Superfluidity or supersolidity as a consequence of off-diagonal long-range order

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We present a general derivation of Hess-Fairbank effect or nonclassical rotational inertial (NCRI), i.e., the refusal to rotate with its container, as well as the quantization of angular momentum, as consequences of off-diagonal long-range order (ODLRO) in an interacting Bose system. Afterwards, the path integral formulation of superfluid density is rederived without ignoring the centrifugal potential. Finally and in particular, for a class of variational wave functions used for solid helium, treating the constraint of single-valuedness boundary condition carefully, we show that there is no ODLRO and, especially, demonstrate explicitly that NCRI cannot be possessed in absence of defects, even though there exist zero-point motion and exchange effect.

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I. INTRODUCTION

It was first suggested by London that the ability of liquid ^{4}He II to flow through narrow capillaries without apparent friction is a consequence of Bose-Einstein condensation (BEC).[1] The concept of BEC was later generalized by Penrose and Onsager to be applicable to interacting particles.[2,3] It was further generalized and systematically investigated by Yang, as the notion of off-diagonal long-range order (ODLRO).[4] Now it is known that the no-friction behavior in narrow capillaries is only one of several phenomena of superfluidity.[5] As elaborated by Leggett,[6] the most basic manifestation of superfluidity is the Hess-Fairbank effect,[7] which was also called "nonclassical rotational inertial" (NCRI) by Leggett.[5] This refers to the refusal of the system to rotate with its container, when its angular velocity is sufficiently low. It is the counterpart of the Meissner effect of superconductivity. Furthermore, the quantization of angular momentum of the superfluid in the rotating container is the counterpart of the magnetic flux quantization in a superconductor.

In the case of superconductivity, the demonstration of Meissner effect and the magnetic flux quantization, as consequences of ODLRO, was made by Yang,[4] and by Sewell and Nieh *et al.* in a more recent alternative approach.[8] Bloch discussed the relation between superconducting persistent current and ODLRO.[9] In the case of superfluidity, Kohn and Sherrington derived the Hess-Fairbank effect as a consequence of ODLRO by using a sophisticated hierarchy of equations of thermal Green functions.[10] For a noninteracting Bose gas and a Gross-Pitaevskii system, Leggett made a clear-cut demonstration of Hess-Fairbank effect and quantization of angular momentum as consequences of BEC.[11] Earlier, in an extremely thorough and insightful discussion,[5] Leggett pointed out that a sufficient condition of superfluidity is a certain topological connectedness property of the many-body wave function, and that at least for zero temperature, ODLRO gives rise to this connectivity and thus superfluidity, but for a finite temperature, whether ODLRO is sufficient for superfluidity in general is not conclusive.

Moreover, Leggett established, from the point of view of connectivity of wave function, that BEC and NCRI behavior can in principle also be exhibited by a solid.[12] Recently, Kim and Chan clearly observed NCRI-like behavior in bulk solid ^{4}He in an annulus channel,[13] shortly after an earlier such observation in solid ^{4}He confined in porous Vycor glass.[14] But a consensus on its origin is yet to be reached.[15–18] The earliest predictions on supersolidity, i.e., superfluid behavior in a solid, were based on BEC of defect states.[19,20] But the concentration of zero-point vacancies is less than 10^{-6} according to the experimental results.[21] Thus an important question is whether it is possible for a pure commensurate sample of solid ^{4}He, i.e., without vacancies or interstitials, to become a supersolid. Negative answers were given recently in a path integral Monte Carlo calculation of exchange frequencies in bulk hcp ^{4}He,[16] and in a general argument about superfluidity density.[17]

Thus from both the fundamental point of view and the perspective of understanding supersolid behavior, it appears still interesting to make a general derivation of the Hess-Fairbank effect and quantization of angular momentum as clear consequences of ODLRO for an interacting Bose system in a rotating container. In this paper, we first make such a derivation. Afterwards, for a reason explained below, we rederive the superfluid density in the path integral formulation,[22] which is the very basis of the analyses of solid ^{4}He in Refs. 16 and 17. Finally, we consider the trial wave functions ever used in variational calculations for solid helium, including the Hartree wave function, the Hatree-Fock wave function, and the Nosanow-Jastrow wave function. It is shown that there is no ODLRO or BEC in these wave functions. Moreover, by examining the dependence of free energy on the rotation velocity of the container, we explicitly demonstrate that a commensurate solid described by such wave functions cannot possess NCRI, in absence of vacancies or interstitials, even if there exist zero-point motion and the exchange effect.

Note that the nonsuperfluidity of the Hartree-Fock wave function made up of localized single particle wave packets has been discussed by Leggett from the point of view of disconnectivity of the wave function long ago.[5] Our approach provides an explicit construction of the rotating wave function under the constraint of the "single-valuedness boundary condition" (SVBC) as called by Leggett,[5] while

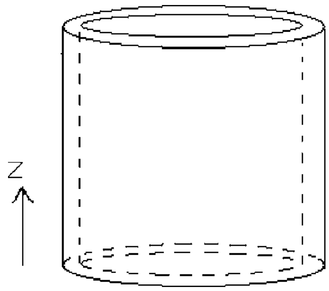

FIG. 1. The cylindrical annular container as often considered in literature and also here. The radius R is much larger than the thickness d. The rotation is along the axis of the two concentric cylinders.

keeping the energy the same as that in the static case. To do this, adjustment on the wave function needs to be made in the exponentially vanishing regions, as argued by Leggett.

II. HAMILTONIANS AND FREE ENERGIES IN THE TWO REFERENCE FRAMES

As usual, consider a Bose system in a container rotating with an angular velocity $\boldsymbol{\omega}$. Thermodynamic equilibrium is determined by the minimization of the free energy in the corotating frame of reference, in which the wall of the container is at rest. In this frame, the Hamiltonian is

$$H = \sum_j \left[\frac{(\mathbf{p}_j - m\boldsymbol{\omega} \times \mathbf{r}_j)^2}{2m} - \frac{1}{2}m(\boldsymbol{\omega} \times \mathbf{r}_j)^2 + U(\mathbf{r}_j) \right] + \frac{1}{2}\sum_{j\neq k} V_{jk}, \tag{1}$$

where the notations are standard, U is the external potential, $V_{jk} \equiv V(|\mathbf{r}_j - \mathbf{r}_k|)$ is the particle-particle interaction and is rotationally invariant. For basic mechanics and thermodynamics of a rotating body and the application to a Bose system, we refer to the standard texts.[23] But we draw attention to the point that for each particle, the radius vector $\mathbf{r}_j$, the canonical momentum $\mathbf{p}_j$, and the angular momentum $\mathbf{l}_j = \mathbf{r}_j \times \mathbf{p}_j$ are, respectively, the same in the laboratory frame and in the corotating frame. It is for this reason that H can be rewritten as

$$H = H_{lab} - \boldsymbol{\omega} \cdot \sum_j \mathbf{l}_j,$$

where

$$H_{\rm lab} = \sum_j [\mathbf{p}_j^2/2m + U(\mathbf{r}_j)] + (1/2)\sum_{j\neq k} V_{jk}$$

is the Hamiltonian in the laboratory frame. This point is quite delicate in the ODLRO study.[24]

For simplicity, as usual, consider a thin cylindrical annular container, with average radius R and thickness $d \ll R$ (Fig. 1). The rotation $\boldsymbol{\omega}$ is, of course, along the cylindrical axis (z axis). Then the centrifugal potential becomes a ω-dependent constant (in the sense that it is independent of the particle configuration), $-\frac{1}{2}M(\omega R)^2$, where M is the total mass of the particles.

It is probably useful to make a synopsis here on the free energies in the two reference frames and their relations with the rotational inertial and the superfluid density. The free energy in the corotating frame can be written as

$$F = F_0 - \frac{1}{2}I_c\omega^2 = a - \frac{1}{2}I\omega^2, \tag{2}$$

where a is a constant, $I_c = MR^2$ is the classical rotation inertial,

$$F_0 \equiv a + \frac{1}{2}(I_c - I)\omega^2.$$

The total angular momentum is $\mathbf{L} = \langle \Sigma_j \mathbf{l}_j \rangle$, hence

$$L_z = I\omega = -\frac{\partial F}{\partial \omega}.$$

In the laboratory frame, the free energy is

$$F_{\rm lab} = F + \boldsymbol{\omega} \cdot \mathbf{L} = F + I\omega^2.$$

Therefore,

$$F_{\rm lab} = F_{\rm lab,0} + \frac{1}{2}I_c\omega^2 = a + \frac{1}{2}I\omega^2,$$

where

$$F_{\rm lab,0} \equiv a - \frac{1}{2}(I_c - I)\omega^2.$$

Consistently, one also has

$$L_z = I\omega = \frac{\partial F_{\rm lab}}{\partial \omega},$$

$$I = -\frac{\partial^2 F}{\partial \omega^2} = \frac{\partial^2 F_{\rm lab}}{\partial \omega^2}.$$

For a normal system, $I = I_c$, thus $F_0 = F_{\rm lab,0} = a$. If F_0 or, equivalently, $F_{\rm lab,0}$ depends on ω, then the system is a superfluid, with NCRI. The superfluid fraction is

$$\frac{\rho_S}{\rho} = 1 - \frac{I}{I_c} = \frac{1}{I_c}\frac{\partial^2 F_0}{\partial \omega^2} = -\frac{1}{I_c}\frac{\partial^2 F_{\rm lab,0}}{\partial \omega^2},$$

where ρ_S and ρ are the superfluid density and the total fluid density, respectively. It should be noted that in equilibrium, it is F, not $F_{\rm lab}$, that is related to the partition function Q as $F = -kT \ln Q$.

III. A DERIVATION OF NCRI FROM ODLRO

Now we make a general derivation that if the system possesses ODLRO, then F_0 in Eq. (2) depends on ω. We use an approach similar to Yang's treatment of superconductivity in a magnetic field.[4]

Using the cylindrical coordinates (z, r, θ) and considering the geometry, the Hamiltonian (1) can be simplified as

$$H = H_0 - \frac{1}{2}M\omega^2 R^2, \tag{3}$$

with

$$H_0 = \sum_j \left[\frac{(p_{\theta j} - m\omega R)^2}{2m} + \frac{p_{zj}^2}{2m} \right] + \frac{1}{2}\sum_{j\neq k} V_{jk} + NU(R),$$

where $p_{\theta j}=(1/R)\partial/\partial\theta_j$. The radial momentum $p_{rj}=\partial/\partial r_j$ is neglected because $d \ll R$. An eigenfunction ψ_α of H satisfies

$$H\psi_\alpha = E_\alpha \psi_\alpha,$$

and the periodic boundary condition, or SVBC,

$$\psi_\alpha(\theta_j + 2\pi, \{\theta_{i\neq j}\}) = \psi_\alpha(\theta_j, \{\theta_{i\neq j}\}) \qquad (4)$$

due to the cylindrical geometry.

Because $-M\omega^2 R^2/2$ is a constant for a given $\boldsymbol{\omega}$, we only need to consider H_0, whose eigenfunctions are completely the same as those of H, i.e.,

$$H_0\psi_\alpha = E'_\alpha \psi_\alpha, \qquad (5)$$

where $E'_\alpha = E_\alpha + M\omega^2 R^2/2$.

By a "gauge" transformation

$$\psi_\alpha = \psi'_\alpha \exp\left(\frac{im\omega R \sum_j \theta_j}{\hbar} \right),$$

ψ'_α satisfies

$$H'_0 \psi'_\alpha = E'_\alpha \psi'_\alpha,$$

where

$$H'_0 = \sum_j \left[\frac{p_{\theta j}^2}{2m} + \frac{p_{zj}^2}{2m} \right] + \frac{1}{2}\sum_{j\neq k} V_{jk} + NU(R).$$

The angular boundary condition becomes

$$\psi'_\alpha(\theta_j + 2\pi, \{\theta_{i\neq j}\}) = e^{-2\pi i m\omega R/\hbar} \psi'_\alpha(\theta_j, \{\theta_{i\neq j}\}). \qquad (6)$$

Now consider the un-normalized density matrix

$$\rho_{dm} = e^{-H_0/kT}.$$

Because $H = H_0 - I_c\omega^2/2$, F_0 in Eq. (2) is given by $F_0 = -kT \ln Q(H_0)$, where $Q(H_0) = \mathrm{Tr}\,\rho_{dm}$. From ρ_{dm}, by tracing over all but one particle, one obtains the (un-normalized) one-particle reduced density matrix ρ_1.

The problem determined by H_0 together with SVBC is equivalent to the description in terms of H'_0 together with Eq. (6). From the ω independence of H'_0 and the boundary condition (6), one knows that

$$\langle \theta' + 2\pi | \rho_1 | \theta \rangle = \langle \theta' | \rho_1 | \theta - 2\pi \rangle = e^{2\pi i m\omega R/\hbar} \langle \theta' | \rho_1 | \theta \rangle. \quad (7)$$

We can now apply Yang's method to the current problem.

Without ODLRO, ρ_1 is vanishingly small except in the regions around $\theta = \theta' \pm 2n\pi$, where $n = 0, 1, \ldots$. As indicated by Eq. (7), the values of ρ_1 in two neighboring regions only differ by a phase factor $e^{\pm 2\pi i m\omega R/\hbar}$.

With ODLRO, these regions with nonvanishing ρ_1 merge into each other, and ρ_1 is nonvanishing everywhere. The above phase relation remains.

Furthermore, with ODLRO, Eq. (7) implies that the dependence of $\langle \mathbf{r}' | \rho_1 | \mathbf{r} \rangle$ on $\mathbf{r} - \mathbf{r}'$ must vary as ω varies. Consequently, $Q(H_0)$ and thus F_0 also vary with ω, as $Q(H_0) = \mathrm{Tr}_1 \rho_1$ and $F_0 = -kT \ln Q(H_0)$. This proves that ODLRO gives rise to superfluidity or NCRI.

IV. QUANTIZATION OF ANGULAR MOMENTUM

We now demonstrate the quantization of angular momentum as a consequence of ODLRO, by employing the method of Bloch in discussing superconducting persistent current,[9] and also as a generalization of an argument by Leggett.[11] As said above, the angular momentum and momentum are, respectively, the same in the laboratory frame and in the corotating frame. But for convenience, here we use the corotating frame.

Consider the one-particle reduced density matrix with r and z coordinates integrated over,

$$\langle \theta' | \rho_1 | \theta \rangle = \int dr \int dz \langle r, \theta', z | \rho_1 | r, \theta, z \rangle,$$

and its Fourier transformation

$$\langle \theta' | \rho_1 | \theta \rangle = \frac{1}{2\pi} \sum_{l',l} e^{(i/\hbar)(l\theta - l'\theta')} \langle l' | \rho_1 | l \rangle, \qquad (8)$$

where l and l' represent angular momenta. Its normalization is

$$\int \langle \theta | \rho_1 | \theta \rangle d\theta = \sum_l \langle l | \rho_1 | l \rangle = N.$$

Conservation of angular momentum in the z direction implies that $\langle l' | \rho_1 | l \rangle = 0$ for $l' \neq l$.

The total angular momentum, along the z direction, for the system under consideration can be given as

$$L_z = \sum_l l \langle l | \rho_1 | l \rangle. \qquad (9)$$

In the Hamiltonian in Eq. (3), $p_{\theta j}$ can be substituted as l_{zj}/R, where l_{zj} is the z-component angular momentum operator of the jth particle. Thus H depends on single particle angular momentum operators through the kinetic term

$$\sum_j (l_{zj} - m\omega R^2)^2 / (2mR^2).$$

Define $\tilde{l} = l - m\omega R^2$. In Eq. (9), if the summation can be replaced as an integral, then one can substitute l as $\tilde{l} + m\omega R^2$ and replace the integral over l as that over $\tilde{l}$. Consequently one obtains $L_z = Nm\omega R^2 + L'_z(\omega)$, where $L'_z(\omega)$ is independent of ω and is thus equal to $L'_z(0)$, which must be vanishing. Therefore

$$L_z = Nm\omega R^2,$$

which is exactly the angular momentum of a classical object. But is it legitimate to replace the summation over angular momentum eigenvalues as an integral?

Let $\Delta\theta$ be the range of $|\theta'-\theta|$ in which $\langle\theta'|\rho_1|\theta\rangle$ remains the same order of magnitude as $\langle\theta|\rho_1|\theta\rangle$, while Δl is the half width of $\langle l|\rho_1|l\rangle$ around $l=l_0$. Then because of Eq. (8), we know

$$\Delta\theta\Delta l \approx \hbar.$$

In the absence of ODLRO, $\Delta\theta \ll 1$, thus

$$\Delta l \gg \hbar.$$

This allows the replacement of the summation over l as an integral, provided that $\langle l|\rho_1|l\rangle$ is smooth.

In contrast, the presence of ODLRO implies that

$$\Delta\theta \approx 1.$$

Therefore,

$$\Delta l \approx \hbar,$$

which is equal to the unit difference of angular momentum eigenvalues. It is thus clear that if there is ODLRO, then one cannot replace the summation as an integral.

For such a probability distribution caused by ODLRO, $\langle l|\rho_1|l\rangle \approx N_0$ for $l\approx l_0$, where N_0 is of the same order of magnitude of N, while $\langle l|\rho_1|l\rangle$ for other values of l are negligible. Thus the total angular momentum is quantized as

$$L_z \approx N_0 l_0,$$

with l_0 determined by minimizing the Hamiltonian. When ω is sufficiently small, $l_0=0$, i.e., the system exhibits Hess-Fairbank effect. When ω is finite, l_0 is finite, but $N_0 l_0$ is less than $Nm\omega R^2$.

V. REDERIVATION OF SUPERFLUID DENSITY IN PATH INTEGRAL FORMALISM

The analyses on solid ^{4}He in Refs. 16 and 17 were based on an elegant path integral formulation of superfluid density in a rotating annulus,[22] with the same geometry as in our consideration above. It was derived by neglecting the centrifugal potential. We believe that the centrifugal potential cannot be neglected. As this formulation of superfluid density is very important and widely used, it may be worthwhile to rederive it without neglecting the centrifugal potential. It turns out that it nicely remains the same, although the centrifugal potential is added to the free energy. But it seems that this is known only after it is checked, so it is reported here.

We rewrite the Hamiltonian in the rotating frame, already given in Eq. (1), as

$$H = \sum_j \frac{(\mathbf{p}_j - m\mathbf{v})^2}{2m} - \frac{1}{2}Nmv^2 + U + V, \tag{10}$$

where, to follow Ref. 22, the rotational velocity ωR is denoted as v. The external potential and the interaction terms are schematically denoted as U and V, respectively. U is absent in Ref. 22, but its addition does not change the equations concerned. This Hamiltonian determines the density matrix ρ_{dm} and the statistical distribution.

One obtains[22]

$$\frac{\rho_N}{\rho}Nm\mathbf{v} = \frac{\mathrm{Tr}(\mathbf{P}\rho_{dm})}{\mathrm{Tr}(\rho_{dm})}, \tag{11}$$

where ρ_N is the normal fluid density, $\mathbf{P}=\Sigma_j \mathbf{p}_j$ is the total momentum. This identity is obtained by considering the momentum in the laboratory frame, as $\mathbf{v}$ is the container velocity in the laboratory frame. Again, note that the canonical momentum is the same in the laboratory and in the corotating frames, while it reduces to the kinematic momentum in the laboratory frame.

Because

$$\mathbf{P} = -\frac{\partial H}{\partial \mathbf{v}},$$

Eq. (11) can be rewritten as

$$\frac{\rho_N}{\rho}Nm\mathbf{v} = -\frac{\partial F}{\partial \mathbf{v}}, \tag{12}$$

where $F=-kT\ln[\mathrm{Tr}(\rho_{dm})]$ is the free energy in the corotating frame. Therefore the superfluid fraction is

$$\frac{\rho_S}{\rho} = 1 + \frac{\partial\left(\frac{F}{N}\right)}{\partial\left(\frac{1}{2}mv^2\right)}.$$

Thus the free-energy change due to the rotation of the container, up to the order of v^2, is

$$\frac{\Delta F}{N} = \frac{mv^2}{2}\left(\frac{\rho_S}{\rho} - 1\right), \tag{13}$$

from which it can be confirmed that the centrifugal potential $mv^2/2$ indeed cannot be ignored, since it is no less than the other term $(\rho_S/\rho)mv^2/2$.

In the path integral calculation

$$e^{-\beta\Delta F} = \frac{\int \rho_{dm}(\mathbf{X},\mathbf{X};\beta;\mathbf{v})d\mathbf{X}}{\int \rho_{dm}(\mathbf{X},\mathbf{X};\beta;\mathbf{v}=0)d\mathbf{X}},$$

where $\mathbf{X}$ represents the configuration of the particles. The "gauge term" $-m\mathbf{v}$ in the kinetic energy term can be transformed away, by adding, in the density matrix elements, a phase factor in winding the periodic system, as in Eqs. (6) and (7). Consequently, one can replace $\rho_{dm}(\mathbf{X},\mathbf{X};\beta;\mathbf{v})$ as the density matrix $\tilde{\rho}_{dm}(\mathbf{X},\mathbf{X};\beta;\mathbf{v})$ corresponding to the Hamiltonian without the "gauge term," while multiplying it by a phase factor due to the total paths $\mathbf{W}L$ of the N particles winding around the system, where $\mathbf{W}$ is the winding number.[22]

$\tilde{\rho}_{dm}=\exp(-\beta\tilde{H})$, where $\tilde{H}=H(\mathbf{v}=0)-Nmv^2/2$. $H(\mathbf{v}=0)$ is just H_0' in Sec. III. We obtain

$$e^{-\beta\Delta F} = \langle e^{i(m/\hbar)\mathbf{v}\cdot\mathbf{W}L} e^{\beta(1/2)Nmv^2}\rangle,$$

where the average is that of the density matrix with $\mathbf{v}=0$. Consequently, up to the order of v^2, we have

$$\Delta F = N\frac{mv^2}{2}\left(\frac{m\langle W^2\rangle L^2}{3\beta\hbar^2 N} - 1\right),$$

which, together with Eq. (13), yields

$$\frac{\rho_S}{\rho} = \frac{m\langle W^2\rangle L^2}{3\beta\hbar^2 N},$$

which is the same as that given in Ref. 22. They remain the same even if v is not a small quantity, for the reason is that v is independent of the particle configuration.

VI. NO ODLRO IN NOSANOW-JASTROW WAVE FUNCTIONS

Now we turn our attention to solid ^{4}He. For a commensurate solid at rest, each atom occupies a lattice site. Because of quantum-mechanical zero-point motion, which is large in solid helium, around the neighborhood of each lattice site, there is a finite region in which the wave function is nonvanishing. With the exchange effect put aside first, the wave function is localized around each lattice site, i.e., it decays from the maximum at the lattice site. Let us denote the wave packet of atom i as $w(\mathbf{r}_i-\mathbf{Q}_i)$, where $\mathbf{r}_i$ is the actual position of the atom, $\mathbf{Q}_i$ represents a lattice site fixed in the solid. The Hartree approximation of the wave function of the solid helium is the product of these single-atom wave functions, i.e.,

$$\Phi_H = \prod_{i=1}^{N} w(\mathbf{r}_i - \mathbf{Q}_i), \tag{14}$$

which was indeed used in the earliest (unsatisfactory) variational calculations of solid helium.[25] Later works, starting by Nosanow,[26] took into account the two-particle short-range correlation by multiplying the Hartree wave function by the Jastrow factor.

To account for the exchange effect due to overlap between neighboring single-particle wave packets, one also needs to consider the wave function symmetrized over all the atoms; the detailed nature of the exchange effect is then determined by the Hamiltonian. With symmetrization, the Hartree approximation is improved to Hartree-Fock approximation

$$\Phi_{\rm HF} = \frac{1}{\sqrt{N!}}\sum_P P\prod_{i=1}^{N} w(\mathbf{r}_i - \mathbf{Q}_i), \tag{15}$$

where P represents $N!$ permutations of the N lattice sites $\{\mathbf{Q}_i\}$. The symmetrization can be made on either the particle positions $\{\mathbf{r}_i\}$ or the lattice sites $\{\mathbf{Q}_i\}$. We choose the latter for easier manipulation below.

The symmetrized Nosanow-Jastrow wave function is

$$\Phi_{\rm SNJ} = K\sum_P P\prod_{i=1}^{N} w(\mathbf{r}_i - \mathbf{Q}_i)\prod_k\prod_{j<k} f_{jk}, \tag{16}$$

where K is the normalization constant,

$$f_{jk} \equiv f[-u(|\mathbf{r}_j - \mathbf{r}_k|)]$$

is the Jastrow (or, to be historically precise, Bijl-Dingle-Jastrow) function. $f[-u(r)]$ attains a maximum larger than 1 at a certain distance r_0, and it is constrained to be $f\to 0$ as $r\to 0$, and $f\to 1$ as $r\to\infty$ or $r>\sigma$ where σ is a parameter. Note that $\Pi_k\Pi_{j<k}f_{jk}$ is automatically symmetric for all particles.

Our consideration is about a thin cylindrical bulk, $\mathbf{r}_i=(R,R\theta_i,z_i)$. Especially, the periodic boundary condition in coordinate θ should be taken into account in an essential way. It implies that the Wannier-like function w must be of the form[27]

$$w(\mathbf{r}-\mathbf{Q}) = A\sum_{\gamma=-\infty}^{\infty}\bar{w}(\mathbf{r}-\mathbf{Q}-\gamma\mathbf{G}), \tag{17}$$

where A is the normalization constant, $\mathbf{G}=2\pi R\hat{\theta}$ represents the circumference, γ represents integers, $\bar{w}$ is the (real) Wannier-like function for the infinite interval. Each $\bar{w}$ extends over a finite range, much smaller than the system size, but finite overlap is allowed. $\pm\infty$ in the summation can be understood as two bounds which can be arbitrarily large. Thus

$$\bar{w}(\mathbf{r})\bar{w}(\mathbf{r}-\mathbf{S}) \approx \bar{w}^2(\mathbf{r})\exp(-|\mathbf{S}|/c), \tag{18}$$

where $\mathbf{S}$ is an arbitrary vector and c is a length scale less than the lattice constant. Consequently, the normalization constant A in Eq. (17) is $A\approx[\Sigma_{\gamma,\gamma'}\exp(-|\gamma-\gamma'|G/c)]^{-1/2}$.

Moreover, it can be found that

$$w(\mathbf{r})w(\mathbf{r}-\mathbf{S}) \leqslant \bar{w}^2(\mathbf{r})\exp(-|\bar{S}_\theta|/c), \tag{19}$$

where $\bar{S}_\theta$ is the θ component of $\mathbf{S}$ modulo $\pm G$ such that $|\bar{S}_\theta|\leqslant G/2$, i.e., $|\bar{S}_\theta|$ is the shortest θ component of the distance between the two physical points represented by $\mathbf{r}$ and $\mathbf{r}-\mathbf{S}$.

We now set out to show that there is no ODLRO or BEC in Φ_H or $\Phi_{\rm HF}$ or $\Phi_{\rm SNJ}$, by examining the one-particle reduced density matrix

$$\rho_1(\mathbf{r},\mathbf{r}') = N\int d\mathbf{r}_2\cdots d\mathbf{r}_N\Phi(\mathbf{r},\mathbf{r}_2,\ldots,\mathbf{r}_N)\Phi(\mathbf{r}',\mathbf{r}_2,\ldots,\mathbf{r}_N)$$

for the ground state wave function Φ of the form of Φ_H or $\Phi_{\rm HF}$ or $\Phi_{\rm SNJ}$.

Though trivial, it is instructive to first consider Φ_H. It is straightforward to integrate out $\mathbf{r}_2,\ldots,\mathbf{r}_N$, and obtain $\rho_1(\mathbf{r},\mathbf{r}')=Nw(\mathbf{r}-\mathbf{Q}_1)w(\mathbf{r}'-\mathbf{Q}_1)$, for which Eq. (19) directly leads to

$$\rho_1(\mathbf{r},\mathbf{r}') \leqslant N\bar{w}^2(\mathbf{r})\exp(-|\overline{x-x'}|/c), \tag{20}$$

where $x=R\theta$ denotes the θ component of $\mathbf{r}$. Of course, $\bar{w}^2(\mathbf{r})\leqslant 1$. Thus $\rho_1(\mathbf{r},\mathbf{r}')\to 0$ as $|\overline{x-x'}|$ approaches the system size, i.e., there is no ODLRO or BEC in Φ_H.

Now consider the Hartree-Fock wave function Φ_{HF}. In the expansion of ρ_1, suppose the lattice sites in the first Φ are denoted as $\{\mathbf{Q}_i\}$ while those in the second Φ are denoted as

$\{\mathbf{Q}_i'\}$. The exponential decay of the overlap between single-particle wave functions, Eq. (19), implies that among the $(N!)^2$ terms in the expansion of ρ_1, one can neglect each term in which $\mathbf{Q}_i \neq \mathbf{Q}_i'$ for at least one of $i=2,\ldots,N$. Consequently, there are only $N!$ remaining terms, in each of which $\mathbf{Q}_i=\mathbf{Q}_i'$ for $i=1,\ldots,N$, then $\mathbf{r}_2,\ldots,\mathbf{r}_N$ are subsequently all integrated out. This $N!$ is cancelled by the $N!$ in the normalization constant. Hence, for large $|\overline{x-x'}|$, $\rho_1(\mathbf{r},\mathbf{r}')$ for Φ_{HF} behaves in the same way as for the Hartree wave function, given in Eq. (20). This proves there is no ODLRO or BEC in Φ_{HF} either.

The argument can be extended to symmetrized Nosanow-Jastrow wave function Φ_{SNJ}, which can be rewritten as

$$\Phi_{SNJ} = K\sum_P P\prod_{i=1}^{N}\left[w(\mathbf{r}_i-\mathbf{Q}_i)\prod_{j<i}f_{ji}\right], \tag{21}$$

where P represents the permutation of the N lattice sites $\{\mathbf{Q}_i\}$. $\Pi_{j<i}f_{ji}$ is a function of $\mathbf{r}_1,\ldots,\mathbf{r}_i$, and reduces to 1 for $i=1$. For each term in the expansion of ρ_1, consider $w(\mathbf{r}_i-\mathbf{Q}_i)w(\mathbf{r}_i-\mathbf{Q}_i')(\Pi_{j<i}f_{ji})^2 \leq \bar{w}^2(\mathbf{r})\exp(-|\overline{Q_{i\theta}-Q_{i\theta}'}|/c)(\Pi_{j<i}f_{ji})^2$, where $Q_{i\theta}$ is the θ component of $\mathbf{Q}_i$. It can be seen that the short-range Jastrow factor does not change the nature of long-range exponential decay. Therefore, the cross terms, in which $\mathbf{Q}_i \neq \mathbf{Q}_i'$ for at least one of $i=1,\ldots,N$, exponentially decay, and are negligible with the remaining terms. Consequently,

$$\rho_1(\mathbf{r},\mathbf{r}') \approx \frac{Nw(\mathbf{r}_1-\mathbf{Q}_1)w(\mathbf{r}_1'-\mathbf{Q}_1)\prod_{i>1}\int w^2(\mathbf{r}_i-\mathbf{Q}_i)\left(\prod_{1<j<i}f_{ji}\right)^2 f_{1i}f_{1i}'d\mathbf{r}_i}{\prod_i\int w^2(\mathbf{r}_i-\mathbf{Q}_i)\left(\prod_{j<i}f_{ji}\right)^2 d\mathbf{r}_i} \tag{22}$$

$$\leq N\bar{w}^2(\mathbf{r}_1)e^{-|\overline{x-x'}|/c}\frac{\prod_{i>1}\int w^2(\mathbf{r}_i-\mathbf{Q}_i)\left(\prod_{1<j<i}f_{ji}\right)^2 f_{1i}f_{1i}'d\mathbf{r}_i}{\prod_i\int w^2(\mathbf{r}_i-\mathbf{Q}_i)\left(\prod_{j<i}f_{ji}\right)^2 d\mathbf{r}_i}, \tag{23}$$

where $f_{1i}' \equiv f[-u(|\mathbf{r}_1'-\mathbf{r}_i|)]$. The fraction factor in Eq. (23) must be bounded by a finite number. Clearly, $\rho_1(\mathbf{r},\mathbf{r}')$ tends to exponentially vanish as $|\overline{x-x'}|$ approaches the system size. Thus there is no ODLRO or BEC in Φ_{SNJ} either. It can be seen that our argument is not disrupted by the thermodynamic limit $N\to\infty$.

Furthermore, the argument can be straightforwardly generalized to a finite temperature, in which each energy eigenfunction is of the form of Φ_H or Φ_{HF} or Φ_{SNJ}. The finite-temperature density matrix is the thermal average of the density matrices of the eigenfunctions. For an infinite sample, w would simply be $\bar{w}$, the conclusion of no ODLRO can still be obtained, in a simpler way.

Therefore, although there is ODLRO or BEC in the Jastrow wave function alone, which describe liquid helium,[28] they are dominated by the localized one-particle wave functions. This is a difference between liquid and solid. The argument extends that of Penrose and Onsager about no BEC in a solid[3] to the case with zero-point motion, exchange effect, as well as short-range correlation.

VII. NO SUPERSOLIDITY IN NOSANOW-JASTROW WAVE FUNCTIONS

As ODLRO is a sufficient condition of NCRI, it is not redundant to demonstrate that there is no NCRI either in Φ_H or Φ_{HF} or Φ_{SNJ}, as we now explicitly do in the following. We adapt the method of Kohn used in discussing electronic insulating state.[27]

Recall that the eigenfunctions and energy spectrum is determined by H_0, as in Eq. (5). The idea is the following. For every eigenfunction $\Psi_\alpha(\omega=0)$ of $H_0(\omega=0)$, where α is the index for different eigenfunctions, be it of the form of Φ_H or Φ_{HF} or Φ_{SNJ}, we show that there is a corresponding eigenfunction $\Psi_\alpha(\omega\neq 0)$ of $H_0(\omega\neq 0)$, and that its eigenvalue remains the same as that of $H_0(\omega=0)$ for $\Psi_\alpha(\omega=0)$.

$H_0(\omega\neq 0)$ is simply related to $H_0(\omega=0)$ by a "gauge" transformation, but one should be cautioned by the requirement of the SVBC,[5,27] Eq. (4). In an infinite internal , for a localized single-particle eigenfunction $\bar{w}(\mathbf{r})$ of a single-particle Hamiltonian, the correct eigenfunction wave function for $\omega\neq 0$ is

$$\bar{w}'(\omega;\mathbf{r}) = \bar{w}(\mathbf{r})\exp\left(\frac{im\omega x}{\hbar}\right),$$

where, as above, $x=R\theta$,

Therefore, for a many-particle eigenfunction $\Psi_\alpha(\omega=0)$ of $H_0(\omega=0)$, given by Φ_H or Φ_{HF} or Φ_{SNJ}, one may construct the corresponding eigenfunction $\Phi_\alpha(\omega\neq 0)$ of $H_0(\omega\neq 0)$ in a similar way, by replacing every single-particle $\bar{w}(\mathbf{r})$ as $\bar{w}'(\mathbf{r})$. The presence of Jastrow factor does not affect this.

On the other hand, by using Eq. (17), $\Psi_\alpha(\omega=0)$ can be written as

$$\Psi_\alpha(\omega=0)=A^N\sum_{\Gamma=-\infty}^{\infty}\bar{\Phi}_\Gamma(\{\mathbf{r}_i\}),$$

where $\bar{\Phi}_\Gamma$ is obtained from $\bar{\Phi}$ by shifting the centers of the single-particle wave packets $\bar{w}$ from $\{\mathbf{Q}_i\}$ to $\{\mathbf{Q}_i+\gamma_i\mathbf{G}\}$, with $\Sigma_i\gamma_i=\Gamma$; here $\bar{\Phi}$ is of the form of $\bar{\Phi}_H=\Pi_{i=1}^N\bar{w}(\mathbf{r}_i-\mathbf{Q}_i)$, or $\bar{\Phi}_{\mathrm{HF}}=(1/\sqrt{N!})\Sigma_P P\Pi_{i=1}^N\bar{w}(\mathbf{r}_i-\mathbf{Q}_i)$, or $\bar{\Phi}_{\mathrm{SNJ}}=K\Sigma_P P\Pi_{i=1}^N\bar{w}(\mathbf{r}_i-\mathbf{Q}_i)\Pi_k\Pi_{j<k}f_{jk}$.

Following the argument in Ref. 27, using the exponential decay of the overlap as given in Eq. (18), and very similar to the argument in last section, it can be shown that for $\Gamma\neq\Gamma'$ and arbitrary α and α', $\Phi_{\alpha,\Gamma}$ and $\Phi_{\alpha',\Gamma'}$ have exponentially vanishing overlap and give vanishing matrix element for an arbitrary one-particle position operator.

Consequently, it can be found that the corresponding eigenfunction of $H_0(\omega)$, satisfying the SVBC, is

$$\Psi_\alpha(\omega)=\sum_{\Gamma=-\infty}^{\infty}\Phi_{\alpha,\Gamma}(\{\mathbf{r}_i\})\exp\left[\frac{im\omega R}{\hbar}\left(\sum_j\theta_j-2\pi\Gamma\right)\right]. \tag{24}$$

Because of exponentially vanishing overlap between $\Phi_{\alpha,\Gamma}$ with different values of Γ, it is clear that

$$H_0(\omega)\Psi_\alpha(\omega)=E_\alpha(\omega)\Psi_\alpha(\omega)$$

with

$$E_\alpha(\omega)=E_\alpha(\omega=0).$$

It is thus proved that every eigenvalue $E_\alpha(\omega)$ of $H_0(\omega)$ is independent of ω. Interestingly, the argument has gone through even in presence of the Jastrow factors.

In fact, the explicit construction of the wavefunction here confirms the principle, established by Leggett,[5] that the system is nonsuperfluid if for the wave function of the rotating system, the SVBC can still be satisfied without causing the energy to be increased by the rotation. Leggett already applied this principle to the Hartree-Fock wave function.

Therefore, for a commensurate quantum solid described by Hartree or Hartree-Fock or Nosanow-Jastrow wave function, even though the exchange effect, large zero-point motion and short-range correlation are taken into account, the free energy is of the form of Eq. (2), with F_0 independent of ω. This indicates that it cannot a supersolid.

In our argument, the localized single-particle wave functions play a crucial role. Obviously, the situation would be different when there exist vacancies or interstitials or both, which makes the wave functions extended. The recent experimental result of Kim and Chan poses a significant challenge. The difficulty might be resolved if an extended factor is found in the actual wave function.

VIII. SUMMARY

To summarize, we have offered some analytic arguments concerning the existence or nonexistence of superfluidity or supersolidity behavior. This work might be useful for further investigations on the cause of supersolidity. It might be helpful in supplementing the understanding of the relevant classic literature, and in clarifying which specific features are counterparts between superfluidity and superconductivity.

Our argument seems to suggest that ODLRO is indeed generically sufficient for superfluidity even in a finite temperature, a question which seems to have remained not entirely resolved previously.

Our discussions start with a synopsis, in Sec. II, on the Hamiltonians and the free energies in the corotating and the laboratory reference frames, as well as their relations with rotational inertial and superfluidity density.

In Secs. III and IV, from the presence of ODLRO, we make a general derivation of the most basic manifestation of superfluidity, namely the Hess-Fairbank effect or NCRI, i.e., the refusal of the Bose system to follow the rotation of the container, by using a method of Yang in treating superconductivity in a magnetic field. We also derive the quantization of angular momentum as a consequence of ODLRO, by borrowing a method of Bloch in studying superconducting persistent current. In Sec. V, we rederive the path integral formulation of the superfluid density without neglecting the centrifugal potential.

In Secs. VI and VII, we consider the variational wave functions which have been used in solid helium calculations, namely, the Hartree, the Hartree-Fock and the symmetrized Nosanow-Jastrow wave functions. The nonsuperfluidity in the Hartree-Fock wave functions was already noted by Leggett from its disconnectivity.[5] We show that there is no ODLRO in these trial wave functions, for both an infinite sample and that confined in a cylindrical annulus. Moreover, by extending a method originally due to Kohn in discussing electronic insulating states, we explicitly demonstrate that there is no NCRI behavior in a commensurate quantum solid described by those trial wave functions, even if there exist large zero-point motion, finite overlap between wave packets and exchange effect. In this argument, the constraint of SVBC in the angular direction is carefully taken into account. The explicit construction of the wavefunction under the rotation is consistent with the early arguments of Leggett in terms of the connectivity properties.[5,12]

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