

Quantum Monte Carlo Simulations of Solid ^4He

P.A. Whitlock¹ and S.A. Vitiello²

¹ Computer and Information Science Department,
Brooklyn College, CUNY Brooklyn, NY 11210, USA
`whitlock@brooklyn.cuny.edu`

² Instituto de Física, Universidade Estadual de Campinas,
13083 Campinas — SP, Brazil
`vitiello@ifi.unicamp.br`

Abstract. Recent experimental investigations [20] of solid ^4He have been interpreted as showing possible superfluidity in the solid at low temperatures, below 0.2 K. A solid behaving this way, exhibiting both long range translational order and superfluidity, has been called a supersolid phase. The existence of a supersolid phase was proposed many years ago [1], and has been discussed theoretically. In this paper we review simulations of the solid state of bulk ^4He at or near absolute zero temperature by quantum Monte Carlo techniques. The techniques considered are variational calculations at zero temperature which use traditional Bijl-Dingle-Jastrow wavefunctions or more recently, shadow wavefunctions; Green's function Monte Carlo calculations at zero temperature; diffusion Monte Carlo, and finally, the finite temperature path integral Monte Carlo method. A brief introduction to the technique will be given followed by a discussion of the simulation results with respect to solid helium.

1 Introduction

After many years of investigation, the properties of the solid phases of bulk, ^4He , were felt to be well understood [3]. At temperatures near absolute zero, ^4He exists in both the solid and fluid states. The crystalline structure is known to exhibit hexagonal closest packing (hcp) rather than the face centered cubic packing expected for a three-dimensional hard sphere system. Even at absolute zero, the atoms exhibit zero point motion around their lattice positions which leads to a very “loose” solid at densities near melting. In the 1960's, Andreev and Lifshitz [1] proposed that such quantum solids could sustain superfluidity. One indicator of the onset of superfluidity is the Bose-Einstein condensate, the fraction of the atoms condensed into the zero momentum state. The condensed atoms acquire quantum mechanical coherence over macroscopic length scales. Quantum Monte Carlo simulations observed a Bose-Einstein condensate of several percent in liquid ^4He systems [34]; but only detected a condensate in a quantum solid when the atoms were interacting with a Yukawa potential [6].

Interest has been recently renewed by the torsional oscillator experiments of Kim and Chan [20]. Ultrahigh-purity ^4He was confined in a torsion cell and subjected to pressures between 26 and 66 bars to reach the solid phase. A non-classical rotational inertia fraction that can be associated with superflow was

observed at temperatures below 230 milliKelvin. These observations have led to renewed interest in the measurements of the Bose-Einstein condensate and other measures of superfluidity in simulations of the properties of solid helium.

^4He systems may be studied theoretically by solving the appropriate Schrödinger or Bloch equation. At absolute zero, the behavior of an N body helium system is described by the eigenfunction of the Schrödinger equation in $3N$ dimensional space:

$$[-\nabla^2 + V(R)]\Psi_0(R) = E_0\Psi_0(R) \quad (1)$$

where $R \equiv \{\mathbf{r}_i \mid i = 1, \dots, N\}$ and the \mathbf{r}_i are the positions of the individual atoms. $V(R)$ represents the interaction potential between the atoms in the system. The term $[-\nabla^2 + V(R)]$ is the Hamiltonian, H , for the system and is written here in dimensionless form. Knowledge of the physical relationships between the atoms can be built into a parametrized mathematical form for a trial wavefunction, $\Psi_T(R)$, an approximation to $\Psi_0(R)$. The variational energy can be minimized with respect to the parameters through the Monte Carlo evaluation of the expectation value of the ground energy, E_0 . This technique is referred to as variational Monte Carlo (VMC). Approaches where the simulation results are subject only to statistical uncertainties are referred to as Quantum Monte Carlo (QMC) methods. In the Green's function Monte Carlo (GFMC) method the integral transform of the Schrödinger equation, (1), is iterated by performing a random walk in the configuration space of the N atoms to yield an asymptotically exact solution. Such a solution can also be obtained by sampling a short time Green's function followed by an extrapolation of the results to account for the time step errors introduced by the approximation. This technique is known as diffusion Monte Carlo (DMC). Finally, finite temperature systems may be studied by considering the Bloch Equation:

$$[-\nabla^2 + V(R) + \partial/\partial t]\varrho_B(R, t) = 0, \quad (2)$$

where $\varrho_B(R, t)$ is the many-body density matrix. Path integrals [12, 16] Monte Carlo (PIMC) simulations can be performed and for small enough temperature intervals, the density matrix can be compared to the ground state eigenfunction from (1).

In the following sections, the results of applying the techniques outlined above to the simulation of solid ^4He will be described.

2 Variational Monte Carlo Methods

Given a trial wavefunction, $\Psi_T(R)$, an estimator for the variational energy,

$$E_T = \frac{\langle \Psi_T | H | \Psi_T \rangle}{\langle \Psi_T | \Psi_T \rangle} \geq E_0, \quad (3)$$

is an upper bound to the true ground state energy E_0 of the system. The lowest variational energy is obtained through a minimization process with respect to the parameters in $\Psi_T(R)$. In the coordinate representation (3) becomes:

$$E_T = \frac{\int dR \Psi_T^*(R) H \Psi_T(R)}{\int dR |\Psi_T(R)|^2} = \int dR \pi(R) E_L(R), \quad (4)$$

where $dR \equiv d^3\mathbf{r}_1 d^3 \dots \mathbf{r}_N$. The last term of the above equation, $E_L(R)$, the local energy, is obtained by multiplying and dividing the numerator of (3) by $\Psi_T(R)$,

$$E_L(R) = \frac{H \Psi_T(R)}{\Psi_T(R)}, \quad (5)$$

and $\pi(R)$ is a normalized probability distribution function,

$$\pi(R) = \frac{|\Psi_T(R)|^2}{\int dR |\Psi_T(R)|^2}. \quad (6)$$

2.1 Trial Wavefunctions

As point out by Feenberg [11] a plausible general form for the exact ground-state wavefunction of a system of N interacting bosons is

$$\Psi(R) = \prod_{i<j} f_2(r_{ij}) \prod_{i<j<k} f_3(i, j, k) \prod_{i<j<k<l} f_4(i, j, k, l) \dots \quad (7)$$

$$= \exp \frac{1}{2} \left[\sum_{i<j} u(r_{ij}) + \sum_{i<j<k} u_3(i, j, k) + \sum_{i<j<k<l} u_4(i, j, k, l) \right] \dots \quad (8)$$

In the liquid phase, the simplest variational function, the so called Bijl-Dingle-Jastrow or Jastrow trial function, considers only a single term of the above expression: $u_2(r_{ij})$. The first computer simulation for a system of helium atoms was performed by McMillan [22] using $u_2(r) = b/r^5$ and reasonable results were obtained. A better approximation to the variational wavefunction which included three-body correlations [28], $u_3(i, j, k)$, led to an improvement of about 10% in the estimated values of the energies.

For the solid phase, the usual approach was to write the trial wavefunction as

$$\psi_{Tsol}(R) = \prod_{i<j} f_2(r_{ij}) \Phi(R), \quad (9)$$

where $\Phi(R)$ is a model function, ideally, a permanent of localized single particle orbitals. However, since the effect of the quantum statistics on the energy is minor, $\Phi(R)$ is left unsymmetrized. Gaussian orbitals were used in simulations performed by Hansen and Levesque [14] with reasonable results. The inclusion of triplet correlations, $f_3(i, j, k)$, in the trial wavefunction lead to an improvement of about 15% in the simulations results [32]. The introduction of higher-order correlations in a trial wavefunction has become feasible by introducing the shadow wavefunction [30], discussed more fully below.

The functional form of correlation factors in a trial wavefunction can be fully optimized. The idea is to write the correlation factors as a sum of the elements of a basis set [31]. For the two-body correlation factor,

$$f(r) = \sum_{n=1}^M c_n f_n(r), \quad (10)$$

where the f_n are functions of the basis set and the c_n are variational parameters. If the basis is well chosen, a small value of M is sufficient to recover all the energy associated with the correlation under consideration. For (10), a very suitable basis is the one obtained by solving for the lowest M energy states of the Schrödinger-like equation involving a pair of helium atoms,

$$\left(-\frac{\hbar}{2m}\nabla^2 + V(r)\right) f_n(r) = \lambda_n f_n(r). \quad (11)$$

The boundary conditions are such that at a distance d , chosen as a cutoff or eventually as a variational parameter, the functions f_n go smoothly to 1 or to a function that gives the correct long range behavior of the system. One of the advantages of this method is to automatically obtain an optimal correlation at small values of r . Since, the wavefunction is small when $r \rightarrow 0$, it is difficult to sample this very important region of configuration space. Thus, the usual Monte Carlo optimization of the trial function, does not perform well at small r .

2.2 Monte Carlo Techniques

The simulation starts by sampling the normalized probability distribution $\pi(R)$ of (6), *i. e.*, by constructing a sequence of points $\{R_i | i = 1, \dots, M\}$ in the configuration space. More formally we require [19] that R_i belong to the sequence with probability given by

$$Pr\{R_i\} = \int_{\Omega} dR \pi(R) \quad (12)$$

for any $\Omega \subset \Omega_0$ of the sample space Ω_0 . The sampling in most cases is performed using the Metropolis [23] algorithm.

If we consider M independent samples, the variational energy is estimated as

$$E_M = \frac{1}{M} \sum_{i=1}^M E_L(R_i). \quad (13)$$

In the limit of large M we have $E_M \rightarrow E_T$. This energy is obtained without any uncontrolled approximations or nonconvergence for any form of the wavefunction and is subject only to statistical uncertainties of $\mathcal{O}(M^{-1/2})$. The statistical error is easily estimated. Variance reduction techniques, *e. g.* importance sampling, can be used to reduce the multiplicative factor that appears in the calculation of the error. Other properties of the system can also be readily estimated.

2.3 Variational Results on Solid ^4He

The earliest variational calculations could not differentiate between a crystal with fcc packing and one with hcp order. Chester [10] showed that a Jastrow

wavefunction, $\Psi_T(R) = \prod_{i<j} f(r_{ij})$, supports a Bose-Einstein condensate. However, this pair product form without the localization provided by $\phi(r)$, as in (9), only crystallizes at a very high density [15]. Therefore the use of gaussian one-body orbitals, $\phi(r)$, was introduced. This, however, precluded the observation of a Bose-Einstein condensate.

Recently, Vitiello considered in great detail the question of the ground-state structure of solid helium using the most recent he-he potential of interaction. Performing careful variational calculations and employing reweighting, he was able to show that the hcp order is favored in the ^4He system [29].

2.4 Shadow Wavefunction Calculations

The construction of trial functions based on the inclusion of auxiliary variables, “shadow particles”, is a very successful approach within the variational methods. These trial functions are particular representations of the Feenberg form [11], where one is able to introduce tractable correlations up to the number of particles

$$\Psi_{Sh}(R) = \prod_{i<j} f(r_{ij}) \prod_{i<j<k} f_{ijk}^{(3)} \cdots \prod_{i<j\dots<w} f_{ij\dots w}^{(N)}. \quad (14)$$

The variational shadow wavefunction is defined in terms of an integral over auxiliary variables $S \equiv \{\mathbf{s}_i | i = 1, \dots, N\}$ in the whole space

$$\Psi_{Sh}(R) = \int \Xi(R, S) dS, \quad (15)$$

where Ξ is a function that includes a factor of the Jastrow form dependent solely on the configuration space coordinates R , a Gaussian coupling between the space variables \mathbf{r}_i and the auxiliary variables \mathbf{s}_i , and a term of the Jastrow form that correlates the \mathbf{s}_i among themselves:

$$\Xi(R, S) = \exp \left(- \sum_{i<j} \frac{1}{2} \left(\frac{b}{r_{ij}} \right)^5 - \sum_i C |\mathbf{r}_i - \mathbf{s}_i|^2 - \sum_{i<j} \gamma V(\delta s_{ij}) \right). \quad (16)$$

In this formulation $\Psi_{Sh}(R)$ depend on the He-He interacting potential and four variational parameters: b , C , γ and δ . Since the auxiliary variables, due to the last term of Eq. (16), are isomorphic to the coordinates of a system of particles interacting through V , we call the auxiliary variables shadow particles.

A trial wavefunction that can correlate all the atoms in the system is important by itself. In addition, there are strong physical motivations to deal with such a class of variational wavefunctions: Feynman’s path integrals in imaginary time and justifications from projection methods.

Shadow wavefunctions have enabled the investigation of disorder phenomena in solid ^4He such as vacancies [24] or the interfacial region between a solid and a liquid at coexistence [25] by variational calculations. This is possible because with the shadow wavefunction approach both the fluid phase and solid phases can be described, without the introduction of single particle orbitals. Moreover the Bose symmetry is manifestly maintained and so relaxation around non-localized defects are allowed.

3 Green's Function Monte Carlo

If the potential energy in (1) is bounded from below $V(R) \geq -V_0$, (1) can be rewritten as:

$$[-\nabla^2 + V(R) + V_0]\Psi_0(R) = (E_0 + V_0)\Psi_0(R). \quad (17)$$

A Green's function,

$$[-\nabla^2 + V(R) + V_0]G(R, R_0) = \delta(R - R_0) \quad (18)$$

can be derived with the same boundary conditions as $\Psi_0(R)$ and used to transform (17) into an integral equation:

$$\Psi_0(R) = (E_0 + V_0) \int G(R, R')\Psi_0(R')dR'. \quad (19)$$

Since the ground-state wavefunction and Green's function for a Bose system are non-negative; the ground state wavefunction and approximations to it may be treated as probability distribution functions. The Green's function may also be used as a distribution function for R conditional on the previous position R' . The integral version of the Schrödinger equation, (19), is solved by a Neumann iteration starting with a zeroth order approximation, such as a trial wavefunction optimized in a variational calculation. A population of points $\{R'\}$ is sampled from $\Psi_T(R')$ and a new set of points $\{R\}$ is sampled from $(E_t + V_0)G(R, R')$ where E_t is an approximation to the ground-state energy. As this process is repeated, at the n^{th} iteration the set of points $\{R'\}$ has been sampled from $\psi^{(n)}$ and the next generation of points, $n+1$, is sampled from:

$$\psi^{(n+1)}(R) = (E_t + V_0) \int G(R, R')\psi^{(n)}(R')dR'. \quad (20)$$

Equation (20) defines one step of a random walk whose asymptotic distribution is $\Psi_0(R)$. Since the simulation system is composed of N atoms with periodic boundary conditions, the Schrödinger equation has a discrete spectrum and the iterations are guaranteed to converge.

The procedure may be made computationally more efficient and the variance reduced by employing an importance sampling transformation [18]. Let $\Psi_T(R)$ be a trial wavefunction which may be the same as $\psi^{(0)}(R)$ and $\bar{\Psi}(R) = \Psi_T(R)\Psi(R)$, then (19) becomes

$$\bar{\Psi}(R) = (E + V_0) \int [\Psi_T(R)G(R, R')/\Psi_T(R)]\bar{\Psi}(R')dR'. \quad (21)$$

The sequence of functions obtained by iteration of the integral equation converges to $\Psi_T(R)\Psi_0(R)$ and E_t is chosen such that the random walk is stable.

Unfortunately, the Green's function, (18), is not known analytically owing to the complexity of the boundary conditions. However, to implement the algorithm represented by (20) or (21), it is not necessary to know the full Green's function;

it is sufficient to develop a method to sample configurations from $G(R, R')$. The Green's function may be written as,

$$G(R, R') = \int_0^\infty G(R, R', \tau) d\tau \quad (22)$$

$G(R, R', \tau)$ is the Green's function for a Bloch equation, (2),

$$(H + \partial/\partial\tau)G(R, R', \tau) = \delta(R - R')\delta(\tau). \quad (23)$$

For a given configuration, R_0 , a finite domain, $D(R_0)$, may be chosen such that the potential of interaction, $V(R)$, is bounded from above within the domain by the constant, $U(R_0)$. A domain Green's function may then be defined:

$$[-\nabla^2 + U(R_1) + \partial/\partial\tau]G_U(R_1, R_0, \tau) = \delta(R_1 - R_0)\delta(\tau) \quad (24)$$

subject to the boundary condition that $G_U(R_1, R_0, \tau) = 0$ whenever R_1 is on the boundary or outside of $D(R_0)$. Physically, (24) represents a diffusion process of a particle in a domain with a constant absorption rate and a perfectly absorbing boundary. Multiplying (18) by $G_U(R_1, R_0, \tau)$ and (24) by $G(R, R_1, \tau)$, integrating both equations over R_1 and subtracting the two resulting equations yields:

$$\begin{aligned} G(R, R_0, \tau) &= G_U(R, R_0, \tau) \\ &+ \int_{\partial D(R_0)} \left(\frac{\partial G_U(R_1, R_0, \tau - \tau_0)}{\partial n} \right) G(R, R_1, \tau_0) dR_1 \\ &+ \int_{D(R_0)} (U(R_0) - V(R_1)) G_U(R_1, R_0, \tau - \tau_0) G(R, R_1, \tau_0) dR_1 \end{aligned} \quad (25)$$

Equation (26) is a linear integral equation for $G(R, R_0, \tau)$ in terms of $G_U(R, R_0, \tau)$. In the second term of the right hand side of (26), the boundary condition for $G_U(R_1, R_0, \tau)$ has been used to convert a volume integral into a surface integral over $\partial D(R_0)$ and the derivative normal to the domain's surface, $\partial/\partial n$ has been introduced. The domain, $D(R_0)$ may be chosen in any convenient way; in particular, as the Cartesian product of three-dimensional spheres or cubes centered at R_0 . $G_U(R, R_0, \tau)$ is known analytically and may be interpreted as a conditional probability distribution function. Thus, points $\{R\}$ may be sampled by a random walk governed by (26) for any given set $\{R_0\}$.

An asymptotically unbiased estimator for the energy is given by

$$E_m = \frac{\int \Psi^n(R) H \Psi_T(R) dR}{\int \Psi^n(R) \Psi_T(R) dR}. \quad (26)$$

Except for statistical sampling and convergence errors, (26) is an exact estimator for the ground state energy. For other properties of the physical system, $F(R)$, that do not commute with the Hamiltonian, a "mixed" estimator may be defined as

$$\langle F \rangle_m = \frac{\int \Psi^n(R) F(R) \Psi_T(R) dR}{\int \Psi^n(R) \Psi_T(R) dR}. \quad (27)$$

If the trial wavefunction $\Psi_T(R)$ is “close” to the actual ground state wavefunction, $\Psi_T(R) = \Psi_0(R) + \delta\psi(R)$, then a linear extrapolation may be used to estimate the exact value to within an order δ^2 :

$$\langle F \rangle_x = 2\langle F \rangle_m - \langle F \rangle_T \quad (28)$$

where $\langle F \rangle_T$ is the variational value calculated with $\Psi_T(R)$. It was shown [34] that this extrapolation process gave the same expected value as the random walk based on the “forward walking” algorithm but with much smaller statistical errors. The extrapolated value was also shown to be independent of the trial wavefunction used.

As in variational calculations, the result of the GFMC simulations is a wavefunction represented as an ensemble of configurations of atomic positions. Through (27) and (28), the Bose-Einstein condensate fraction can be obtained for the helium system. The fraction of particles in the zero-momentum state is given by the asymptotic limit of $n(\mathbf{r})$,

$$n_0 = \lim_{r \rightarrow \infty} n(\mathbf{r}). \quad (29)$$

The one-body density matrix, $n(\mathbf{r})$, is a measure of the change in the wavefunction for given displacement r and is the fourier transform of the momentum distribution, $n(\mathbf{k})$:

$$\begin{aligned} n(\mathbf{r}) &= \int e^{i\mathbf{k}\cdot\mathbf{r}} n(\mathbf{k}) d\mathbf{k} \\ &= \left\langle \frac{\Psi(r_1, r_2, \dots, r_i + r, \dots, r_n)}{\Psi(r_1, r_2, \dots, r_i, \dots, r_n)} \right\rangle. \end{aligned} \quad (30)$$

The first calculation of the Bose-Einstein condensate in solid ${}^4\text{He}$ using the GFMC method [7] involved the trial wavefunction of Eq. (9) and the Lennard-Jones potential of interaction [4]. It was of course recognized that the form of the trial wavefunction that was used as an importance function might bias the results and, not surprisingly, the condensate fraction was less than 1%. Additional calculations [34], showed that the Lennard Jones potential itself was inadequate to describe the helium system. A further investigation of the Bose-Einstein condensate concluded that Ceperley, *et. al.* [6] observed a condensate because they used a translationally invariant wavefunction for the importance function. The GFMC simulations were repeated using a more realistic form for the potential of interaction, the HFDHE2 potential [2] and improved wave-functions [17]. However, no condensate fraction within statistical error was observed in the solid phase [35, 36].

In a variational calculation using a shadow wavefunction, when the density of a system of helium atoms reaches the appropriate value, a state with translationally broken symmetry is spontaneously produced. Thus, it was natural to introduce shadow wavefunctions as importance functions in GFMC calculations. In order to perform these calculations, Whitlock and Vitiello [33] made an extension to the GFMC method such that the shadow degrees of freedom were updated using the Metropolis algorithm according to the probability distribution of (16). Despite good results for some of the properties of the system, the

variance of the calculation did not encourage further attempts to compute the condensate fraction in the solid phase. However the idea of using the shadow wavefunction ideas in a QMC method seems promising.

3.1 Diffusion Monte Carlo

The time dependent Schrödinger equation in imaginary time $t \rightarrow it/\hbar$,

$$\frac{\partial \psi(R, t)}{\partial t} = -(-\nabla^2 + V(R) - E_t)\psi(R, t), \quad (31)$$

is equivalent to the classical diffusion equation with sources represented by $V(R)$. In (31), the Hamiltonian H has been written as the sum of the kinetic energy T , $-\nabla^2$, plus the potential energy $V(R)$ displaced by a trial energy E_t , which does not change the description of the state of the system.

In a short time approximation, the Green's function for (31) can be written to $\mathcal{O}(t)$ as,

$$G(R, R', \delta t) \approx \langle R | e^{-V(R)\delta t/2} e^{-T\delta t} e^{-V(R')\delta t/2} e^{E_t\delta t} | R' \rangle. \quad (32)$$

It is possible to rewrite the above expression as the product of a rate term,

$$w(R, R', \delta t) = \exp(-(V(R) + V(R'))\frac{\delta t}{2} + E_t\delta t), \quad (33)$$

times a propagator, identified as the Green's function for ordinary diffusion,

$$G_d(R, R', \delta t) = \langle R | e^{-T\delta t} | R' \rangle = (4\pi\delta t)^{-3N/2} \exp\left(-\frac{(R - R')^2}{4\delta t}\right). \quad (34)$$

In a simulation, for each R' in a given set of configurations, a new R is easily sampled from G_d and weighted by $w(R, R', \delta t)$. By repeating these steps and performing a suitable extrapolation to $t \rightarrow 0$, the results will yield an estimate of the ground-state energy if $E_t \approx E_0$. This is shown by writing the formal solution of the time dependent Schrödinger equation as

$$\psi(R, t) = \sum_i \varphi_i(R) e^{-i(E_i - E_t)t/\hbar}, \quad (35)$$

where the $\varphi_i(R)$ are an orthogonal basis set.

The method presented so far is very inefficient due to the branching process and because the random walk may explore unimportant regions of the configuration space. Here again an importance sampling transformation as in (21) allows the simulations to converge faster and more efficiently. If (31) is multiplied by a trial wavefunction ψ_T , it can be written in the coordinate representation as

$$\frac{\partial \bar{\psi}(R, t)}{\partial t} = -(-\nabla^2 + \nabla \cdot \mathbf{F}(\mathbf{R}) + \mathbf{F}(\mathbf{R}) \cdot \nabla - (E_t - E_L(R))\bar{\psi}(R, t), \quad (36)$$

where $\bar{\psi}(R, t) = \psi_T(R)\psi(R, t)$, $E_L(R)$ is the local energy and $\mathbf{F}(R) = 2\nabla \ln \psi_T(R)$. If we compare the above expression with equation (31), it still includes

a branching process, given by $\mathcal{V} = E_L(R) - E_t$. The diffusion process has a superimposed drift velocity given by the two last terms of the expression, $-\nabla^2 + \nabla \cdot \mathbf{F}(R) + \mathbf{F}(R) \cdot \nabla$.

By taking the short time approximation, as before we can write:

$$\bar{G}(R, R', \delta t) = \bar{W}(R, R', \delta t) \bar{G}_d(R, R', \delta t), \quad (37)$$

where

$$\bar{W}(R, R', \delta t) = \exp\left(-\frac{(E_L(R) + E_L(R'))\delta t}{2} + E_t\delta t\right), \quad (38)$$

and

$$\bar{G}_d(R, R', \delta t) = (4\pi\delta t)^{-3N/2} \exp\left(-\frac{(R - R' - \delta t\mathbf{F}(R))^2}{4\delta t}\right). \quad (39)$$

Simulations that include importance sampling converge to $\psi_T\psi$. Instead of computing $V(R)$, now we calculate E_L which approaches a constant as $\psi_T(R)$ goes to the true eigenfunction of the system. This is important since the simulations become much more stable. Moreover, the drift guides the random walk to the important regions of the configuration space.

4 Path Integral Monte Carlo

All static and, in principle, dynamic properties of a many-body quantum system, such as ${}^4\text{He}$, at thermal equilibrium, may be obtained from the density matrix, $\varrho(R, R', \beta)$, the solution to the Bloch equation, (2). β represents an inverse temperature or “imaginary time”, $\beta = 1/kT$. The solution to the Bloch equation can be written in the coordinate representation as:

$$\varrho(R, R', \beta) = \langle R | e^{-\beta H} | R' \rangle \quad (40)$$

For distinguishable particles, the density matrix is non-negative for all values of its arguments and can be interpreted as a probability distribution function. If two density matrices are convoluted together, a density matrix at a lower temperature results:

$$\langle R | e^{-(\beta_1 + \beta_2)H} | R' \rangle = \int \langle R | e^{-\beta_1 H} | R'' \rangle \langle R'' | e^{-\beta_2 H} | R' \rangle dR''. \quad (41)$$

The integral over R'' may be evaluated using a generalization of the Metropolis sampling algorithm [26, 8]. Starting at a sufficiently high temperature, the density matrix may be accurately written as an expansion in one and two-body density matrices. Then, multiple convolutions can be performed to reduce the temperature to near absolute zero.

The density matrix for a boson system such as ${}^4\text{He}$ is obtained from the distinguishable particle density matrix by using the permutation operator to project out the symmetric component,

$$\langle R | e^{-(\beta H)} | R' \rangle_B = \frac{\sum_{\wp} \langle \wp R | e^{-(\beta H)} | R' \rangle}{N!} \quad (42)$$

The sum over permutations is performed by a Monte Carlo technique.

To calculate the momentum distribution requires obtaining the off-diagonal parts of the density matrix. In one method, an atom is displaced off the diagonal by a distance \mathbf{r} while the other atoms and permutation are held fixed while $n(\mathbf{r})$, (30), is computed. This method is very accurate at small r . In a second method, one atom is again off the diagonal, but the distance between the two ends of the path for that atom is allowed to vary. This allows the calculation of $n(\mathbf{r})$ at large r [9].

Ceperley and Bernu [5] have found that the superfluid density observed in PIMC simulations of solid ^4He are strongly affected by the size of the system simulated. A 48 atom system exhibits a 1.2% superfluid density at 55 bars pressure while a 180 atom systems has zero superfluid density. They conclude that the phenomenon observed by Kim and Chan can not be explained by vacancies or interstitials in the equilibrium bulk ^4He system.

4.1 Path Integral Ground State Calculations

Ground state expectations values at finite temperatures can be efficiently calculated by using a path integral ground state Monte Carlo method [27]. The integral equation in imaginary time equivalent to the Schrödinger equation is

$$\psi(R, t) = \int G(R, R', t - t_0) \psi(R', t_0) dR'. \quad (43)$$

In the above equation, $G(R, R', t)$ is the propagator of (23). As was seen in the previous section, this propagator is viewed as density matrix operator corresponding to an inverse temperature β and simulated by path integrals.

The difference in the present method compared to PIMC is that a truncated path on a trial wavefunction is considered instead of periodic boundary conditions in imaginary time as the trace of $G(R, R', t)$ requires. Since the ground state eigenfunction can be obtained by filtering a suitable trial function ψ_T

$$\psi_0(R) = \lim_{t \rightarrow \infty} \psi(R, t) = \lim_{t \rightarrow \infty} \int G(R, R', t) \psi_T(R') dR', \quad (44)$$

the ground state expectation value of any operator can be written as

$$\langle \mathcal{O} \rangle = \frac{\langle \psi_0 | \mathcal{O} G(t) \mathcal{O} G(t') | \psi_T \rangle}{\langle \psi_0 | G(t) G(t') | \psi_T \rangle}. \quad (45)$$

If the convolution of the density matrix of (41) is divided into N time steps, $\beta/N = t/N = \delta t$,

$$G(R, R', t) = \int dR_1 dR_2 \cdots dR_{N-1} \rho(R, R_1, \delta t) \rho(R_1, R_2, \delta t) \rho(R_{N-1}, R', \delta t) \quad (46)$$

and substituted in (45), we obtain

$$\langle \mathcal{O} \rangle = \frac{\int \prod_{i=0}^N dR_i \mathcal{O}(R_N) \psi_T(R_0) \left(\prod_{i=0}^{N-1} \rho(R_i, R_{i+1}, \delta t) \right) \psi_T(R_N)}{\int \prod_{i=0}^N dR_i \psi_T(R_0) \left(\prod_{i=0}^{N-1} \rho(R_i, R_{i+1}, \delta t) \right) \psi_T(R_N)}, \quad (47)$$

where $R_0 = R$, $R_M = R'$ and R_M is an internal time slice. For a converged calculation, if the operator is placed on the extreme edges of the path one gets a mixed estimator. If R_M is in the middle, the exact expectation value of the ground state is obtained. The paths are sampled using the Metropolis algorithm. Samples that do not include coordinates of the trial wavefunction are performed as in PIMC.

Galli and Reatto [13] have employed this formalism using the shadow wavefunction as $\Psi_T(R)$ to study confined solid ^4He . Their model system contains a large static spherical object that uses a purely repulsive potential to prevent the helium atoms from reaching the center of the simulation cell. As a consequence of the periodic boundary conditions this correspond to a static lattice of hard core spheres. They observe that the freezing pressure increases to about 38 atm. This behavior is comparable to that found in experiments of ^4He confined in vycor [21]. In addition they observe that the disorder induced by the mismatch between the ^4He crystalline structure and the static hard spheres induces delocalization. This is a necessary condition to have off-diagonal long range order in the system. Also, the presence of a Bose-Einstein condensate requires delocalization of the atoms. These results could be relevant in explaining the observation of a supersolid phase for ^4He in vycor [21].

However, to date, no quantum Monte Carlo studies have observed delocalization or Bose-Einstein condensation in the pure bulk solid ^4He .

References

1. A.F. Andreev and L.M. Lifshitz: *Soviet Phys. JETP* **29** (1969) 1107
2. R.A. Aziz, V.P.S. Nain, J.S. Carley, W.L. Taylor, and G.T. McConville: An accurate intermolecular potential for helium. *J. Chem. Phys.* **70** (1979) 4330–4342
3. K.H. Bennemann and J.B. Ketterson, eds.: *The Physics of Liquid and Solid Helium*. Wiley, New York (1976)
4. J. de Boer and A. Michels: Contribution to the Quantum Mechanical Theory of the Equation of State and the Law of Corresponding States. Determination of the Law of Force of Helium. *Physica (Utrecht)* **5** (1938) 945–957
5. D.M. Ceperley and B. Bernu: Ring Exchanges and the Supersolid Phase of ^4He . *Phys. Rev. Lett.* **93** (2004) 155303-1–4
6. D.M. Ceperley, G.V. Chester, and M.H. Kalos: Monte Carlo study of the ground state of bosons interacting with Yukawa potentials. *Phys. Rev. B* **17** (1978) 1070–1081
7. D.M. Ceperley, G.V. Chester, M.H. Kalos, and P.A. Whitlock: Monte Carlo Studies of Crystalline Helium. *Journal de Physique* **39 Colloque C6** (1978) 1298–1304
8. D.M. Ceperley and E.L. Pollock: Path-integral computation of the low-temperature properties of liquid ^4He . *Phys. Rev. Lett.* **56** (1986) 351–354
9. D.M. Ceperley and E.L. Pollock: The momentum distribution of normal and superfluid liquid ^4He . *Can. J. Phys.* **65** (1987) 1416
10. G.V. Chester: Speculations on Bose-Einstein Condensation and Quantum Crystals. *Phys. Rev. A* **2** (1970) 256–258
11. E.Feenberg: Ground state of an interacting boson system. *Ann. Phys. (N.Y.)* **84** (1974) 128
12. R.P. Feynman: The lambda-Transition in Liquid Helium. *Phys. Rev.* **90** (1953) 1116–1117

13. D.E. Galli and L.Reatto: The shadow path integral ground state method: study of confined solid ^4He . *J.Low Temp. Phys.* **136** (2004) 343–359
14. J.P. Hansen and D. Levesque: Ground state of solid helium-4 and -3. *Phys. Rev.* **165** (1968) 293–299
15. J.P. Hansen and E.L. Pollock: Ground-State Properties of Solid Helium-4 and -3. *Phys. Rev. A* **5** (1972) 2651–2665
16. M. Kac: Probability and Related Topics in Physical Science. Interscience, New York (1959)
17. M.H. Kalos, M.A. Lee, P.A. Whitlock, and G.V. Chester: Modern potentials and the properties of condensed ^4He . *Phys. Rev. B* **24** (1981) 115–130
18. M.H. Kalos, D.Levesque, and L.Verlet: Helium at zero temperature with hard-sphere and other forces. *Phys. Rev.A* **9** (1974) 2178–2195
19. M.H. Kalos and P.A. Whitlock: *Monte Carlo Methods Volume I: Basics*. John Wiley, New York (1986).
20. E. Kim and M.H.W. Chan: Observations of Superflow in Solid Helium. *Science* **305** (2004) 1941–1944
21. E.Kim and M.H.W. Chan: Probable observation of a supersolid helium phase. *Nature* **427** (2004) 225–227
22. W.L. McMillan: Ground state of liquid ^4He . *Phys. Rev.* **138** (1965) A442–A451
23. N.Metropolis, A.W. Rosenbluth, M.N. Rosenbluth, A.H. Teller, and E.Teller: Equation of state calculations by fast computing machines. *J.Chem. Phys.* **21** (1953) 1087–1092
24. F.Pederiva, G.V. Chester, S.Fantoni, and L.Reatto: Variational study of vacancies in solid ^4He with shadow wave functions. *Phys. Rev. B* **56** (1997) 5909–5917
25. F.Pederiva, A.Ferrante, S.Fantoni, and L.Reatto: Homogeneous nucleation of crystalline order in superdense liquid ^4He . *Phys. Rev. B* **52** (1995) 7564–7571
26. E.L. Pollock and D.M. Ceperley: Simulation of quantum many-body systems by path-integral methods. *Phys. Rev. B* **30** (1984) 2555–1568.
27. A.Sarsa, K.E. Schmidt, and W.R. Magro: A path integral ground state method. *J.Chem. Phys.* **113** (2000) 1366–1371
28. K.E. Schmidt, M.H. Kalos, M.A. Lee, and G.V. Chester: Variational Monte Carlo calculations of liquid ^4He with triplet correlations. *Phys. Rev. Lett.* **45** (1980) 573–576
29. S.A. Vitiello: Relative stability of hcp and fcc crystalline structures of ^4He , *Phys. Rev. B* **65** (2002) 214516–214520
30. S.A. Vitiello, K. Runge, and M.H. Kalos: Variational calculations for solid and liquid ^4He with a “shadow” wavefunction. *Phys. Rev. Lett.* **60** (1988) 1970–1972
31. S.A. Vitiello and K.E. Schmidt: Optimization of ^4He wave functions for the liquid and solid phases. *Phys. Rev. B* **46** (1992) 5442–5447
32. S.A. Vitiello and K.E. Schmidt: Variational Methods for ^4He using a modern he-he potential. *Phys. Rev. B* **60** (1999) 12342–12348
33. S.A. Vitiello and P.A. Whitlock: Green’s function Monte Carlo algorithm for the solution of the Schrödinger equation with the shadow wave function. *Phys. Rev. B* **44** (1991) 7373–7377
34. P.A. Whitlock, D.M. Ceperley, G.V. Chester, and M.H. Kalos: Properties of liquid and solid ^4He . *Phys. Rev. B* **19** (1979) 5598–5633
35. P.A. Whitlock and R.M. Panoff: One-body density matrix and the momentum density in ^4He and ^3He . Proc. of the 1984 Workshop on High-Energy Excitations in Condensed Matter, ed. R.N. Silver. LA-10227-C Vol II (1984)
36. P.A. Whitlock and R.M. Panoff: Accurate momentum distributions from computations on ^3He and ^4He . *Can. J. Phys.* **65** (1987) 1409–1415