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The coherent-state wave function for solid ^{3}He

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Abstract
A new class of variational wave functions describing many-body systems with spin-dependent correlations is used to study solid ^{3}He. The idea of spin coherent states is used to construct a variational coherent-state wave function for solid ^{3}He as an antisymmetrized Jastrow–Nosanow wave function that also contains spin-dependent correlations. We investigate this wave function by a variational Monte Carlo method. The addition of triplet (three-body) correlations produces a ground-state energy per particle that is a considerable improvement upon other variational results, but still appreciable discrepancies with the experiment remain. We speculate that such discrepancies point to a non-negligible effect of more-than-three-body correlations for both liquid and solid ^{3}He.

1. Introduction

The physics of ^{3}He and ^{4}He has always been a subject of great interest in quantum statistical mechanics and many-body theory. Helium atoms, as components of liquid or solid helium, can be considered as structureless, spherical particles interacting via a two-body potential. The attractive part of the potential causes helium gas to condense into a liquid phase (at a temperature $T_0 = 3.2$ K for ^{3}He and 4.2 K for ^{4}He, at normal pressure). In addition, on decreasing temperature below T_0, neither ^{3}He nor ^{4}He solidifies unless pressure is applied. This is a genuine quantum effect caused in part by the strong zero-point motion arising from the small atomic mass and in part by the weakness of the attractive part of the interaction, due to the high symmetry of the atoms. Moreover, quantum effects are responsible for the strikingly different behaviour of the Fermi ^{3}He and the Bose ^{4}He systems, which emphasizes the role played by the exchange symmetry for such low-temperature quantum fluids.

A transition to the crystalline state can only occur at higher pressure. At low temperature the systems undergo phase transitions to superfluid phases of different origins. The Bose ^{4}He undergoes a Bose–Einstein condensation in the liquid phase at the λ-temperature (2.17 K at normal pressure), while for ^{3}He, which is a Fermi liquid, the transition occurs at a much lower temperature (some mK) due to a mechanism of pairing that can be described by BCS theory. The phase diagram of ^{3}He is richer and more complicated than that of ^{4}He.

Realistic pair potentials have been extracted from experiments and simulation data to represent the interaction between helium atoms in the condensed systems, from the Lennard-Jones (LJ) potential adopted in early studies to the more accurate HFDHE2 potential developed and refined by Aziz *et al* [1].

The HFDHE2 potential has become the potential of choice for helium studies and its wide acceptance has been due in part to Green's function Monte Carlo (GFMC) results [2, 3] that have shown a good agreement with the low-temperature experimental equation of state for ^{4}He. Small inconsistencies with theoretical results and experimental data have been detected and this has prompted revisions of the HFDHE2 potential, with much of the work done by the Aziz group itself [4]. These recent minor revisions have improved the quality of but not greatly altered the description of the interaction between helium atoms at low temperature. In this work we will continue to use the HFDHE2 potential to facilitate comparison with existing calculations in the literature and because the GFMC work has shown that the HFDHE2 potential provides an accurate description of the interaction of helium atoms.

For ^{3}He the situation is less satisfactory, because the quantum Monte Carlo (QMC) results are not as accurate as for ^{4}He. Difficulties associated with the antisymmetric nature of Fermi wave functions are well known and the Fermi sign problem manifests itself as an exponential increase in statistical error as the calculation proceeds. GFMC simulations for liquid ^{3}He have been performed in the fixed-node approximation [5] (employing nodes from accurate variational wave functions); these give an upper bound for the exact energies.

While for solid ^{4}He an unsymmetrized Jastrow–Nosanow (JN) wave function works reasonably well, it is less satisfactory for solid ^{3}He, as first shown by the variational Monte Carlo (VMC) calculations of Hansen and Levesque [6]. In these calculations, the crystalline order of the solid phases is imposed through one-body Gaussian terms that explicitly localize the particles in the vicinity of the lattice sites of a perfect lattice. However, it is important to mention that the one-body Gaussian terms of the unsymmetrized JN wave function violate both the translational symmetry of the Hamiltonian and the statistics (Bose/Fermi) of the wave function.

Several other calculations for solid ^{3}He have been performed with an antisymmetrized version of the JN wave function [7], obtained by replacing the unsymmetrized simple product of localized Gaussian orbitals [8] with a determinant of the same orbitals. Although this wave function has the correct symmetry and statistics, the energy per particle is always higher in this approach than in the unsymmetrized case.

Solid ^{3}He is very interesting also in view of its magnetic properties [9]; it is experimentally well known that below a certain temperature of the order of mK, a nuclear-spin ordering of the up–up–down–down (u2d2) form becomes stable—that is, there is a stacking of two planes of the body-centred-cubic (bcc) crystal with 'up' spins, followed by two planes with 'down' spins. Just as in electronic systems where the underlying interaction is independent of spin, the magnetic effects in solid ^{3}He are produced by the Pauli principle and exchange interaction. Even though the Hamiltonian of the system is considered independent of spin, including spin-exchange terms in the wave function may allow one to describe the physical correlations in a simpler way than by just using spatial correlations.

A wave function without spin-dependent correlations can be easily written as the correlation factor times two determinants of spatial orbitals: one for 'up' spins and one for 'down' spins. The reason for this simplification is that neither the correlation operator nor the Hamiltonian can flip the spins. The introduction of spin-dependent correlations makes this simple analysis fail, since now the spin correlations introduce spin exchanges which flip the spins of particles. The inclusion of spin-correlation operators into the wave function

severely restricts the system size and it is difficult to construct a low-variance method for performing such calculations.

Until recently, this has remained a long-standing problem in many areas of physics, including that of quantum liquids and nuclear physics. This difficulty seems to be overcome by a different new approach for dealing with spin-dependent correlations in variational calculations [10]. In this approach, the wave function is constructed using spin coherent states to represent the quantum spin states of particles, which are then parametrized by a continuous variable that looks like a classical spin vector, and, in particular, spin operators can now be represented as simple integrals over these classical spin variables. Thus, correlation operators that had previously proven cumbersome in variational calculations can be replaced by integrals over c-valued functions. With this in mind, Lawson *et al* [10] have presented a coherent-state wave function (CSWF) for liquid ^{3}He and have performed explicit VMC calculations showing that the CSWF for liquid ^{3}He gives very good results at the level of the best wave functions which include either spin and/or backflow correlations.

It is the intent of this paper to extend the spin-coherent-state formalism to solid ^{3}He and present new results obtained by a VMC calculation.

Variational calculations yielding a good ground-state trial function are an essential preliminary to a reliable GFMC calculation, because improved trial wave functions significantly reduce the statistical error by initiating the iterative calculation nearer to the ground state. A good trial wave function is especially crucial to a successful attack on the fermion problem for solid ^{3}He where not many results are available, and we believe that a CSWF for solid ^{3}He has all the physical ingredients to be a very good starting trial wave function.

The CSWF for solid ^{3}He is constructed as an antisymmetrized JN wave function that incorporates spin correlations among the ^{3}He particles, and in addition we add triplet (three-body) correlations to bring the equilibrium density and energy closer to the experimental values.

2. The coherent-state wave function for solid ^{3}He

In the coherent-state formulation, the spin coherent states are a family of spin states created by applying the rotation operator $\hat{R}(\theta, \phi)$ to the maximally spin-polarized state $|S, S\rangle$:

$$|\Omega\rangle = \hat{R}(\theta, \phi)|S, S\rangle = \mathrm{e}^{\mathrm{i}\phi\hat{S}_z}\mathrm{e}^{\mathrm{i}\theta\hat{S}_y}|S, S\rangle \tag{1}$$

where $|\Omega\rangle$ is a unit vector on the sphere specified by polar and azimuthal angles $0 \leqslant \theta \leqslant \pi$, $0 \leqslant \phi < 2\pi$ and the state $|S, S\rangle$ is the eigenstate of $\hat{S}_z$ with the largest possible eigenvalue. With this definition, there is a one-to-one correspondence between the coherent states and points on the unit sphere except for the case of the south pole.

For spin $\sigma = 1/2$ particles which is the case that we will consider here, the expansion is especially simple:

$$|\Omega\rangle = \omega_\uparrow(\Omega)|\uparrow\rangle + \omega_\downarrow(\Omega)|\downarrow\rangle \tag{2}$$

where the coefficients are given by

$$\omega_\uparrow(\Omega) = \langle\uparrow|\Omega\rangle = \cos\left(\frac{\theta}{2}\hbar\right)\exp\left(\frac{\mathrm{i}}{2}\phi\hbar\right) \tag{3}$$

and

$$\omega_\downarrow(\Omega) = \langle\downarrow|\Omega\rangle = \sin\left(\frac{\theta}{2}\hbar\right)\exp\left(-\frac{\mathrm{i}}{2}\phi\hbar\right). \tag{4}$$

In the coherent spin representation any spin operator $\hat{O}$ can be represented in a form that looks like a diagonal operator:

$$\hat{O} = \int \frac{\mathrm{d}\vec{\Omega}}{2\pi} \, |\Omega\rangle f(\Omega) \langle\Omega| \tag{5}$$

where $f(\Omega)$ is, in general, a non-unique, c-valued function of the angles (θ, ϕ) and $\mathrm{d}\vec{\Omega} = \mathrm{d}\theta \sin(\theta)\, \mathrm{d}\phi$ is an element of solid angle. In general, if the operator $\hat{O}$ is linear in the quantum spin $\hbar\vec{\sigma}$, then the corresponding $f(\Omega)$ is also linear in $\vec{\Omega}$; for example, $\vec{\sigma}_i \cdot \vec{\sigma}_j$ goes over to $\vec{\Omega}_i \cdot \vec{\Omega}_j$.

We describe solid ^{3}He by an antisymmetrized JN wave function that contains explicitly the spin-dependent correlations through the coherent spin representation and is written as

$$|\Psi\rangle = \int \mathrm{d}\vec{\Omega}(N) \, |\Omega(N)\rangle \exp\left[\sum_{i<j}^{N} u(|\vec{r}_i - \vec{r}_j|)\right] \exp\left[\sum_{i<j}^{N} u_\sigma(|\vec{r}_i - \vec{r}_j|)\vec{\Omega}_i \cdot \vec{\Omega}_j\right] \langle\Omega(N)|\Phi\rangle \tag{6}$$

where $|\Phi\rangle = \mathrm{Det}\{\varphi_{\vec{s}_j}(\vec{r}_i)\}$ is the antisymmetrized determinant of Gaussian orbitals localized around the sites of a solid lattice. The two-body Jastrow correlation pseudopotential, $u(r)$, is taken to be of McMillan form [11]:

$$u(r) = -\frac{1}{2}\left(\frac{b}{r}\right)^5 \tag{7}$$

where b is chosen variationally.

We use a shorthand notation where $|\Omega(N)\rangle$ represents the many-spin state $|\Omega_1 \cdots \Omega_N\rangle$, $\mathrm{d}\vec{\Omega}(N)$ is the whole set of variables $\mathrm{d}\vec{\Omega}_1 \cdots \mathrm{d}\vec{\Omega}_N$ and $\langle\Omega(N)|\Phi\rangle$ is the modified determinant of Gaussian orbitals within the coherent spin representation. For each spin-$\sigma = 1/2$ particle, the spin state is specified as being 'up' $|\uparrow\rangle$ or 'down' $|\downarrow\rangle$ and the full overlap $\langle\Omega(N)|\Phi\rangle$ is expressed as a determinant of modified single-particle orbitals of the form

$$\langle\Omega(N)|\Phi\rangle = \mathrm{Det}(M_{ij}) \tag{8}$$

where $M_{ij} = \varphi_{\vec{s}_j}(\vec{r}_i)\langle\Omega_i|\sigma_j\rangle$ and

$$\sigma_j = \begin{cases} \uparrow & j = 1, \ldots, N/2 \\ \downarrow & j = N/2+1, \ldots, N. \end{cases} \tag{9}$$

The single-particle states $\varphi_{\vec{s}_j}(\vec{r}_i)$ where particle i occupies the jth solid lattice site $\vec{s}_j$ are taken as Gaussian orbitals, $\varphi_{\vec{s}_j}(\vec{r}_i) = \exp[-C(\vec{r}_i - \vec{s}_j)^2]$, where the localization strength C is a parameter to be optimized variationally. The spin-dependent pseudopotential has been taken to be of the backflow form [10] and is written as

$$u_\sigma(r) = -\lambda \exp\left[-\left(\frac{r - r_0}{w}\right)^2\right]\left(\frac{L/2 - r}{L/2}\right)^3 \tag{10}$$

where L is the size of the cubic simulation box and N is the number of particles used in the simulation. At the two-body level, spin-singlet pairs and spin-triplet pairs are correlated differently using the CSWF. The effect can be similar to backflow, which correlates states with different wave vectors differently. Recent calculations have shown that spin correlations can give results quantitatively similar to backflow [12]. The fact that the energy per particle obtained from the CSWF for liquid ^{3}He agrees very well when compared to the Jastrow–Slater (JS) wave function with backflow correlations (JSB) indicates that the CSWF provides a good representation of the true spin correlations.

The inclusion of the triplet correlations in the CSWF follows the same formalism as was given by Schmidt *et al* [13], where we use a modified Jastrow pseudopotential instead of the original one:

$$\tilde{u}(r) = u(r) + \frac{\lambda_T}{2}\xi^2(r)r^2 \tag{11}$$

and we then multiply the CSWF of equation (6) for the modified Jastrow pseudopotential by a term of the form

$$\exp\left[-\frac{\lambda_T}{4}\sum_{l=1}^{N}\vec{G}(\vec{r}_l)\cdot\vec{G}(\vec{r}_l)\right]$$

where

$$\vec{G}(\vec{r}_l) = \sum_{j\neq l}^{N}\xi(|\vec{r}_l - \vec{r}_j|)(\vec{r}_l - \vec{r}_j). \tag{12}$$

The parametrization of $\xi(r)$ is done as follows:

$$\xi(r) = \exp\left[-\left(\frac{r - r_T^0}{w_T}\right)^2\right]\left(\frac{r - R_T}{R_T}\right)^3 \tag{13}$$

where in total there are three new variational parameters that describe the triplet correlations: the strength λ_T, the peak position r_T^0 and the width w_T of the Gaussian factor of the triplet function. The cut-off R_T should be chosen equal to $L/3$ in order to avoid counting different images of the same triplet, but as $\xi(r)$ is very short ranged and is almost zero at $L/3$, even larger cut-off values, as reported in literature, can be used without trouble.

3. Results and discussion

As an explicit test of this wave function, we present the results of a VMC calculation for bcc solid ^{3}He. This is an appropriate test system because it has been the subject of extensive numerical investigation [14] and, in addition, there is strong evidence that spin-dependent correlations can play a major role in determining its ground-state properties. We computed the energy per particle of bcc solid ^{3}He at several densities by considering the standard Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^2 + \sum_{i<j}^{N} v(|\vec{r}_i - \vec{r}_j|) \tag{14}$$

where $v(r)$ is the two-body HFDHE2 Aziz potential. The choice of this potential is due to its wide and successful application both to the liquid phase and to the solid phase of ^{4}He. It is believed, although we are not aware of any proof, that the potential between ^{3}He atoms should be almost the same as that for ^{4}He atoms.

We performed VMC simulations at several densities of bcc solid ^{3}He for $N = 16$ and $N = 54$ particles. Finite-size effects on the binding energy per particle have been estimated at the equilibrium density and have been found to be of about 0.15 K. Unlike the simulations for liquid ^{3}He [10], those for solid ^{3}He were statistically stable for $N = 54$ particles as well. The simulations were performed using the Metropolis algorithm [15]. Initial coordinates are chosen for each particle; typically they are either on a lattice or are a result of a previous Monte Carlo run. The particles are then moved one by one to new trial positions. For a simulation with N particles, the size of the cubic simulation box was taken as $L = (N/\rho)^{1/3}$, compatible with the density ρ, and periodic boundary conditions were always considered.

We started the simulation from an initial configuration of bcc type with either antiferromagnetic (AF) or u2d2 nuclear-spin ordering, and optimized the variational parameters of the CSWF. For $N = 16$ particles the optimal value for the Jastrow pseudopotential parameter was $b = 2.84$ Å; for the spin–spin pseudopotential parameters the optimal values were $\lambda = -5$, $r_0 = 2.4$ Å, $w = 1.3$ Å and for the Gaussian orbital $C = 0.40$ Å^{-2}.

When we extended the simulation to $N = 54$ particles we had to reoptimize these variational parameters; however, we always found the same energy per particle (within the statistical error) whether we had AF or u2d2 spin ordering. This is to be expected since the difference in energy amongst different spin configurations does not exceeds a few mK per particle. The CSWF for bcc solid ^{3}He allows us to incorporate spin correlations into the wave function and has the advantage of not freezing the spin structure, so the problems encountered with the Shadow–Slater-backflow (ShSB) wave function by Pederiva *et al* [16] when exchange moves of particles with different spin assignments were turned on were not observed.

In principle, analogous problems would arise whenever a frozen spin structure was used, so the main advantage of using the CSWF is the possibility that it affords for allowing spins to arrange their structure.

In table 1 we report the energy per particle for bcc solid ^{3}He at several densities obtained from a VMC simulation with $N = 54$ particles using the CSWF. The inclusion of the triplet correlations into the trial variational many-body wave function was done by modifying the Jastrow pseudopotential and adding the triplet term as previously explained.

Table 1. Total energy per particle at several densities corresponding to bcc solid ^{3}He obtained from a VMC simulation with $N = 54$ particles using the coherent-state wave function (CSWF) and the CSWF with triplet correlations (CSWF + T).

N	ρ (Å^{-3})	Potential	Wave function	E/k_B (K)
54	0.025 091	HFDHE2	CSWF	0.98 ± 0.03
54	0.025 091	HFDHE2	CSWF + T	0.42 ± 0.04
54	0.026 349	HFDHE2	CSWF	1.54 ± 0.03
54	0.026 349	HFDHE2	CSWF + T	0.91 ± 0.04
54	0.027 373	HFDHE2	CSWF	2.55 ± 0.03
54	0.027 373	HFDHE2	CSWF + T	1.67 ± 0.04

To find the optimal variational parameters for Jastrow and triplet correlations we used the Euler Monte Carlo (EMC) method of Moroni *et al* [17], which combines the reweighting method for variance minimization with a technique which makes use of the derivatives of the local energy with respect to the expansion parameters. In table 1 we also show the energy per particle obtained when we added the triplet correlations into the wave function (CSWF + T) for the same densities. As can be seen from the results in table 1, the triplet correlations play an important role for solid ^{3}He, lowering the energy per particle by more than 0.5–0.6 K.

In table 2 we show the energy per particle for bcc solid ^{3}He at density $\rho = 0.026\,349$ Å^{-3} obtained from a VMC simulation with $N = 54$ particles using firstly the CSWF and secondly the CSWF + T wave function (with added triplet correlations). We compare our results with the respective results of Pederiva *et al* [16], who used a ShSB wave function that also contains triplet correlations.

Finally, in table 3 we show the optimal values of the variational parameters of the CSWF with and without triplet correlations used in our VMC simulation of bcc solid ^{3}He with $N = 54$ particles. Setting to zero the triplet correlations, we recalculated the energy corresponding to the CSWF. As the backflow + triplet correlations were optimized together, the Jastrow correlations may still need reoptimization once we turn off the triplet correlations, although

Table 2. Total energy per particle at density $\rho = 0.026\,349$ Å^{-3} ($\rho\sigma^3 = 0.440$, $\sigma = 2.556$ Å) for bcc solid ^{3}He. All of the VMC results are obtained from a simulation with $N = 54$ particles using the coherent-state wave function (CSWF) and the CSWF with triplet correlations (CSWF + T). We compare our results with the results of Pederiva *et al* [16] using the Shadow–Slater-backflow (ShSB) wave function when the initial configuration of spins has a normal antiferromagnetic order (ShSB–NAF) and when an exchange of particles with different spin assignments is tried (ShSB + exchange). In all cases we use the HFDHE2 potential.

N	ρ (Å^{-3})	Potential	Wave function	E/k_B (K)
54	0.026 349	HFDHE2	CSWF	1.54 ± 0.03
54	0.026 349	HFDHE2	CSWF + T	0.91 ± 0.04
54	0.026 349	HFDHE2	ShSB–NAF	1.382 ± 0.023
54	0.026 349	HFDHE2	ShSB + exchange	2.405 ± 0.042

Table 3. The variational parameters of the CSWF and CSWF + T used in the simulation of bcc solid ^{3}He with $N = 54$ particles.

N	Wave function	b (Å)	λ	r_0 (Å)	w (Å)	c (Å^{-2})	λ_T (Å^{-2})	r_T^0 (Å)	w_T (Å)
54	CSWF	2.86	−2.1	1.8	1.3	0.35	—	—	—
54	CSWF + T	2.86	−2.1	1.8	1.3	0.35	−3.22	1.758	1.61

even when we do not do this, we clearly see a strong triplet contribution on lowering the energy per particle.

In figure 1 we show two different spin-dependent pseudopotentials $u_\sigma(r)$ that we use to see the influence of different spin pseudopotentials on the spin-resolved radial distribution functions. The first one (solid line) is chosen to have its peak at an interparticle distance less than 2 Å where the chance of finding two particles is very small because of the hard-core repulsion of the HFDHE2 pair potential, while the second (dashed line) is peaked at an interparticle distance of about 3 Å. For these two different spin–spin pseudopotentials we computed the spin-resolved radial distribution functions, $g^{\uparrow\uparrow}(r)$ and $g^{\uparrow\downarrow}(r)$, and the total radial distribution function, $g(r) = g^{\uparrow\uparrow}(r) + g^{\uparrow\downarrow}(r)$, at several densities. The spin-parallel

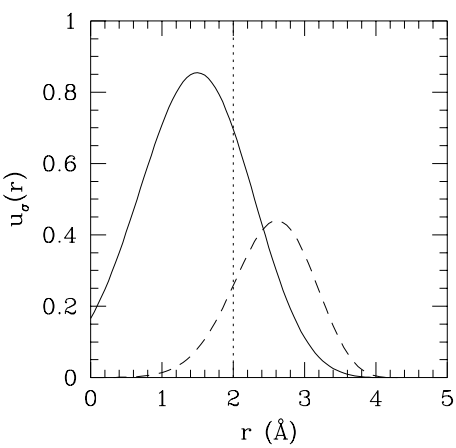

Figure 1. Two different spin–spin pseudopotentials $u_\sigma(r)$ used in a VMC simulation with $N = 16$ particles to test the influence of different forms of spin-correlation pseudopotentials on the spin-resolved radial distribution function for bcc solid ^{3}He at density $\rho = 0.025\,091$ Å^{-3}.

and spin-antiparallel radial distribution functions $g^{\uparrow\uparrow}(r)$ and $g^{\uparrow\downarrow}(r)$ are plotted in figure 2 for bcc solid ^{3}He at the density $\rho = 0.025\,091$ Å^{-3}. We see that at distances where the spin-dependent correlation pseudopotential is more effective (dashed line), both spin orderings, ($\uparrow\uparrow$) and ($\uparrow\downarrow$), are affected and the tendency is to increase the spin-parallel radial distribution function $g^{\uparrow\uparrow}(r)$, by simultaneously decreasing the spin-antiparallel radial distribution function $g^{\uparrow\downarrow}(r)$. The overall equation of state of liquid and solid ^{3}He is shown in figure 3. For the sake of completeness we have also included some results for liquid ^{3}He, although our main interest was the study of bcc solid ^{3}He. We show the energy per particle for bcc solid ^{3}He for several densities obtained from a VMC simulation with $N = 54$ particles using the CSWF and the CSWF + T wave functions.

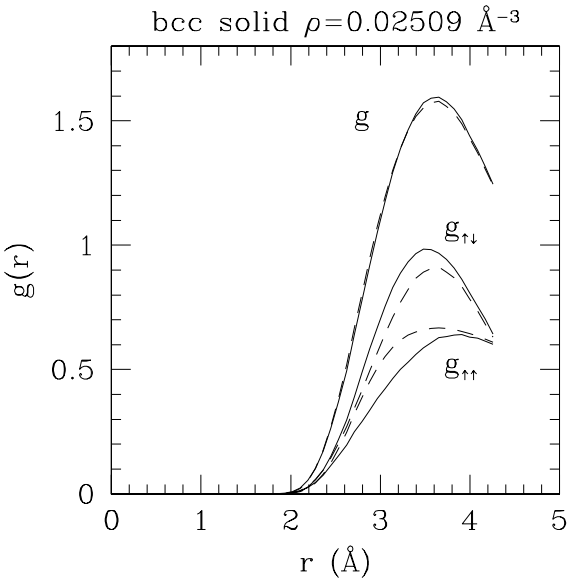

Figure 2. The spin-parallel ($g^{\uparrow\uparrow}(r)$), spin-antiparallel ($g^{\uparrow\downarrow}(r)$) and total ($g(r)$) radial distribution functions for bcc solid ^{3}He at density $\rho = 0.025\,091$ Å^{-3} obtained using the CSWF with the two different spin–spin pseudopotentials (solid and dashed lines) shown in figure 1.

The VMC results for the CSWF + T wave function constitute a sizable improvement upon the ShSB wave function, although there is still a significant discrepancy with the experimental results for bcc solid ^{3}He taken from Pandorf and Edwards [18].

Previous diffusion Monte Carlo (DMC) calculations for bcc solid ^{3}He carried out using an unsymmetrized JN wave function [19] and fixed-node DMC calculations [17] for liquid ^{3}He have given an energy per particle well above the experimental values. Such discrepancies are too large to be attributed to imperfections in the potential. In the context of solid ^{3}He studies, these results seem to suggest that the bcc solid ^{3}He phase is correctly stabilized only by an antisymmetrized ground-state wave function that may be not very different from the CSWF + T wave function that we are using.

In the case of liquid ^{3}He studies it has been suggested that the discrepancies between fixed-node DMC simulations, fixed-node GFMC simulations [20] and experiment arise from the nodal surface of the trial JSB wave function not being accurate enough. However, in recent work by Casulleras and Boronat [21] it is shown that the fixed-node method combined with the released-node technique and a systematic method for analytically improving the nodal surface constitutes a very efficient strategy for improving the calculation of the energy and

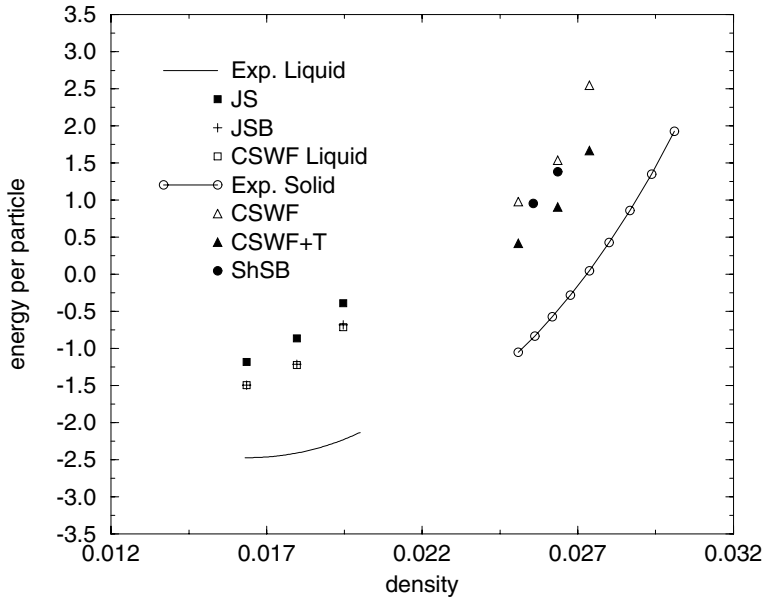

Figure 3. The equation of state of liquid and solid ^{3}He. The density is expressed in Å^{-3} while the energy per particle is expressed in K. The experimental energy per particle for liquid ^{3}He is taken from Aziz and Pathria [24]. The energies per particle for liquid ^{3}He with a Jastrow–Slater (JS), a Jastrow–Slater-backflow (JSB) and a coherent-state wave function (CSWF liquid) are the results of a VMC simulation with $N = 14$ particles, as reported by Lawson *et al* [10]. The experimental energy per particle for bcc solid ^{3}He is taken from Pandorf and Edwards [18]. The open and filled triangles represent the VMC results of this work for bcc solid ^{3}He obtained using respectively the CSWF and the CSWF with triplet correlations (CSWF + T). Filled circles represent the results of Pederiva *et al* [16] obtained using the Shadow–Slater-backflow (ShSB) wave function which contains the triplet correlations implicitly because of its structure. All results for bcc solid ^{3}He refer to simulations with $N = 54$ particles.

related quantities up to a desired accuracy. The combination of the above methods into a DMC calculation for liquid ^{3}He allowed them to perform a very accurate microscopic calculation of the equation of state for liquid ^{3}He, including obtaining a prediction for the negative-pressure region and the spinodal density. The fact that this general approach has successfully dealt with liquid ^{3}He suggests that it could also be useful for other Fermi systems including solid ^{3}He. As far as the fixed-node framework is concerned, the choice of an accurate trial wave function used for importance sampling constitutes the most crucial step. VMC calculations for liquid and solid ^{4}He with shadow-type wave functions [22] strongly indicate the relevance of many-body correlations for improving the trial wave function. The relevance of four- and five-body correlations has been recently investigated for small clusters [23]. At this point we speculate that a CSWF + T wave function that incorporates triplet correlations may constitute a very good trial wave function for use in importance sampling in a fixed-node DMC simulation for solid ^{3}He.

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