

A Wave Function Describing Superfluidity in a Perfect Crystal

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Abstract. We propose a many-body wave function that exhibits both diagonal and off-diagonal long-range order. Incorporating short-range correlations due to interatomic repulsion, this wave function is shown to allow condensation of zero-point lattice vibrations and phase rigidity. In the presence of an external velocity field, such a perfect crystal will develop non-classical rotational inertia, exhibiting the supersolid behavior. In a sample calculation we show that the superfluid fraction in this state can be as large as of order 0.01 in a reasonable range of microscopic parameters. The relevance to the recent experimental evidence of a supersolid state by Chan and Kim is discussed.

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1. Introduction

Superfluidity (including superconductivity) has remained at the center of attention of low temperature physics since it was discovered at the beginning of last century. By now it is well known that both superfluidity in liquids and gases and superconductivity in electron systems can all be characterized by the appearance of off-diagonal long-range order (ODLRO)[1]. In contrast to the diagonal long-range order (DLRO), ODLRO is a quantum phenomenon with long-range phase coherence, not describable in classical mechanical terms. On the other hand, Yang has pointed out the possibility that ODLRO may occur in a solid, coexisting with DLRO [1]. The possibility for such a supersolid has been explored theoretically or numerically in 1970's by a number of authors [2, 3, 4, 6, 5]. In particular, Leggett [4] has suggested to study superfluidity in a quantum solid in terms of non-classical rotational inertia (NCRI). These have stimulated efforts to search for superfluidity in solid helium in the following decades [7]. Recent experiments of Chan and Kim have shown evidence of NCRI in solid ^4He , either confined in porous medium [8] or in a bulk [9], with the observed values of the superfluid fraction (SFF) of the order 0.01. The experimental progress recently drew much attention to revisiting the theory of supersolids [10, 11, 12].

In contrast to the efforts concentrated on defects or vacancies, in this paper we shall consider a *perfect crystal* of ^4He , where the number, N , of atoms precisely equals that of the sites, and the single-particle density profile has a discrete translation symmetry. We shall show that (i) a many-body wave function can be constructed which indeed exhibits both DLRO and ODLRO, (ii) in this state short-range correlations due to interatomic hard-core repulsion lead to a condensation of zero-point lattice vibrations with long-range phase rigidity, (iii) in the presence of an external velocity field, this state shows NCRI, and the associated SFF is estimated to be of order 0.01 in a reasonable range of parameters. Finally we point out our wave function has features consistent with the experiments [8, 9].

2. Many-body wave function for a perfect supersolid

We start with the construction of a wave function that describes a perfect supersolid. In a normal crystal individual atoms are localized and oscillate around their equilibrium positions, which form a lattice, so that the density profile is periodic, resulting in DLRO. For helium atoms, their small mass makes the zero-point oscillations significant. Normally the zero-point motion of individual atoms is incoherent, as in the Einstein picture of lattice dynamics. This is what happens in normal solid helium (under pressure). We propose that at sufficiently low temperature, due to Bose statistics of ^4He atoms and short-range correlations arising from interatomic hard-core repulsion, the zero-point motion of individual atoms may become phase-locked and, therefore, an ODLRO and phase rigidity will be developed across the whole system. We shall not address the question of under precisely what conditions this will happen, but be

concentrated on constructing a wave function that demonstrates that the coexistence of DLRO and ODLRO is possible in principle.

We use a localized wave function, $\phi(\mathbf{r} - \mathbf{R}_i)$, to describe the zero-point motion of the atom around a lattice point \mathbf{R}_i . Then the coherent zero-point motion of the atoms in the crystal can be described by the following symmetrized product of single particle wave functions:

$$\mathcal{S} \prod_{i=1}^N \phi(\mathbf{r}_i - \mathbf{R}_i), \quad (1)$$

with \mathcal{S} the symmetrization operator with respect to r_i . The symmetrization \mathcal{S} in Eq. (1), which is absent for an Einstein crystal, incorporates the fact that all atoms are identical bosons. The superposition involved in \mathcal{S} of permuted products of $\phi(\mathbf{r}_i - \mathbf{R}_j)$ takes for granted that the zero-point lattice vibrations of individual atoms must be *coherent*; otherwise it would not make sense to superpose the permuted terms. Moreover, as in the description of helium superfluid, we should also include a Jastrow factor to incorporate short-range pair correlations. Normally the Jastrow factor is taken to be

$$\prod_{i<j} J(r_{ij}) \equiv \prod_{i<j} \exp\{-\gamma v(r_{ij})\}, \quad (2)$$

with $\gamma > 0$ and the exponents proportional to the interatomic potential $v(r_{ij})$ of the Lennard-Jones type, with a hard-core repulsion plus a weak attractive part. Usually the product of wave function (1) and (2) is used to describe a perfect quantum solid, namely

$$\Psi = \mathcal{S} \prod_{i=1}^N \phi(\mathbf{r} - \mathbf{R}_i) \prod_{i<j} J(r_{ij}). \quad (3)$$

Provided that the characteristic width, a , of the localized wave packet ϕ is much smaller than the hard-core size λ , the wave function (3) can be approximated by

$$\Psi_0 = \frac{1}{\sqrt{N!}} \prod_{i=1}^N \left(\sum_{j=1}^N \phi(\mathbf{r}_i - \mathbf{R}_j) \right) \prod_{k<l} J(r_{kl}), \quad (4)$$

since the Jastrow factor almost annihilates the cross terms in which two atoms are in the same localized wave packet at one site. However, when a becomes comparable to λ , the wave function (4) incorporates some new features and may exhibit qualitatively different behavior than the wave function (3). The above arguments motivate us to propose Ψ_0 as our model wave function to describe, at least approximately, a perfect supersolid, and we will proceed to show that this wave function allows appreciable Bose-Einstein condensation in a density periodic state.

3. Proof of Bose-Einstein condensation

From previous experience with ^4He superfluid it is known that the Jastrow factor can have a Bose-Einstein condensation into the zero-momentum state [15, 13, 14, 3, 16].

Similarly by expanding the Jastrow factor in Eq. (4):

$$\Psi_0 = \prod_{i=1}^N \left(\frac{1}{\sqrt{N}} \sum_{j=1}^N \phi(\mathbf{r}_i - \mathbf{R}_j) \right) (\sqrt{n_0} + \dots), \quad (5)$$

a non-vanishing zero-mode part ($n_0 \neq 0$) would give rise to macroscopic occupation in a single particle state, which has a periodic density modulation. (The value of the condensate fraction n_0 depends on the microscopic details, and in the superfluid case it was estimated to be of the order 0.01 [16].) Now let us proceed to prove that the wave function (4), which is of the general form: ($u(r_{ij}) = \gamma v(r_{ij})$)

$$\Psi_0 \sim \prod_{k=1}^N f(\mathbf{r}_k) \prod_{i<j} J(r_{ij}) = \prod_{k=1}^N f(\mathbf{r}_k) \prod_{i<j} \exp\{-u(r_{ij})\}, \quad (6)$$

has a Bose-Einstein condensation on the single-particle state $f(\mathbf{r})$, provided that $|f(\mathbf{r})|$ nowhere vanishes and has an upper bound. Assume the same conditions used in Ref.[13, 14]: There exists a positive constant ϕ such that the function $u(r_{ij})$ satisfies $\sum_{i=1}^t u(r_{is}) \geq -\phi$, for all t, s, r_1, r_2, \dots satisfying $\sum_{i<j \leq t} u(r_{ij}) < \infty$. The proposition is the resulting one-particle density matrix possesses ODLRO:

$$\lim_{|\mathbf{r}-\mathbf{r}'| \rightarrow \infty} \langle \mathbf{r} | \rho_1 | \mathbf{r}' \rangle = n_0 f^*(\mathbf{r}) f(\mathbf{r}'), \quad (7)$$

with n_0 finite and positive, where

$$\langle \mathbf{r} | \rho_1 | \mathbf{r}' \rangle = \frac{N}{Q_N} \int \prod_{i=2}^N d\mathbf{r}_i \Psi_0^*(\mathbf{r}, \mathbf{r}_2, \dots) \Psi_0(\mathbf{r}', \mathbf{r}_2, \dots) \quad (8)$$

with Q_N the normalization constant of Ψ . Eq. (7) implies that the wave function (6) has a Bose condensation (macroscopic occupation) in the single particle state $f(r)$.

To prove Eq.(7), we notice in the infinite volume limit,

$$n_0 = \lim_{V \rightarrow \infty} \frac{1}{V^2} \int d\mathbf{r} d\mathbf{r}' \frac{\langle \mathbf{r} | \rho_1 | \mathbf{r}' \rangle}{f^*(\mathbf{r}) f(\mathbf{r}')} = \frac{N}{V^2} \frac{\zeta_{N+1}}{Q_N}, \quad (9)$$

where ζ_{N+1} is defined as

$$\zeta_{N+1} = \int \frac{d\mathbf{r} d\mathbf{r}'}{f^*(\mathbf{r}) f(\mathbf{r}')} \prod_{i=2}^N d\mathbf{r}_i \Psi_0^*(\mathbf{r}, \mathbf{r}_2, \dots) \Psi_0(\mathbf{r}', \mathbf{r}_2, \dots). \quad (10)$$

Note that the Jastrow functions in ζ_{N+1} are given by

$$J(r_{ab}) \prod_{k=2}^N J(r_{ak}) J(r_{bk}) \prod_{2 \leq i < j} J^2(r_{ij}) \quad (11)$$

where $\mathbf{r}_a = \mathbf{r}, \mathbf{r}_b = \mathbf{r}'$. The use of the inequality $\sum_{i=1}^t u(r_{is}) \geq -\phi$ allows us to give a lower bound for ζ_{N+1} :

$$\zeta_{N+1} \geq \frac{e^{-\phi-\Delta}}{\kappa} Q_{N+1}, \quad (12)$$

where $\Delta = \min u(r)$ and $\kappa = \max |f(\mathbf{r})|^4$. Therefore the condensate fraction (9) has a lower bound:

$$n_0 \geq \frac{n^2 e^{-\phi-\Delta}}{z \kappa}, \quad (13)$$

where the density $n \equiv N/V$ is fixed in the thermodynamic limit, and z denotes the limit

$$z = \lim_{V, N \rightarrow \infty} \frac{(N+1)Q_N}{Q_{N+1}}. \quad (14)$$

Note Q_N can be interpreted as the partition function

$$\int \prod_{i=1}^N d\mathbf{r}_i \exp \left\{ - \sum_{i < j} u(|\mathbf{r}_i - \mathbf{r}_j|) + 2 \sum_i \ln |f(\mathbf{r}_i)| \right\} \quad (15)$$

of a system of classical particles interacting through the two-body potential $k_B T_{eff} u(r)$ and in an external potential $2k_B T_{eff} \ln |f(\mathbf{r})|$ with fugacity z . For our wave function (4), $f(r) \equiv \sum_j \phi(\mathbf{r} - \mathbf{R}_j)$ is periodic, positive and everywhere nonvanishing, so the external potential is also finite everywhere. Hence, the thermodynamic limit of this classical system exists, and fugacity z is finite if $n < n_c$, where n_c is the close-packing density. In this way we have proved that at $T = 0$ our many-body wave function (4) has a finite condensate fraction n_0 , leading to ODLRO, Eq.(7), a periodic density profile.

4. Non-Classical Rotational Inertia

Next we study the response of our perfect supersolid to an external velocity field. Suppose that there are N bosonic atoms enclosed in a cylindrical annulus with internal radius R and thickness $h \ll R$. When the cylinder is rotated at a constant angular velocity ω about its axis, the free energy $F(\omega)$ measured in the rest frame is of the form [4]

$$F(\omega) = F(0) + \frac{1}{2} I_0 \omega^2 - \Delta F(\omega), \quad (16)$$

where $F(0)$ is the free energy for $\omega = 0$, and $I_0 = NmR^2$ is the classical rotational inertia. The last term is the NCRI, which is related to the SFF α via

$$\Delta F(\omega) = \frac{1}{2} I_0 \omega^2 \alpha. \quad (17)$$

In the rotating frame (with the azimuthal angles $\varphi_i \rightarrow \varphi_i + \omega t$), after the gauge transformation

$$\Phi \rightarrow \exp \left(-i \sum_{i=1}^N \frac{m\omega R^2 \varphi_i}{\hbar} \right) \Phi, \quad (18)$$

the Schrödinger equation reads [4]

$$i\hbar \frac{\partial}{\partial t} \Phi = \left[\sum_i \left(-\frac{\hbar^2}{2m} \nabla_i^2 + V + \frac{m\omega^2 R^2}{2} \right) + \sum_{ij} U_{ij} \right] \Phi. \quad (19)$$

Apart from an additive term, $Nm\omega^2 R/2$, in energy, Φ satisfies the same equation as Φ_0 in the absence of rotation, however the boundary conditions are changed to

$$\Phi(\varphi_i = 0) = \exp \left(-i2\pi \frac{m\omega R^2}{\hbar} \right) \Phi(\varphi_i = 2\pi). \quad (20)$$

One can therefore conclude that the energy levels are periodic functions of ω . However the free-energy is insensitive to the twisted boundary conditions, either when it is in the

normal state [17] or the wave function of all the particles are localized. Only when (at least) one extended single-particle state is macroscopically occupied by N_0 atoms, the SFF is finite and given by

$$\alpha = \frac{1}{I_0} \frac{\partial^2 \Delta F(\omega)}{\partial \omega^2}. \quad (21)$$

This idea is similar to that explaining flux quantization in superconductors [18].

For the superfluid component, we have

$$\Delta F(\omega) = N_0 \min \int_0^L dx \frac{\hbar^2}{2m} |\nabla \theta|^2 \rho, \quad (22)$$

where $\sqrt{\rho} e^{i\theta}$ is the order parameter $\langle x | \rho_1 | x \rangle$, and L is the length of the sample. Here as a sample calculation, we only consider a one dimensional lattice along the circumference x -direction. The one-particle density ρ has a periodic structure:

$$\rho(x) = \frac{1}{N} \sum_{i=1}^N A(x - R_i), \quad (23)$$

where $|R_i - R_{i-1}| = d$, and the function A , for simplicity, is taken to be a localized Gaussian packet:

$$A(x) = \frac{1}{\sqrt{\pi a^2}} \exp\left(-\frac{x^2}{a^2}\right). \quad (24)$$

The phase $\theta(x)$ is non-uniform, but satisfies

$$\theta(L) = \theta(0) + \frac{m\omega RL}{\hbar}. \quad (25)$$

Write $\theta = \theta_0 + \delta\theta$, where $\theta_0 = c_0 x$ with $c_0 = m\omega R/\hbar$. It is natural to assume that $\delta\theta$ has a periodic dependence on x with period d . To minimize $\Delta F(\omega)$, the phase gradient becomes large only in regions with low density. Therefore the SFF is expected to be less than the condensate fraction and to increase with decreasing density modulation. We apply a simple variational method to prove this. By fixing a global phase we set

$$\delta\theta\left(\frac{d}{2}\right) = \delta\theta\left(-\frac{d}{2}\right) = \delta\theta\left(\frac{(2k+1)d}{2}\right) = 0, \quad (26)$$

For $\delta\theta$ in the interval $[-d/2, d/2]$, we take

$$\delta\theta = c_0 d \left[c_1 \frac{x}{d} + c_3 \left(\frac{x}{d}\right)^3 + c_5 \left(\frac{x}{d}\right)^5 \right] \quad (27)$$

as a trial function, in which the parameters should satisfy the constraint that $c_5 = -16c_1 - 4c_3$. Noting that $N_0 \hbar^2 c_0^2 / m = n_0 I_0 \omega^2$, the SFF α can be expressed as

$$\frac{\alpha}{n_0} = N \min_{c_1, c_3} \int_{-d/2}^{d/2} dx \left| (1 + c_1) + 3c_3 \left(\frac{x}{d}\right)^2 + 5c_5 \left(\frac{x}{d}\right)^4 \right|^2 \rho. \quad (28)$$

The right-hand side of Eq.(28) is quadratic in c_1 and c_3 and can be easily minimized. The resulting SFF is a function of the Lindermann radio a/d . We plot it in Fig. 1. The

phase θ as a function of x is shown in Fig. 2 for three typical values of a/d . Our results show that the SFF is vanishingly small when $a/d < 0.1$. When $a/d > 0.1$, the SFF experiences a rapid increase and reaches the condensate fraction n_0 when a/d is around 0.35. Our result, obtained analytically by a simple variational calculation, is consistent with the previous numerical result obtained for three dimensional fcc lattice [6, 11].

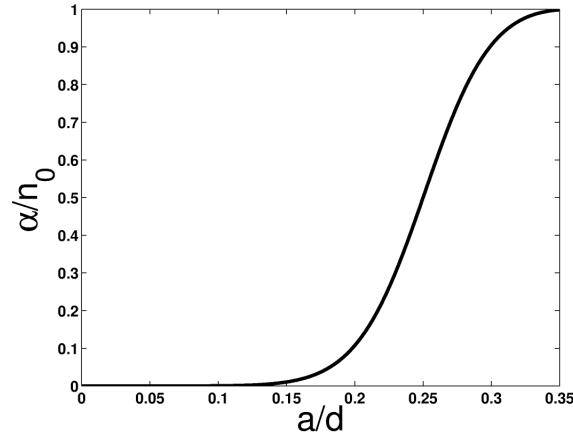


Figure 1. The ratio of SFF α to condensate fraction n_0 as a function of Lindermann's ratio a/d .

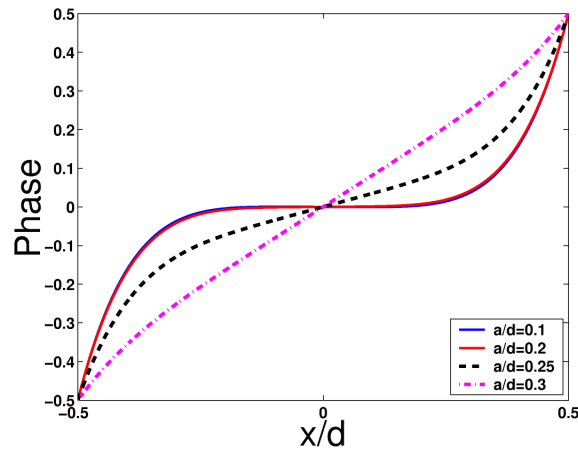


Figure 2. The phase θ (in units of c_0) as a function of x/d in one period for three values of Lindermann's ratio a/d .

5. Summary

In summary, we have suggested that in a perfect quantum bosonic solid, under favorable conditions, a conspiracy of Bose statistics, significant zero-point fluctuations and short-range correlation due to interatomic hard-core repulsion may lead to ODLRO and

macroscopic phase coherence, coexisting with crystalline DLRO and leading to the supersolid behavior, e.g. the appearance of NCRI under vessel rotation. We have proposed a many-body wave function and proved that indeed both DLRO and ODLRO coexist in such a state. The interatomic potential of the Lennard-Jones type, having a large hard core and being mostly attractive outside, with favorable parameters is arguably credential to choose our state before other non-supersolid states. We note that with this mechanism for supersolid the more closely packed the lattice is, the larger the SFF α is. Also the presence of a small number of vacancies or impurities (e.g. ^3He) is harmful to condensation of zero-point vibrations, and thus reduces the SFF. Observationally, these two features may be exploited as qualitative indication of the underlying mechanism suggested here for supersolid behavior.

The mechanism for supersolid proposed in this note (section 2) can be understood intuitively in the language of path integral. Consider, say, a one dimensional lattice of spacing d . If $d - 2a < \lambda$, where a is the amplitude of zero-point vibration, then the probability amplitude for two nearby atoms oscillating completely out of phase will become negligible due to huge potential energy of the hard-core repulsion. Therefore, it is the phase-locked trajectories of oscillating atoms that have lower potential energy and dominate the path integral, namely only nearly in-phase zero-point motion of all atoms in the crystal are favorable. It should be noticed that these phase-locked trajectories are quantum fluctuating pathes describing the ground state in the framework of path integral, which should be distinguished from the acoustic phonon excitation. It is these phase-locked trajectories that give rise to long-range phase coherence or phase rigidity as described by the first factor in Eq.(4). We call this phenomenon as *condensation of zero-point lattice vibrations*.

In recent experiments of Chan and Kim [8, 9] that show NCRI of solid ^4He , their sample is claimed to be ultrahighly pure (with a stated ^3He impurity of 0.3 parts of per million). Also parameterwise we note [19] that in solid ^4He the hard core radius is a big fraction (> 0.65) of the lattice spacing; and the ratio a/d can be as big as 0.22 in a variety of situations. As mentioned above, all these features are favorable to our suggested mechanism and to get an appreciable SFF. It is arguable that the condensation fraction n_0 is of the order 0.01 as estimated in Ref. [16]; then in accordance with our estimation, Fig. 1, the SFF of our state is appreciable and may reach the order of 0.01 if a/d is not less than 0.25. (A likely explanation of why Ref. [4] found the SFF $\alpha \leq 10^{-4}$ is that the estimate used an analogy of the exchange effect for ^3He in a normal rather than supersolid phase.) Since the SFF depends sensitively on the microscopic parameters, to measure the lattice constant and the NCRI at the same time would be very desirable.

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References

- [1] C. N. Yang, *Rev. Mod. Phys.* **34**, 694 (1962); Sec. 25.
- [2] A.F. Andreev and I.M. Lifshitz, *Sol. Phys. JETP* **29**, 1107 (1969).
- [3] G. V. Chester, *Phys. Rev. A* **2**, 256 (1970).
- [4] A. J. Leggett, *Phys. Rev. Lett.* **25**, 1543 (1970).
- [5] J. Fernandez, M. Puma, *J. Low Tem. Phy.* **17**, 131 (1974).
- [6] W. M. Saslow, *Phys. Rev. Lett.* **36**, 1151 (1976).
- [7] M. W. Meisel, *Physica B* **178**, 121 (1992).
- [8] E. Kim and M. H. W. Chan, *Nature* **427**, 225 (2004).
- [9] E. Kim and M. H. W. Chan, *Science* **305**, 1941 (2004).
- [10] D. Ceperley, B. Bernu, *Phys. Rev. Lett.* **93**, 155303 (2004).
- [11] M. W. Saslow, *Phys. Rev B*, **71**, 092502 (2005).
- [12] M. Tiwari and A. Datta, cond-mat/0406124; D. Weiss, cond-mat/0407043; N. Prokof'ev and B. Svistunov, *Phys. Rev. Lett.* **94**, 155302 (2005); Shun-ichiro Koh, cond-mat/0411713.
- [13] L. Reatto, *Phys. Rev.* **183**, 334 (1969)
- [14] L. Reatto and G. V. Chester, *Phys. Rev.* **155**, 88 (1967)
- [15] L. Reatto, *Phys. Rev.* **183**, 334 (1969).
- [16] J. Fernandez and H. Gersch, *Phys. Rev. A* **7**, 239 (1973).
- [17] A. J. Leggett, *Rev. Mod. Phys.* **73**, 307 (2001).
- [18] N. Byers and C. N. Yang, *Phys. Rev. Lett.* **7**, 46 (1961).
- [19] See, for example, H. R. Glyde, *Excitations in Liquid and Solid Helium*, Clarendon Press, Oxford (1994).