Path Integral Ground State study of 2D solid \(^4\)He

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We have studied a two-dimensional triangular commensurate crystal of \(^4\)He with the exact \(T = 0\) K Path Integral Ground State (PIGS) Monte Carlo method. We have projected onto the true ground state both a Jastrow-Nosanow wave function, in which equilibrium positions are explicitly given and no Bose–Einstein (BEC) is present, and a translationally invariant shadow wave function, in which the solid phase emerges through a spontaneously broken symmetry process and it has BEC. We find a remarkable convergence to the same properties, both the diagonal ones as well as the off-diagonal one-body density matrix \(\rho_1\). This supplies a strong evidence that no variational bias are present in the PIGS method. We find no BEC in the commensurate 2D \(^4\)He crystal at \(T = 0\) K, \(\rho_1\) shows an exponential decay in the large distance range. The structure found in \(\rho_1\) is due to virtual vacancy–interstitial pairs and this shows up in the momentum distribution.

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Quantum Monte Carlo methods have provided a very powerful tool in exploring the physics of strongly interacting many-body quantum systems. As far as the properties of Bose fluids and solids are concerned, Path Integral Monte Carlo (PIMC) methods have been proved to evaluate “exact” and “unbiased” expectation values on the thermal equilibrium state at finite temperature \([1]\); “exact” means that the obtained results are the true expectation values within the statistical error, while “unbiased” means that the only required input is the interatomic potential. At zero temperature, different “exact” techniques are available, as the Green’s function Monte Carlo \([2]\) (GFMC), the Diffusion Monte Carlo \([3]\) (DMC), the Reptation Monte Carlo \([4]\) or the Path Integral Ground State \([5]\) (PIGS) methods. All such methods, though “exact” in suitable limits, rely on variational models for the ground state wave function (wf) of the system. These variational models play a relevant role in the importance sampling employed by these methods; although, in principle, the final results should not be affected by the particular choice of the trial wf, in practice, the possibility that some bias could survive, especially in systems with complex broken symmetries like in the solid phase, has not been established. In this paper we will show the robustness of the results given by the PIGS method with respect to the choice of the variational wf by studying a model for \(^4\)He in two dimensions in the solid phase. In fact, we find the same physical properties of the system, within the statistical noise, starting from two radically different wfs. One, a Jastrow–Nosanow \([6]\) wf (JNWF), has been built in the crystal lattice via Gaussian localization factors, it is not Bose–symmetric and has no Bose–Einstein condensation (BEC). The other, a shadow \([7]\) wf (SWF), is translationally invariant, with crystalline order arising as spontaneously broken symmetry, and it has BEC \([8,9,10]\). We have chosen to study this model in 2D for different reasons. The reduced dimensionality allows us to study correlations to much larger distances than in 3D, even more than 20 lattice parameters. Fluctuations are expected to be stronger in 2D so this is a more stringent test for convergence given the different symmetry properties of the starting variational wfs. Finally, the 2D system is a model which is relevant for adsorbed \(^4\)He atoms on a smooth substrate like graphite.

With the present study we address also the important question of the supersolid state of matter \([11,12,13,14,15,16]\). PIMC computations give strong evidence that in a 3D commensurate solid \(^4\)He (number of atoms equal to the number of lattice sites) there is no superfluid response and no BEC \([17,18]\). The PIMC computations are at finite temperature and the lowest \(T\) is of order 0.1 K which is above the experimental transition temperature of crystals of good quality \([12]\). By computing the density matrix \(\rho_1(\vec{r},\vec{r'})\) of crystalline \(^4\)He at \(T = 0\) K, we find that there is no BEC in a 2D crystal. Preliminary results indicate that this is true also in 3D.

Dealing with low temperature properties, \(^4\)He atoms are described as structureless zero–spin bosons, interacting through a realistic two–body potential, that we assume to be the HFDHE2 Aziz potential \([19]\). The aim of the PIGS method is to improve a variationally optimized trial wf by constructing a path in the Hilbert space of the system which connects the given wf to the true ground state of the system; during this “path”, the correct correlations among the particles arise through the “imaginary time evolution operator” \(e^{-\tau \hat{H}}\), where \(\hat{H}\) is the Hamiltonian operator. Being \(\phi\) a trial wf with non–zero overlap with the exact ground state \(\psi_0\), this \(\psi_0\) is obtained as the \(\tau \to \infty\) limit of \(\psi_\tau = e^{-\tau \hat{H}} \phi\) suitably normalized. This \(\psi_\tau\) can be written analytically by discretizing the path in imaginary time and exploiting the factorization property \(e^{-(\tau_1+\tau_2)\hat{H}} = e^{-\tau_1\hat{H}} e^{-\tau_2\hat{H}}\). In this way, \(\psi_\tau\) turns out to be expressed in term of convolution integrals which involve the “imaginary time propagator” \(\langle \hat{R} | e^{-\delta \tau \hat{H}} | \hat{R}' \rangle\) for a \(\delta \tau\), that can be small enough such that very accurate approximants are known \([1,20]\). This maps the quan-
An appealing feature peculiar to the PIGS method is that, in \( \psi \), the variational ansatz acts only as a starting point, while the full path in imaginary time is governed by \( e^{-\tau H} \), which depends only on the Hamiltonian operator.

As a trial \( \psi \), we used both a JNWF and a SWF. The JNWF is written as the product of two–body correlations and of Gaussian one–body terms which localize the particles around the assumed lattice positions \( \varphi \). In the SWF, beyond the explicit two–body factors, additional correlations are introduced via auxiliary (shadow) variables which are integrated out \( \rho \). Nowadays, SWF gives the best variational description of solid and liquid \( ^4\text{He} \) \([21]\). In both the cases, the variational parameters have been chosen to minimize the expectation value of the Hamiltonian operator. In what follows, we will refer to PIGS when we deal with the projection of the JNWF, and to SPIGS \([22]\) (Shadow Path Integral Ground State) when we project the SWF.

Because of the Bose statistics obeyed by the atoms, when using \( \psi \), as an approximation of the true ground state \( \psi_0 \), one has, in principle, also to account for permutations in the propagator \( \langle R | e^{-\delta\tau \hat{H}} | R' \rangle \) \([1, 3]\). Permutation moves are necessary when the JNWF, which is not Bose–symmetric, is used. On the other hand permutation moves are not necessary whenever the trial \( \psi \) is already Bose–symmetric, as the SWF. However, also for SPIGS, adding permutation moves turns out to be useful in improving the efficiency and the ergodicity of the sampling, mainly in reaching the large–distance range of \( \rho \).

In our algorithm we have introduced two different permutation samplings: cycles of inter–particles exchanges and swap moves. The first, which may involve an arbitrary number of particles, are described in detail in Ref. \([24]\). In a PIGS or SPIGS calculation of \( \rho_1 (\vec{r}, \vec{r'} \rangle \), the efficiency can be further improved by introducing particular two–particles permutations cycles involving always one of the two positions \( \vec{r} \) and \( \vec{r}' \): the swap moves \([18]\). These moves improve very much the efficiency of the computation of \( \rho_1 \) and their acceptance rate is remarkably high: in the present 2D system, by using a staging \([23]\) method to sample the free (kinetic) part of the imaginary time propagator, we have found an acceptance rate for this swap move which is nearly 15% in the liquid phase and in the solid phase at densities close to the melting.

The 2D \( ^4\text{He} \) system phase diagram is known from accurate finite temperature PIMC simulations \([20]\); at zero temperature both DMC \([27]\) and GFMC \([28]\) have been used to investigate its properties mainly for the liquid phase. We have performed SPIGS and PIGS simulations of a 2D \( ^4\text{He} \) commensurate triangular crystal at \( \rho = 0.0765 \text{ Å}^{-2} \), slightly above the melting density. In order to control the reliability of our results we have tested their dependence on both the “projection time” \( \tau \) and the “time step” \( \delta\tau \). For a fixed value of \( \tau = 0.075 \text{ K}^{-1} \), we have done calculations with \( \delta\tau = 1/40, 1/80, 1/160 \) and \( 1/320 \text{ K}^{-1} \) and we have used the pair–product approximation \([1]\) for the imaginary time propagator. Reducing \( \delta\tau \) below \( 1/40 \text{ K}^{-1} \) affects only marginally the results; for example, by using \( 1/320 \text{ K}^{-1} \), the obtained energy is only 1% lower than the one with \( 1/40 \text{ K}^{-1} \). So we have adopted in most of the computations \( \delta\tau = 1/40 \text{ K}^{-1} \) as a reasonable compromise between accuracy and computational effort. These tests provide also a robust check of the ergodicity of the sampling algorithm since a lower value of \( \delta\tau \) for given \( \tau \) means a bigger number of small time projections (convolution integrals) so that one is dealing with polymers of increasing length. We have then increased \( \tau \) till convergence in the results has been achieved.

Diagonal properties, like the energy, have been computed in a box which hosts \( N = 120 \) particles with periodic boundary conditions. In Fig. 1 we give the energy per particle \( E/N \) and Debye–Waller factor \( e^{-2W} \) as functions of the projection time \( \tau \) obtained from PIGS and SPIGS for a commensurate 2D \( ^4\text{He} \) crystal with \( N = 120 \) particles at \( \rho = 0.0765 \text{ Å}^{-2} \). Error bars are smaller than the used symbols. The dotted lines indicate the convergence values \( \epsilon_0 = 1.308 \pm 0.002 \text{ K} \) and \( e^{-2W} = 0.214 \pm 0.002 \), solid lines are exponential fits to guide the eye.
structure factor we have extracted the Debye-Waller factor; we have found that both SPIGS and PIGS converge to the same value $e^{-2W} = 0.214 \pm 0.002$ (Fig. 1) and, as in the energy case, SPIGS shows a faster convergence. It is important to note that the energy convergence does not allow to deduce a priori the convergence of other physical properties: the convergence must be checked independently for each observable.

In order to study whether the 2D commensurate solid $^4$He has BEC, we have computed the one-body density matrix $\rho_1(\vec{r},\vec{r}')$ for both SPIGS and PIGS. We have found that both SPIGS and PIGS converge to the same value $e^{-2W} = 0.214 \pm 0.002$ (Fig. 1) and, as in the energy case, SPIGS shows a faster convergence. It is important to note that the energy convergence does not allow to deduce a priori the convergence of other physical properties: the convergence must be checked independently for each observable.

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of interatomic potentials does the commensurate crystal have BEC and supersolidity?

The convergence in the results obtained starting from radically different wfs is a remarkable result because supplies strong evidence for the absence of any variational bias in the PIGS method. Moreover, even if not shown in this letter, we have also obtained convergence of diagonal bias in the PIGS method. Moreover, even if not shown in this letter, we have also obtained convergence of diagonal properties, such as the static structure factor and the radial distribution function, by projecting a simple Jastrow wf which has just the minimal information on the short range behavior and displays no crystalline order at the considered density.

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