}_j) - \frac{1}{2}\sum_{i<j<l}\nu_{\rm FC}^{(3)}(\vec{r}_i, \vec{r}_j, \vec{r}_l)\right), \tag{21}$$

$$\nu_{\rm FC}(r) = \lambda(r) + (2/r^2)\mu'(r), \tag{22}$$

$$\begin{aligned}\nu_{\rm FC}^{(3)}(\vec{r}_i, \vec{r}_j, \vec{r}_l) = {} & 2\left(\frac{\mu'(r_{ij})}{r_{il}^2} + \frac{\mu'(r_{il})}{r_{ij}^2}\right)\cos\theta_i \\ & + 2\left(\frac{\mu'(r_{ji})}{r_{jl}^2} + \frac{\mu'(r_{jl})}{r_{ji}^2}\right)\cos\theta_j \\ & + 2\left(\frac{\mu'(r_{lj})}{r_{li}^2} + \frac{\mu'(r_{li})}{r_{lj}^2}\right)\cos\theta_l,\end{aligned} \tag{23}$$

where θ_i is the angle corresponding to the i vertex of the triangle determined by $\vec{r}_i$, $\vec{r}_j$, and $\vec{r}_l$ and similarly for θ_j and θ_l, λ and μ read

$$\lambda(r) = \frac{1}{N}\sum_{\vec{k}}\frac{1}{\mathfrak{N}_k}e^{i\vec{k}\cdot\vec{r}}, \tag{24}$$

$$\mu(r) = \frac{1}{N}\sum_{\vec{k}}\frac{A_k}{\mathfrak{N}_k}e^{i\vec{k}\cdot\vec{r}}, \tag{25}$$

and $\mu'(r) = d\mu(r)/dr$. The normalization factor $\mathfrak{N}_k$ is

$$\mathfrak{N}_k = S(k) + kA_k I_9(k) + k^2A^2 I_{10}(k), \tag{26}$$

where I_9 and I_{10} are three- and four-particle integrals which have been evaluated for ^{4}He by Feynman-Cohen and more recently by Padmore and Chester[29] and there one can also find the values of A_k.

From these data one can determine $\lambda(r)$ and $\mu(r)$ but for our purpose a qualitative description is enough. The k dependence of $\mathfrak{N}_k$ is similar to the one of the structure factor $S(k)$ but the first maximum is more pronounced by roughly 50%. Therefore $\lambda(r)$ has the same behavior as $\nu(r)$, Eq. (12), but with an enhanced structure at $r \sim 2\sigma$ (see Fig. 1). A_k is negative and has a minimum roughly in correspondence to the first minimum of $S(k)$; as a result $A_k/\mathfrak{N}_k$ has almost the same behavior as $S^{-1}(k)$ in the roton region and we can take $\mu(r) \sim -A_{\rm rot}\nu_0(r)$. $A_{\rm rot}$ is the value of A_k at the roton minimum. Therefore $\mu'(r)$ is large and positive at short distances, has a negative minimum at $r \sim 1.6\sigma$ and a positive maximum at $r \sim 2.6\sigma$. In conclusion our computation gives the two-particle term $\nu_{\rm FC}$, Eq. (22), with the same features of the Feynman form ν_0, Eq. (12). The three-particle term (23) has a negative minimum for equilateral configurations with the interparticle distance slightly larger than the position of the first maximum of $g(r)$ of the fluid. This is shown in Fig. 6 where we plot $\nu_{\rm FC}^{(3)}$ for the equilateral configuration as function of the interparticle distance. Since we are interested only in distances of order of nn distance or larger, in drawing the figure we have neglected the short-distance repulsive part of $\mu(r)$ and we have taken

$$\mu(r) = -(0.15/4\pi\rho)\exp[-(r-\lambda)^2/\Lambda^2]$$

with the values $\lambda = 2\sigma$ and $\Lambda = 0.6\sigma$ modeled on our variational results for the Lennard-Jones system[26] and we have taken into account that at the roton minimum $A_k \sim -1/4\pi\rho$.

We conclude that the roton backflow induces three-particle correlations which favor equilateral configurations as found in the solid phase. The presence of such correlations has been suggested

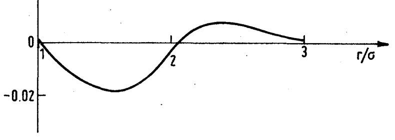

FIG. 6. $\nu_{FC}^{(3)}(r,r,r)$ as a function for r for the choice of $\mu(r)$ discussed in the text. It includes also the second-order contribution in addition to the first-order one [Eq. (23)].

before[7,20] on the basis of the observed discrepancies between variational and experimental data. Our result is in agreement with that suggestion and gives to it a microscopic interpretation. The presence of such three-particle correlations should be confirmed by a variational calculation based on the wave function

$$\psi(\vec{r}_i \cdots \vec{r}_N) = \prod_{i<j} \exp[-\tfrac{1}{2}u(\vec{r}_i - \vec{r}_j)] \times \prod_{i<j<l} \exp[-\tfrac{1}{2} w(\vec{r}_i, \vec{r}_j, \vec{r}_l)] \tag{27}$$

with the three-particle pseudopotential w modeled on the Feynman-Cohen form (23). We note that form (23) differs qualitatively from a form suggested[30] on the basis of the results of the weak coupling system.

The present results for hard spheres and the similar results that we find for the Lennard-Jones system[26] concern Bose systems with strongly repulsive core and, as already discussed, we believe that a roton feature is present in the ground state of any such system at high density. Recently some interest has risen on soft-core systems, as a rough guide on the properties of neutron matter. Variational and exact calculations[31] have been performed for Bose systems interacting with the Yukawa potential and also in this case the Jastrow function gives, near the solidification line, much less short-range order than the exact calculation. The elementary excitations of such systems are not known but it is found that the computed short-range order can be as large as the one of liquid ^{4}He and therefore we expect a phonon-roton spectrum to be present also in this case. Actually the Feynman excitation spectrum $\epsilon(k) = \hbar^2 k^2/2mS(k)$ has in this case an even more-pronounced structure because the maximum of $S(k)$ is located at a smaller k value ($k\sigma \simeq 3$) than in ^{4}He ($k\sigma \simeq 5$). For this reason we expect that the roton structure is present also in the ground state of such a soft-core system and we have in progress such calculation.

Our calculations indicate that no Jastrow wave function with spherically symmetric pseudopotential is satisfactory for the solid phase of Bose particles. The relation between pseudopotential and excitation spectrum suggests the investigation of the Jastrow wave function with an angular-dependent pseudopotential as a wave function of the solid phase.

Also in liquid ^{3}He the short-range correlations[24] determined experimentally are more pronounced than the theoretical prediction[5] obtained on the basis of a wave-function product of a Slater determinant and of a Jastrow term. This suggests that also in this case the Jastrow term contains a rotonlike structure. Really no roton excitation is expected in ^{3}He because of the presence of the particle-hole continuum but some effect of short-range correlations can be expected on the excitation spectrum, for instance, as a k dependence of the effective mass. The experimental situation in this respect is not definite yet. A variational calculation to test the presence of a rotonlike structure in the ground state of ^{3}He should give useful information.

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