

Off-diagonal long-range order and supersolidity in a quantum solid with vacanciesYu Shi,^{1,*} Yin Yang,² and Shao-Ming Fei³¹*Department of Physics, Fudan University, Shanghai 200433, China*²*School of Mathematics and Statistics, Huazhong University of Science and Technology, Wuhan 430074, China*³*School of Mathematical Sciences, Capital Normal University, Beijing 100048, China*

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We consider a lattice of bosonic atoms, whose number N may be smaller than the number of lattice sites M . We study the Hartree-Fock wave function built up from localized wave functions $w(\mathbf{r})$ of single atoms, with nearest-neighboring overlap. The zero-momentum particle number is expressed in terms of permanents of matrices. In one dimension, it is analytically calculated to be $\alpha N(M-N+1)/M$, with $\alpha = |\int w(\mathbf{r}) d\Omega|^2 / [(1+2a)l]$, where a is the nearest-neighboring overlap and l is the lattice constant. α is on the order of 1. The result indicates that the condensate fraction is proportional to and of the same order of magnitude as that of the vacancy concentration, hence there is off-diagonal long-range order or Bose-Einstein condensation of atoms when the number of vacancies $M-N$ is a finite fraction of the number of the lattice sites M .

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I. INTRODUCTION

Supersolidity refers to the superfluidlike behavior of a solid, in particular, the nonclassical rotational inertia (NCRI) or missing moment of inertia, as a consequence of Bose-Einstein condensation (BEC) or off-diagonal long-range order (ODLRO).¹⁻⁴ A few years ago, Kim and Chan⁵ observed NCRI in bulk solid ⁴He in torsional oscillators, which was subsequently confirmed by several other experimental groups.⁶⁻¹⁰ Heat capacity exhibits a peak near the onset of NCRI.¹¹ Superfluidlike mass flow was seen close to the melting temperature,¹² and on melting curve,¹³ being carried by liquid regions at the interface.¹⁴ Recently, it has also been observed off the melting curve by injecting atoms from superfluids.¹⁵ Increase in shear modulus was observed at low temperatures¹⁶ but similar phenomenon in solid ³He is not accompanied by NCRI, indicating that elastic stiffening alone cannot produce NCRI.¹⁷

BEC of zero-point vacancies in the ground state of solid Helium is the basis in some proposals of supersolidity mechanism.¹⁸⁻²⁰ Path integral Monte Carlo studies indeed found that solid ⁴He is commensurate without BEC.²¹ It was argued that zero-point vacancies or interstitials are necessary for supersolidity.²² Analytical calculations based on insulatorlike trial wave functions also showed that a commensurate solid cannot be a supersolid.^{4,23-25} But on the other hand, zero-point vacancies are found in variational studies using Jastrow or Shadow wave function,²⁶ vacancy-induced BEC was also found by using shadow wave functions.²⁷ A recent diffusion Monte Carlo study of commensurate solid ⁴He using another trial wave function found a condensate fraction $\sim 10^{-4}$ and a superfluid fraction $< 10^{-5}$.²⁸

Vacancy-based mechanism was disfavored by some researchers for the reasons that ⁴He is believed to be commensurate while the vacancies tend to be phase separated because of attraction.²⁹⁻³¹ Nevertheless, the interaction between vacancies may be more complicated.³² On the other hand, disorders such as dislocations, grain boundary, and glassiness indeed appear to be important.^{10,13,31,33-35} Grain boundaries does not seem to be the fundamental origin of NCRI, which

has also been observed in large crystals.³⁶ In considering disorder or glassiness, there are theories combining this aspect with superfluidity,³⁷⁻⁴¹ as well as theories without resorting to superfluidity.^{42,43}

With all these results, the issue whether the ground state of solid ⁴He is commensurate or incommensurate and the mechanism of NCRI in solid ⁴He are still open questions.⁴⁴ It is possible that intrinsic zero-point vacancy is the fundamental origin of supersolidity while assisted by the extrinsic disorders. This possibility is consistent with the finding in simulations that the gap for vacancy creation can be closed under a moderate stress.⁴⁵ Most recently, Anderson put forward a Gross-Pitaevskii theory of dilute gas of vacancies to account for the supersolidity, arguing that every pure Bose solid's ground state is a supersolid based on vacancies.⁴⁶

As a theoretical approach shedding light on supersolid mechanism, it is interesting to consider phenomenological trial wave functions of a quantum solid and examine whether they give rise to ODLRO and supersolidity. One of the trial wave functions is metal-like, which is a product of copies of the same extended single-atom wave function, each being a superposition of localized wave functions at all lattice sites. This is a BEC state, even in the case of a perfect crystal. First studied in 1970s, this wave function suffers the shortcoming that the probability amplitude of a configuration with one particle on each site tends to vanish when $N \rightarrow \infty$.²⁴ Recently, it was reconsidered with multiplication of Jastrow factors, which suppress multiple occupancy in a same site.⁴⁷ However, it still has the shortcoming that the equality between the lattice site and the number of atoms is a coincidence.³¹ In the trial wave function used in the recent diffusion Monte Carlo study which found BEC,²⁸ the single-particle part is replaced as a product of wave functions on all lattice sites, each being superposition of wave functions of all possible single occupations of this site.

Another trial wave function is insulatorlike, with the single-particle part being a symmetrized product of the localized single-atom wave functions. There is no ODLRO in such a wave function, even though there is wave function overlap between nearest-neighboring atoms.²³ The nonexistent

ence of ODLRO was further proved in the cases that two particles cannot come too close²⁴ and that the sum of overlap integrals of a single-atom wave function with its neighboring ones is less than unity.²⁵ Recently, the nonexistence of ODLRO or NCRI was generally shown for the case that the overlap between the neighboring atoms decays exponentially or faster, with the decay constant much smaller than the system size, with or without Jastrow factors.⁴

On the basis of the insulatorlike wave function, Imry and Schwartz²⁴ introduced vacancies in the case that there is no overlap between single-atom local wave functions. They found the zero-momentum particle number to be

$$N_0 = N(M - N + 1) \frac{\left| \int w(\mathbf{r}) d\Omega \right|^2}{\Omega}, \quad (1)$$

where M is the number of total lattice sites, N is the number of atoms, $w(\mathbf{r})$ is the single-atom wave function, and Ω is the volume. $M \approx L^d$, $\Omega \approx Ml^d$, where L is the number of atoms on each side of the lattice, d is the dimension, and l is the lattice constant.

But nearest-neighbor overlap is crucial in a quantum solid. Moreover, there is some inconsistency in discussing BEC under the assumption that there is no overlap between neighboring atomic wave functions. If the overlap is zero, $|\int w(\mathbf{r}) d\Omega|^2$ also becomes zero. Then Eq. (1) becomes not useful, as $N_0=0$. To see this clearly, one can fiducially assume the single-atom wave function to be Gaussian, as indeed used in variational calculations of solid ⁴He,^{48,49} i.e.,

$$w(\mathbf{r}) = \frac{1}{(\sqrt{\pi\xi})^{d/2}} \exp\left[-\frac{1}{2}\left(\frac{r}{\xi}\right)^2\right], \quad (2)$$

where d is the dimension of the lattice. Then

$$\left| \int w(\mathbf{r}) d\Omega \right|^2 = (2\sqrt{\pi\xi})^d. \quad (3)$$

The nearest-neighbor overlap is

$$a = \int w(\mathbf{r})w(\mathbf{r}-\mathbf{l})d\Omega = \exp\left[-\frac{1}{4}\left(\frac{l}{\xi}\right)^2\right]. \quad (4)$$

Therefore the overlap $a \rightarrow 0$ means $\xi \rightarrow 0$ or $\xi \ll l$. But then $|\int w(\mathbf{r})d\Omega|^2 \rightarrow 0$ or $|\int w(\mathbf{r})d\Omega|^2/l^d \ll 1$. Therefore, it is indispensable to consider nearest-neighbor overlap.

In this paper, we consider the Hartree-Fock wave function of a quantum solid with vacancies in presence of nearest-neighbor overlap of single-atom wave functions. We obtain an analytical expression for the zero-momentum particle number N_0 , in terms of permanents of matrices. This expression formally reduces to Eq. (1) if the nearest-neighbor overlap integral a is set to be 0. We have made the analytical calculation of N_0 in one dimension. Our result on N_0 indicates that there is ODLRO when the number of vacancies is a finite fraction of the number of lattice sites, in presence of nearest-neighbor overlap between single-atom wave functions.

The rest of this paper is organized as follows. In Sec. II, we consider the Hartree-Fock wave function for a quantum

solid with vacancies, constructed in terms of localized single-atom wave functions. We obtain the analytical expression for the zero-momentum particle number, which is expressed in terms of the permanents of matrices. In Sec. III, we make a calculation in the case that the overlap integral between neighboring atoms is zero, reproducing the formula obtained by Imry and Schwartz. In Sec. III, we make the calculation for the case that the overlap integral is nonzero. Part of the mathematical derivation is presented in the appendix. The summary and discussions are made in Sec. IV.

II. TRIAL WAVE FUNCTION AND THE EXPRESSION FOR ZERO-MOMENTUM PARTICLE NUMBER IN TERMS OF PERMANENTS OF MATRICES

We consider the following Hartree-Fock wave function of a bosonic solid with vacancies:

$$\Psi(\mathbf{r}_1 \cdots \mathbf{r}_N) = \mathcal{A} \sum_I \sum_{P_I} \prod_{i=1}^N w[\mathbf{r}_i - P_I(\mathbf{R}_i)], \quad (5)$$

where w is the localized single-atom wave function, which is real and nonnegative, I represents a selection of N sites $\{\mathbf{R}_{I_1} \cdots \mathbf{R}_{I_N}\}$ from the total M sites, P_I represents the $N!$ permutations of these selected N sites, the summation over I represents $M!/N!(M-N)!$ different choices of the N sites. The normalization constant \mathcal{A} is obtained as

$$\mathcal{A}^{-2} = \sum_I \sum_{I'} \sum_{P_I} \sum_{P_{I'}} \prod_i Q[P_I(\mathbf{R}_i) - P_{I'}(\mathbf{R}_i)], \quad (6)$$

where

$$Q(\mathbf{R} - \mathbf{R}') \equiv \int w(\mathbf{r} - \mathbf{R})w(\mathbf{r} - \mathbf{R}')d\Omega. \quad (7)$$

In our consideration,

$$Q(\mathbf{R} - \mathbf{R}') = \begin{cases} 1: & \text{if } \mathbf{R} - \mathbf{R}' = 0, \\ a: & \text{if } |\mathbf{R} - \mathbf{R}'| = l, \\ 0: & \text{if } |\mathbf{R} - \mathbf{R}'| > l. \end{cases} \quad (8)$$

\mathcal{A}^{-2} can be rewritten as

$$\mathcal{A}^{-2} = N! \sum_I \sum_{I'} \mathcal{P}[\Delta(I, I')], \quad (9)$$

where $\mathcal{P}[\Delta(I, I')]$ is the permanent of an $N \times N$ submatrix $\Delta(I, I')$ of the $M \times M$ matrix Q , whose elements are

$$Q_{ij} \equiv Q(\mathbf{R}_i - \mathbf{R}_j),$$

where \mathbf{R}_i and \mathbf{R}_j run over all the lattice sites. The submatrix $\Delta(I, I')$ is formed by choosing, from Q , N rows according to the set I and N columns according to the set I' .

The permanent of an $N \times N$ matrix Δ is defined as

$$\mathcal{P}(\Delta) = \sum_{i_1 \cdots i_N} \epsilon^{i_1 \cdots i_N} \Delta_{i_1} \cdots \Delta_{i_N}, \quad (10)$$

where $\epsilon^{i_1 \cdots i_N} = 1$ when every two indices are different from each other, otherwise $\epsilon^{i_1 \cdots i_N} = 0$. In other words, a permanent

is like a determinant, except that all the terms in the expansion are positive, rather than with a sign alternation.

In this paper, the calculation is limited to a one-dimensional lattice. The lattice sites are numbered from left to right as $1, 2, \dots, M$. \mathcal{Q} is trigonal with $Q_{ii}=1$, $Q_{i,i+1}=Q_{i+1,i}=a$ while the other elements are 0. Therefore \mathcal{Q} is

$$\mathcal{Q} = A_M,$$

here we introduce a square matrix A_n , n being a positive integer, written schematically as

$$A_n \equiv \begin{pmatrix} 1 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ a & 1 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & a & 1 & a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 1 & a & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a & \ddots & \ddots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a & \ddots & \ddots & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & a & 1 & a & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & a & 1 & a & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 1 & a \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 1 \end{pmatrix}_{n \times n}, \quad (11)$$

where the subscript $n \times n$ indicates that it is an $n \times n$ matrix.

For the many-body trial wave function [Eq. (5)], the one-particle reduced density matrix is

$$\begin{aligned} \rho(\mathbf{r}, \mathbf{r}') &= N \int \Psi(\mathbf{r}, \mathbf{r}_2, \dots, \mathbf{r}_N) \Psi(\mathbf{r}', \mathbf{r}_2, \dots, \mathbf{r}_N) d\Omega_2 \cdots d\Omega_N \\ &= N A^2 \sum_I \sum_{I'} \sum_{P_I} \sum_{P_{I'}} w[\mathbf{r} - P_I(\mathbf{R}_{I_1})] \\ &\quad \times w[\mathbf{r}' - P_{I'}(\mathbf{R}_{I'_1})] \prod_{i \neq 1} Q[P_I(\mathbf{R}_{I_i}) - P_{I'}(\mathbf{R}_{I'_i})] \\ &= A^2 N! \sum_I \sum_{I'} \sum_{i \in I, j \in I'} w(\mathbf{r} - \tilde{\mathbf{R}}_i) w(\mathbf{r}' - \tilde{\mathbf{R}}_j) W_{ij}, \quad (12) \end{aligned}$$

where the summation over i and j run over the rows and columns of submatrix $\Delta(I, I')$, $\tilde{\mathbf{R}}_i \equiv P_I(\mathbf{R}_{I_i})$, and $\tilde{\mathbf{R}}_j \equiv P_{I'}(\mathbf{R}_{I'_j})$, for which $Q(\tilde{\mathbf{R}}_i - \tilde{\mathbf{R}}_j)$ is just the (i, j) th element Δ_{ij} of the submatrix $\Delta(I, I')$, W_{ij} is the minor of Δ_{ij} . Here the minor W_{ij} of Δ_{ij} is defined as the permanent of the submatrix of Δ obtained by removing the i th row and the j th column.

The number of particles at the zero-momentum state is thus

$$N_0 = \frac{1}{\Omega} \int \rho(\mathbf{r}, \mathbf{r}') d\Omega d\Omega' = \frac{X_N(\mathcal{Q})}{Y_N(\mathcal{Q})} \frac{\left| \int w(\mathbf{r}) d\Omega \right|^2}{\Omega}, \quad (13)$$

where

$$X_N(\mathcal{Q}) \equiv \sum_I \sum_{I'} \sum_{i \in I, j \in I'} W_{ij}, \quad (14)$$

$$Y_N(\mathcal{Q}) \equiv \sum_I \sum_{I'} \mathcal{P}[\Delta(I, I')]. \quad (15)$$

$X_N(\mathcal{Q})$ is the summation of the permanents of the minors of all the elements of all the $N \times N$ submatrices Δ 's of \mathcal{Q} . $Y_N(\mathcal{Q})$ is the summation of the permanents of all the $N \times N$ submatrices Δ 's of \mathcal{Q} .

III. CASE WITHOUT NEAREST-NEIGHBORING OVERLAP

First let us reconsider the case without overlap between neighboring single-atom wave functions, i.e., $a=0$ and show that Eq. (13) formally reduces to Eq. (1).

In this case,

$$\mathcal{Q} = \mathcal{I}_M,$$

where \mathcal{I}_M represents the $M \times M$ unit matrix. Thus in obtaining a submatrix $\Delta(I, I')$, once N rows are chosen, there is only one choice of N columns to give rise to a nonvanishing permanent. Namely, the ordering numbers, in the parent matrix \mathcal{I}_M , of the chosen columns must be equal to those of the chosen rows, i.e., $\Delta(I, I')$ must be a unit matrix in order to have nonvanishing permanent. Consequently,

$$Y_N(\mathcal{I}_M) = \frac{M!}{N!(M-N)!}, \quad (16)$$

which is just the number of ways of choosing N rows. Note that the order of the chosen rows and the order of the chosen columns both remain the same as in the parent matrix.

In order to calculate $X_N(\mathcal{I}_M)$, we need to find out all nonzero minors for all submatrices Δ 's of \mathcal{I}_M . Note that $\mathcal{P}(\Delta) = 0$ does not mean Δ has no nonzero minors. Given that the parent matrix is a unit matrix \mathcal{I}_M , in order that Δ has one or more nonzero minors, Δ must be either a unit matrix \mathcal{I}_N or diagonal with only one "0" diagonal element. In the former case, there are $M!/N!(M-N)!$ ways of making up the unit submatrix $\Delta = \mathcal{I}_N$, which has N nonzero minors, each equal to 1. In the latter case, one first choose $N-1$ rows and $N-1$ columns, with the same ordering numbers in the parent matrix \mathcal{I}_N , to make up $N-1$ diagonal elements "1." The number of ways of doing this is $M!/(N-1)!(M-N+1)!$. To choose the remaining one row and one column, their ordering numbers in the parent matrix \mathcal{I}_N must be different, such that the remaining diagonal element in Δ is "0." The number of ways of doing this is $(M-N+1)(M-N)$. Each Δ so obtained only has one nonzero minor, which is equal to 1. Therefore,

$$\begin{aligned} X_N(\mathcal{I}_M) &= \frac{M!}{N!(M-N)!} N \\ &\quad + \frac{M!}{(N-1)!(M-N+1)!} (M-N)(M-N+1) \\ &= \frac{M!}{N!(M-N)!} N(M-N+1). \quad (17) \end{aligned}$$

Substituting Eqs. (16) and (17) into Eq. (13) indeed recovers Eq. (1).

IV. CASE WITH NEAREST-NEIGHBORING OVERLAP

With nearest-neighboring overlap, the zero-momentum particle number is

$$N_0 = \frac{X_N(A_M) |\int w(\mathbf{r}) d\Omega|^2}{Y_N(A_M) \Omega}, \quad (18)$$

where the matrix A_M is as defined in Eq. (11).

For an arbitrary matrix $S_{m \times n}$, we introduce $Y_k(S_{m \times n})$ and $X_k(S_{m \times n})$, with $k \leq \min(m, n)$. $Y_k(S_{m \times n})$ is the sum of the permanents of all the $k \times k$ submatrices of $S_{m \times n}$. $X_k(S_{m \times n})$ is the sum of the permanents of all the minors of all the $k \times k$ submatrices of $S_{m \times n}$.

First, we note the existence of the relation

$$X_k(A_n) = (n - k + 1)^2 Y_{k-1}(A_n) \quad (19)$$

for the following reason. Every minor of a $k \times k$ submatrix of A_n is in fact a $(k-1) \times (k-1)$ submatrix of A_n while a $(k-1) \times (k-1)$ submatrix is a minor of many different $k \times k$ submatrices. For a given $(k-1) \times (k-1)$ submatrix of A_n , one can add an additional row and an additional column of the A_n , making up a $k \times k$ submatrix of A_n , of which the concerned $(k-1) \times (k-1)$ submatrix of A_n is a minor. There are $(n-k+1)^2$ ways to do this. Hence a $(k-1) \times (k-1)$ submatrix is a minor of $(n-k+1)^2$ different $k \times k$ submatrices of A_n , thus we obtain the relation (19).

Therefore,

$$\frac{X_k(A_n)}{Y_k(A_n)} = \frac{(n - k + 1)^2 Y_{k-1}(A_n)}{Y_k(A_n)}. \quad (20)$$

In Appendix A, we obtain that for $n \geq 2$,

$$\begin{aligned} Y_2(A_n) &= (1 + 2a)^2 \frac{n(n-1)}{2} - (5a^2 + 4a)n + 7a^2 + 4a \\ &= (1 + 2a)^2 \frac{n(n-1)}{2!} \left[1 + O\left(\frac{1}{n}\right) \right], \end{aligned} \quad (21)$$

where $O(1/n)$ represents a term on the order of $1/n$.

In Appendix B, we obtain that for any $3 \leq k < n$,

$$\begin{aligned} Y_k(A_n) &= \sum_{l=k-1}^{n-1} Y_{k-1}(A_l) + 2 \sum_{s=1}^{k-2} a^s \sum_{l=k-s}^{n-s-1} Y_{k-s}(A_l) \\ &+ a^2 \sum_{l=k-2}^{n-2} Y_{k-2}(A_l) + (1 + 2a) 2a^{k-1} (n-k)(n-k+1). \end{aligned} \quad (22)$$

From this relation, we know that $Y_k(A_n) > Y_{k-1}(A_{n-1})$, $Y_{k-1}(A_{n-1})$ being merely one term in the first summation in right-hand side (RHS) of Eq. (22). Consequently, in the summation over s , $2 \sum_{l=k-s}^{n-s-1} Y_{k-s}(A_l)$, which also depends on a , by which a^s is multiplied, decreases with the increase in s . Since $a < 1$, RHS of Eq. (22) converges with respect to a . Also note that the last term is of the power of a^{k-1} .

Therefore, $Y_k(A_n)$ can be written as

$$\begin{aligned} Y_k(A_n) &= \left[\sum_{l=k-1}^{n-1} Y_{k-1}(A_l) + 2a \sum_{l=k-1}^{n-2} Y_{k-1}(A_l) \right] [1 + O_{\leq}(a)] \\ &= \left[(1 + 2a) \sum_{l=k-1}^{n-1} Y_{k-1}(A_l) - 2a Y_{k-1}(A_{n-1}) \right] [1 + O_{\leq}(a)], \end{aligned} \quad (23)$$

where $O_{\leq}(a)$ denotes a term at most on the order of a .

In the following, we show by induction that

$$Y_k(A_n) = (1 + 2a)^k \frac{n!}{k! (n-k)!} [1 + O_{\leq}(a)]. \quad (24)$$

Suppose that the similar identity is valid for $Y_{k-1}(A_l)$, with $k-1 \leq l < n$, i.e.,

$$Y_{k-1}(A_l) = (1 + 2a)^{k-1} \frac{l!}{(k-1)! (l-k+1)!} [1 + O_{\leq}(a)]. \quad (25)$$

Then

$$\begin{aligned} (1 + 2a) \sum_{l=k-1}^{n-1} Y_{k-1}(A_l) &= \frac{(1 + 2a)^k}{(k-1)!} \sum_{l=k-1}^{n-1} \frac{l!}{(l-k+1)!} [1 + O_{\leq}(a)]. \end{aligned} \quad (26)$$

Using the identity⁵⁰

$$\sum_{j=1}^p j(j+1) \cdots (j+q) = \frac{1}{q+2} \frac{(p+q+1)!}{(p-1)!}, \quad (27)$$

we obtain

$$\sum_{l=k-1}^{n-1} \frac{l!}{(l-k+1)!} = \frac{1}{k} \frac{n!}{(n-k)!}, \quad (28)$$

Hence Eq. (26) becomes

$$(1 + 2a) \sum_{l=k-1}^{n-1} Y_{k-1}(A_l) = (1 + 2a)^k \frac{n!}{k! (n-k)!} [1 + O_{\leq}(a)]. \quad (29)$$

On the other hand, according to the assumption [Eq. (25)] and the above result [Eq. (29)], we have

$$\begin{aligned} 2a Y_{k-1}(A_{n-1}) &= 2a (1 + 2a)^{k-1} \frac{(n-1)!}{(k-1)! (n-k)!} [1 + O_{\leq}(a)] \\ &= \frac{2a}{1 + 2a} \frac{k}{n} \left[(1 + 2a) \sum_{l=k-1}^{n-1} Y_{k-1}(A_l) \right] [1 + O_{\leq}(a)] \\ &= O(a) \frac{k}{n} \sum_{l=k-1}^{n-1} Y_{k-1}(A_l), \end{aligned} \quad (30)$$

where $k/n \leq 1$.

Substituting Eqs. (29) and (30) into Eq. (23) yields Eq. (24), hence the proof completes.

Then we substitute the proved identity [Eq. (24)] into Eq. (20), obtaining

$$\frac{X_k(A_n)}{Y_k(A_n)} \approx \frac{k(n-k+1)}{1+2a}, \quad (31)$$

if $a \ll 1$.

Therefore, according to Eq. (18), the zero-momentum particle number is

$$N_0 \approx \frac{N(M-N+1)}{1+2a} \frac{\left| \int w(\mathbf{r}) d\Omega \right|^2}{\Omega}. \quad (32)$$

This identity formally reduces to that obtained by Imry and Schwartz long ago when we set $a=0$. But $|\int w(\mathbf{r}) d\Omega|^2 \neq 0$ only if $a \neq 0$.

On the other hand, in case $n \gg k$, no matter whether $a \ll 1$, we can also obtain the identity [Eq. (31)] and thus the result [Eq. (32)]. This condition does not correspond to the physical situation concerning solid ^4He , as that would mean most of the lattice sites are empty. For completeness, we give the mathematical proof for this case in Appendix C.

V. SUMMARY AND DISCUSSIONS

To summarize, we have studied the Hartree-Fock wave function of a lattice of atoms with $N \leq M$, where M and N are the numbers of lattice sites and atoms, respectively. The Hartree-Fock wave function is constructed in terms of localized wave functions of single atoms, with nearest-neighbor overlap.

In one dimension, under this wave function, we have obtained the zero-momentum particle number as given in Eq. (32), which can be rewritten as

$$N_0 = \alpha \frac{N(M-N+1)}{M}, \quad (33)$$

where

$$\alpha = \frac{\left| \int w(\mathbf{r}) d\Omega \right|^2}{(1+2a)l} \quad (34)$$

is a finite fraction on the order of 1.

To be specific, let us again use the Gaussian wave function for $w(\mathbf{r})$, as given in Eq. (2). Then in one dimension,

$$\alpha = \frac{2\sqrt{\pi}\frac{\xi}{l}}{\left[1 + 2 \exp\left(-\frac{1}{4}\left(\frac{l}{\xi}\right)^2\right) \right]}, \quad (35)$$

which is on the order of 1 when ξ/l is a finite fraction around 0.36, which is obtained from the Lindemann ratio $\delta \approx 0.29$ for solid ^4He ,⁴⁹ using $\delta \equiv \sqrt{\langle r^2 \rangle} / l = \sqrt{3/2} \xi / l$ under the Gaussian wave function [Eq. (2)]. For $d=3$, $1/(1+2a)$ should be replaced by another function $f(\alpha)$ of α , which should still be on the order of 1. Anyway, $\alpha = (2\sqrt{\pi}\xi/l)^3 f(\alpha)$ must be on the order of 1.

Therefore there is BEC of atoms, i.e., N_0 is a finite fraction of N , when the number of vacancies $M-N$ is a finite fraction of the number of lattice sites M . This condition also implies that the number of atoms N is a finite fraction of M .

Interestingly, the condensate fraction N_0/N is proportional to and on the order of vacancy concentration $(M-N)/M$,

$$\frac{N_0}{N} = \alpha \frac{M-N}{M}. \quad (36)$$

Currently, the experimental upper bound of vacancy concentration is about 0.4%.²⁶ Hence a Hartree-Fock wave function for a solid with zero-point vacancy implies that the condensate fraction is about 0.004α , which is very reasonable.

Moreover, for such low vacancy concentration, one has

$$\frac{N_0}{M-N} \approx \alpha, \quad (37)$$

i.e., α equals the number of condensed atoms per vacancy. This is well consistent with the result of variational simulation based on Shadow wave function, which gives 0.23 condensed atoms per vacancy at 54 bar.²⁷

The Hartree-Fock wave function could be the ground state of a mean-field theory. Although it is not multiplied by the Jastrow factor, the double occupancy is excluded by construction. Our calculation is done for one dimension. In three dimensions, there should not be qualitative difference in order of magnitude from the result for one dimension. Hence our result is qualitatively informative for solid ^4He , suggesting that its supersolidity based on BEC of atoms induced by zero-point vacancy is possible.

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APPENDIX A: $Y_2(A_n)$

Here we calculate $Y_2(A_n)$ ($n \geq 2$), i.e., the sum of the permanents of all the 2×2 submatrices of A_n .

In addition to the definition of A_n as given in Eq. (11), we shall also use matrices

$$B_{n-1} \equiv \begin{pmatrix} a & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & a & 1 & a & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 1 & a & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \ddots & \ddots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \ddots & \ddots & a & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & a & 1 & a & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & a & 1 & a \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 1 \end{pmatrix}_{(n-1) \times (n-1)}, \quad (A1)$$

$$C_{(n-2) \times (n-1)} \equiv \begin{pmatrix} a & 1 & a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & a & 1 & a & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 1 & a & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a & 1 & a & 0 & 0 & 0 \\ 0 & 0 & 0 & \ddots & \ddots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & \ddots & \ddots & 1 & a & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & a & 1 & a \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 1 \end{pmatrix}_{(n-2) \times (n-1)} \quad (A2)$$

The permanent of an $n \times n$ matrix S is equal to

$$\mathcal{P}(S) = \sum_j S_{ij} W_{ij}, \quad (A3)$$

where W_{ij} is the minor of the S_{ij} . Using this property, we can expand $Y_2(A_n)$ as

$$Y_2(A_n) \equiv Y_2 \begin{pmatrix} 1 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ a & 1 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & a & 1 & a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 1 & a & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a & \ddots & \ddots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a & \ddots & \ddots & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & a & 1 & a & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & a & 1 & a & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 1 & a \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 1 \end{pmatrix}_{n \times n} \quad (A4)$$

$$= Y_1(A_{n-1}) + aY_1(B_{(n-1) \times (n-1)}) + aY_1(C_{(n-2) \times (n-1)}) + Y_2(A_{n-1}) = Y_2(A_{n-1}) + Y_1(A_{n-1}) + 2aY_1(A_{n-2}) + 3a^2,$$

where we have used $Y_1(B_{(n-1) \times (n-1)}) = 2a + Y_1(A_{n-2})$ and $Y_1(C_{(n-2) \times (n-1)}) = a + Y_1(A_{n-2})$, which are straightforward.

In this way, we obtain the following set of identities:

$$Y_2(A_n) - Y_2(A_{n-1}) = Y_1(A_{n-1}) + 2aY_1(A_{n-2}) + 3a^2,$$

$$Y_2(A_{n-1}) - Y_2(A_{n-2}) = Y_1(A_{n-2}) + 2aY_1(A_{n-3}) + 3a^2,$$

⋮

$$Y_2(A_3) - Y_2(A_2) = Y_1(A_2) + 2aY_1(A_1) + 3a^2. \quad (A5)$$

Adding these identities together gives rise to

$$Y_2(A_n) - Y_2(A_2) = Y_1(A_{n-1}) + (1 + 2a) \sum_{j=2}^{n-2} Y_1(A_j) + 2aY_1(A_1) + 3a^2(n-2). \quad (A6)$$

Clearly $Y_2(A_2) = 1 + a^2$ and $Y_1(A_j) = j + 2(j-1)a$. Hence it can be obtained that

$$Y_2(A_n) = (1 + 2a)^2 \frac{n(n-1)}{2} - (5a^2 + 4a)n + 7a^2 + 4a, \quad (A7)$$

which is also satisfied when $n=2$, as $Y_2(A_2) = 1 + a^2$.

APPENDIX B: $Y_k(A_n)$

We now calculate $Y_k(A_n)$ for $3 \leq k < n$, in a way similar to the calculation of $Y_2(A_n)$ above.

Similar to Eq. (A4), we obtain

$$Y_k(A_n) \equiv Y_k \begin{pmatrix} 1 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ a & 1 & a & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & a & 1 & a & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a & 1 & a & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & a & \ddots & \ddots & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & a & \ddots & \ddots & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & a & 1 & a & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & a & 1 & a & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 1 & a \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & a & 1 \end{pmatrix}_{n \times n} \quad (B1)$$

$$= Y_{k-1}(A_{n-1}) + aY_{k-1}(B_{(n-1) \times (n-1)}) + aY_{k-1}(C_{(n-2) \times (n-1)}) + Y_k(A_{n-1}).$$

Expansion of $Y_{k-1}(B_{(n-1) \times (n-1)})$ gives

$$Y_{k-1}(B_{(n-1) \times (n-1)}) = aY_{k-2}(A_{k-2}) + Y_{k-1}(C_{(n-1) \times (n-2)}^T). \quad (B2)$$

For any matrix S , $Y_{k-1}(S^T) = Y_{k-1}(S)$. Hence we have

$$Y_k(A_n) = Y_k(A_{n-1}) + Y_{k-1}(A_{n-1}) + a^2Y_{k-2}(A_{n-2}) + 2aY_{k-1}(C_{(n-2) \times (n-1)}). \quad (B3)$$

Iterative expansion of $Y_{k-1}(C_{(n-2) \times (n-1)})$ yields

$$Y_{k-1}(C_{(n-2) \times (n-1)}) = Y_{k-1}(A_{n-2}) + aY_{k-2}(C_{(n-3) \times (n-2)}) = \dots = \sum_{s=1}^{k-2} a^{s-1} Y_{k-s}(A_{n-s-1}) + a^{k-2} Y_1(C_{(n-k) \times (n-k+1)}), \quad (B4)$$

where $Y_1(C_{(n-k) \times (n-k+1)}) = (n-k) + a + 2(n-k-1)a$.

Therefore,

$$Y_k(A_n) - Y_k(A_{n-1}) = Y_{k-1}(A_{n-1}) + a^2Y_{k-2}(A_{n-2}) + 2aY_{k-1}(C_{(n-2) \times (n-1)}) = Y_{k-1}(A_{n-1}) + a^2Y_{k-2}(A_{n-2}) + 2 \sum_{s=1}^{k-2} a^s Y_{k-s}(A_{n-s-1}) + 2a^{k-1}[(n-k) + a + 2(n-k-1)a]. \quad (B5)$$

Hence

$$Y_k(A_n) - Y_k(A_{n-1}) = Y_{k-1}(A_{n-1}) + a^2Y_{k-2}(A_{n-2}) + 2 \sum_{s=1}^{k-2} a^s Y_{k-s}(A_{n-s-1}) + 2a^{k-1}[a + (n-k) + 2(n-k-1)a],$$

$$\begin{aligned}
 Y_k(A_{n-1}) - Y_k(A_{n-2}) &= Y_{k-1}(A_{n-2}) + a^2 Y_{k-2}(A_{n-3}) \\
 &+ 2 \sum_{s=1}^{k-2} a^s Y_{k-s}(A_{n-s-2}) \\
 &+ 2a^{k-1} [a + (n-1-k) + 2(n-k-2)a], \\
 &\vdots
 \end{aligned}$$

$$\begin{aligned}
 Y_k(A_{k+2}) - Y_k(A_{k+1}) &= Y_{k-1}(A_{k+1}) + a^2 Y_{k-2}(A_k) \\
 &+ 2 \sum_{s=1}^{k-2} a^s Y_{k-s}(A_{k+1-s}) + 2a^{k-1} [a + 2 + 2a],
 \end{aligned}$$

$$\begin{aligned}
 Y_k(A_{k+1}) - Y_k(A_k) &= Y_{k-1}(A_k) + a^2 Y_{k-2}(A_{k-1}) \\
 &+ 2 \sum_{i=1}^{k-2} a^i Y_{k-s}(A_{k-s}) + 2a^{k-1} [a + 1].
 \end{aligned} \tag{B6}$$

Adding these identities together leads to

$$\begin{aligned}
 Y_k(A_n) - Y_k(A_k) &= \sum_{l=k}^{n-1} Y_{k-1}(A_l) + a^2 \sum_{l=k-1}^{n-2} Y_{k-2}(A_l) \\
 &+ 2 \sum_{s=1}^{k-2} a^s \sum_{l=k-s}^{n-s-1} Y_{k-s}(A_l) \\
 &+ 2a^{k-1} \sum_{s=0}^{n-k-1} [a + (n-k-s) + 2(n-k-1-s)a].
 \end{aligned} \tag{B7}$$

Since $Y_m(A_n)$ exists only when $m \leq n$, we have

$$Y_k(A_k) = Y_{k-1}(A_{k-1}) + a^2 Y_{k-2}(A_{k-2}). \tag{B8}$$

Therefore,

$$\begin{aligned}
 Y_k(A_n) &= \sum_{l=k-1}^{n-1} Y_{k-1}(A_l) + 2 \sum_{s=1}^{k-2} a^s \sum_{l=k-s}^{n-s-1} Y_{k-s}(A_l) \\
 &+ a^2 \sum_{l=k-2}^{n-2} Y_{k-2}(A_l) + (1+2a)2a^{k-1}(n-k)(n-k+1).
 \end{aligned} \tag{B9}$$

APPENDIX C: CALCULATION OF N_0 IN THE CASE OF $n \gg k$

Here we show that the identity [Eq. (31)] and thus the result [Eq. (32)] are also valid if $n \gg k$, no matter whether $a \ll 1$ or not. Mathematically, $n \gg k$ means $n \rightarrow \infty$ while k remains finite.

In the following, we show by induction that

$$Y_k(A_n) = (1+2a)^k \frac{n!}{k!(n-k)!} \left[1 + O(a)O\left(\frac{1}{n}\right) \right]. \tag{C1}$$

Suppose that the similar identity is valid for $Y_{k-s}(A_l)$, with $s \geq 1$ and $k-s \leq l < n$, i.e.,

$$Y_{k-s}(A_l) = (1+2a)^{k-s} \frac{l!}{(k-s)!(l-k+s)!} \left[1 + O(a)O\left(\frac{1}{l}\right) \right]. \tag{C2}$$

In the second term in the exact identity [Eq. (B9)] for $Y_k(A_n)$, $2a^s$ is multiplied by $\sum_{l=k-s}^{n-s-1} Y_{k-s}(A_l)$, which can be evaluated by using the assumption [Eq. (C2)] to be

$$\begin{aligned}
 \sum_{l=k-s}^{n-s-1} Y_{k-s}(A_l) &= \frac{(1+2a)^{k-s} n^{s-1}}{(k-s)!} \sum_{l=k-s}^{n-s-1} \frac{l!}{(l-k+s)!} \left[1 + O(a)O\left(\frac{1}{l}\right) \right] = \frac{(1+2a)^{k-s}}{(k-s+1)!(n-k-1)!} (n-s)! \\
 &= \left[\sum_{l=k-1}^{n-2} Y_{k-1}(A_l) \right] \frac{(k-2) \cdots (k-s+1)}{(1+2a)^{s-1}} \frac{1}{(n-1) \cdots (n-s+1)},
 \end{aligned} \tag{C3}$$

where we have used the identity [Eq. (27)].

In the third term in Eq. (B9), $2a^2$ is multiplied by $\sum_{l=k-2}^{n-2} Y_{k-2}(A_l)$, which can be similarly evaluated to be

$$\begin{aligned}
 \sum_{l=k-2}^{n-2} Y_{k-2}(A_l) &= \frac{(1+2a)^{k-2}}{(k-2)!} \sum_{l=k-2}^{n-2} \frac{l!}{(l-k+2)!} \left[1 + O(a)O\left(\frac{1}{l}\right) \right] \\
 &= \frac{(1+2a)^{k-2} (n-1)!}{(k-1)!(n-k)!} \\
 &= \left[\sum_{l=k-1}^{n-2} Y_{k-1}(A_l) \right] \frac{k}{(1+2a)} \frac{1}{(n-k)},
 \end{aligned} \tag{C4}$$

where we have also used the identity [Eq. (27)].

Besides, the last term in Eq. (B9) is $O(a^{k-1})O(n^2) \ll Y_{k-1}(A_{n-1}) = O(n^k)$ if $k \ll n$.

Therefore,

$$\begin{aligned}
 Y_k(A_n) &= \left[\sum_{l=k-1}^{n-1} Y_{k-1}(A_l) + 2a \sum_{l=k-1}^{n-2} Y_{k-1}(A_l) \right] \\
 &\times \left[1 + O(a)O\left(\frac{1}{n}\right) \right],
 \end{aligned} \tag{C5}$$

where $O(1/n) \ll 1$, $O(a)$ is on the order of a , which we do not need to specify.

Using the assumption [Eq. (C2)] for $s=1$, we obtain

$$\begin{aligned} (1+2a) \sum_{l=k-1}^{n-1} Y_{k-1}(A_l) &= (1+2a)^k \sum_{l=k-1}^{n-1} \frac{l!}{(k-1)!(l-k+1)!} \left[1 + O\left(\frac{1}{l}\right) \right] \\ &= \frac{(1+2a)^k}{(k-1)!} [F + O(G)], \end{aligned} \quad (\text{C6})$$

where

$$F = \sum_{l=k-1}^{n-1} \frac{l!}{(l-k+1)!}, \quad (\text{C7})$$

$$G = \sum_{l=k-1}^{n-1} \frac{(l-1)!}{(l-k+1)!}. \quad (\text{C8})$$

Using the identity [Eq. (27)], we obtain

$$F = \frac{1}{k} \frac{n!}{(n-k)!}, \quad (\text{C9})$$

$$G = \frac{1}{k-1} \frac{(n-1)!}{(n-k)!}. \quad (\text{C10})$$

Hence Eq. (C6) becomes

$$(1+2a) \sum_{l=k-1}^{n-1} Y_{k-1}(A_l) = \frac{(1+2a)^k}{k!} \frac{n!}{(n-k)!} \left[1 + O(a)O\left(\frac{1}{n}\right) \right]. \quad (\text{C11})$$

On the other hand, according to Eqs. (C2) and (C11),

$$\begin{aligned} 2aY_{k-1}(A_{n-1}) &= \frac{2a(1+2a)^{k-1} (n-1)!}{(k-1)! (n-k)!} \left[1 + O(a)O\left(\frac{1}{n}\right) \right] \\ &= \frac{2a}{1+2a} \frac{k}{n} \left[(1+2a) \sum_{l=k-1}^{n-1} Y_{k-1}(A_l) \right] \\ &= \left[(1+2a) \sum_{l=k-1}^{n-1} Y_{k-1}(A_l) \right] O(a)O\left(\frac{1}{n}\right) \end{aligned} \quad (\text{C12})$$

for the reason that $k \ll n$.

Therefore,

$$\begin{aligned} \sum_{l=k-1}^{n-1} Y_{k-1}(A_l) + 2a \sum_{l=k-1}^{n-2} Y_{k-1}(A_l) &= (1+2a) \sum_{l=k-1}^{n-1} Y_{k-1}(A_l) - 2aY_{k-1}(A_{n-1}) \\ &= (1+2a) \sum_{l=k-1}^{n-1} Y_{k-1}(A_l) \left[1 + O(a)O\left(\frac{1}{n}\right) \right]. \end{aligned} \quad (\text{C13})$$

By using Eqs. (C11) and (C13), Eq. (C5) leads to the identity [Eq. (C1)], which is thus proved. Substituting this proved identity into Eq. (20), we obtain Eq. (31) and thus also Eq. (32).

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