Insulator-Superfluid transition of spin-1 bosons in an optical lattice in magnetic field

A. A. Svidzinsky and S. T. Chui
Bartol Research Institute, University of Delaware, Newark, DE 19716
(December 6, 2018)

We study the insulator-superfluid transition of spin-1 bosons in an optical lattice in a uniform magnetic field. Based on a mean-field approximation we obtained a zero-temperature phase diagram. We found that depending on the particle number the transition for bosons with antiferromagnetic interaction may occur into different superfluid phases with spins aligned along or opposite to the field direction. This is qualitatively different from the field-free transition for which the mean-field theory predicts a unique (polar) superfluid state for any particle number.

I. INTRODUCTION

The insulator-superfluid transition is an example of quantum phase transitions which take place at zero temperature. At the transition point the quantum ground state of the system changes in some fundamental way. This is accomplished by changing some parameter in the Hamiltonian of the system. Possible examples are transition between different quantized plateaus in a quantum-Hall effect under the change of magnetic field, transition between different phases in high-$T_c$ superconductor compounds under the variation of doping, metal-insulator transition in a conductor under the change of disorder, or phase transitions in baryonic matter under the change of density (e.g., transition from nuclear matter to a uniform liquid of neutrons, protons and electrons at the interface between a crust and a core of a neutron star).

Originally the insulator-conductor transition has been studied in Fermi systems. However, analogous phenomena occur for a system of bosons, for example, in $^4$He absorbed in porous media or granular superconductors in which the Cooper pairs may be considered as bosons. For pure Bose systems at zero temperature the conducting phase is the superfluid, so that the insulator-conductor transition corresponds to the onset of superfluidity. In the context of insulator-superfluid transition in liquid $^4$He the problem has been studied in [1,2]. Recently such a problem attracted much attention due to experimental realization of Bose-Einstein condensation (BEC) of atoms in magnetic and optical traps. It has been proposed that the insulator-superfluid transition might be observable when an ultracold gas of atoms with repulsive interactions is trapped in a periodic optical lattice [3]. Recently the transition in $^{87}$Rb condensate in a three-dimensional simple-cubic potential was realized experimentally by changing the potential depth [4]. An artificial optical lattice has a great advantage in that the system is basically defect-free which provides ideal conditions for study the quantum phase transitions.

In the insulator phase the atoms are localized (by the effect of the potential) in the lattice sites so that fluctuations in the atom number on each site are suppressed. In such a state there is no phase coherence across the lattice. In addition the Mott insulator phase is characterized by the existence of an energy gap for the creation of particle or hole excitations, i.e., for the addition of particles to, or removal of particles from, the system. In a periodic potential the bosons can move from one lattice site to the next by quantum tunneling. The heights of the barriers can readily be adjusted since they are proportional to the intensity of the laser beam. The competition between the tunneling amplitude (kinetic energy) and the atom-atom interactions controls the point of the phase transition. When the tunneling coupling becomes large compared to the atom-atom interactions a delocalized wavefunction minimizes the dominant kinetic energy and the system undergoes a phase transition into the superfluid state. Recent theoretical studies include a delocalizing transition of BEC in optical lattices [5], the superfluid density and the quasi-momentum distribution [6,7], the superfluid to Mott insulator transition with high filling factors (multiband situation) [8], commensurate-incommensurate transition [9], as well as Monte Carlo simulations for the Bose-Hubbard systems [10,11].

An advantage of an optical trap is that it liberates the spin degrees of freedom and makes possible condensation of spinor bosons. For example, $^{23}$Na, $^{39}$K and $^{87}$Rb atoms (with nuclear spin $I = 3/2$ and electrons at $s$ orbits) at low temperatures behave as simple bosons with a hyperfine spin $f = 1$. Optically trapped BEC creates a possibility to study a variety of phenomena in spinor many boson systems which posses extremely rich physics. The insulator-superfluid transition in spinor BEC is one of the possible novel phenomena. Recently the insulator-superfluid transition of spin-1 bosons interacting antiferromagnetically in an optical lattice was investigated theoretically [12,13], as well
as the transition in a multicomponent BEC system [14] and spin-2 Bose atoms [15]. In this paper we study the phase transition of spin-1 bosons in the presence of an external magnetic field. Magnetic field lifts a degeneracy of the antiferromagnetic ground state and enriches the phase diagram. We show that magnetic field results in a qualitatively new effect. Depending on the field value the transition for bosons with antiferromagnetic interparticle interaction may occur into different superfluid phases with spins aligned along or opposite to the field direction.

II. BASIC FORMALISM

We consider a dilute gas of trapped bosonic atoms with hyperfine spin \( f = 1 \). The system is described by the following Hamiltonian [16]:

\[
\hat{H} = \hat{H}_S + \hat{H}_A, \quad \text{where the spin symmetric and asymmetric parts are}
\]

\[
\begin{align*}
\hat{H}_S &= \sum_\alpha d^3r \Psi_\alpha^+ \left( -\frac{\nabla^2}{2M} + V_{fr} \right) \Psi_\alpha + \frac{\Lambda_s}{2} \sum_{\alpha,\beta} \int \Psi_\alpha^+ \Psi_\beta^+ \Psi_\alpha \Psi_\beta d^3r, \\
\hat{H}_A &= \frac{\Lambda_a}{2} \int d^3r \left( \Psi_1^+ \Psi_1^+ \Psi_1 \Psi_1 + \Psi_3^+ \Psi_3^+ \Psi_3 \Psi_3 + 2 \Psi_1^+ \Psi_3^+ \Psi_1 \Psi_3 \right) \\
&\quad + 2 \Psi_0^+ \Psi_0^+ \Psi_0 \Psi_0.
\end{align*}
\]

(1)

(2)

here \( \Psi_\alpha \) (\( \alpha = -1, 0, 1 \)) is the atomic field annihilation operator associated with atoms in the hyperfine spin state \( \{ f = 1, m_f = \alpha \} \). \( V_{fr} = V_0(\sin^2 kx + \sin^2 ky + \sin^2 kz) \) is the optical lattice potential which is assumed to be the same for all three spin components, \( k = 2\pi/\lambda \), \( \lambda \) is the wavelength of the laser light, \( V_0 \) is the tunable depth of the potential well. The coefficients \( \Lambda_s, \Lambda_a \) are related to scattering lengths \( a_0 \) and \( a_2 \) of two colliding bosons with total angular momenta 0 and 2 by \( \Lambda_s = 4\pi\hbar^2(a_0 + 2a_2)/3M \) and \( \Lambda_a = 4\pi\hbar^2(a_2 - a_0)/3M \), where \( M \) is the mass of the atom [17]. For scattering of \( ^{23}\text{Na} \) \( a_2 = 54.7a_B \) and \( a_0 = 49.4a_B \), where \( a_B \) is the Bohr radius [18]. This suggests \( \Lambda_a > 0 \) (antiferromagnetic interaction). For \( ^{87}\text{Rb} \) \( a_2 = (107 \pm 4)a_B \) and \( a_0 = (110 \pm 4)a_B \) [17], that is \( \Lambda_a < 0 \) and the interaction is ferromagnetic.

For single atoms the energy eigenstates are Bloch wave functions. An appropriate superposition of Bloch states yields a set of Wannier functions which are localized on the individual lattice sites. Expanding the field operators in the Wannier basis

\[
\hat{\Psi}_\alpha(r) = \sum_i \hat{a}_{\alpha i} w(r - r_i),
\]

(3)

where \( \hat{a}_{\alpha i} \) correspond to the bosonic annihilation operators on the \( i \)th lattice site, and keeping terms in first order in the hopping matrix element, the Hamiltonian (1), (2) reduces to the Bose-Hubbard Hamiltonian

\[
\hat{H}_S = -J \sum_{<i,j>} \sum_\alpha \hat{a}_{\alpha i}^+ \hat{a}_{\alpha j} + \lambda_s \sum_i \hat{N}_i (\hat{N}_i - 1),
\]

(4)

\[
\hat{H}_A = \lambda_a \sum_i (\hat{a}_{i1}^+ \hat{a}_{i1}^+ \hat{a}_{i1} \hat{a}_{i1} - 2\hat{a}_{i1}^+ \hat{a}_{i1} \hat{a}_{i1} \hat{a}_{i1} - 2\hat{a}_{i1}^+ \hat{a}_{i1} \hat{a}_{i1} \hat{a}_{i1}^+ + 2\hat{a}_{i1}^+ \hat{a}_{i1} \hat{a}_{i1}^+ \hat{a}_{i1}^+ + 2\hat{a}_{i1}^+ \hat{a}_{i1}^+ \hat{a}_{i1} \hat{a}_{i1} + 2\hat{a}_{i1}^+ \hat{a}_{i1} \hat{a}_{i1}^+ \hat{a}_{i1}^+ + 2\hat{a}_{i1}^+ \hat{a}_{i1} \hat{a}_{i1}^+ \hat{a}_{i1}^+),
\]

(5)

where \( \hat{N}_i = \sum_\alpha \hat{a}_{\alpha i}^+ \hat{a}_{\alpha i} \) is the number of atoms at lattice site \( i \), \( <i,j> \) stands for the nearest-neighbor sites, \( 2\lambda_{s,a} = \Lambda_{s,a} \int d^3r |w|^4 \) corresponds to the strength of the on-site interaction between atoms and

\[
J = - \int d^3r w^*(r - r_i) \left( -\frac{\nabla^2}{2M} + V_{fr} \right) w(r - r_j) > 0
\]

is the hopping matrix element between adjacent sites \( i,j \). This describes tunneling of atoms and is related to the kinetic energy. The parameter \( J \) exponentially depends on the strength of periodic potential \( V_0 \) and can be varied experimentally by several orders of magnitude. One should mention that when number of particles in each well \( N \) is large enough the parameters \( \lambda_{s,a} \) can be reduced by a factor \( N^{-3/5} \). This occurs when condensates in each well reach the Thomas-Fermi regime. However, in experiments on 3D optical lattices \( N \lesssim 100 \) and the Thomas-Fermi regime is
usually not achieved. Higher filling factor can be realized in 2D and 1D lattices [19,20]. Also, equation (3) suggests that atoms in different spin states are approximately described by the same coordinate wave function which is the case when the spin symmetric interaction is strong compared with the asymmetric part: \(|\lambda_s| \gg |\lambda_a|\) [16]. This is relevant to experimental conditions for \(^{23}\text{Na}\) and \(^{85}\text{Rb}\) atoms [18,17]. Introducing the operators

\[ \hat{L}_+ = \sqrt{2}(\hat{a}_1^+ \hat{a}_0 + \hat{a}_0^+ \hat{a}_1), \quad \hat{L}_- = \sqrt{2}(\hat{a}_0^+ \hat{a}_1 + \hat{a}_1^+ \hat{a}_0), \quad \hat{L}_z = \hat{a}_1^+ \hat{a}_1 - \hat{a}_1 \hat{a}_1^+, \quad \hat{L}^2 = \hat{L}_+ \hat{L}_- + \hat{L}_z^2 - \hat{L}_z \]

which obey the angular momentum commutation relations \([\hat{L}_+, \hat{L}_-] = 2\hat{L}_z, [\hat{L}_z, \hat{L}_\pm] = \pm \hat{L}_\pm\) one can obtain [16]

\[ \hat{H}_A = \lambda_a \sum_i (\hat{L}_i^2 - 2\hat{N}_i). \]  

(6)

The operators \(\hat{L}_i\) and \(\hat{L}_z\) commute with \(\hat{N}_i\) and each other.

To study the phase transitions, it is more convenient to perform calculations in the grand-canonical ensemble, so we add the term with the chemical potential \(\mu\). We also include an external uniform magnetic field \(B\) along the \(z\) axis [21]. Then the Hamiltonian becomes

\[ \hat{H} = -J \sum_{<i,j>} \sum_\alpha \hat{a}_{\alpha i}^+ \hat{a}_{\alpha j}^+ \hat{a}_{\alpha j} \hat{a}_{\alpha i} + \sum_\alpha \left[ \lambda_s \hat{N}_i(\hat{N}_i - 1) + \lambda_a (\hat{L}_i^2 - 2\hat{N}_i) - \mu \hat{N}_i - b \hat{L}_z i \right], \]

(7)

where \(b = g \mu_B B\) which we assume to be positive, \(g\) is a Landé factor of an atom and \(\mu_B\) is the Bohr magneton. As we will see later the most interesting effects occur when the magnetic energy \(g \mu_B B\) is less than or comparable with the energy of spin asymmetric interaction. For such values of magnetic field the energy of spin symmetric interaction is much larger than \(g \mu_B B\) and, hence, the description of atoms in different spin states by the same coordinate wave function is justified for such magnetic field.

The consistent mean-field theory we will use corresponds to the following decomposition of the hopping terms [22–24]:

\[ \hat{a}_{\alpha i}^+ \hat{a}_{\alpha j}^+ = <\hat{a}_{\alpha i}^+ \hat{a}_{\alpha j}^+ > \hat{a}_{\alpha j} \hat{a}_{\alpha i} > - <\hat{a}_{\alpha i}^+ > <\hat{a}_{\alpha j}^+ > = \psi_{\alpha}(\hat{a}_{\alpha i}^+ + \hat{a}_{\alpha j}^+) - \psi_{\alpha}^2, \]

(8)

where \(\psi_{\alpha} = <\hat{a}_{\alpha i}^+ > = <\hat{a}_{\alpha i} >\) is the three component superfluid order parameter. In such a decomposition we omit the higher-order fluctuations \((\hat{a}_{\alpha i}^+ - \psi_{\alpha})(\hat{a}_{\alpha j} - \psi_{\alpha})\). Also we assume the order parameter to be real and neglect the Josephson-type tunneling term. Then Eq. (7) yields

\[ \hat{H} = zJ N_s \sum_\alpha \psi_{\alpha}^2 + \sum_\alpha \left[ \lambda_s \hat{N}_i(\hat{N}_i - 1) + \lambda_a (\hat{L}_i^2 - 2\hat{N}_i) - \mu \hat{N}_i - b \hat{L}_z i - zJ \sum_\alpha \psi_{\alpha}(\hat{a}_{\alpha i}^+ + \hat{a}_{\alpha i}) \right], \]

(9)

where \(z = 2d\) is the number of nearest-neighbor sites, \(d\) is the space dimension and \(N_s\) is the total number of lattice sites. This Hamiltonian is diagonal with respect to the site index \(i\), so one can use an effective onsite Hamiltonian \(\hat{H}_{i}^{\text{eff}}\)

\[ \hat{H}_{i}^{\text{eff}} = \lambda_s \hat{N}_i(\hat{N}_i - 1) + \lambda_a (\hat{L}_i^2 - 2\hat{N}_i) - \mu \hat{N}_i - b \hat{L}_z i + zJ \sum_\alpha \psi_{\alpha}^2 - zJ \sum_\alpha \psi_{\alpha}(\hat{a}_{\alpha i}^+ + \hat{a}_{\alpha i}). \]

(10)

One should note that the simple mean-field approximation we use may not catch some interesting features discussed in [12] for a field-free transition. However, our simple approximation is good enough to describe a new effect we predict for a transition in magnetic field and, hence, there is no need to consider more complicated theories.

### III. Perturbation Expansion Over the Superfluid Order Parameter

We will treat the last two terms in Eq. (10) as a perturbation. For the second order phase transition the order parameter \(\psi_{\alpha}\) continuously changes from zero (in insulator phase) to a finite value (in superfluid phase). Hence, in the vicinity of phase transition the order parameter is infinitesimally small and, therefore, to find the transition point the last two terms in Eq. (10) can be treated as a perturbation. In zero order approximation (we drop the site index \(i\) since the effective Hamiltonian is diagonal with respect to the lattice sites)

\[ \hat{H}_0^{\text{eff}} = \lambda_s \hat{N}(\hat{N} - 1) + \lambda_a (\hat{L}^2 - 2\hat{N}) - \mu \hat{N} - b \hat{L}_z. \]

(11)
The eigenstates of $\hat{H}_0^{\text{eff}}$ are states with defined total number of atoms in the site $N$ (an integer number), the total spin per site $l$ and its projection $m$ along the magnetic field. We denote the eigenstates as $|N, l, m>$. The corresponding eigenvalues are

$$E_0 = \lambda_s N(N - 1) + \lambda_a [l(l + 1) - 2N] - \mu N - bm.$$  \hspace{1cm} (12)

For $b > 0$ the state with $m = l$ corresponds to the lowest energy. We assume that all the atoms in the well are in the same orbital state, which is the ground state for the confining potential. Then the symmetry of the bosonic wave function and the structure of the operator $\hat{L}$ enforces a constraint on $l$. The allowable values of $l$ are $l = 0, 2, 4, ..., N$ if $N$ is even and $l = 1, 3, 5, ..., N$ if $N$ is odd (also $m = 0, \pm 1, \pm 2, \ldots, \pm l$ for any allowable $l$). This result is known in cavity QED; the details of the proof are provided in Appendix A of Ref. [25]. The eigenfunctions $|N, l, m>$ in terms of the Fock states $|n_1,n_0,n_{-1}>$ with defined number of particles $n_a$ with the spin projection $\alpha$ are given by

$$|N, l, m> = \sum_k A_k |k; N - 2k - m, k + m >,$$  \hspace{1cm} (13)

where $A_k$ satisfy the recursion relation

$$A_{k+1}\sqrt{(k + 1)(k + m + 1)(N - 2k - m - 1)(N - 2k - m)} + A_{k-1}\sqrt{k(k + m)(N - 2k - m + 1)(N - 2k - m + 2)} +$$

$$+A_k [k(N - 2k - m + 1) + (N - 2k - m)(k + m + 1)] = [(l + 1) - (m(m + 1))]A_k/2.$$  \hspace{1cm} (14)

In some particular cases this equation has simple solutions. E.g., if $m = l$ the coefficients are

$$A_k = (-1)^k \sqrt{(k + l)!} \sqrt{(N - l - 2k - 1)!!} \lambda_s N N \lambda_a A_0,$$  \hspace{1cm} (15)

while for $m = l - 1$

$$A_k = (-1)^k \sqrt{(k + l)!} \sqrt{(N - l - 2k)!!} \lambda_s N N \lambda_a A_0.$$  \hspace{1cm} (16)

The coefficient $A_0$ can be obtained from the normalization condition $\sum_k A_k^2 = 1$.

\section{Mott ground state of spin-1 bosons}

The ground state of $\hat{H}_0^{\text{eff}}$ depends on the relation between $\lambda_s$, $\lambda_a$, $b$ and $\mu$. It is determined by minimizing the energy (12) with the constraint $N + l = \text{even}$. We assume $\lambda_s > 0$. When $\lambda_a < 0$ the ground state is $|N, N, N>$, it is a ferromagnetic state in which all bosons occupy the $m = 1$ state. The number of particles $N$ is determined from the condition

$$2(N - 1)(\lambda_s + \lambda_a) < \mu + b < 2N(\lambda_s + \lambda_a).$$  \hspace{1cm} (17)

When $\lambda_a > 0$ the nature of the ground state depends on magnetic field. For $b = 0$ the ground state is antiferromagnetic. However, the number of particles per site depends on the relation between $\lambda_s$ and $\lambda_a$. There are two possibilities:

1) $\lambda_s > 2\lambda_a$, then the particle number is determined from

$$\begin{cases} 2(N - 1)\lambda_s - 4\lambda_a < \mu < 2N\lambda_s, & N = 0, 2, 4, ..., \; l = 0 \\ 2(N - 1)\lambda_s < \mu < 2N\lambda_s - 4\lambda_a, & N = 1, 3, 5, ..., \; l = 1 \end{cases}.$$  \hspace{1cm} (18)

The number of particles at each site increases by +1 any time the chemical potential $\mu$ crosses the points $2\lambda_s - 4\lambda_a$, $4\lambda_s - 6\lambda_a$, $4\lambda_s - 6\lambda_a$, ...

2) $\lambda_s < 2\lambda_a$, then states with even $N$ are the only possibility and

$$2(N - 3)\lambda_s - 2\lambda_a < \mu < (2N + 1)\lambda_s - 2\lambda_a, \quad N = 0, 2, 4, ..., \; l = 0.$$  \hspace{1cm} (19)
The particle number increases by +2 each time the chemical potential $\mu$ crosses the points $\lambda_s - 2\lambda_a$, $5\lambda_s - 2\lambda_a$, $9\lambda_s - 2\lambda_a$, $13\lambda_s - 2\lambda_a$, ..., For $\lambda_a > 0$ and $b = 0$ the insulator-superfluid transition has been studied in detail in [13]. For $\lambda_a, b > 0$ and given $N$ the number $l$ is determined by the parity of $N$ and the condition

$$(2l - 1)\lambda_a < b < (2l + 3)\lambda_a.$$  

When $b > \lambda_a(2N - 1)$ the ground state is ferromagnetic with $l = N$. Let us define $l_{\text{max}}$ so that $\lambda_a(2l_{\text{max}} - 1) < b < \lambda_a(2l_{\text{max}} + 1)$. Then for $b > 0$ the particle number is determined from (we assume $\lambda_s > \lambda_a > 0$)

$$N \leq l_{\text{max}} - 1: \quad 2(N - 1)(\lambda_s + \lambda_a) < \mu + b < 2N(\lambda_s + \lambda_a),$$

$$N \geq l_{\text{max}}: \quad 2(N - 1)\lambda_a - 2\lambda_a + (-1)^{N+l_{\text{max}}}(2l_{\text{max}}\lambda_a - b) < \mu < 2N\lambda_s - 2\lambda_a - (-1)^{N+l_{\text{max}}}(2l_{\text{max}}\lambda_a - b).$$

**B. Phase diagram**

We calculate the phase boundary between the insulator and the superfluid states for $b > 0$ using second-order perturbation theory. The idea is to find the energy as a function of the superfluid order parameter $\psi_\alpha$: $E = E_0 + B_1 \psi_1^2 + B_0 \psi_0^2 + B_{-1} \psi_{-1}^2 + \ldots$, where coefficients $B_\alpha$ depend on the system’s parameters. In the insulator phase all $B_\alpha > 0$ and, hence, $\psi_\alpha = 0$ minimizes the energy. Phase transition into a superfluid state occurs when one of the coefficients $B_\alpha$ becomes negative. In Appendix A we calculate the necessary matrix elements of the perturbation operator between the ground state $|N,l,l>\rangle$ and excited states of $H_{\text{eff}}$. Here we list the nonzero matrix elements:

$$<N + 1, l + 1, l|\hat{a}_0^+|N, l, l> = \sqrt{\frac{N + l + 3}{2l + 3}}, \quad <N - 1, l + 1, l|\hat{a}_0|N, l, l> = \sqrt{\frac{N - l}{2l + 3}},$$

$$<N + 1, l + 1, l|\hat{a}^+_0|N, l, l> = \sqrt{\frac{(l + 1)(N + l + 3)}{2l + 3}}, \quad <N - 1, l + 1, l - 1|\hat{a}_1|N, l, l> = -\sqrt{\frac{N - l}{(2l + 3)(2l + 1)}},$$

$$<N - 1, l - 1, l - 1|\hat{a}_1|N, l, l> = \sqrt{\frac{l(N + l + 1)}{2l + 1}}, \quad <N + 1, l + 1, l - 1|\hat{a}^+_1|N, l, l> = \sqrt{\frac{N + l + 3}{(2l + 3)(2l + 1)}},$$

$$<N + 1, l - 1, l - 1|\hat{a}^+_1|N, l, l> = -\sqrt{\frac{l(N - l + 2)}{2l + 1}}, \quad <N - 1, l + 1, l + 1|\hat{a}_{-1}|N, l, l> = -\sqrt{\frac{(N - l)(l + 1)}{2l + 3}}.$$  

The second order perturbation theory results in the following expression for the energy correction to the $|N,l,l>\rangle$ state in terms of the superfluid order parameter $\psi_\alpha$:

$$E = \lambda_s N(N - 1) + \lambda_a [l(l + 1) - 2N] - \mu N - bl + zJ \sum_\alpha \psi_\alpha^2 -$$

$$\frac{(zJ)^2 \psi_1^2}{(2l + 3)(2l + 1)} \left[ \frac{(l + 1)(N + l + 3)(2l + 1)}{2N\lambda_s + 2l\lambda_a - b - \mu} + \frac{N - l}{2(1 - N)\lambda_s + 2(l + 2)\lambda_a + b + \mu} + \frac{l(N + l + 1)(2l + 3)}{2(1 - N)\lambda_s - 2(l - 1)\lambda_a + b + \mu} \right] -$$

$$\frac{(zJ)^2 \psi_0^2}{2l + 3} \left[ \frac{N + l + 3}{2N\lambda_s + 2l\lambda_a - \mu} + \frac{N - l}{2(1 - N)\lambda_s + 2(l + 2)\lambda_a + \mu} \right] -$$

$$\frac{(zJ)^2 \psi_{-1}^2}{(2l + 3)(2l + 1)} \left[ \frac{N + l + 3}{2N\lambda_s + 2l\lambda_a + b - \mu} + \frac{l(N - l + 2)(2l + 3)}{2N\lambda_s - 2(l + 1)\lambda_a + b - \mu} + \frac{(N - l)(l + 1)(2l + 1)}{2(1 - N)\lambda_s + 2(l + 2)\lambda_a - b + \mu} \right].$$  \hspace{1cm} (17)

The leading correction to the energy is quadratic in $\psi_\alpha$, which demonstrates close analogy of the approach with Schrieffer-Wolff transformation. The idea of such canonical transformation is to eliminate the perturbation term in the Hamiltonian to first order [26]. Phase transition into a superfluid state with $\psi_\alpha \neq 0$ occurs when the coefficient
in front of $\psi_0^2$ becomes negative. For $b = 0$ and $\lambda_s > 0$ the superfluid transition occurs into a polar (spin–0) state; the result is valid for both even and odd number of particles per site [13]. In such a transition the order parameter $\psi_0$ becomes nonzero.

When $b > 0$ the situation changes substantially. One can see from Eq. (17) that as soon as the ground state corresponds to $l \neq 0$ the coefficient in front of $\psi_0^2$ in the expression for $E$ becomes smaller than the coefficient in front $\psi_0^2$. At the same time the terms containing $\psi_1$ and $\psi_{-1}$ compete with each other. Depending on the value of $b$ and the chemical potential (particle number) the system undergoes a transition into a superfluid state with $\psi_1 \neq 0$ or $\psi_{-1} \neq 0$.

The coefficient in front of $\psi_0^2$ becomes zero when

$$\frac{(2l + 3)(2l + 1)}{zJ} = \frac{(l + 1)(N + l + 3)(2l + 1)}{2N\lambda_s + 2l\lambda_a - b - \mu} + \frac{N - l}{2(1 - N)\lambda_s + 2(l + 2)\lambda_a + b + \mu} +$$

$$+ \frac{l(2l + 1)(2l + 3)}{2(1 - N)\lambda_s - 2(l - 1)\lambda_a + b + \mu},$$

while for the coefficient in front of $\psi_{-1}^2$ the condition is

$$\frac{(2l + 3)(2l + 1)}{zJ} = \frac{(N + l + 3)}{2N\lambda_s + 2l\lambda_a - b - \mu} + \frac{(N - l)(l + 1)(2l + 1)}{2(1 - N)\lambda_s + 2(l + 2)\lambda_a - b - \mu} +$$

$$+ \frac{l(N - l + 2)(2l + 3)}{2N\lambda_s - 2(l + 1)\lambda_a + b - \mu}.$$  \hfill (18)

The lowest value of $J$ from Eqs. (18), (19) determines the point of phase transition. In Fig. 1 we plot the phase boundary in the $J - \mu$ plane for the insulator-superfluid transition in a magnetic field. In our estimates we take $\lambda_s = 0.4\lambda_a$ and $b = 4.25\lambda_a$. For $J = 0$ (no tunneling) the system is in the ground state for a single well. The number of particles per site $N$ as well as the total spin $l$ depend on the chemical potential $\mu$. Solid line corresponds to a transition into superfluid phase with $\psi_1 \neq 0$, while along the dash line the transition occurs into a state with $\psi_{-1} \neq 0$. The phase boundaries between different superfluid phases with either non-zero $\psi_1$ or $\psi_{-1}$ are beyond the scope of the present paper and are not shown. In Fig. 2 we plot the phase diagram for $\lambda_s = 0.4\lambda_a$ and $b = 6\lambda_a$. The possibility of the phase transition into different superfluid states can be understood as follows. In the insulator phase particle permutation symmetry imposes the constraint $N + l = $ even; the parity of $l$ is fixed by the parity of $N$. However, the interaction energy $\lambda_a l(l + 1) - \beta l$ can be lower for $l$ with the opposite parity. The symmetry constraint is relaxed in the superfluid phase. Due to the appearance of a coherent superfluid component the particle number per site is no longer fixed. Effectively the superfluidity removes the restriction on the $l$’s parity and, as a result, the superfluid order parameter may correspond to different projections of spins along the magnetic field in order to decrease the excessive interaction energy. The effect takes place for small magnetic field or large particle number per site when $\lambda_s(2N - 1) > b$. The coefficient $\lambda_a$ can be estimated as $\lambda_a = (\pi^2/3)E_R[(a_2 - a_0)/\lambda]|V_0/E_R|^{1/4}$, where $E_R = 2\pi^2\hbar^2/ML^2$ is the recoil energy [12]. For $^{23}$Na atoms $a_2 - a_0 \approx 5.3a_B$ and typical experimental parameters $\lambda = 0.985\mu_m$, $E_R = 4.4 \times 10^{-7}K$, $V_0 \sim 12E_R$, $N \approx 3$ we obtain the following limitation on the magnetic field $B < 10^{-4}G$. Since the current capability of magnetic shielding can reach $10^{-5}G$, the low magnetic field regime is attainable. Experimentally the transition into different superfluid phases may be detected, for example, by creating a weak gradient of magnetic field. In such a case the superfluids with different magnetization will move in opposite directions.

For $b > \lambda_a(2N - 1)$ or $\lambda_a < 0$ the ground state is ferromagnetic with $l = N$. In this case the coefficient in front of $\psi_0^2$ in the expression for $E$ is smallest among the coefficients in front of $\psi_1^2, \psi_0^2, \psi_{-1}^2$. This means that the order parameter $\psi_1$ always appears first and the system undergoes a transition into ferromagnetic superfluid with $\psi_1 \neq 0$. The transition occurs when

$$zJ = \frac{(2N(\lambda_s + \lambda_a) - b - \mu)(b + \mu - 2(N - 1)(\lambda_s + \lambda_a))}{2(\lambda_s + \lambda_a) + b + \mu}, \quad 2(N - 1)(\lambda_s + \lambda_a) < b + \mu < 2N(\lambda_s + \lambda_a).$$

In Figs. 1 and 2 the ferromagnetic state is realized for small particle numbers per site ($N < 2$ and $N < 3$).

One should mention that we neglected possible presence of slowly varying (at the length scale of the lattice period) component of the trapping potential. Such potential effectively provides a scan over $\mu$ of the phase diagram at fixed values of $J/\lambda_s$ and $\lambda_s/\lambda_a$. Also at higher value of the tunneling amplitude $J$ additional phase transitions between different superfluid states may occur. Their description requires estimate of the next order terms in the energy and lies beyond the scope of our paper. One of the interesting question for future studies is superfluidity of “holes” which
might occur when some sites remain empty after filling the optical lattice by atoms. Also, thermal fluctuations may become important at nonzero temperature and destroy long-range phase coherence of superfluid. As a result, the transition can first occur into a conductor phase (with no long-range coherence) and only later into a superfluid state.

This work was supported by NASA, Grant No. NAG8-1427.

APPENDIX A: CALCULATION OF MATRIX ELEMENTS

In the presence of magnetic field the ground state of zero-order Hamiltonian (11) is $|N, l, l\rangle$. Let us consider matrix elements of the perturbation operator $\hat{a}_1^+ + \hat{a}_0$ between the ground state and the other eigenstates. To calculate matrix elements we consider the eigenstates of the Hamiltonian (11) in a form [28]

$$|N, l, l\rangle = \frac{1}{\sqrt{f(N, l)}} (\hat{a}_1^+) (\hat{\Theta}^+)^{(N-l)/2}) |\text{vac}\rangle,$$

where $\hat{\Theta}^+ = \hat{a}_0^+ - 2\hat{a}_1^+ \hat{a}_{-1}^+$ and $f$ is a normalization factor

$$f(N, l) = l! \left( \frac{N-l}{2} \right)^l (N+l+1)!!.\]

States with lower magnetic quantum numbers can be obtained by operating $\hat{L}_- = \sqrt{2}(\hat{a}_0^+ \hat{a}_1 + \hat{a}_{-1}^+ \hat{a}_0)$, $\hat{L}_+ = \sqrt{2}(\hat{a}_1^+ \hat{a}_0 + \hat{a}_{-1}^+ \hat{a}_-)$ to $|N, l, l\rangle$ and using $\hat{L}_- |N, l, m\rangle = \sqrt{(l+m)(l-m+1)} |N, l, m-1\rangle$, $\hat{L}_+ |N, l, m\rangle = \sqrt{(l+m+1)(l-m)} |N, l, m+1\rangle$. Another useful operator is $\hat{L}_z = \hat{a}_1^+ \hat{a}_1 - \hat{a}_{-1}^+ \hat{a}_{-1}$, $\hat{L}_z |N, l, m\rangle = m |N, l, m\rangle$. We note the properties

$$[\hat{L}_z, \hat{\Theta}^+] = 0, \quad [\hat{L}_z, \hat{\Theta}^-] = 0, \quad [\hat{L}_-, (\hat{a}_1^+) l] = \sqrt{2l} \hat{a}_0^+ (\hat{a}_1^+) l^{-1}, \quad [\hat{L}_-, \hat{a}_0^+] = \sqrt{2} \hat{a}_1^+,$$

$$\hat{\Theta}^+ |N, l, l\rangle = \sqrt{(N-l+2)(N+l+3)} |N+2, l, l\rangle, \quad \hat{L}_- |\text{vac}\rangle = 0, \quad \hat{L}_z |\text{vac}\rangle = 0,$$

$$[\hat{a}_1, (\hat{\Theta}^+) n] = -2n \hat{a}_{-1}^+ (\hat{\Theta}^+) n^{-1}, \quad [\hat{a}_0, (\hat{\Theta}^+) n] = 2n \hat{a}_0^+ (\hat{\Theta}^+) n^{-1}, \quad [\hat{a}_{-1}, (\hat{\Theta}^+) n] = -2n \hat{a}_1^+ (\hat{\Theta}^+) n^{-1},$$

$$[\hat{L}_+, \hat{a}_{-1}^+] = \sqrt{2} \hat{a}_0^+, \quad [\hat{L}_+, \hat{a}_1] = -\sqrt{2} \hat{a}_0, \quad [\hat{L}_z, \hat{a}_{-1}^+] = -\hat{a}_{-1}^+, \quad [\hat{L}_z, \hat{a}_1] = -\hat{a}_{-1},$$

where $[\hat{a}, \hat{b}]$ stands for the commutator of $\hat{a}$ and $\hat{b}$. Then using (A1) we obtain

$$\sqrt{f(N-1, l-1)} \hat{a}_0^+ |N-1, l-1, l-1\rangle = \hat{a}_0^+ (\hat{a}_1^+) l^{-1} (\hat{\Theta}^+) (N-l)/2 |\text{vac}\rangle = \frac{1}{\sqrt{2l}} [\hat{L}_-, (\hat{a}_1^+) l] (\hat{\Theta}^+) (N-l)/2 |\text{vac}\rangle,$$

$$= \frac{1}{\sqrt{2l}} \sqrt{f(N, l)} \hat{L}_- |N, l, l\rangle = \frac{1}{\sqrt{f(N, l)}} \hat{L}_- |N, l, l\rangle = \sqrt{f(N, l)} \sqrt{N, l, l+1} >,$$

or

$$\hat{a}_0^+ |N, l, l\rangle = \frac{\sqrt{(N-1)(N+1)}}{2l+3} |N+1, l+1, l+1\rangle.$$

Further

$$\hat{a}_1^+ |N, l, l\rangle = \frac{1}{\sqrt{f(N, l)}} (\hat{a}_1^+) l+1 (\hat{\Theta}^+) (N-l)/2 |\text{vac}\rangle = \sqrt{f(N+1, l+1)} f(N, l) |N+1, l+1, l+1\rangle =$$

$$\frac{\sqrt{(l+1)(N+1)}}{2l+3} |N+1, l+1, l+1\rangle.$$
\[ \hat{a}_{-1}|N, l, l> = \frac{1}{\sqrt{f(N, l)}}(\hat{a}_L^+)^{\dagger}\hat{a}_{-1}(\hat{\Theta}^+)^{(N-l)/2}|\text{vac}> = -\frac{(N-l)}{\sqrt{f(N, l)}}(\hat{a}_L^+)^{\dagger+1}(\hat{\Theta}^+)^{(N-l-2)/2}|\text{vac}> = -(N-l)\sqrt{f(N-1, l+1)/f(N, l)}|N-1, l+1, l+1> = -(\frac{N-l}{2l+3})|N-1, l+1, l+1> . \tag{A4} \]

\[ \hat{a}_0|N, l, l> = \frac{1}{\sqrt{f(N, l)}}(\hat{a}_L^+)^{\dagger}\hat{a}_0(\hat{\Theta}^+)^{(N-1-l)/2}|\text{vac}> = \frac{(N-l)}{\sqrt{f(N, l)}}(\hat{a}_L^+)^{\dagger+1}(\hat{\Theta}^+)^{(N-l-2)/2}|\text{vac}> = (N-l)\sqrt{f(N-2, l)/f(N, l)}\hat{a}_0|N-2, l, l> = \sqrt{\frac{N-l}{2l+3}}|N-1, l+1, l> . \tag{A5} \]

Now let us find \( \hat{a}_{-1}^+ |N, l, l> \). Using
\[ \sqrt{2}\hat{a}_0^+ |N, l, l> = \hat{L}_+ \hat{a}_{-1}^+ |N, l, l> , \]
we obtain
\[ \hat{a}_{-1}^+ |N, l, l> = \sqrt{\frac{N+l+3}{(2l+3)(2l+1)}}|N+1, l+1, l-1> + B|N+1, l-1, l-1> , \tag{A6} \]
where \( B \) is a coefficient. Other terms such as \( |N+1, m, m> \) do not enter Eq. (A6). This can be proven by applying \( \hat{L}_z \) to Eq. (A6) and using the property \( \hat{L}_z \hat{a}_{-1}^+ |N, l, l> = (l-1)\hat{a}_{-1}^+ |N, l, l> \). To find the coefficient \( B \) one can apply \( \hat{a}_{-1} \) to Eq. (A6) and consider the matrix element \( <N, l, l|\hat{a}_{-1}^+ \hat{a}_{-1}^+ |N, l, l> = 1 + <N, l, l|\hat{a}_{-1}^+ \hat{a}_{-1}^+ |N, l, l> = 1 + (N-l)(l+1)/(2l+3) \). As a result, we obtain \( B = -\sqrt{\frac{l(N-l+2)}{2l+1}} \). Hence
\[ \hat{a}_{-1}^+ |N, l, l> = \sqrt{\frac{N+l+3}{(2l+3)(2l+1)}}|N+1, l+1, l-1> - \sqrt{\frac{l(N-l+2)}{2l+1}}|N+1, l-1, l-1> . \tag{A7} \]

Finally, let us calculate \( \hat{a}_1 |N, l, l> \). Using
\[ -\sqrt{2}\hat{a}_0 |N, l, l> = \hat{L}_+ \hat{a}_1 |N, l, l> , \]
we find
\[ \hat{a}_1 |N, l, l> = -\sqrt{\frac{N-l}{(2l+3)(2l+1)}}|N-1, l+1, l-1> + C|N-1, l-1, l-1> . \]

The coefficient \( C \) can be obtained by applying \( \hat{a}_1^+ \) and considering the matrix element \( <N, l, l|\hat{a}_1^+ \hat{a}_1^+ |N, l, l> \). Ultimately
\[ \hat{a}_1 |N, l, l> = -\sqrt{\frac{N-l}{(2l+3)(2l+1)}}|N-1, l+1, l-1> + \sqrt{\frac{l(N+l+1)}{2l+1}}|N-1, l-1, l-1> . \tag{A8} \]
FIG. 1. Phase diagram of spin-1 bosons in an optical lattice in $J - \mu$ plane for a fixed value of magnetic field $b = 4.25\lambda_a$ and $\lambda_a = 0.4\lambda_s$. Solid line corresponds to a transition from an insulator into superfluid phase with $\psi_1 \neq 0$, while along the dash line the transition occurs into a state with $\psi_{-1} \neq 0$. 

FIG. 1. Phase diagram of spin-1 bosons in an optical lattice in $J - \mu$ plane for a fixed value of magnetic field $b = 4.25\lambda_a$ and $\lambda_a = 0.4\lambda_s$. Solid line corresponds to a transition from an insulator into superfluid phase with $\psi_1 \neq 0$, while along the dash line the transition occurs into a state with $\psi_{-1} \neq 0$. 

9
FIG. 2. The same as in Fig. 1, but for $b = 6\lambda_a$ and $\lambda_a = 0.4\lambda_s$. 