Bose Einstein Condensation in solid $^4$He

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We have computed the one-body density matrix $\rho_1$ in solid $^4$He at $T = 0$ K using the Shadow Wave Function (SWF) variational technique. The accuracy of the SWF has been tested with an exact projector method. We find that off-diagonal long range order is present in $\rho_1$ for a perfect hcp and bcc solid $^4$He for a range of densities above the melting one, at least up to 54 bars. This is the first microscopic indication that Bose Einstein Condensation (BEC) is present in perfect solid $^4$He. At melting the condensate fraction in the hcp solid is $5 \times 10^{-7}$ and it decreases by increasing the density. The key process giving rise to BEC is the formation of vacancy–interstitial pairs. We also present values for Leggett’s upper bound on the superfluid fraction deduced from the exact local density.

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The supersolid state, a solid with superfluid properties, is moving out from theoretical speculations as a result of the observation of non classical rotational inertia (NCRI) in solid $^4$He in Vycor and very recently in the bulk. The initial theoretical suggestion of the supersolid state was based on the possible presence of vacancies in the ground state of a Bose quantum solid. In addition these vacancies have to be mobile in order to give rise to Bose Einstein Condensation (BEC) of $^4$He atoms. Experimentally no evidence has been found for the presence of vacancies at very low temperature and this is in agreement with the results of microscopic theory which gives an energetic cost of about 15 K for the formation of a vacancy in bulk solid $^4$He. However it was almost immediately recognized that the presence of ground state vacancies is only one possible mechanism for NCRI and what is really needed is that atoms are not localized at the lattice sites but are delocalized via exchange or other processes. This gives the possibility of having in the wave function (wf) a phase which governs collectively the motion of the atoms. The existence of a supersolid state in $^4$He is therefore strictly related to the question of localization or delocalization of particles and, of course, this is a topic of general interest. This is the case, for instance, of cold alkali atoms in a periodic potential. Experiments with $^4$He give access to the superfluid fraction $\rho_s/\rho$ which turns out to be at most of order 2%. Theoretically only upper bounds on $\rho_s$ have been obtained up to now and no microscopic theory has given evidence for a supersolid phase. The commonly accepted view is that one can have a finite $\rho_s$ in a three dimensional system if there is BEC in the system so a central quantity to compute is the off diagonal one–body density matrix $\rho_1(\vec{r}, \vec{r}')$, whose Fourier transform represents the momentum distribution.

In this article we address the computation of $\rho_1$ for solid $^4$He at $T = 0$ K based on a variational wf, a shadow wf (SWF). In a previous computation we have found that the presence of vacancies in the solid induces a BEC which is proportional to the concentration of vacancies. On the other hand the large energy of formation of a vacancy makes the probability of having such defects at low temperature vanishing small. Here we study in the perfect solid the large distance behavior of $\rho_1(\vec{r}, \vec{r}')$, specifically if $\rho_1$ has a non zero limit at large distance (off diagonal long range order, ODLRO) which implies BEC. With perfect solid we mean that the number of maxima in the local density $\rho(\vec{r})$ is equal to the number of $^4$He atoms. The use of SWF is specially useful in the present context because with such wf the crystalline order is an effect of the spontaneously broken symmetry so that local disorder processes like exchange of two or more particles, creation of vacancy–interstitial pairs (VIP) or more complex processes are in principle allowed. The major finding of our computation is the presence of a small but finite condensate for a range of densities above melting. The variational theory is very useful to describe strongly interacting systems like liquid or solid $^4$He but it is always open to debate how much the results depend on the ansatz on the wf, specially for quantities other than the energy. In order to give indication on the reliability of our SWF we present some results on quantities like the degree of local order, of localization and of the local density obtained also from an exact computation based on a projection algorithm (SPIGS), a Path Integral Ground State method which uses a SWF as the starting wf.

In a SWF the correlations between atoms are introduced both explicitly by a Jastrow factor and also in an implicit way by coupling with a set of subsidiary variables, which are called “shadow” variables (one shadow for each quantum particle), which are integrated over. All expectation values are computed by a Monte Carlo (MC) method and the statistical sampling of $|\Psi|^2$ maps the quantum system of $N$ particles in a system of $N$ special interacting triatomic “molecules” which consist of a $^4$He atom and two shadows. The accuracy of the SWF technique is well documented and it has been possible to treat also disorder phenomena in a quantum solid, like a vacancy or even the interfacial region between a solid and a liquid at coexistence. As functional form for the correlating factors contained in the SWF we have taken the ones used in ref, as interatomic interaction we have used a standard Aziz potential.
TABLE I: Upper bounds \( f_s^+ \) for the superfluid fraction in hcp bulk solid \( ^4\text{He} \). He computed at different densities with the SWF technique, the SPIGS method and the GM for \( \rho(\vec{r}) \). \( P \) is the pressure from the SPIGS equation of state. \( \sigma \) is the standard deviation of the Gaussians used in the GM.

| \( \rho (\text{Å}^{-3}) \) | \( P \) (bar) | SWF | SPIGS | GM | \( f_s^+ \) | \( f_s^+ \) | \( f_s^+ \) | \( \sigma (\text{Å}) \) |
|------------------|---------|-----|------|----|----------|----------|----------|---------|
| 0.0290           | 29.3    | 0.287 | 0.384 | 0.380 | 0.543   |
| 0.0310           | 53.6    | 0.255 | 0.299 | 0.297 | 0.503   |
| 0.0330           | 87.8    | 0.209 | 0.230 | 0.222 | 0.467   |
| 0.0353           | 141.9   | 0.141 | 0.164 | 0.166 | 0.436   |
| 0.0400           | 316.9   | 0.077 | 0.080 | 0.079 | 0.381   |
| 0.0440           | 553.5   | 0.042 | 0.042 | 0.041 | 0.345   |

A SWF can be interpreted as a first projection step in imaginary time of a Jastrow wave function via a variationally optimized imaginary time propagator. With SPIGS one goes beyond the variational theory by adding successive projection steps in the imaginary time propagation with the full Hamiltonian and in this way we are able to compute exact expectation values on the ground state without extrapolations. With these two Quantum MC methods no a priori equilibrium positions for the solid phase are required, the Bose symmetry is manifestly maintained and atoms can be delocalized.

The equation of state given by SWF is in good agreement with the results of SPIGS, for instance at melting with the results of SPIGS, for instance at melting the main Bragg peak of the hcp solid is about 17% higher than the experimental value of \( \rho(\vec{r}) \). The accuracy is lost when we consider the local density \( \rho(\vec{r}) \); in the region of the minima of \( \rho(\vec{r}) \) deviations greater than 100% are found.

The one-body density matrix \( \rho_1(\vec{r}, \vec{r}', \sigma) \) is given by the overlap between the normalized many-body ground state \( \psi(\vec{r}, \vec{r}'; \sigma) \) and \( \psi(\vec{r}, \vec{r}'; \sigma) \) for \( \sigma \) and, in any case, it is only an upper bound so it is not very conclusive. A word of caution on the GM is in order. If this model gives an excellent representation for the integrated density \( \rho(z) \), the accuracy is lost when we consider the local density \( \rho(\vec{r}) \): in the region of the minima of \( \rho(\vec{r}) \) deviations greater than 100% are found.

It is possible to interpret the integrand in Eq. (1) as a probability density; then \( \rho_1 \) can be computed by sampling the integrand in Eq. (1) and by histogramming the occurrence of the distance \( d = |\vec{r} - \vec{r}'| \). In the following we will call “half” particles the particles with coordinates \( \vec{r} \) and \( \vec{r}' \) because they have just \( \frac{1}{2} \) the correlation strength with the other \( N-1 \) particles (with coordinates \( \vec{r}_2, ..., \vec{r}_N \)) and no direct correlation between them. The method of computation has been described in Ref. 12. Absence of ODLRO corresponds to the two “half” particles forming a “molecule” whereas presence of ODLRO corresponds to a finite probability of dissociation up to infinite distances.

We have computed \( \rho_1(\vec{r} - \vec{r}') \) along the nearest neigh-
FIG. 1: $\rho_1(\vec{r} - \vec{r}')$ at different densities for hcp and bcc perfect $^4$He crystals and for the same crystals with a finite concentration $x_v$ of vacancies.

In Fig.1 we report $\rho_1$ for a perfect hcp crystal at different densities at and above melting and for a bcc crystal at $\rho = 0.02898 \AA^{-3}$. It is clear that at melting and at $\rho = 0.031 \AA^{-3}$ $\rho_1$ reaches a plateau at large distance whereas at $\rho = 0.033 \AA^{-3}$ $\rho_1$ steadily decreases with increasing distance. By averaging the tail in $\rho_1$ for distances greater than 14 Å, we find at the melting density a condensate fraction $n_c = (5.0 \pm 1.7) \times 10^{-6}$ in a perfect hcp and $(7.6 \pm 1.7) \times 10^{-6}$ in a perfect bcc crystal. This is the first microscopic indication that BEC is present in perfect solid $^4$He. At $\rho = 0.031 \AA^{-3}$ we find $n_c = (2.0 \pm 0.4) \times 10^{-6}$ and at $\rho = 0.033 \AA^{-3}$ the tail is so much depressed that the size of the simulation box is too small to conclude if ODLRO is present; in this case we can only say that the condensate fraction, if any, is lower than $10^{-9}$. The simulation box which has been used to compute $\rho_1$ is cubic and contains $N = 432$ $^4$He atoms for the bcc crystal, it is elonged in the $\Gamma K$ direction and contains $N = 360$ $^4$He atoms for the hcp crystal. By changing the size of the boxes at fixed density we have checked that our results for $\rho_1$ have no finite size effect within the statistical errors of our computations. This is shown in the inset of Fig.1 for the hcp crystal at $\rho = 0.029 \AA^{-3}$; by averaging the tail in $\rho_1$ for distances greater than 14 Å, we find $n_c = (3.9 \pm 1.7) \times 10^{-6}$ for $N = 288$ and $n_c = (5.7 \pm 2.0) \times 10^{-6}$ for $N = 432$, to be compared with the value given above: $n_c = (5.0 \pm 1.7) \times 10^{-6}$ for $N = 360$. In ref.13 we found that a finite concentration of vacancies $x_v$ induces a condensate fraction which depends linearly on $x_v$. In Fig.1 we show also $\rho_1$ when a vacancy is present both in hcp and bcc. Taking into account the value of $x_v$ of the computation we estimate that at $\rho = 0.029 \AA^{-3}$ the condensate fraction due to a finite concentration of vacancies is equal to the one in a perfect hcp crystal when $x_v \simeq 1.5 \times 10^{-5}$.

All the computed $\rho_1$ show oscillations which reflect the crystalline order in the system. However these oscillations are not the same in the perfect and in the defected solid. We find that when a vacancy is present the maxima of the oscillations in $\rho_1$ correspond to multiples of the nn distance $d_{nn}$. This is an indication that in presence of a vacancy the main mechanism which contributes to the separation of the two “half” particles is that one of them moves through the crystal following the vacancy which is very mobile. The different positions of the maxima in $\rho_1$ for the perfect crystal suggest a different microscopic process for the ODLRO in this case. By analysing the particle configurations sampled in our runs we find that the secondary peak of $\rho_1$, located at about 5 Å, always corresponds to a configuration in which the two “half” particles occupy two nn lattice positions slightly distorted by the presence of one interstitial $^4$He atom between them. In Fig.2 we show 100 successive configurations of the particles which corresponds to this event. In the formalism of second quantization $\rho_1(\vec{r} - \vec{r}')$ is equal to the expectation value of the composite event where one $^4$He atom is destroyed at $\vec{r}'$ and one is created at $\vec{r}$; then it is possible to interpret the event in Fig.2 as the creation of a VIP. The same process is found in bcc crystal. After this first step the two “half” particles have a finite probability of moving away one from another by exchange processes with the other atoms and this gives rise to the other maxima of $\rho_1$ at larger distance. By analysing the particle configurations corresponding to these other maxima we find that a VIP is present in all the configurations. Similar processes were considered in Ref.14 as a necessary condition for the supersolid phase, but there it is argued that VIP cannot be present. Our results disagree with this hypothesis. In order to characterize the anisotropy of $\rho_1$ as function of $\vec{d}$ we have computed $\rho_1$ when the two “half” particles are no more constrained to lie on the nn direction but can freely move in a plane. In Fig.3 one can see that $\rho_1$ in a perfect bcc crystal is strongly anisotropic for distances up to about 6 Å, and the maxima of $\rho_1$ are in the direction of nn. However at greater distances $\rho_1$ becomes nearly isotropic and we conclude that our estimation of the BEC fraction is not affected by the pre-
vious restriction on $d$. Similar results are obtained for hcp. It is interesting to notice that when a vacancy is present the anisotropy of $\rho_1$ persists up to greater distances (data not shown). Also in Fig. 1 one can see that the oscillations of $\rho_1$ are more persistent with increasing distance in the crystal with a vacancy; this is another indication that different microscopic processes are at the origin of the ODLRO in the perfect and in the defected solid $^4$He. The exchange of atoms and VIPs are present not only in $\rho_1$ but also in $|\Psi|^2$. At melting about every $2 \times 10^9$ MC steps an atom has a displacement larger than $d_n$ and in many cases this is associated with the presence of an interstitial. In principle one can devise an algorithm based on SPIGS to compute $\rho_1$ exactly. However at present this appears to be a major computational problem. In any case we have given solid evidence that SWF overestimates the degree of local order so that we should expect that the SWF results for the BEC fraction are an underestimation of the exact values.

In conclusion we have shown that solid $^4$He at $T = 0$ K has BEC at melting density and above at least up to 54 bars whereas we find a vanishing BEC at 90 bars. Thus BEC should be at the basis of the NCRI observed experimentally. Our result has been obtained from an advanced variational theory the accuracy of which has been tested with a projector method on the exact ground state. The key process giving rise to ODLRO is the formation of a VIP. Such defects have a finite probability to be present in the ground state of the system; they are not permanent excitations but simply rare fluctuations of the perfect crystal induced by the large zero-point motion. In other words the number of atoms is equal to the number of lattice sites and, at the same time, atoms are delocalized. Since the ground state is the vacuum of the elementary excitations of the system we conjecture that a branch of low energy excitations different from phonons should be present in solid $^4$He. Such excitations should have an important role in determining the critical temperature. It is a possibility that this branch is related to some experimental results which have been interpreted in term of an excitation with energy of about 2 K.

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