The Shadow Path Integral Ground State Method:
Study of Confined Solid $^4$He

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We have studied the zero temperature phase diagram of confined $^4$He by means of a new exact projector Quantum Monte Carlo method: the Shadow Path Integral Ground State (SPIGS). This method is able to compute exact ground state expectation values without extrapolations and with a Shadow Wave Function (SWF) as trial variational state for the importance sampling. Thanks to the ability of SWF in describing the solid phase via spontaneously broken translational symmetry, this is an important extension which opens the possibility to study disorder phenomena in the solid phase by an exact method at zero temperature. We have applied this technique to study $^4$He confined in a lattice of big static objects with a purely repulsive interaction with $^4$He atoms. We have studied the equation of state of this system finding that a well defined liquid–solid transition is still present but with an increased freezing pressure. In the case we have studied this pressure goes from 25.2 atm for pure bulk system to about 38 atm. This is similar to what is experimentally found in $^4$He confined in porous material like vycor. We have found also that the disorder due to the mismatch between the crystal structure and the spherical geometry of the object induces delocalization of $^4$He atoms.

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1. INTRODUCTION

The study of the effect induced by confining a quantum system is one of the key themes of present-day condensed matter physics. In fact it is known that the interplay of the confining potential with the interparticle interaction may yield completely new phenomena, as well as strongly enhancing correlations effects. The interest in studying disordered solid phases of $^4$He has very recently gained strong importance from the first probable experimen-
tal evidence of the existence of a supersolid phase for solid $^4$He confined in porous medium. In this experiment a drop in the rotational inertia of solid $^4$He confined in vycor has been observed from torsional oscillator technique below a certain critical temperature; this has been interpreted with a probable entry into the supersolid phase.

From a theoretical point of view the first discussion on a possible supersolid phase, that is a phase were a broken translational symmetry coexists with Bose–Einstein condensation (BEC), was presented by Chester. Penrose and Onsager showed few years before that a perfect crystal with localized particles is incompatible with BEC; however Chester argued that the situation could be different if a solid phase is present but particles can exchange their positions. In fact wave functions exist with such properties and there was a proof that these wave functions have BEC. The non classical response to rotation of such solid was discussed by Leggett. A mechanism for such a state was suggested before by Andreev and Lifshitz in terms of a ground state for the solid phase of $^4$He which contains a finite concentration of vacancies. Searches for zero-point vacancies in the seventies and eighties has been unsuccessful and this is in agreement with later results of microscopic theory which predicts a ground state for the solid phase of $^4$He without vacancies. However this is not the only possibility to have a supersolid phase; BEC could arise in a quantum solid also at finite temperature when the concentration of thermal vacancies is large enough, or the disorder in the crystal structure, needed to sustain a BEC transition, can be induced by a confinement of the quantum system; this is the kind of system which we have studied in the present work.

Previous theoretical analysis on a possible supersolid phase were somehow speculative in their nature; in the last years, the possibility to predict on a quantitative basis the physical properties of a disordered quantum solid has been reached with the development of accurate simulations methods. Some year ago the first microscopic calculation of the vacancy activation energy in solid $^4$He has been obtained from the variational Shadow Wave Function (SWF) technique. More recently it has been shown that a finite concentration of vacancies in solid $^4$He is able to induce Off-Diagonal Long Range Order (ODLRO) in the one-body density matrix, the synonymous of BEC for a strongly interacting boson system, but also the excitation spectrum of a vacancy and accurate description of longitudinal acoustic phonons have been obtained within a development of this variational theory. A recently introduced projection Quantum Monte Carlo method, the Shadow Path Integral Ground State (SPIGS), uses a SWF as a trial function for importance sampling; this is very important because it opens the possibility to study by exact methods at $T = 0$ K also disorder phenomena in the solid.