

Coordinated wave function for the ground state of liquid ^4He

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(Received 11 June 2015; revised manuscript received 19 November 2015; published 14 December 2015)

We present a variational ansatz for the ground state of a strongly correlated Bose system. This ansatz goes beyond the Jastrow-Feenberg functional form and explicitly enforces coordination shells in the structure of the wave function. We apply this ansatz to liquid helium-4 with a simple three-variable parametrization of the pair functions. The optimized wave function is found to give an excellent description of the mid-range correlations in the fluid. We also demonstrate the possibility to use this ansatz to study inhomogeneous systems. The phase separation and free surface emerge naturally in this wave function, even though it is constructed of short-range two-body functions and does not contain one-body terms. Because no explicit description of the surface is necessary, this provides a powerful description tool for cluster states.

DOI: [10.1103/PhysRevB.92.214507](https://doi.org/10.1103/PhysRevB.92.214507)

PACS number(s): 67.25.D-, 31.15.xt, 02.70.Ss

I. INTRODUCTION

Interest in the microscopic nature of the ground state of liquid ^4He has drawn attention for over half a century and has shaped the development of many aspects of the quantum many-body theory [1]. The question continues to be of interest, especially as new correlated bosonic systems are becoming the subject of experiment, including the cold atomic gases [2–5]. An explicit and numerically efficient expression for the many-body wave function also has a practical use in computer calculations. A good approximation to the ground state reduces the numerical costs and improves the statistical accuracy of the true ground state results obtained with the diffusion Monte Carlo [6,7] as well as the path-integral ground state Monte Carlo [8–11] methods.

The variational ansatz for liquid ^4He has followed the path of improving the Jastrow-Feenberg form of the wave function [12,13],

$$\begin{aligned} \psi(\mathbf{r}_1, \dots, \mathbf{r}_N) \\ = \prod_{i < j} e^{\frac{1}{2}u_2(\mathbf{r}_i - \mathbf{r}_j)} \prod_{i < j < k} e^{\frac{1}{2}u_3(\mathbf{r}_i - \mathbf{r}_j, \mathbf{r}_j - \mathbf{r}_k, \mathbf{r}_k - \mathbf{r}_i)} \dots, \quad (1) \end{aligned}$$

where N is the number of atoms, and the k -body correlation factors u_k must have proper symmetry under the exchange of particles. Because each successive term in Eq. (1) increases the numerical complexity by an additional factor of N , one is in practice limited to two- and three-body terms. Limiting Eq. (1) to two-body factors results in the Jastrow function [14,15]. In an early work, McMillan [16] and Schiff and Verlet [17] used a Jastrow function with the two-body function $u_2 = -(b/r)^5$. Parameter b was determined variationally. The McMillan function captures the most significant features of the system caused by the core of the interparticle potential, and it continues to be used successfully as a guiding function for projector Monte Carlo [11,18,19]. Successive improvements in the ground state of helium refined the two- and, later, three-body factors in the form [Eq. (1)]. Published progress on this topic is too numerous to cover in any detail here. Relevant to this work, we note the addition of the mid-range correlation

[20,21] which among other things allowed to replicate the first correlation peak of the pair distribution function $g(r)$, the addition of long-range terms in the two-body function u_2 that allows to account for the long-wavelength zero-point phonons [22,23], the computation of u_2 based on the maximum overlap with the true ground state [24,25], and finally, a detailed optimization of the pair factors expanded in terms of the pair scattering eigenstates [26,27] which along with the inclusion of the three-body factors allowed to account for nearly all the correlation energy. The success of the above works came at the expense of the increased complexity and the number of variational parameters that are needed to accurately describe the functions u_k . The general functional form of Eq. (1), though, remained unchanged [28].

The development of the shadow wave function (SWF) methods [29,30] has to a large degree overtaken the development of the wave function for liquid helium. The SWF allows to account for the correlations missed by the Jastrow function and results in an excellent description in terms of both energy and structure [31,32] of ^4He . Relevant to this work, we notice that SWF can support self-bound states of liquid ^4He [33]. Shadow wave function accounts for correlations via integrals on auxiliary (shadow) variables. The inclusion of the shadow variables may be seen as going beyond the Jastrow-Feenberg form of Eq. (1). However, the integrals on the shadow variables must be taken numerically by a Monte Carlo scheme, and in this sense the shadow wave function is not explicit, partially limiting its adoption in quantum Monte Carlo.

We will present a variational ansatz for the ground state of liquid ^4He which is built upon the Jastrow wave function but goes beyond the general functional form of Eq. (1). This ansatz allows us to explicitly control the mid-range structure of the liquid and results in a stark improvement of the atomic pair distribution already with a three-parameter wave function. The wave function is presented in Sec. II, and the computational results are shown in Sec. III. Section IV presents results for inhomogeneous systems, followed by a discussion.

II. THE COORDINATED WAVE FUNCTION

A. Variational ansatz

Our proposed wave function consists of a product of the Jastrow function [limiting Eq. (1) to two-body terms] and of

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the additional term which we refer to as the ‘‘coordination term.’’ The wave function has the following form,

$$\psi_{JC}(\mathbf{r}_1, \dots, \mathbf{r}_N) = \prod_{i < j} e^{\frac{1}{2}u_2(|\mathbf{r}_i - \mathbf{r}_j|)} \prod_i \sum_{j \neq i} y_2(|\mathbf{r}_i - \mathbf{r}_j|). \quad (2)$$

The factors $y_2(r)$ must vanish at large distances. At short distances, y_2 is expected to rise to a constant.

The effect of the coordination term in Eq. (2) can be seen by inspection. Suppose the function $y_2(r)$ vanishes for distances r beyond the mean interparticle distance. In this case, $y_2(r_{ij})$ will have significant value only for the pairs of immediate neighbors $\langle i, j \rangle$. On the other hand, the number of neighbors for each atom is limited by the presence of the repulsive core and by the Jastrow part of the wave function. Thus the overall number of nonvanishing terms $y_2(r_{ij})$ in the system is, roughly speaking, fixed. Under such a restraint, the product of sums in the coordination part of Eq. (2) is maximized when all sums are equal to each other. That is, *the nonvanishing values of $y_2(r_{ij})$ are distributed equally between the products*. The wave function ψ_{JC} , while constructed only of pairwise functions, has a ‘‘global’’ property in that it explicitly demands that each atom in the system has an equal expected number of immediate neighbors. As we will see, this allows to improve the mid-range properties of the system independently of the Jastrow factor.

B. Inspiration and origin

The inspiration for the coordinated wave function ψ_{JC} comes from the symmetrized Bose-solid wave function proposed by Cazorla *et al.* [34]. This symmetrical solid wave function does an excellent job describing the quantum Bose solid, both variationally [35] and as a guiding function for the importance sampling in quantum Monte Carlo simulations of Bose solids [36–39]. In fact, one will recognize that Eq. (2) is the wave function of Cazorla *et al.*, except that the site locations of a crystalline structure are here replaced by the positions of atoms themselves.

The solid wave function of Ref. [34] forces atoms to be located in the vicinity of one of the externally specified lattice sites while at the same time imposing the global restraint by favoring single site occupancy. In the liquid, the translational symmetry is not broken, and there are no preferred positions; instead, the atoms in Eq. (2) are ‘‘localized’’ around their neighbors. As the overlap of atomic cores is prohibited by the Jastrow term, this creates the coordination shells.

An important distinction between ψ_{JC} of Eq. (2) and the symmetrized Nosanow-Jastrow wave function of Ref. [34] is in the nature of the sum factors. As discussed in Ref. [35], factors that bind atoms to the lattice sites in the solid wave function of Ref. [34] can be seen as a generalized symmetrical form of the one-body factor; the coordination part of Eq. (2), however, is by the same criterion a full N -body term.

C. Separability

If the particles of the system are divided into subgroups separated by a large distance, the wave function ought to reduce to the product of the wave functions for the individual subgroups [40]. While such a cluster property is obviously satisfied by the Jastrow function, it is less transparent for the

coordination term. Suppose all particles are divided into two groups, or clusters, A and B . Let the corresponding number of particles be N_A and N_B , $N_A + N_B = N$. The distance between these clusters is sufficiently large such that the function y_2 vanishes for any pair of particles from across the two groups,

$$\forall i \in A, j \in B : y_2(|\mathbf{r}_i - \mathbf{r}_j|) = 0.$$

In this case, the coordination sum for any particle in a subgroup reduces to the sum on that subgroup only, and the coordination term separates,

$$\begin{aligned} \psi_C(\mathbf{r}_1, \dots, \mathbf{r}_N) &= \prod_i \sum_{j \neq i} y_2(|\mathbf{r}_i - \mathbf{r}_j|) \\ &= \left(\prod_{i \in A} \sum_{j \neq i} y_2(|\mathbf{r}_i - \mathbf{r}_j|) \right) \\ &\quad \times \left(\prod_{i \in B} \sum_{j \neq i} y_2(|\mathbf{r}_i - \mathbf{r}_j|) \right) \\ &= \left(\prod_{i \in A} \sum_{\substack{j \neq i \\ j \in A}} y_2(|\mathbf{r}_i - \mathbf{r}_j|) \right) \\ &\quad \times \left(\prod_{i \in B} \sum_{\substack{j \neq i \\ j \in B}} y_2(|\mathbf{r}_i - \mathbf{r}_j|) \right) \\ &= \psi_C(\underbrace{\mathbf{r}_{i'_1}, \dots, \mathbf{r}_{i'_{N_A}}}_{i' \in A}) \times \psi_C(\underbrace{\mathbf{r}_{i''_1}, \dots, \mathbf{r}_{i''_{N_B}}}_{i'' \in B}) \\ &= \psi_C(A)\psi_C(B). \end{aligned}$$

Thus a wave function for the two clusters reduces to the product of the wave functions for the individual clusters.

D. Computational complexity

The evaluation of the coordinated wave function of Eq. (2) requires the computation of $O(N^2)$ interparticle distances, and the overall computational cost also scales as the second order in the number of particles. The scaling holds for the application of the Hamiltonian and other relevant operators. To see this, we write Eq. (2) as

$$\psi_{JC}(\mathbf{r}_1, \dots, \mathbf{r}_N) = \prod_{i < j} e^{\frac{1}{2}u_2(|\mathbf{r}_i - \mathbf{r}_j|)} \prod_i S_i(\mathbf{r}_1, \dots, \mathbf{r}_N),$$

with

$$S_i(\mathbf{r}_1, \dots, \mathbf{r}_N) = \sum_{j \neq i} y_2(|\mathbf{r}_i - \mathbf{r}_j|).$$

In order to compute all N sums S_i , one needs to compute $N(N-1)/2$ values of $y_2(|\mathbf{r}_i - \mathbf{r}_j|)$ so long as the sums are stored in memory. This is not a taxing requirement, given one must in any case store $3N$ atomic coordinates. Once the sums are computed, the computation of the product $\prod_i S_i$ only requires N operations.

Similar considerations apply to the computation of the Hamiltonian and other relevant expressions. For quantum

Monte Carlo, one generally needs to compute the contribution to the local kinetic energy $\sum_i \frac{\nabla_i^2 \psi}{\psi}$ and the “quantum velocity” vector $\frac{2\nabla_i \psi}{\psi}$. The relation

$$\frac{\nabla^2 \psi}{\psi} = \nabla^2 \log \psi + (\nabla \log \psi)^2 \quad (3)$$

allows us to separate the contributions from the Jastrow and the coordination terms. The later is labeled below as ψ_c . We also use a label $(\cdot)_{s,t}$ for the t th spatial dimension corresponding to particle s ; that is, $1 \leq t \leq D$, and s spans from 1 to N . It is convenient to define vectors \mathbf{v} and \mathbf{u} ,

$$v_{s,t} = \frac{1}{S_s} \sum_{i \neq s} y_2'(r_{si}) \frac{x_{s,t} - x_{i,t}}{r_{si}}, \quad (4)$$

$$u_{s,t} = \sum_{i \neq s} y_2'(r_{si}) \frac{1}{S_i} \frac{x_{s,t} - x_{i,t}}{r_{si}}. \quad (5)$$

The quantum velocity is obtained by

$$\nabla_{s,t} \log \psi_c = (\mathbf{u} + \mathbf{v})_{s,t}. \quad (6)$$

The second derivative, summed on the spatial dimension, can be written as

$$\begin{aligned} & \sum_{t=1}^D \nabla_{s,t}^2 \log \psi_c \\ &= \sum_{i \neq s} \left\{ \left[y_2''(r_{si}) + \frac{D-1}{r_{si}} y_2'(r_{si}) \right] \right. \\ & \quad \left. \times \left(\frac{1}{S_s} + \frac{1}{S_i} \right) - \left[\frac{y_2'(r_{si})}{S_i} \right]^2 \right\} - \sum_t v_{s,t}^2. \quad (7) \end{aligned}$$

Notice the cancellation between v^2 terms from Eqs. (6) and (7) suggested by Eq. (3).

Written in the above form, it is clear that the relevant calculations involve the order of N^2 operations with a storage requirement of only the first order in N . The calculation may proceed as follows. First, one loops through $N(N-1)/2$ pairs of particles and computes the sums S . Then the loop is repeated, this time summing the contributions to the vectors \mathbf{v} and \mathbf{u} given by Eqs. (4) and (5) and the contribution to the second derivative given by the first sum on the r.h.s. of Eq. (7). To complete the calculation of the kinetic energy, one needs to perform N additional operations to compute the second sum in the r.h.s. of Eq. (7) and to sum the square of the gradient vector according to Eq. (3) [41]. Thus the computations with the coordinated wave function of Eq. (2) scale only as the second order in the number of particles, although the usual loop over the particle pairs needs to be repeated twice.

E. The form of the pair and coordination factors

To test the coordinated wave function of Eq. (2), we have decided to limit the Jastrow term to the simple McMillan form [16] with $u_2 = -(b/r)^5$. As this term aims to capture the short-range correlations in the fluid, the mid-range correlations are left to be treated with the coordination term. Having only one variational parameter in the Jastrow product simplifies the parametrization of the wave function. However, the simple

form of the McMillan factor misses over 1 K of the correlation energy, most of it due to its imperfection at short distances. One should not hope to recover this energy with any improvement to the mid-range correlations.

For calculations, we used the following form of the pairwise functions,

$$u_2(r) = -\frac{1}{2} \left(\frac{b}{r} \right)^5 - \frac{1}{2} \left(\frac{b}{2L_c - r} \right)^5 + \left(\frac{b}{L_c} \right)^5 \quad (8)$$

$$y_2(r) = 1 - \exp \left[- \left(\frac{\delta}{R(r)} \right)^m \right] \quad (9)$$

$$R(r) = \frac{r}{1 - (r/L_c)^4}, \quad (10)$$

where b , m , and δ are the three variational parameters, and L_c is the cutoff distance of the calculation given by half the dimension of the simulation box.

The coordination function y_2 was chosen to provide a reasonably sharp cutoff beyond a certain distance δ . At the same time, we found it quite important to have a “flat” y_2 at small distances, as otherwise the derivative of y_2 interferes with the energy terms produced by the derivatives of the pair factors u_2 . Because of this effect, using y_2 of a Gaussian or exponential form results in wide flat energy plateaus in the space of variational parameters. Instead, the form given by Eq. (9) assures that y_2 reaches a constant at small distances. The relevant small distances are given by the parameter b , and the condition can be formulated as

$$\exp[-(\delta/b)^m] \ll 1.$$

Satisfying the above condition effectively decouples the optimization of u_2 and y_2 , allowing for a clear interpretation of both terms and for a straight-forward variational optimization. Indeed, we found that variationally optimized parameters b, δ , and m fulfill the above condition to about 10^{-3} .

As is beneficial for a variational calculation, both Jastrow and the coordination terms are symmetrized to result in zero gradient of the wave function at the computational cutoff L_c . The pair term in Eq. (8) is symmetrized in the traditional manner, while the coordination factor y_2 employs a scaling function $R(r)$ to assure that y_2 vanishes smoothly at the cutoff distance $r = L_c$. The use of the scaling function allows for a robust implementation of the cutoff at L_c , yet introduces minimal disturbance to y_2 at the relevant distances $r \approx \delta$, as in our case $(\delta/L_c)^4 < 10^{-2}$. We found that using scaling function provides a convenient way for symmetrizing the wave function.

III. RESULTS

A. Variational optimization

We carried the variational optimization with three-dimensional 512-atom ${}^4\text{He}$ system at the equilibrium density [43] of liquid ${}^4\text{He}$, $\rho_0 = 0.365\sigma^{-3} = 21.8 \text{ nm}^{-3}$. Here and below, we use the reduced unit of length equal to $\sigma = 2.556 \text{ \AA}$. All observables were computed on Markov chains generated by the Metropolis method [44] with single-particle updates. We used a GPU cluster to speed up the calculations using a modification of the QL quantum Monte Carlo package [45]. The coordinated wave function of Eq. (2) was taken

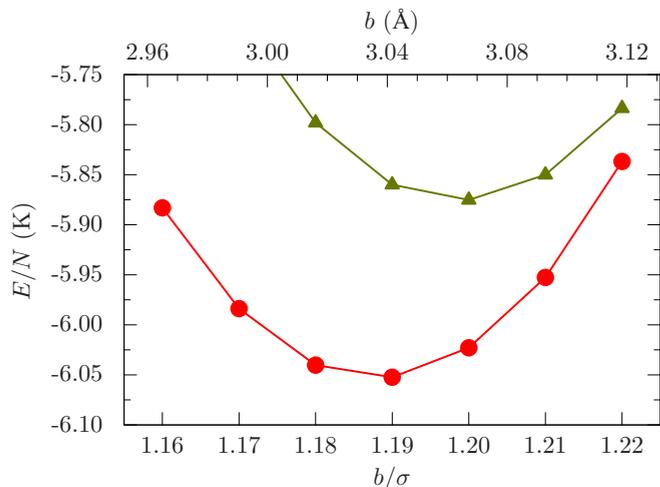


FIG. 1. (Color online) Variational energy (per particle) for the coordinated wave function given by Eqs. (2) and (8)–(10) (bullets) and the Jastrow function with the McMillan pair factor given by Eq. (8) (triangles). Both energies are shown as a function of parameter b which enters the two-body correlation factors. For each value of b , the coordinated function was optimized with respect to its parameters m and δ . For the unit of distance, we use $\sigma = 2.556 \text{ \AA}$. The energies were computed for 512-particle systems interacting with Aziz-II [42] pairwise potential. Statistical errors are smaller than the symbol size.

in three-parameters form given by Eqs. (8–10). The system Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m} \sum_i \nabla_i^2 + \sum_{i<j} V(r_{ij})$$

was used with the pair potential by Aziz [42].

The three variational parameters b , m , and δ were optimized on a grid. Figure 1 shows variational energy as a function of parameter b , given optimal m and δ for each value of b . The results are compared to the (noncoordinated) Jastrow function with the McMillan factor given by Eq. (8). Optimal value of the parameter b for the coordinated function was found to be $b = 1.19\sigma$, slightly below the optimal value of the noncoordinated function $b = 1.20\sigma$. As expected, we found little variation in optimal value of δ with respect to changing the value of parameter b . In the range shown in Fig. 1, optimal δ varies less than two percent. We also notice relatively weak correlation between parameters δ and m near the variational minimum.

The optimized values of variational parameters are shown in Table I. The table also shows the value of optimized energy extrapolated to the thermodynamic limit. For comparison, Table I also lists the energy for the Jastrow function with the McMillan factor. This energy differs slightly from the one obtained by McMillan [16], which can be prescribed to the difference in the interaction potential. As expected, one will notice that the gain in the correlation energy is mild and amounts to just under 200 mK. This is in part due to the fact that the missing mid-range correlations are not responsible for a large amount of energy, but also because the presence of the coordination term ever so slightly offsets the correlation hole which in turn carries an energy penalty.

TABLE I. Optimized parameters of the coordinated and noncoordinated Jastrow wave functions with the McMillan factor. Distances are specified in units of $\sigma = 2.556 \text{ \AA}$. Lowest line shows the thermodynamic limit extrapolation of the per-particle energy, with up to 1920 particles used for the calculation. The interaction was modeled with the Aziz pair potential from Ref. [42].

	Coordinated	Noncoord.
b/σ	1.19	1.20
δ/σ	1.60	
m	6.55	
E/N (K)	-6.05 (1)	-5.88 (1)

B. Structural properties of the coordinated function

As both the potential energy and the wave function are built from the pairwise functions, the properties of the system are captured by the pair distribution function. The computed pair distribution function $g(r)$ is shown in Fig. 2, along with the results for the McMillan function and an unbiased (pure) estimate for the $g(r)$ obtained with the diffusion Monte Carlo (DMC). The unbiased DMC estimator for $g(r)$ was obtained with the ancestry tracking algorithm of Casulleras and Boronat [46]. Such an unbiased estimator is computed from the projected ground state and can be expected to reflect accurately on the experimental values [46–48]. In properly converged calculations, pure DMC results do not depend on the DMC guiding function. However, it is worth pointing out that the guiding function for the DMC calculation was in fact the Jastrow function with the McMillan factor, and it did not contain the coordination factor. In all three cases shown in Fig. 2, the calculations were performed with 512-particle

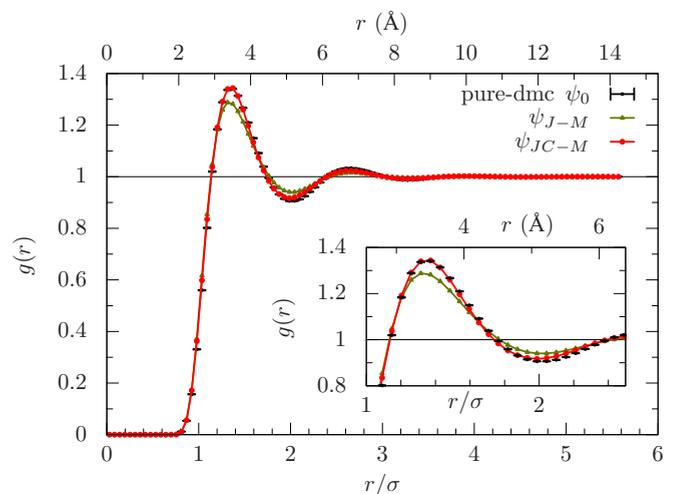


FIG. 2. (Color online) Pair distribution function $g(r)$ as a function of the interparticle distance, obtained for a 512-atom system. For the unit of distance, we use $\sigma = 2.556 \text{ \AA}$. Unconnected black error bars: unbiased (pure) estimator obtained with DMC, as described in the text. Connected green triangles: Jastrow function with the McMillan pair factor as specified in Eq. (8). Connected red bullets: energy-optimized three-parameter coordinated wave function ψ_{JC} with the McMillan factor, given by Eqs. (2) and (8)–(10). Error bars for both VMC calculations are smaller than their corresponding symbol sizes. The inset shows the details of the first correlation peak.

TABLE II. The degree to which the computed pair distribution functions $g(r)$ capture the unbiased estimate $g^*(r)$. The values are computed as $|g(r_m) - g^*(r_m)|/|1 - g^*(r_m)|$, where r_m are the locations of extrema of $g^*(r)$. The simulation conditions are described in Fig. 2.

	1st max	1st min	2nd max	2nd min	3rd max	3rd min
Coordinated	1.0	0.9	0.7	0.6	0.4	0.4
Noncoord.	0.8	0.6	0.5	0.3	0.2	0.2

systems at the equilibrium density of ${}^4\text{He}$, $\rho = 0.365\sigma = 21.8 \text{ nm}^{-3}$. The variational parameters were chosen by energy optimization, as specified above, and are given in Table I.

It is notable that the coordinated wave function reproduces accurately the first correlation peak in the pair distribution function. The inset in Fig. 2 shows the detail of the first maximum. The first correlation minimum is reproduced slightly less accurately. The following oscillations in the pair distribution function are also reproduced better by the coordinated wave function, albeit with decreasing accuracy. The position of the maxima and minima in the pair distribution was also considerably improved by the coordination term. The details are given in Table II. However, the absolute value of these successive oscillations is minute, and they are at distances where the pair potential is vanishing rapidly. Thus their influence to the overall energy is nonsignificant.

IV. INHOMOGENEOUS SYSTEMS

Jastrow wave functions based on short-range pair factors cannot support the formation of a self-bound state. That is, a simulation in a sufficiently large box will result in a low-density uniform gas with near-zero potential and kinetic energy. Helium liquid, however, is self-bound. To describe inhomogeneous systems, one generally adds one-body factors which bind the liquid phase to a desired shape [48–51]. This has obvious disadvantages if the surface shape is complex and may pose additional challenges when one needs to maintain the translational symmetry in the system [52]. Parametrization of the surface adds to the required number of the variational variables. Self-binding may also be enforced through the use of long-range terms in the two-body factors, such as introduced in Ref. [53], with an additional term in the two-body function $u_2(r)$ proportional to the distance between the particles r . Such a wave function serves well as a trial wave function for a projector Monte Carlo calculation, yet variationally, the kinetic per-particle energy of a system with $u_2 \sim -\alpha r$ for large r is divergent with the increasing number of particles N as $\sim (\hbar^2/m)\rho_0^{1/3}N^{2/3}\alpha$, where ρ_0 is the bulk density. This presents a number of challenges, as at the very least α must be N dependent.

The coordinated wave function has an unexpected feature in that by design it supports a self-bound state of the atoms. Upon inspection, one will notice that the coordination sum factors in Eq. (2) in fact vanish in the limit of low-density, uniformly distributed gas. Thus the coordination term requires

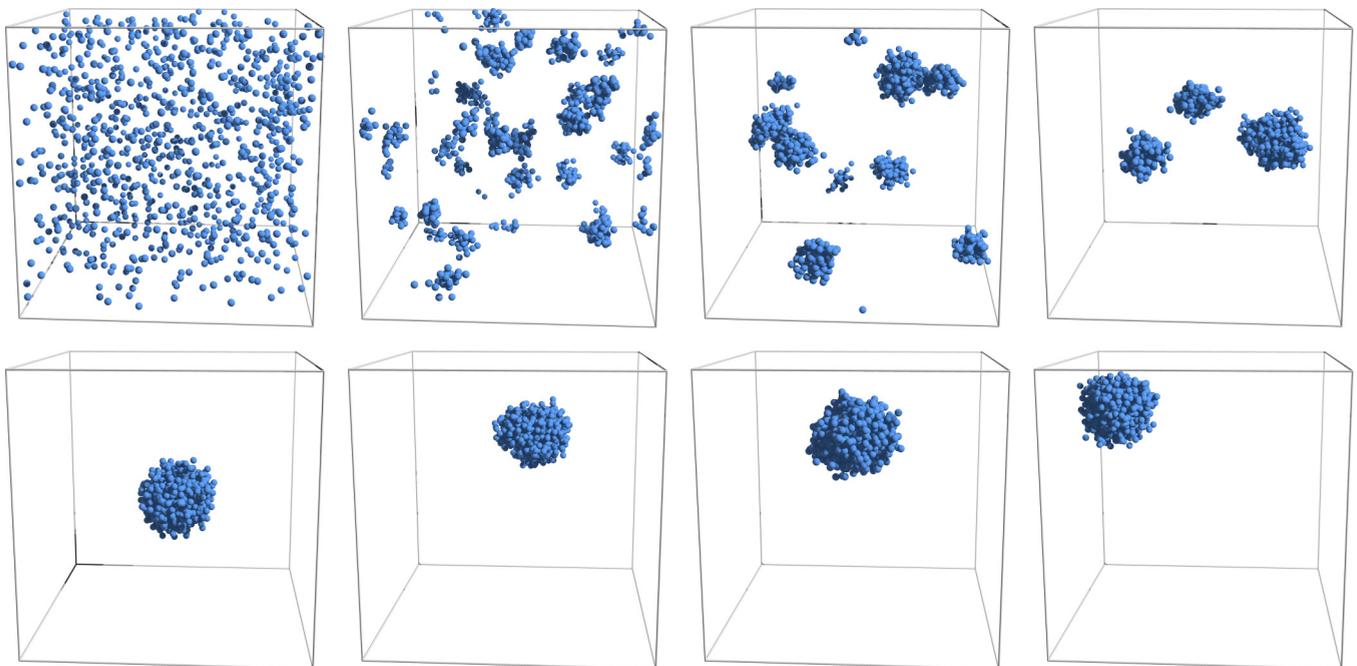


FIG. 3. (Color online) Progression of Markov chain during Metropolis sampling of a system with $N = 1000$ atoms with the coordinated wave function. The size of the cubic box is equal to $L = 100 \sigma = 256 \text{ \AA}$, which would correspond to a very dilute homogeneous system. Top row, left to right, shows the initial state of the system (with atoms distributed randomly and uniformly) and the system correspondingly after 10^3 , 10^4 , and 10^5 macroudates. After 10^5 updates, the Markov chain reaches droplet configuration which is then sampled throughout the (periodic) simulation cell. The bottom row, left to right, shows configurations after 2×10^5 , 3×10^5 , 10^6 , and 2×10^6 macroudates. Wave-function parameters are $b = 1.19\sigma$, $\delta = 4.60\sigma$, $m = 6.55$. Metropolis sampling was carried via single-particle updates, with a fixed Gaussian distribution of displacements which resulted in the acceptance ratio of above 20% in the homogeneous phase to below 35% in the condensed phase. Each “macroudate” equals N single-particle Metropolis attempts.

that atoms form clusters, so far as function $y_2(r)$ falls off sufficiently rapidly with distance. The size and number of the clusters is determined by the variational parameters and particle density. For instance, a gas of dimers already has a nonzero coordination term. Increasing the range of y_2 (which in our case translates to increasing δ or decreasing m) increases the size of the clusters. The parameters also provide control over the structure of the surface.

We have carried a variational calculation with the coordinated wave function with 1000 atoms in a simulation box that resulted in particle density $10^{-3} \sigma^{-3} \approx 0.06 \text{ nm}^{-3}$. The Jastrow wave function results in a ground state of dilute gas with close to zero energy. However, the coordinated wave function resulted in a bound state for a wide range of parameters m and δ . Only small δ resulted in the unbound states albeit with positive energy. We also find that the extent of function y_2 controls the average cluster size and thus the energy. Variational optimization of m and δ results in a state with a single liquid droplet.

To demonstrate the robustness of the inhomogeneous simulation, we carried Monte Carlo sampling of the coordinated wave function with parameters $m = 6.55$ and $\delta = 4.50\sigma$ (i.e., with y_2 having larger extent than for the bulk). The initial coordinates of the 1000 particles were randomly distributed in the simulation box. The sampling sequence is presented in Fig. 3. Soon after the start, the Markov chain arrives at configurations with multiple small clusters. As the clusters merge, a single droplet is eventually formed. The center of mass of the system is not fixed, and the droplet continues to sample the entire simulation cell.

The inner structure of the droplets and clusters depend strongly on the two-body function u_2 . However, Jastrow function with the McMillan factor underestimates the equilibrium density of the bulk ^4He . Without the fixed density constraint, it is to be expected that the inhomogeneous simulation should result in lower densities of the condensed phase. This was indeed observed. For example, the droplet shown in Fig. 3 has inner density that is less than 70% of the bulk equilibrium helium density. Thus the droplet calculation presented here should be seen as a demonstration of principle. The details of their structure, which require a more detailed Jastrow term, will be the subject of further investigation.

V. CONCLUSION

We have considered a wave-function ansatz for a strongly correlated Bose system that goes beyond the Jastrow-Feenberg expansion. Originating from a symmetrical solid wave function proposed by Cazorla *et al.* [34], it is a Bose-liquid wave function which explicitly promotes the creation of the coordination shells around atoms. The function is translationally and exchange symmetric. It is fully explicit and is computationally

hard as $O(N^2)$, making it well suitable for treatment with quantum Monte Carlo.

To demonstrate the coordination effect, we have studied the wave function with the one-parameter McMillan factor for the Jastrow term and a two-parameter coordination function. The resulting three-parameter wave function was straightforward to optimize variationally. The short-range nature of the McMillan factor allowed us to directly observe the effects of the coordination terms on the mid-range structure of the liquid. Indeed, the optimized wave function results in superior description of mid-range correlations in the system. Comparing with an unbiased estimate for the pair distribution function obtained with the diffusion Monte Carlo, we find that the first correlation peak is reproduced almost exactly. Moreover, the structure of the pair distribution function is improved consistently throughout larger distances as well.

As was first demonstrated in Ref. [20], the first correlation peak can be reproduced rather exactly with the Jastrow function. However, this required eight variational parameters, and already the description of the first minimum was significantly lacking. Other approaches to accurately describe the mid-range structure with the Jastrow factors alone have also been reported [54]. In our case, the addition of the coordination term allows us to separate the short- and middle-range correlations, which can be accounted for correspondingly by the Jastrow and the coordination terms.

By construction, the coordinated wave function supports a self-bound state. Consequently, the simulation of inhomogeneous systems does not require the addition of one-body terms. Moreover, inhomogeneity and surface formation at low densities result directly from the variational optimization of the bulk wave function. Since the variational ansatz does not require knowledge of the surface geometry, this also provides a powerful tool for cluster states of matter. However, we find that a satisfactory description of the inhomogeneous phase of helium requires improvements in the Jastrow pair term, which was here limited to the McMillan form for simplicity.

The separation of the mid-range correlations into the coordination term which was demonstrated here means that the Jastrow pair term in the coordinated wave function only needs to account for the short-range correlations and possibly for the well-understood long-range correlations arising from zero-point phonons. This makes it promising that an accurate short-range pair term can be designed in the future with a simple parametrization.

ACKNOWLEDGMENTS

The author acknowledges the computer resources and assistance provided by the Spanish Supercomputing Network (Red Española de Supercomputación), and by the Barcelona Supercomputing Center. We are also thankful to the Nvidia corporation for the provided hardware and technical expertise.

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