### Excitation spectrum of a supersolid

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The quantum-lattice-gas model is used to describe the solid phase of a system consisting of Bose particles. The Hamiltonian is diagonalized in the spin-wave approximation and a twobranch excitation spectrum is obtained. When the system exhibits a Bose-Einstein (BE) condensation (i.e., in the supersolid phase), the excitation is a coupled density—order-paramet oscillation. The lower branch is proportional to  $k(\omega \sim k)$  and is mixed with the phonon spectrum; the upper branch has a gap and is proportional to  $k^2$  ( $\omega \sim \omega_0 + bk^2$ ,  $b > 0$ ). The magnitude of the gap  $\omega_0$  is a pressure-dependent quantity and is estimated to be in the range of 0 (at the superfluid—supersolid transition) to  $10^{12}$  per sec (at the supersolid—normal-solid transition) In the normal-solid phase (no BE condensation) these two branches do not couple to,density oscillations and cannot be observed by neutron scattering experiments. Therefore the existence of the upper branch by neutron scattering experiments may be used as a criterion for the existence of a supersolid.

#### I. INTRODUCTION

In the past decade there has been numerous theoretical speculation $^{1-11}$  concerning the possibility of a Bose-Einstein (BE) condensation in a quantum solid, and whether this BE condensed phase exists in a real physical system such as solid 4He. So far there has been no report on the experimental observation of such a BE condensed solid (supersolid). But before any experimentalist can do research in this aspect, one must answer the following fundamental question first: What physical properties characterize a supersolid and how to detect them experimentally? It is the purpose of this paper to provide some of the answers to the above questions and hopefully this would help the experimentalists in their research for a supersolid.

The properties of a supersolid have been studied by The properties of a supersolid have been studied by Andreev and Lifshitz,<sup>2</sup> Saslow,<sup>12</sup> and Liu<sup>13</sup> from macroscopic symmetric considerations. They used a macroscopic theory, in close analogy to the theory of two-fluid hydrodynamics<sup>14, 15</sup> of superfluid liquid  ${}^{4}$ He, to study the possibility of a persistent flow of defects, and entropy flux, etc. While the validity of their theory remains to be proven by experiments, we give a microscopic approach in this paper. The model we use is quantum-lattice-gas (QLG) model. This model has been successfully used by several authors to describe the superfluid transition and the phonon spectrum, <sup>16</sup> and other properties<sup>17, 18</sup> of liquid <sup>4</sup>He. The same model has also been used by several auspectrum, <sup>16</sup> and other properties<sup>17, 18</sup> of liquid <sup>4</sup>He.<br>The same model has also been used by several au<br>thors <sup>4, 8, 9, 11, 19</sup> to describe the properties of a Bose solid. In this paper, we use the spin-wave analysis to derive the excitation spectrum of a Bose solid, and find that the experimentally observable spectrum is

distinctly different for a supersolid and for a normal Bose solid. We think this may be the simplest method to detect a supersolid.

The excitation spectrum of the QLG model in the supersolid phase has been calculated by Mullin<sup>8</sup> and by Liu and Fisher. $9$  However we think it is appropriate to rederive and to reexamine the result more thoroughly here because of the following two reasons. Firstly, neither of the results of Mullin, or of Liu and Fisher seems to be satisfactory. Secondly, and more importantly, the physical nature of the excitation spectrum has been overlooked and it deserves a new explanation here. We explain these two points more thoroughly in the following'.

(i) The spectrum obtained by Mullin has two branches  $\left[\omega \sim k^2 \text{ and } \omega \sim \text{const} + O(k^2) \text{ for small }\right]$  $k$ ]. However, Mullin used a set of parameters which correspond to a limiting point in the parameter space which would support a stable supersolid phase.<sup>4</sup> Therefore his result is not a general one. Liu and Fisher used a correct set of parameters and also obtained a two-branch spectrum [ $\omega \sim k$ , and  $\omega \sim \text{const}+O(k^2)$  for small k]. The lower branch is now proportional to k rather than  $k^2$ . However their result is also unsatisfactory because as the supersolid-normal-solid phase transition is approached, the lower branch does not change form and is still proportional to  $k$ , which is incorrect. We recalculate and obtain a two-branch spectrum similar to theirs but with a different proportionality constant for the lower branch. This new proportionality constant goes to zero as the supersolid-normal-solid transition line is approached, and the spectrum becomes that obtained by Mullin for a normal solid.<sup>19</sup>

(ii) The QLG model is mathematically equivalent

to the antisotropic Heisenberg model.<sup>16,20</sup> Therefore the spin-wave analysis can be used to obtain the low-temperature excitation spectrum. However the magnetic analogy is a fictitious one and care must be taken in the explanation of the excitation spectrum. In the QLG model (see Sec. II below), the space is divided into cells and to each cell there associates a "spin" operator  $\vec{\sigma}$ . At the ground state, all the "spins" prefer to align along a direction different from the z direction for a supersolid  $(\sigma_z)$  is related to the number density of each cell and  $\langle \sigma_x \rangle$  or  $\langle \sigma_y \rangle$  is the BE condensation order parameter). For the lowlying excited states, the spins deviate slightly from the preferred direction and a spin-wave-like excitation<sup>21</sup> is obtained. From this picture we see that this type of excitation is a coupled density-orderparameter oscillation ( $\sigma_z$  varies from cell to cell, and  $\langle \sigma_x \rangle \neq 0$  and also varies from cell to cell). Therefore this spectrum can be excited by phonon excitation (e.g., neutron scattering). For a normal Bose solid the situation is completely different. At the ground state, all the "spins" align in the <sup>z</sup> direction. And the "spin-wave" excitation corresponds to a situation where  $\sigma_z$  = const is independent of the position of the cell and  $\langle \sigma_x \rangle = \langle \sigma_y \rangle = 0$  (no BE condensation). Therefore in the normal solid this type of excitation does not couple to density oscillations and<br>cannot be observed by neutron scatterings.<sup>22</sup> cannot be observed by neutron scatterings.<sup>22</sup>

For a supersolid the spectrum has two branches which are coupled density-order-parameter oscillations. The lower branch  $(\omega \sim k)$  is mixed with the phonon spectrum and will modify the sound velocity. The upper branch  $(\omega \sim \omega_0 + bk^2)$  has a gap and a positive effective mass  $(b > 0)$ . Because of the similarity of the excitation spectrum, it is tempting to identify this mode as one of the types of "defectons" discussed by Andreev and Lifshitz.<sup>2</sup> This branch can also be excited by neutron scatterings. For a normal Bose solid, the spectrum has also two branches,  $19$  but they do not couple to density oscillations and cannot be observed by neutron scattering experiments. Therefore the presence (or absence) of the upper branch by neutron scattering experiments may be used as a criterion for the existence (or nonexistence) of a supersolid. $^{23}$ 

In Sec. II, we give a brief description of the QLG model. In Sec. III, the spin-wave analysis is employed to derive the excitation spectrum. Discussions and conclusions are given in Sec. IV.

# II. QUANTUM-LATTICE-GAS MODEL

In order to have a close comparison with the result of Liu and Fisher,<sup>9</sup> we adopt their conventions and notations. We consider a bcc lattice which decomposes into two interpenetrating simple cubic sublattices  $\alpha$  and  $\beta$ . In a "perfect" crystalline state, all the

lattice points (or "cells") of the sublattice  $\alpha$  are occupied, and those of  $\beta$  sublattice are empty. We call  $\alpha$  "regular" sites and  $\beta$  "interstitial" sites. The scheme of the second quantization is adopted, and the operators  $a_i^{\dagger}$  and  $a_i$  are defined as the creation and annihilation operator at the *i*th cell, respectively. These being Bose operators, it is assumed that they obey the usual commutation relations for different cells,

$$
[a_i, a_j]_- = [a_i, a_j^+]_- = 0 \text{ for } i \neq j .
$$
 (1)

In the lattice-gas model, there is also a restriction that no cell can contain more than one particle at a time. This simulates the hard-core potential and can be accomplished by the Fermi anticommutation relations when they refer to the same cell,

$$
[ai, ai]+ = [ai+, ai+]+ = 0 ,[ai, ai+]+ = 1 .
$$
 (2)

The commutation relations Eqs. (1) and (2) characterize the operaters in. the model. They have the same relations as the commutation relations of a collection of spin units, with each unit fixed at a lattice site and spin magnitude  $\frac{1}{2}$ . In terms of the Pauli matrices  $\vec{\sigma}_i$  we have

$$
a_j^{\dagger} = \frac{1}{2} \sigma_j^{(+)} = \frac{1}{2} (\sigma_j^x + i \sigma_j^y) ,
$$
  
\n
$$
a_j = \frac{1}{2} \sigma_j^{(-)} = \frac{1}{2} (\sigma_j^x - i \sigma_j^y) ,
$$
  
\n
$$
n_j = a_j^{\dagger} a_j = \frac{1}{2} (1 + \sigma_j^z) .
$$
  
\n(3)

Here  $n_i$  is the number operator for the *j*th cell. If we approximate the kinetic-energy operator of the system as the finite difference<sup>16</sup> of the operators of the nearest-neighbor (NN) and next-nearestneighbor (NNN) cells, and consider only the NN and NNN interactions, the Hamiltonian has the form,<sup>9</sup>

$$
\mathbf{3c} = \sum_{\langle ij \rangle} t_{ij} a_i^{\dagger} a_j + \frac{1}{2} \sum_{\langle ij \rangle} V_{ij} n_i n_j
$$
  
=  $I_0 + \frac{1}{8} \sum_{\langle ij \rangle} V_{ij} \sigma_i^z \sigma_j^z$   

$$
- \frac{1}{4} \sum_{\langle ij \rangle} t_{ij} (\sigma_i^x \sigma_j^x + \sigma_i^y \sigma_j^y) - \sum_i \sigma_i^z H_z \qquad (4)
$$

Here  $\langle ij \rangle$  stands for NN and NNN pairs,  $V_{ij}$ 's are the potential energy, and  $t_{ij}$ 's are related to kinetic energy.  $I_0$  is the part of the Hamiltonian which is independent of the  $\sigma$ 's and  $H_z$  is the external field. Readers are advised to consult Ref. 9. for the details. Let

$$
t_{\alpha\beta} = \frac{1}{4}J_1, \quad t_{\alpha\alpha} = \frac{1}{3}J_2 \quad ,
$$
  

$$
V_{\alpha\beta} = -\frac{1}{2}J'_1, \quad V_{\alpha\alpha} = -\frac{2}{3}J'_2 \quad ,
$$
 (5)

and take into account the fact that for each site there

are eight NN and six NNN sites, we have

$$
\mathbf{K} = I_0 - \frac{1}{16} J'_1 \sum_{\langle ij \rangle} \sigma_{\alpha i}^z \sigma_{\beta j}^z - \frac{1}{12} J'_2 \sum_{\langle ij \rangle} (\sigma_{\alpha i}^z \sigma_{\alpha j}^z + \sigma_{\beta i}^z \sigma_{\beta j}^z) - \frac{1}{16} J_1 \sum_{\langle ij \rangle} (\sigma_{\alpha i}^x \sigma_{\beta j}^x + \sigma_{\alpha i}^y \sigma_{\beta j}^y)
$$
  

$$
- \frac{1}{12} J_2 \sum_{\langle ij \rangle} (\sigma_{\alpha i}^x \sigma_{\alpha j}^x + \sigma_{\alpha i}^y \sigma_{\alpha j}^y + \sigma_{\beta i}^z \sigma_{\beta j}^x + \sigma_{\beta i}^y \sigma_{\beta j}^y) - \sum_{i} (\sigma_{\alpha i}^z + \sigma_{\beta i}^z) H_z .
$$
 (6)

## III. SPIN-WAVE ANALYSIS

Consider a BE condensed solid in which the BE condensation order parameters  $\langle \sigma_{\alpha}^{x} \rangle$  and  $\langle \sigma_{\beta}^{x} \rangle$  are nonzero.<sup>8, 9, 11</sup>. At the ground state all the spins of the  $\alpha$  sublattice align along the same direction (denoted as the  $\zeta$  direction) which makes an angle  $\theta$  with the z direction. In order for the spin-wave analysis to be applicable we transform to the new axes  $\xi \eta \zeta$  for the  $\alpha$  sublattice, we have

$$
\sigma_{\alpha i}^{x} = \sigma_{\alpha i}^{\xi} \cos \theta + \sigma_{\alpha i}^{\xi} \sin \theta \quad , \qquad \sigma_{\alpha i}^{y} = \sigma_{\alpha i}^{\eta} \quad , \qquad \sigma_{\alpha i}^{z} = -\sigma_{\alpha i}^{\xi} \sin \theta + \sigma_{\alpha i}^{\xi} \cos \theta \quad . \tag{7}
$$

Similarly we have to transform to a new coordinate axes  $\xi' \eta' \zeta'$  for the  $\beta$  sublattice in which the  $\zeta'$  direction, the direction of the magnetization for the  $\beta$  sublattice, makes an angle  $\phi$  with the z direction. Equation (6) then takes the form

$$
\mathbf{3}\mathbf{C} = I_0 + H_z \sum_i (\sigma_{\alpha i}^i \cos\theta - \sigma_{\alpha i}^i \sin\theta + \sigma_{\beta i}^{i'} \cos\phi - \sigma_{\beta i}^{i'} \sin\phi)
$$
  
+ 
$$
\sum_{\langle ij \rangle} [A_{11} \sigma_{\alpha i}^i \sigma_{\beta j}^i + A_{33} \sigma_{\alpha i}^i \sigma_{\beta j}^{i'} + A_{13} \sigma_{\alpha i}^i \sigma_{\beta j}^{i'} + A_{31} \sigma_{\alpha i}^i \sigma_{\beta j}^{i'} + A_{22} \sigma_{\alpha i}^i \sigma_{\beta j}^{j'} + B_{11} \sigma_{\alpha i}^i \sigma_{\alpha j}^{i'} + B_{33} \sigma_{\alpha i}^i \sigma_{\alpha j}^{i'} + B_{13} \sigma_{\alpha i}^i \sigma_{\beta j}^{i'} + B_{22} \sigma_{\alpha i}^i \sigma_{\alpha j}^{i'}] ,
$$
  
+ 
$$
B_{13} (\sigma_{\alpha i}^i \sigma_{\alpha j}^i + \sigma_{\alpha i}^i \sigma_{\alpha j}^i) + B_{22} \sigma_{\alpha i}^i \sigma_{\alpha j}^{i'} + B_{11}^{i} \sigma_{\beta i}^i \sigma_{\beta j}^{i'} + B_{33}^{i} \sigma_{\beta i}^i \sigma_{\beta j}^{i'} + B_{13}^{i} \sigma_{\beta i}^i \sigma_{\beta j}^{i'} + B_{22}^{i} \sigma_{\beta i}^{i'} \sigma_{\beta j}^{i'}].
$$
\n(8)

I

where

$$
A_{11} = -\frac{1}{16} (J'_1 \sin\theta \sin\phi + J_1 \cos\theta \cos\phi) ,
$$
  
\n
$$
A_{33} = -\frac{1}{16} (J'_1 \cos\theta \cos\phi + J_1 \sin\theta \sin\phi) ,
$$
  
\n
$$
A_{13} = -\frac{1}{16} (-J'_1 \sin\theta \cos\phi + J_1 \cos\theta \sin\phi) ,
$$
  
\n
$$
A_{21} = -\frac{1}{16} (-J'_1 \cos\theta \sin\phi + J_1 \sin\theta \cos\phi) ,
$$
  
\n
$$
A_{22} = -\frac{1}{16} J_1 ,
$$
  
\n
$$
B_{11} = -\frac{1}{12} (J'_2 \sin^2\theta + J_2 \cos^2\theta) ,
$$
  
\n
$$
B_{33} = -\frac{1}{12} (J'_2 \cos^2\theta + J_2 \sin^2\theta) ,
$$
  
\n
$$
B_{13} = -\frac{1}{12} (J_2 - J'_2) \sin\theta \cos\theta ,
$$
  
\n
$$
B_{22} = -\frac{1}{12} J_2 ,
$$
  
\n
$$
B_{33} = -\frac{1}{12} (J_2 - J'_2) \sin\theta \cos\theta ,
$$
  
\n
$$
B_{34} = -\frac{1}{12} (J_2 - J'_2) \sin\theta \cos\theta ,
$$
  
\n
$$
B_{41} = -\frac{1}{12} (J_2 - J'_1) \sin\theta \cos\theta ,
$$
  
\n
$$
B_{51} = -\frac{1}{12} (J_2 - J'_2) \sin\theta \cos\theta ,
$$
  
\n
$$
B_{61} = -\frac{1}{12} (J_2 - J'_1) \sin\theta \cos\theta ,
$$
  
\n
$$
B_{72} = -\frac{1}{12} J_2 ,
$$
  
\n
$$
B_{81} = -\frac{1}{12} (J_2 - J'_1) \sin\theta \cos\theta ,
$$
  
\n
$$
B_{92} = -\frac{1}{12} (J_2 - J'_2) \sin\theta \cos\theta ,
$$
  
\n

and a similar set of equations for  $B'_{ij}$  if we replace  $\theta$ by  $\phi$  in the last four equations in Eq. (9).

To diagonalize Eq. (8) we make the transformations

$$
\sigma_{\alpha i}^{\xi} + i \sigma_{\alpha i}^{\eta} = \frac{2}{\sqrt{N}} \sum_{\vec{k}} \exp[-i \vec{k} \cdot \vec{R}_{\alpha i}] \tilde{a}_{\vec{k}} ,
$$

$$
\sigma_{\alpha i}^{\xi} - i \sigma_{\alpha i}^{\eta} = \frac{2}{\sqrt{N}} \sum_{\vec{k}} \exp[i \vec{k} \cdot \vec{R}_{\alpha i}] \tilde{a}_{\vec{k}}^{\dagger} , \qquad (10)
$$

$$
\sigma_{\alpha i}^{\zeta} = 1 - \frac{2}{N} \sum_{\vec{k}, \vec{k}} \exp[i(\vec{k} - \vec{k}') \cdot \vec{R}_{\alpha i}] \tilde{a}^{\dagger}_{\vec{k}} \tilde{a}_{\vec{k}'}
$$

and a similar set of equations for the  $\beta$  sublattice if we make the substitutions  $\xi \eta \zeta \rightarrow \xi' \eta' \zeta', \alpha_i \rightarrow \beta_i$  $\tilde{a}_{\vec{k}} \rightarrow \tilde{b}_{\vec{k}}$ , and  $\tilde{a}_{\vec{k}}^+ \rightarrow \tilde{b}_{\vec{k}}^+$ . Equation (8) become

$$
\mathcal{K} = \mathcal{K}_{0} + \sum_{\vec{k}} \left[ A_{\vec{k}} \tilde{a}_{\vec{k}} \tilde{a}_{\vec{k}} + B_{\vec{k}} \tilde{b}_{\vec{k}} \tilde{b}_{\vec{k}} + C_{\vec{k}} (\tilde{a}_{\vec{k}} \tilde{b}_{-\vec{k}} + \tilde{a}_{\vec{k}} \tilde{b}_{-\vec{k}}^{\dagger}) + D_{\vec{k}} (\tilde{a}_{\vec{k}} \tilde{b}_{\vec{k}} + \tilde{a}_{\vec{k}} \tilde{b}_{\vec{k}}) + \frac{1}{2} E_{\vec{k}} (\tilde{a}_{\vec{k}} \tilde{a}_{\vec{k}} \tilde{a}_{-\vec{k}} + \tilde{a}_{\vec{k}} \tilde{a}_{-\vec{k}}^{\dagger}) + \frac{1}{2} F_{\vec{k}} (\tilde{b}_{\vec{k}} \tilde{b}_{-\vec{k}} + \tilde{b}_{\vec{k}} \tilde{b}_{-\vec{k}}^{\dagger}) \right],
$$
\n(11)

where we have made use of the commutation relations

$$
[\tilde{a}_{\overrightarrow{k}}, \tilde{a}_{\overrightarrow{k}'}^{\dagger}]_{-} = \delta_{\overrightarrow{k}, \overrightarrow{k}'}, \quad [\tilde{b}_{\overrightarrow{k}}, \tilde{b}_{\overrightarrow{k}'}^{\dagger}]_{-} = \delta_{\overrightarrow{k}, \overrightarrow{k}'}, \quad [\tilde{a}_{\overrightarrow{k}}, \tilde{b}_{\overrightarrow{k}'}^{\dagger}]_{-} = [\tilde{a}_{\overrightarrow{k}}, \tilde{b}_{\overrightarrow{k}'}^{\dagger}]_{-} = [\tilde{a}_{\overrightarrow{k}}, \tilde{b}_{\overrightarrow{k}'}^{\dagger}]_{-} = [\tilde{a}_{\overrightarrow{k}}, \tilde{b}_{\overrightarrow{k}'}^{\dagger}]_{-} = 0
$$
\n(12)

 $\mathfrak{X}_0$  is the  $\vec{k}$ -independent part of the Hamiltonian and

$$
A_{\overline{k}} = -2H_z \cos\theta - 16A_{33}
$$
  
\n
$$
-12B_{33} + (B_{11} + B_{22})\Delta_{\overline{k}}
$$
  
\n
$$
B_{\overline{k}} = -2H_z \cos\phi - 16A_{33}
$$
  
\n
$$
-12B'_{33} + (B'_{11} + B'_{22})\Delta_{\overline{k}}
$$
  
\n
$$
C_{\overline{k}} = (A_{11} - A_{22})\gamma_{\overline{k}}, \quad D_{\overline{k}} = (A_{11} + A_{22})\gamma_{\overline{k}}
$$
  
\n
$$
E_{\overline{k}} = (B_{11} - B_{22})\Delta_{\overline{k}}, \quad F_{\overline{k}} = (B'_{11} - B'_{22})\Delta_{\overline{k}}
$$
  
\n
$$
\gamma_{\overline{k}} = \sum_{\overline{b}_1} e^{i\overline{k} \cdot \overline{b}_1}, \quad \Delta_{\overline{k}} = \sum_{\overline{b}_2} e^{i\overline{k} \cdot \overline{b}_2}, \quad (13)
$$

where  $\vec{\delta}_1$  and  $\vec{\delta}_2$  are NN and NNN lattice vectors, respectively. In the derivation of Eq. (11), we neglect third- and higher-order terms of  $\tilde{a}_{\overline{k}}$  and  $\tilde{b}_{\overline{k}}$ , etc. We also require the coefficients of the firstorder terms to be  $zero^{24}$ .

$$
-H_{z}\sin\theta + 6B_{13} + 8A_{13} = 0,
$$
  

$$
-H_{z}\sin\phi + 6B'_{13} + 8A_{31} = 0.
$$
 (14)

These two equations determine  $\theta$  and  $\phi$  for a given value of  $H_z$ .  $H_z$  represents pressure for a quantum solid (and is the magnetic field for a magnetic system).

By using the equation of motion  $i\tilde{\sigma}_{\overline{k}} = [\tilde{\sigma}_{\overline{k}}, H]_-,$ and assuming  $\tilde{a}_{\overline{k}} \sim e^{-i\omega t}$ , etc., we get from Eqs. (11) and (12)

$$
\omega_{\pm}^{2}(\vec{k}) = \frac{1}{2} (A^{2} + B^{2} - E^{2} - F^{2} - 2C^{2} + 2D^{2})
$$
  
\n
$$
\pm \frac{1}{2} \{ (A^{2} - B^{2} - E^{2} + F^{2})^{2}
$$
  
\n
$$
+ 4[(A - E)(D + C) + (B + F)(D - C)]
$$
  
\n
$$
\times [(B - F)(D + C) + (A + E)(D - C)]^{1/2},
$$
  
\n(15)

where  $A = A_{\overrightarrow{k}} = A_{-\overrightarrow{k}}$ , etc. This is exactly the result obtained by Liu and Fisher,<sup>25</sup> if we eliminate  $H_z$  by Eq.  $(14)$ . However, in the small-k limit we get a result different from theirs

$$
\omega_{+}^{2}(\vec{k}) = J_{1}^{2} (S_{\beta}/S_{\alpha} - S_{\alpha}/S_{\beta})^{2}
$$
  
+ 
$$
[J_{1}^{2} + \frac{1}{3}J_{1}J_{2}(S_{\alpha}/S_{\beta} + S_{\beta}/S_{\alpha}) - \frac{1}{12}(J_{2} - J_{2}')J_{1}S_{\alpha}S_{\beta}]k^{2}\delta_{1}^{2} + O(k^{4})
$$
 (16)

and

$$
\omega_{-}^{2}(k) = (J_{2} - J_{2}')[\frac{1}{4}J_{1}S_{\alpha}S_{\beta} + \frac{1}{6}J_{2}(S_{\alpha}^{2} + S_{\beta}^{2})]
$$

$$
\times k^{2}|\delta_{1}|^{2} + O(k^{4}),
$$

$$
S_{\alpha} = \sin\theta, \quad S_{\beta} = \sin\phi
$$

It is easily seen from Eq.  $(16)$  that in the supersolid phase  $\omega - \kappa$ . But as the supersolid-normal-solid transition is approached  $\omega$ . becomes proportional to  $k^2$ , because at the transition  $\theta = 0$  and  $\phi = \pi$  and  $S_{\alpha} = S_{\beta} = 0$ , while the result obtained by Liu and Fisher indicates that the lower branch is still proportional to  $k$  at the transition which is incorrect.

### IV. DISCUSSIONS AND CONCLUSIONS

In order that the spectrum of Eqs.  $(15)$  or  $(16)$  has any physical meaning, the system described by the Hamiltonian Eq. (6) must exhibit a stable supersolid phase for a certain range of  $H_z$ . The stability conditions at absolute zero have been studied by Matsuda and Tsuneto,<sup>4</sup> and they are<sup>1</sup>

$$
-(J_1 + J'_1) > J_2 - J'_2 > 0 \t\t(17)
$$

of which, the second inequality  $(J_2 - J_2' > 0)$  can be considered as the condition that there exist a finite fraction of lattice vacancies in the ground state.<sup>26</sup> Therefore  $J_2 - J_2' < 0$  corresponds to the case where ground-state lattice vacancies do not exist and the system does not exhibit a stable supersolid phase.

As mentioned in the Introduction, the ground state of a supersolid has the following pictures: For the  $\alpha$ sublattice, the mean number of particles per cell  $n_{\alpha} = \frac{1}{2}(1 + \cos \theta)$  is less than one, and the BE condensation order parameter  $\zeta_{\alpha} = \langle \sigma_{\alpha}^{x} \rangle = \sin \theta$  is nonzero. Similarly for the  $\beta$  sublattice,  $n_{\beta}$  $=\frac{1}{2}(1+\cos\phi)$  and  $\zeta_{\beta} = \langle \sigma_{\beta}^2 \rangle = \sin\phi \neq 0$ . For lowlying excited states,  $(n_{\alpha}, \zeta_{\alpha})$  and  $(n_{\beta}, \zeta_{\beta})$  oscillate about a mean value, respectively. Therefore this is a coupled density —order-parameter oscillation. The lower branch of Eq. (16) has an acousticlike spectrum  $\omega \sim k$ , in which  $(n_{\alpha}, \zeta_{\alpha})$  and  $(n_{\beta}, \zeta_{\beta})$  oscillate in phase. This mode is mixed with the phonon spectrum and may modify the sound velocity. The upper branch has a gap and is proportional to  $k^2$  ( $\omega \sim \omega_0$ +  $bk^2$ ), in which  $(n_{\alpha}, \zeta_{\alpha})$  and  $(n_{\beta}, \zeta_{\beta})$  oscillate 180° out of phase. This is different from an opticalphonon spectrum because in the supersolid phase  $S_{\alpha}$ and  $S_{\beta}$  are small positive quantities and  $J_1$  and  $J_2$  are positive numbers, therefore  $b > 0$ . Because this mode exists (or, more precisely, can be detected) only when there are ground-state lattice defects (in this case lattice vacancies) and because of the similarly of the excitation spectrum, it is tempting to identify this mode as one of the types of "defectons" discussed by Andreev and Lifshitz.<sup>2</sup> This mode is an order-parameter oscillation and it is quite possible that the system may exhibit some types of super fluidity as discussed by some authors.<sup>2,1</sup>

Two remarks about the two branches in Eq. (16): (i) As the system undergoes a phase transition

from a supersolid phase to a superfluid phase, the angles  $\theta$  and  $\phi$  change from  $\theta \neq \phi \neq 0$  to  $\theta = \phi \neq 0$ , the upper branch disappears. The spectrum has only one branch with  $\omega \sim k$  as that obtained by Matsubara and Matsuda.<sup>16</sup>

(ii) When the pressure increases, or the parameters of Eq. (6) do not support a stable supersolid phase, the system will exhibit a normal-solid phase in which  $\theta = 0$  and  $\phi = \pi$ . The spectrum in this phase can be obtained either by a direct calculation from Eq. (11), or by examining Eq. (16). At the transition  $\theta \rightarrow 0$ and  $\phi \rightarrow \pi$ , the lower branch becomes proportional to  $k<sup>2</sup>$  (which is in contrast to that obtained by Liu and Fisher<sup>9</sup>), while the upper branch still has a gap. The magnitude of the gap can be calculated from Eq. (14) by eliminating  $H_z$ . In the limit  $\theta \rightarrow 0$  and  $\phi \rightarrow \pi$  $(\cos\theta \rightarrow 1, \cos\phi \rightarrow -1)$ , we easily find

$$
\frac{S_{\alpha}}{S_{\beta}} = \frac{J_2' - J_1' - J_2}{J_1} \pm \left[ \frac{(J_2' - J_1' - J_2)^2}{J_1^2} - 1 \right]^{1/2}
$$
  
 $\theta \to 0, \quad \phi \to \pi$ 

and

as

$$
\omega_{+}(\vec{k}) = 2J_{1}\left[\frac{(J_{2}^{2} - J_{1}^{2} - J_{2})^{2}}{J_{1}^{2}} - 1\right]^{1/2} + O(k^{2}) \quad . \quad (18)
$$

The two-branch spectrum of a normal solid has been obtained by Mullin.<sup>19</sup> In the normal-solid phase

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the excitations correspond to a situation where  $\sigma_{\alpha}^{z}$ and  $\sigma^z_{\beta}$  are constants, respectively, and do not couple to density oscillations. Therefore in normal Bose solids this type of excitation cannot be observed by neutron scatterings.

In conclusion we have shown that in a supersolid there exists a two-branch spectrum. which is the excitation of a coupled density-order-parameter oscillation. The lower branch ( $\omega \sim k$ ) is mixed with the phonon spectrum. The upper branch has a gap and is proportional to  $k^2$  ( $\omega \sim \omega_0 + bk^2$ ,  $b > 0$ ). The magnitude of the gap  $\omega_0$  is a pressure-dependent quantity (as the angles  $\theta$  and  $\phi$  are pressure-dependent quantities). The gap  $\omega_0$  is zero at the superfluidsupersolid transition line and increases as the pressure increases. It is of the order of  $J_1$  (estimated to be a few degrees kelvin) at the supersolid-normalsolid transition line. Therefore we would estimate  $\omega_0$ to be in the range of 0 to  $10^{12}$  per sec depending on the pressure. These two branches cannot be observed by neutron scattering experiments in a normal Bose solid. Therefore the existence of the upper branch by neutron scattering experiments may be used as a criterion for the existence of a supersolid.

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 $2<sup>1</sup>A$  spin wave is an excitation in which the longitudinal component (referred to the preferred direction of magnetization) of the spin is a constant independent of time and site position; only the transverse components of the spin oscillate and propagate through the lattice. See, for example, C. Kittel, Introduction to Solid State Physics, 5th ed. (Wiley, New York, 1976), pp. <sup>468</sup>—469.

- $22$ It is possible that this excitation can be observed by other means. For example it may have a contribution to the specific heat of a normal Bose solid. However the observed excess specific heat in solid <sup>3</sup>He may be irrelevant to this excitation, because the QLG model cannot be applied to a Fermi system.
- $23$ This has been pointed out by Mullin in Ref. 8. However he did not explain why this mode cannot be observed in a normal solid. See also Ref. 19.
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- $26$ This can be easily obtained by comparing Eq. (17) and Ref. 11. In Ref. 11 the conditions for the existence of a supersolid are  $-J'_1 + J'_2 >> \frac{3}{8}J_1$  and existence of ground-state lattice vacancies, The above inequality is equivalent to the first inequality of Eq. (17), since  $J_1 \gg J_2 > 0$ .