Shadow wave function for many-boson systems

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(Received 8 February 1988)

Some properties of a new class of variational wave functions for boson systems are studied. This study extends the Jastrow class, and many-body correlations are implicitly introduced by a coupling of the particle coordinates to subsidiary shadow variables. We prove that the new wave function has Bose-Einstein condensation both in the liquid and in the solid phase. The maximum-overlap criterion for this wave function with the exact ground state is developed. The kind of Jastrow correlations implicitly contained in the new wave function is studied and we formulate a theory of correlations based on the reference interaction site model.

I. INTRODUCTION

The variational theory of the ground state of many-boson systems based on the Jastrow trial wave function (WF) and on its generalizations has had great success[1] when we compare its results with the properties of ^{4}He or with the results of exact simulations. Still some fundamental aspects escape our understanding. The outstanding problem is the freezing process and how the equilibrium positions in a highly quantum system develop. Until now these equilibrium positions had to be assumed *a priori* and inserted in the WF in an *ad hoc* way. It is true that in this way we can compute rather accurately the liquid-solid transition in ^{4}He, for instance, but we would like to see these equilibrium positions emerging in a dynamical way from a translational invariant WF. This is not only for a question of principle but also because it would open the possibility of detailed studies of disorder phenomena in quantum solids.

Recently[2] a shadow WF has been introduced which has, in addition to a Jastrow term, a factor in which the correlations between the particles are mediated by subsidiary variables, the shadows. We write this function in the following form:

$$\psi_S(\mathbf{r}_1 \cdots \mathbf{r}_N) = \exp{-\frac{1}{2}\left[\sum_{i<j} u(r_{ij})\right]} S(\mathbf{r}_1 \ldots \mathbf{r}_N)/Q_N^{1/2} , \quad (1)$$

$$S(\mathbf{r}_1 \ldots \mathbf{r}_N) = \int d\xi_1 \ldots d\xi_N$$
$$\times \exp{-\left[\sum_{i<j} w(\xi_{ij})\right]} \prod_k \chi(|\mathbf{r}_k - \xi_k|) , \quad (2)$$

where $\chi(r)$ is a normalized function of finite range and Q_N is the normalization constant. Clearly the shadow variables $\{\xi_i\}$ induce some extra correlations between the $\{r_i\}$ and this can be considered a way of introducing Jastrow terms of higher order as implied by the cluster expansion of $\ln S(\mathbf{r}_1 \cdots \mathbf{r}_N)$.

The physical basis of why (2) should be a good repre-

sentation of these higher-order terms can be obtained by considering the discretized path-integral representation[3] of the density matrix and the isomorphism between a Jastrow function and the Boltzmann factor of classical particles. When $S \equiv 1$ in (1) we have the standard Jastrow function and $u(r_{ij})$ represents the complete direct action between particles i and j. $u(r)$ has exactly the same role as the pair potential energy divided by $k_B T$ in a classical system. However, in the path-integral representation, to each variable $\mathbf{r}_i$ a sequence of positions $\mathbf{r}_i^{(\mu)}$ is associated so that each particle[4] is represented by a kind of "polymer" and $\mathbf{r}_i^{(\mu)}$ are the positions of the "monomers." Therefore, the actual position $\mathbf{r}_i$ of a particle implies the virtual presence in its neighborhood of the remaining part of the "polymer" and clearly this will induce additional correlations between the particles which cannot be reduced to the Jastrow form. When the density is large the important configurations of the "polymers" presumably are rather compact and in fact from path-integral computations[5]; it is found that the distribution of the "monomers" around the center of mass of this "polymer" is Gaussian-like and the correlations between different centers of mass are very much classical-like. From this picture the shadow WF (1,2) naturally emerges with ξ_i having the role of the centers of mass and χ representing the probability distribution of a "monomer," i.e., of the real particle, around this center of mass.

Monte Carlo computations with this new WF have already been performed[2] and it has been shown that ψ_S can satisfactorily describe both the liquid and the solid phase. This is the first realistic translationally invariant wave function of a quantum solid. Which phase is stable depends on the values of the parameters contained in u, w, and χ. In this paper we consider some aspects of this shadow WF. In Sec. II we discuss the presence of a Bose-Einstein condensate. In Sec. III we consider the criterion of maximum overlap for ψ_S and we obtain the Jastrow WF which has the maximum overlap with ψ_S of Ref. 2. In Sec. IV we formulate a theory of correlations for ψ_S in the fluid phase on the basis of an analogy with the problem of a classical system of triatomic molecules. Section V contains some additional considerations on the shadow wave function.

II. BOSE-EINSTEIN CONDENSATION

A Jastrow WF always has Bose-Einstein condensation (BEC) if $u(r)$ vanishes at large distance.[6] Here we extend the proof to the case of the shadow WF. The density of particles in the condensate $n_0 = N_0/V$ can be written[6] in the form

$$n_0 = \lim_{N,V \to \infty} \frac{\rho}{V} \frac{\mathcal{Q}_{N+1}}{\mathcal{Q}_N} , \tag{3}$$

where $\rho = N/V$ and $\mathcal{Q}_N$ is the normalization constant

$$Q_N = \int dR_N d\Xi_N d\Xi'_N \prod_k \chi(|\mathbf{r}_k - \xi_k|) \prod_l \chi(|\mathbf{r}_l - \xi'_l|) \exp\left[-\sum_{i<j} [u(r_{ij}) + w(\xi_{ij}) + w(\xi'_{ij})] \right] , \tag{4}$$

where $dR_N = d\mathbf{r}_1 \ldots d\mathbf{r}_N$ and $d\Xi_N = d\xi_1 \ldots d\xi_N$. The term $\mathcal{Q}_{N+1}$ derives from the spatial integration of the off-diagonal single-particle density matrix and it reads

$$\mathcal{Q}_{N+1} = Q_N \int dR_{N+1} \psi_S(\mathbf{r}_1, \mathbf{r}_3, \ldots, \mathbf{r}_{N+1}) \psi_S(\mathbf{r}_2, \mathbf{r}_3, \ldots, \mathbf{r}_{N+1}) . \tag{5}$$

In (5) each particle from 3 to $N+1$ has two shadow variables but particles 1 and 2 have only one. In order to have a more symmetrical form we can introduce two additional shadow variables bonded to particles 1 and 2 without changing the value of Q since $\chi(r)$ is normalized. Then we get

$$\mathcal{Q}_{N+1} = \int dR_{N+1} d\Xi_{N+1} d\Xi'_{N+1} \prod_k \chi(|\mathbf{r}_k - \xi_k|) \prod_l \chi(|\mathbf{r}_l - \xi_l|) \exp\left[-\sum_{i<j} u(r_{ij}) \right]$$

$$\times \exp\left[u(r_{12}) + \tfrac{1}{2} \sum_{i=3}^{N+1} [u(r_{1i}) + u(r_{2i})] \right] \exp\left[-\sum_{\substack{i<j \\ i\neq 2}} w(\xi_{ij}) - \sum_{\substack{i<j \\ i\neq 1}} w(\xi'_{ij}) \right] . \tag{6}$$

Let us assume that the WF is short range, i.e., positive constants A, b, ϵ and A', b', ϵ' exist, such that

$$|u(r)| < Ar^{-3-\epsilon} \text{ for } r > b$$

and

$$|w(\xi)| < A'\xi^{-3-\epsilon} \text{ for } \xi > b' . \tag{7}$$

In addition we assume that $u(r)$ and $w(\xi)$ have a hard core:

$$u(r) = \infty \text{ for } r \leq a$$

and

$$w(\xi) = \infty \text{ for } \xi \leq a' . \tag{8}$$

Under these conditions[6] two positive constants exist, which we call ϕ and ϕ', such that

$$\sum_{i=1}^{t} u(\mathbf{r}_i - \mathbf{s}) \geq -\phi, \quad \sum_{i=1}^{t} w(\xi_i - \mathbf{s}) \geq -\phi' \tag{9}$$

for all $t, \mathbf{s}, \mathbf{r}_1 \ldots \mathbf{r}_t, \xi_1 \ldots \xi_t$ satisfying, respectively,

$$\sum_{\substack{i,j \\ i<j\leq t}} u(r_{ij}) < \infty \text{ and } \sum_{\substack{i,j \\ i<j\leq t}} w(\xi_{ij}) < \infty . \tag{10}$$

In view of (9) we can get a lower bound for $\mathcal{Q}_{N+1}$ by replacing the second exponential term in (6) by $e^{-\phi-\Delta}$ where

$$\Delta = -\min_r [u(r)] . \tag{11}$$

In addition, from the second of (9) we have

$$\exp\left[-\phi' - \sum_{i=1,3,\ldots,N+1} w(\xi_i - \xi_2) \right] < 1 , \tag{12}$$

$$\exp\left[-\phi' - \sum_{i=2,3,\ldots,N+1} w(\xi_i - \xi_1) \right] < 1 , \tag{13}$$

so that a new lower bound for $\mathcal{Q}_{N+1}$ is obtained by multiplying the integrand of (6) with the two exponential factors in (12) and (13). Thus, we finally get,

$$\mathcal{Q}_{N+1} > e^{-\phi-2\phi'-\Delta} \int dR_{N+1} d\Xi_{N+1} d\Xi'_{N+1} \prod_k \chi(|\mathbf{r}_k - \xi_k|) \prod_l \chi(|\mathbf{r}_l - \xi'_k|) \exp\left[-\sum_{\substack{i,j \\ i<j}} [u(r_{ij}) + w(\xi_{ij}) + w(\xi'_{ij})] \right]$$

$$= e^{-\phi-2\phi'-\Delta} \mathcal{Q}_{N+1} \tag{14}$$

and we can write the inequality

$$n_0 > \frac{\rho^2}{z} e^{-\phi-2\phi'-\Delta} \tag{15}$$

for the BEC. Here z, given by

$$z = \lim_{N,V \to \infty} [(N+1)Q_N/\mathcal{Q}_{N+1}] , \tag{16}$$

is formally equal to the molecular activity of a suitable system of classical particles. In fact, let us consider a system of classical triatomic molecules formed by a central

particle to which two shadow particles, let us call them red and blue, are bonded. In the isolated molecule the distribution probability of each shadow around the central particle is taken to be $X(z)$ and these two shadows do not have any mutual interaction. The intermolecular interaction divided by temperature consists of a particle-particle interaction $u(r)$ and of an interaction $w(\xi)$ between shadows of the same color. No interaction between particle-shadow and shadow-shadow of different colors is present. This represents a well-defined system of flexible molecules, Q_N is its partition function and z is the molecular activity. Conditions (7) and (8) are sufficient for the existence of a thermodynamic limit and $z < \infty$ for densities for which there is no overlap of the cores. Notice that the hard-core diameters a and a' in (8) are finite but otherwise as small as we like. Therefore, this condition places only a very small restriction and we conclude that short-range shadow wave functions possess BEC.

The true WF has a long-range component due to the zero-point motion of phonons.[7] Thus $u(r)$ has a long range r^{-2} tail and the previous proof does not apply. However, we can carry over the trick used for a pure Jastrow function[6] in the present case and reach the same conclusion: the shadow wave function has BEC also when it contains the long-range phonon contribution. Here we have considered a three-dimensional system. The conclusion remains true in two dimensions when the phonon part decays like r^{-1} but not in one dimension where the phonon part has the range of the size of the system.[7]

Since the shadow WF describes either a liquid or a solid depending on the choice of $u(r)$ and $w(\xi)$, the solid phase described by ψ_S has BEC. n_0 vanishes only if $w(\xi)$ is such that the shadows are completely localized. $w(\xi)$ is not necessarily a continuous function (see Sec. IV), and in particular, it could be the hard-sphere function: $w(\xi) = \infty$ for $\xi < a'$, $w(\xi) = 0$ for $\xi > a'$. If the diameter a' is such that the shadows are in contact, i.e., $na'^3 = \sqrt{2}$, $z = \infty$ since there is no space to accommodate an additional molecule and $Q_{N+1} = 0$. In this case the shadows form a perfect static lattice and ψ_s coincides with the standard Jastrow-Slater form for the solid phase with localization factors, apart from a trivial integration over the center of mass of the crystal.

III. MAXIMUM OVERLAP FOR SHADOW WAVE FUNCTIONS

Maximization of the overlap integral between the exact ground state of the system and a trial wave function gives rise[8] to a variational principle distinct from the common one based on the expectation value of the Hamiltonian. The maximum overlap principle for Jastrow-like functions leads to some equality between suitable correlation functions and this criterion has found[9] some useful applications. Therefore it is interesting to extend this principle to the shadow WF.

Let $\psi_0(\mathbf{r}_1 \ldots \mathbf{r}_N)$ be the exact ground state of the system and consider the family of shadow functions $\psi_S(\mathbf{r}_1 \ldots \mathbf{r}_N \mid u,w,X)$. The overlap integral

$$\langle \psi_S \mid \psi_0 \rangle = \int dR_N \, d\Xi_N \psi_0(\mathbf{r}_1 \ldots \mathbf{r}_N) P(\mathbf{r}_1 \ldots \mathbf{r}_N, \xi_1 \ldots \xi_N)/Q_N^{1/2} , \tag{17}$$

$$P(\mathbf{r}_1 \ldots \mathbf{r}_N, \xi_1 \ldots \xi_N) = \prod_k X(\mid \mathbf{r}_k - \xi_k \mid) \exp\left[-\sum_{\substack{i,j \\ i<j}} \left[\tfrac{1}{2}u(r_{ij}) + w(\xi_{ij})\right]\right] \tag{18}$$

is a functional of u, w, and X. Minimization of $\langle \psi_S \mid \psi_0 \rangle$ with respect to these functions is a straightforward extension of the computation given in detail in Ref. 8 for a Jastrow function and we give only the final result. We find that $\langle \psi_S \mid \psi_0 \rangle$ is maximum for the functions $\bar{u}$, $\bar{w}$, and $\bar{X}$ such that the following equalities between correlation functions are satisfied:

$$n_{PP}^{(mxd)}(\mathbf{r}_1,\mathbf{r}_2 \mid \bar{u},\bar{w},\bar{X}) = n_{PP}^{(S)}(\mathbf{r}_1,\mathbf{r}_2 \mid \bar{u},\bar{w},\bar{X}) , \tag{19}$$

$$n_{SS}^{(mxd)}(\xi_1,\xi_2 \mid \bar{u},\bar{w},\bar{X}) = n_{SS}^{(S)}(\xi_1,\xi_2 \mid \bar{u},\bar{w},\bar{X}) , \tag{20}$$

$$s_{PS}^{(mxd)}(\mathbf{r},\xi \mid \bar{u},\bar{w},\bar{X}) = s_{PS}^{(S)}(\mathbf{r},\xi \mid \bar{u},\bar{w},\bar{X}) , \tag{21}$$

where $n_{PP}(\mathbf{r}_1,\mathbf{r}_2)$ is the two-body interparticle distribution function, i.e., the probability density of finding one particle in $\mathbf{r}_1$ and another in $\mathbf{r}_2$ and $n_{SS}(\xi_1,\xi_2)$ is the analogous intershadow distribution function for shadows of the same color. s_{PS} is the *intra*molecular particle-shadow correlation function. The index (S) means correlation functions computed with respect to the weight $P(R_N,\Xi_N)P(R_N,\Xi'_N)$ whereas (mxd) denotes a mixed average, i.e., average taken with respect to the weight $\psi_0(R_N)P(R_N,\Xi_N)$ suitably normalized. The mixed aver-

ages are exactly the ones computed[1] in a Green's-function Monte Carlo (GFMC) computation when ψ_S is used as importance sampling function.

ψ_S contains both direct calculations of a Jastrow kind between the particles given by the pseudopotential $u(r)$ in (1) and indirect ones mediated by the shadows. Part of these correlations are still of the Jastrow kind but in general also non-Jastrow terms are present. It is interesting to ask which is their best representation in terms of a Jastrow function. To this end we can apply the maximum overlap principle to $\langle \psi_J(u') \mid \psi_S \rangle$ considered as functional of the Jastrow pseudopotential u' for fixed ψ_S. This gives the condition

$$g^{(mxd)}(r \mid u') = g^{(J)}(r \mid u') , \tag{22}$$

where we have assumed that the system is in the fluid phase so that the correlation functions depend only on the modulus of the interparticle distance and here we have used the radial distribution function (RDF): $n(r) = \rho^2 g(r)$. Now (mxd) indicates a mixed average with respect to $\psi_J \psi_S$. If $\psi_J - \psi_S$ can be considered as a small perturbation with respect to ψ_S one finds to linear order

in this difference that $g_{PP}^{(S)}=2g^{(mxd)}-g^{(J)}$ so that the maximum overlap condition becomes

$$g_{PP}^{(S)}(r)=g^{(J)}(r\mid u')\ ,\qquad(23)$$

i.e., the pseudopotential u' must be such to give rise to the same RDF given by the shadow WF.

We have already solved[9] functional equations of the kind of (23) via an iterative predictor-corrector method when the RDF to be reproduced was derived from a GFMC computation. We have applied the same method to solve (23) when $g_{PP}^{(S)}$ is the RDF computed by Vitiello and co-workers[2] for the shadow WF:

$$u(r)=(b/r)^5,\quad w(\xi)=(b_{sh}/\xi)^5\ ,$$
$$\chi(z)=\pi^{-3/2}C^{3/2}e^{-Cr^2}\ .\qquad(24)$$

Minimization of the energy (the HFDHE2 potential of Aziz *et al.*[10] was used) at the equilibrium density $\rho\sigma^3=0.365$ ($\sigma=2.556$ Å) of liquid ^{4}He gives[2] the parameters $b=1.13$, $b_{sh}=1.40$, $C=4$. All lengths are in units of σ. Our method to solve (23) consists of a number of iterations in which the modified hypernetted chain equation is used to predict u' followed by a Monte Carlo simulation in which the exact $g^{(J)}$ for the estimated u' is computed. The iterations are repeated until (23) is satisfied to within a set limit of error.

In Fig. 1 three pseudopotentials are plotted, the direct interparticle one $u(r)$ (the McMillan form with $b=1.13$), the maximum overlap $u'(r)$, and the best McMillan form for a pure Jastrow WF ($b=1.20$). The coupling to the shadows induces a stronger repulsive pseudopotential at short distance. In addition one can notice that u' has a structure at $r/\sigma \sim 2.1$, the position of the first minimum beyond the main maximum of $g(r)$. This feature was found also in some previous variational computation[11,12] and here it arises from the many-body correlations induced by the shadows. The conjecture that this structure
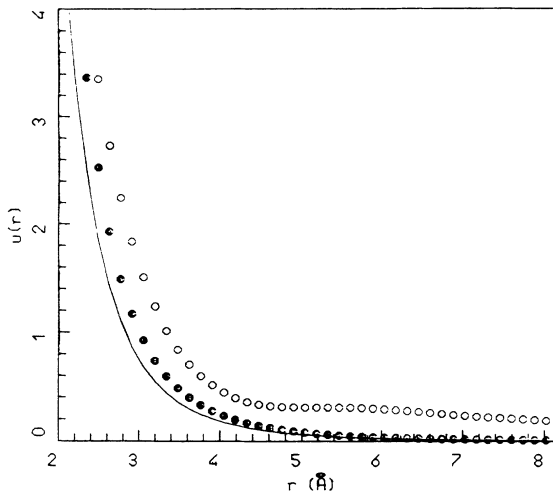

FIG. 1. Pseudopotential of the Jastrow component in the shadow WF of Ref. 2 (McMillan form with $b=1.13$, solid line), maximum-overlap pseudopotential with this shadow WF (○) and pseudopotential of the best pure Jastrow WF (McMillan form with $b=1.20$, ●).

arises from three-body correlations was previously made.[11]

IV. THEORY OF CORRELATIONS FOR THE SHADOW WAVE FUNCTION

The most important correlation functions one would like to compute with the shadow wave function are the single-particle $n_P(\mathbf{r})$ and the two-particle $n_{PP}(\mathbf{r}_1,\mathbf{r}_2)$ distribution functions. These, in the first place, are needed for the computation of the expectation value of the Hamiltonian. If the interparticle interaction is $v(r)$, so that the Hamiltonian reads

$$H_N=-\frac{\hbar^2}{2m}\sum_i \nabla_i^2+\sum_{\substack{i,j\\i<j}} v(r_{ij})\ ,\qquad(25)$$

the expectation value of the potential energy is given by

$$\langle\psi_S\mid V\mid\psi_S\rangle=\tfrac{1}{2}\int d\mathbf{r}_1 d\mathbf{r}_2 n_P(\mathbf{r}_1)n_P(\mathbf{r}_2)g_{PP}(\mathbf{r}_1,\mathbf{r}_2)v(r_{12})\ ,\qquad(26)$$

where we have written

$$n_{PP}(\mathbf{r}_1,\mathbf{r}_2)=n_P(\mathbf{r}_1)n_P(\mathbf{r}_2)g_{PP}(\mathbf{r}_1,\mathbf{r}_2)\ .$$

In this section we drop the index (S) on the correlation functions since all of them are computed with ψ_S^2. The kinetic energy is the sum of two terms

$$\langle\psi_S\mid T\mid\psi_S\rangle=T_1+T_2\ ,\qquad(27)$$

$$T_1=\frac{\hbar^2}{8m}\int d\mathbf{r}_1 d\mathbf{r}_2 n_P(\mathbf{r}_1)n_P(\mathbf{r}_2)g_{PP}(\mathbf{r}_1,\mathbf{r}_2)\nabla^2 u(r)\ ,\qquad(28)$$

$$T_2=-N\frac{\hbar^2}{4m}\left\langle\frac{2}{r}\bar{X}'(r)+\bar{X}''(r)\right.$$
$$\left.+\bar{X}'(r)\left[\bar{X}'(r)-\frac{\mathbf{r}\cdot\mathbf{t}}{rt}\bar{X}'(t)\right]\right\rangle_S\ ,\qquad(29)$$

where $\bar{X}=\ln X$, $\mathbf{r}=\mathbf{r}_1-\boldsymbol{\xi}_1$, $\mathbf{t}=\mathbf{r}_1-\boldsymbol{\xi}'_1$ and the average is taken with respect to ψ_S^2. If X is a Gaussian as in (24) T_2 is simply given by

$$T_2=\frac{3}{2}\frac{\hbar^2}{m}CN\ .\qquad(30)$$

It is interesting to notice that the intershadow pseudopotential $w(r)$ does not enter explicitly the expression for the energy so that $w(r)$ can be a discontinuous function like the hard-sphere one.

The potential energy (26) and the kinetic energy term T_1 has the same form appropriate for a Jastrow function, the only difference being that g_{PP} is the RDF deriving from the shadow WF. The T_2 term is absent in the case of ψ_J but it is present in the case of the Slater-Jastrow function commonly used to describe the solid phase.

In the case of a fluid phase the single-particle distribution $n_P(\mathbf{r})$ is constant equal to the average density and $g_{PP}(\mathbf{r}_1\mathbf{r}_2)$ depends only on the radial distance $\mid\mathbf{r}_1-\mathbf{r}_2\mid$ so that the integrals in (26) and (28) become one-dimensional integrals over this radial distance. This is the situation we consider from now on. We have already mentioned

that this problem is isomorphous to the statistical problem of a classical molecular fluid of flexible triatomic molecules. The intermolecular interaction is of the intersite type so that a particularly convenient theory is the interaction site description developed for molecular fluids by Chandler and coworkers.[13]

In order to be more compact let us introduce the notation $r_i^{(\alpha)}$, $i=1\ldots N$, and $\alpha=1,2,3$. i is the index of a particle with its two shadows (the "molecule"), $\alpha=1$ represents the real particle of the ith "molecule," $\alpha=2$ is the red shadow, and $\alpha=3$ is the blue shadow. The unnormalized distribution function in the configuration space of the $\{r_i^{(\alpha)}\}$ variables is

$$\mathcal{P}(\{r_i^{(\alpha)}\})=\exp\left[-\sum_{\alpha,\gamma}\sum_{\substack{i,j\\i<j}}u_{\alpha\gamma}(\mathbf{r}_i^{(\alpha)}-\mathbf{r}_j^{(\gamma)})\right.$$
$$\left.-\sum_{\alpha,\gamma}\sum_i t_{\alpha\gamma}(\mathbf{r}_i^{(\alpha)}-\mathbf{r}_i^{(\gamma)})\right]\ ,\quad(31)$$

where we have introduced two matrices, $\underline{u}$ for the intermolecular interactions and $\underline{t}$ for the intramolecular ones. These are given by

$$\underline{u}=\begin{bmatrix}u(r)&0&0\\0&w(r)&0\\0&0&w(r)\end{bmatrix}\ ,$$

$$\underline{t}=\begin{bmatrix}0&-\ln\mathcal{X}(r)&-\ln\mathcal{X}(r)\\-\ln\mathcal{X}(r)&0&0\\-\ln\mathcal{X}(r)&0&0\end{bmatrix}\quad(32)$$

in terms of the functions introduced in (1) and (2). It is convenient to introduce two kinds of distribution functions, the intramolecular ones

$$s_{\alpha\gamma}(r)=(1-\delta_{\alpha\gamma})\langle\delta(\mathbf{r}-\mathbf{r}_1^{(\alpha)}+\mathbf{r}_1^{(\gamma)})\rangle\ ,\quad(33)$$

and the intermolecular ones

$$g_{\alpha\gamma}(r)=V^2\left[1-\frac{1}{N}\right]\langle\delta(\mathbf{r}_1^{(\alpha)})\delta(\mathbf{r}-\mathbf{r}_2^{(\gamma)})\rangle\ ,\quad(34)$$

where the averages are taken with the weight (31). Due to the particular nature of the interaction matrices (32) only two of the $s_{\alpha\gamma}$ are distinct and four of the $g_{\alpha\gamma}$ are distinct and the matrices of the distribution functions have the structure

$$\underline{s}(r)=\begin{bmatrix}0&s_{PS}&s_{PS}\\s_{PS}&0&s_{SS'}\\s_{PS}&s_{SS'}&0\end{bmatrix}\ ,$$

$$\underline{g}=\begin{bmatrix}g_{PP}&g_{PS}&g_{PS}\\g_{PS}&g_{SS}&g_{SS'}\\g_{PS}&g_{SS'}&g_{SS}\end{bmatrix}\ .\quad(35)$$

Intershadow correlations between shadows bound to the same particle are given by $s_{SS'}$ and between shadows of different particles are given by g_{SS} for shadows of the same color and by $g_{SS'}$ for shadows of different color. In

a similar way s_{PS} and g_{PS} give the particle-shadow correlations.

The reference-interaction-site model[13] (RISM) develops a theory of correlations via a matrix of direct correlation functions $c(r)$ defined by an Ornstein-Zernlike–like relation

$$\underline{h}(r)=(\underline{\omega}\otimes\underline{c}\otimes\underline{\omega})_r+\rho(\underline{\omega}\otimes\underline{c}\otimes\underline{h})_r\ ,\quad(36)$$

where

$$h_{\alpha\gamma}(r)=g_{\alpha\gamma}(r)-1\ ,$$
$$\omega_{\alpha\gamma}(r)=\delta_{\alpha,\gamma}\delta(\mathbf{r})+s_{\alpha\gamma}(\mathbf{r})\ ,\quad(37)$$

and $\otimes$ indicates both a convolution and a product between matrices. It is easy to verify that $\underline{c}$ has the same structure (35) of $\underline{g}$.

In order to have a self-contained theory of correlations it is necessary to supplement the previous definitions by a closure relation. For instance the Percus-Yevick (PY) closure is

$$c_{\alpha\gamma}(r)=(1-e^{u_{\alpha\gamma}(r)})g_{\alpha\gamma}(r)\ ,\quad(38)$$

and similarly one can introduce the hypernetted chain (HNC) closure. As in the case of a simple liquid these closures correspond to a resummation of a suitable class of diagrams in a cluster expansion of $g_{\alpha\gamma}$. In the molecular case,[13] however, not all the resummed diagrams are proper, some of them are not allowed in the exact expansion. In any case the closure (38) has been useful for classical molecular liquids so that some cancellation must take place. It is difficult to say *a priori* how accurate this equation is in the present case and an answer will require a number of numerical tests of the equations.

A closure like (38) is not enough unless we know the two intramolecular functions s_{PS} and $s_{SS'}$. Since shadows of different colors do not have a direct mutual interaction, a reasonable approximation is to consider only the correlation induced by the presence of a link to the same particle so that

$$s_{SS'}(r)=\int d\mathbf{r}'s_{PS}(\,|\,\mathbf{r}-\mathbf{r}'\,|\,)s_{PS}(r')\ .\quad(39)$$

A Gaussian approximation for s_{PS} should be appropriate, in particular when $\mathcal{X}(r)$ is itself a Gaussian, and the remaining single parameter can be determined in a self-consistent way in terms of the cavity function as it has been done in the case of flexible classical molecules.[13]

The main interest is in the interparticle RDF $g_{PP}(r)$ on which the observable properties like the energy and the structure factor depend. The question we ask is if we can get a simple representation of the higher-order correlations induced by the shadows in terms of a Jastrow term. This is the same problem considered in Sec. III but here we consider this from the point of view of the integral equation. Let us consider a standard Jastrow function with pseudopotential $u^+(r)$. In the PY approximation we have the relation

$$u^+(r)=\ln\left[1-\frac{c^+(r)}{g^+(r)}\right]\ ,\quad(40)$$

where c^+ and g^+ are the correlation functions for this Jastrow function. If u^+ has to reproduce the correlations of the shadow WF we must have $g^+(r) = g_{PP}(r)$. For the shadow WF the role of c^+ is approximately given by the (11) component of the matrix $\underline{\omega} \otimes \underline{c} \otimes \underline{\omega}$ which is

$$c_{PP}(r) + 4(s_{PS} \otimes c_{PS})_r$$
$$+ 2(s_{PS} \otimes c_{SS} \otimes s_{PS})_r + 2(s_{PS} \otimes c_{SS'} \otimes s_{PS})_r . \quad (41)$$

In the PY approximation (38) $c_{PS} = 0$ and $c_{SS'} = 0$ so that the effective Jastrow pseudopotential is

$$u^+(r) = \ln \left[1 - \frac{c_{PP}(r) + 2(s_{PS} \otimes c_{SS} \otimes s_{PS})_r}{g_{PP}^{(r)}} \right] . \quad (42)$$

In (41) and (42) $\otimes$ represents a convolution only.

We have computed this effective Jastrow pseudopotential for the shadow WF of Vitiello et al.[2] g_{PP} is the interparticle RDF computed by them with a Monte Carlo simulation; we have computed $c_{PP}(r)$ from the Ornstein-Zernlike relation starting from the simulated g_{PP} suitably extended[9] to large distance beyond the simulation box side. We have approximated s_{PS} with $X(r)$ assuming that the many-body renormalization of the intramolecular distribution is not large at the equilibrium density of ^{4}He. Finally c_{SS} has been approximated by the direct correlation function of a Jastrow function with a pseudopotential equal to the intershadow term, i.e., $w(r) = (b_{sh}/r)^5$ with $b_{sh} = 1.40$. This has been computed with the modified HNC (MHNC) equation which is known to be a very accurate integral equation. The general structure of $u^+(r)$ is similar to the maximum overlap pseudopotential obtained in Sec. III: u^+ is strongly repulsive at short distance and there is a shoulder around $r/\sigma = 2$. The detailed shape of u^+ depends on the precise choice of c_{SS} and s_{PS} so we have to wait for the results of simulation for these functions before we can get quantitative results.

V. FINAL CONSIDERATIONS

We believe that the shadow wave function represents an important advance in the variational theory of quantum systems. In a sense it gives a way of interpolating between a simple Jastrow function when $w(r)$ in (2) is vanishingly small to the standard Slater-Jastrow function with localizing factors when $w(r)$ is the hard-sphere function at close packing. However, the path-integral analogy already mentioned in the Introduction indicates that ψ_S is more than an interpolation form; it is a way of incorporating in the wave function some of the complex non-Jastrow terms which must be present in the exact ground state in terms of just three functions [$u(r)$, $w(r)$, and $X(r)$]. It is easy to predict that much of the theoretical development based on Jastrow functions will be extended to the new wave function. Here we have discussed the presence of a Bose-Einstein condensate, the maximum overlap between shadow WF and the exact ψ_0 and between shadow WF and Jastrow WF and the development of a theory of correlations for ψ_S. Now we want

to touch briefly upon two other questions. The first is the question of the self-bound state. ^{4}He has a self-bound ground state (N particles form a droplet) whereas quantum hard spheres, for instance, do not. This difference does not show up with the usual Jastrow functions because these do not possess a proper volume but a finite density must be imposed with a suitable boundary condition. In fact, the Jastrow pseudopotential[14] reflects the short-range part of the interatomic potential $v(r)$, but there is no signal of the attractive well, for instance, of the Lennard-Jones potential. Also the shadow WF of Vitiello et al. does not describe a self-bound state: in the molecular analogy all the intermolecular forces are repulsive. We believe, however, that the intershadow pseudopotential w must reflect some aspects of $v(r)$. Again the path-integral analogy is useful. The interaction between single beads of different "polymers" is reduced by the factor $1/n$, where n is the number of beads of a "polymer," so that the attractive well of $v(r)$ is washed out and only the hard part plays a role. This is the contribution contained in the Jastrow term $u(r)$ in ψ_S. However, at the level of "polymers" all the interbead interactions add up so that the attractive part of $v(r)$ should show up at this level. The intershadow pseudopotential $w(r)$ is a way to represent the correlations between "polymers" and therefore it should have an attractive well if $v(r)$ has one. This idea should be tested by a variational computation and the form we suggest is

$$w(r) = \delta v(r/l) , \quad (43)$$

i.e., a rescaled pair interaction both with respect to the intensity by means to δ and to the length scale by means of l. A WF giving self-binding will be important for the study of the free surface of liquid helium, for instance.

It is known that the best Jastrow function falls short of the exact ground-state energy by about 10%, i.e., about 0.7 K per particle is missing at the equilibrium density of liquid ^{4}He. Most of this difference can be recovered[15] with an extended function $\psi = \psi_J \psi_{\text{triplet}}$ with a special form for the triplet term:

$$\psi_{\text{triplet}} = \prod_i \exp \left[-\frac{\lambda}{4} \mathbf{G}_j \cdot \mathbf{G}_j \right] , \quad (44)$$

$$\mathbf{G}_j = \sum_{i(\neq j)} l(r_{ji}) \mathbf{r}_{ji} , \quad (45)$$

where $l(r)$ is a short-range function.

The shadow WF implicitly contains three-body terms and the question is if it can represent the triplet term (44). This triplet can be considered a product of Gaussian in $\mathbf{G}_j$, and by introducing the Fourier representation

$$\exp \left[-\frac{\lambda}{4} \mathbf{G}_j \cdot \mathbf{G}_j \right] = \int d\xi_j e^{i\xi_j \cdot \mathbf{G}_j} e^{-\xi_j^2/\lambda} , \quad (46)$$

we obtain

$$\psi_{\text{triplet}} = \int d\Xi_N \exp \left[-\lambda^{-1} \sum_j \xi_j^2 \right] \prod_j \cos(\xi_j \cdot \mathbf{G}_j) . \quad (47)$$

The integrand in (47) is not a function of definite sign but if the main contribution to (47) derives from regions

where $\xi_j \cdot \mathbf{G}_j < 1$, we can approximate $\cos(\xi_j \cdot \mathbf{G}_j)$ by $\exp\{-|\xi_j \cdot \mathbf{G}_j|^2/2\}$. In fact, it can be shown that

$$\psi_{\text{triplet}} = \int d\Xi_N \exp\left[-\lambda^{-1}\sum_j \xi_j^2\right]\exp\left[-\frac{1}{2}\sum_j |\xi_j \cdot \mathbf{G}_j|^2\right] \tag{48}$$

is equal to the form (44) where the exponential function is replaced by $(1+\lambda G^2)^{-1/2}$. The structure of (48) differs from the shadow function (2) because there is a coupling between each shadow variable and the positions of two particles via $\xi_j \cdot \mathbf{G}_j$. This suggests that a more general shadow WF which incorporates these triplet terms is

$$\psi = \exp\left[-\frac{1}{2}\sum_{\substack{i,j \\ i<j}} u(r_{ij})\right]\int d\Xi_N \exp\left[-\sum_{i<j} w(r_{ij})\right]\prod_k \left[\chi(|\mathbf{r}_k - \xi_k|)\exp\left[-\frac{\lambda}{2}|(\mathbf{r}_k - \xi_k)\cdot\mathbf{G}_k|^2\right]\right], \tag{49}$$

where the Gaussian in ξ^2 in (48) has been replaced by the more general function χ and each integrated ξ_i variable by $\xi_j - \mathbf{r}_j$.

It has been shown[2] that the shadow WF can give a solid phase with an energy even lower than the standard localized WF. Our proof that this WF has Bose-Einstein condensation raises again the question of the existence of BEC in the solid phase. If the initial suggestion[16] was based on a WF which very badly represented a quantum solid, now we have a WF which presently gives the best variational description of solid ^{4}He. It will be interesting to compute the size of this condensate.

ACKNOWLEDGMENTS

[1]See, for instance, D. M. Ceperley and M. H. Kalos, in *Monte Carlo Methods in Statistical Physics*, edited by K. Binder (Springer, Berlin, 1979).

[2]S. Vitiello, K. Runge, and M. H. Kalos, Phys. Rev. Lett. **60**, 1970 (1988).

[3]R. P. Feynman and A. R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, New York, 1965).

[4]Here we are neglecting the effects of exchange between particles which give rise to crosslinking between the "polymers." We do not believe that this has an important role for the present considerations. In order to take into account approximately these effects, one should take the sum in (2) over the permutations of the ξ_k variables.

[5]K. Runge and L. Reatto (unpublished).

[6]L. Reatto, Phys. Rev. **183**, 334 (1969).

[7]L. Reatto and G. V. Chester, Phys. Rev. **155**, 88 (1967).

[8]L. Reatto, Phys. Rev. B **26**, 130 (1982).

[9]G. L. Masserini and L. Reatto, Phys. Rev. B **35**, 6756 (1987).

[10]R. A. Aziz, V. P. S. Nain, J. S. Carley, W. L. Taylor, and G. T. McConville, J. Chem. Phys. **70**, 4330 (1970).

[11]C. De Michelis and L. Reatto, Phys. Lett. **50A**, 275 (1974).

[12]C. C. Chang and C. E. Campbell, Phys. Rev. B **15**, 4238 (1977).

[13]D. Chandler, in *The Liquid State of Matter*, edited by E. W. Montroll and J. L. Lebowitz (North-Holland, Amsterdam, 1982); D. Chandler, Mol. Phys. **31**, 1231 (1976).

[14]M. H. Kalos, D. Levesque, and L. Verlet, Phys. Rev. A **9**, 2178 (1974).

[15]K. Schmidt, M. H. Kalos, M. A. Lee, and G. V. Chester, Phys. Rev. Lett. **45**, 573 (1980).

[16]G. V. Chester, Phys. Rev. A **2**, 256 (1970).