Quantum phase diagrams and time-of-flight pictures of spin-1 Bose systems in honeycomb optical lattices

Jun Zhang and Ying Jiang

1 Department of Physics, College of Sciences, Shanghai University, Shanghai, People’s Republic of China
2 Shanghai Key Laboratory of High Temperature Superconductors, Shanghai, People’s Republic of China
3 Key Lab for Astrophysics, Shanghai, People’s Republic of China

E-mail: yjiang@shu.edu.cn

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Abstract
By treating the hopping parameter as a perturbation, with the help of cumulant expansion and the re-summing technique, the one-particle Green’s function of a spin-1 Bose system in a honeycomb optical lattice is calculated analytically. By the use of the re-summed Green’s function, the quantum phase diagrams of the system in ferromagnetic cases as well as in antiferromagnetic cases are determined. It is found that in antiferromagnetic cases the Mott insulating states with even filling factor are more robust against the hopping parameter than that with odd filling factor, in agreement with results via other different approaches. Moreover, in order to illustrate the effectiveness of the re-summed Green’s function method in calculating time-of-flight pictures, the momentum distribution function of a honeycomb lattice spin-1 Bose system in the antiferromagnetic case is also calculated analytically and the corresponding time-of-flight absorption pictures are plotted.

Keywords: Bose–Einstein condensates, quantum phase transition, quantum gases on optical lattices

1. Introduction
Since it was proposed theoretically [1, 2] and realized experimentally [3], spinor Bose–Einstein condensate has opened a new avenue to investigate magnetic systems by utilizing ultracold atomic gases [4]. Immediately after the realization of optical lattice [5], confining spinor bosons in optical lattices becomes one of the hottest research topics in the field of cold atoms and has been extensively investigated [6–10], although the experimental realization of the optical lattice spinor Bose system has been achieved only very recently [11].

As is known, for atoms trapped in a magneto-optical trap, the spin degree of freedom is frozen and the atoms become effectively spinless. However, the quantum gases will keep their spin degree of freedom if they are trapped by purely optical means. Such an additional spin degrees of freedom, together with other tunable parameters, makes the spinor Bose lattice systems unique for studying quantum magnetic properties of matter (for review, see [12–14], even for quantum information processing [15].

Among spinor Bose systems in optical lattices, spin-1 lattice Bose gases should be the simplest one and have attracted lots of attention. Such systems can be depicted by the extended Bose–Hubbard Hamiltonians [1, 2] with spin-dependent terms which will dramatically change the properties of the system [12]. In fact, the nature of on-site spin–spin interaction can be either ferromagnetic (87Rb) [16]
or antiferromagnetic ($^2$Na) [3], depending on the relative magnitudes of the $s$-wave scattering lengths in spin-0 and spin-2 channels [17]. The possibility of appearance of different quantum phases in such systems has been predicted both analytically and numerically [6, 7, 18–22]. To determine the quantum phase boundaries, a variety of methods have also been applied, such as mean-field methods [23–25], strong coupling expansion [27], and Monte Carlo simulations [26, 28] et al. However, most of these efforts have been only devoted to small Bravais lattice systems.

With the progress of experimental techniques, scalar Bose gases trapped in a non-Bravais honeycomb optical lattice has been accomplished [29]. Due to its complexity, trapping a spinor Bose gas in the honeycomb lattice has been only realized most recently [11]. However, theoretical studies on the quantum phase transitions of spinor Bose systems in honeycomb lattice are less explored. In this paper, by utilizing a generalized Green’s function method [30], together with cumulants expansion [31] and re-summed Green’s function technique [32, 33], we will investigate the quantum phase transitions of the spin-1 Bose system in a honeycomb optical lattice. As a demonstration of the usefulness of the generalized Green’s function method, the time-of-flight absorption pictures of the system in anti-ferromagnetic cases will also be presented. Our analytical results may serve as a reference object for the upcoming experiments.

The paper is arranged as follows. In section 2, the spinor Bose–Hubbard model is introduced, and the possible ground states of the pure local part of the spinor Bose–Hubbard Hamiltonian are discussed. In section 3, by the use of the cumulants expansion as well as the re-summed Green’s function technique, the one-particle Green’s function of a spinor Bose–Hubbard system in a honeycomb lattice is constructed. The phase boundary equations for both anti-ferromagnetic and ferromagnetic cases are presented in section 4, where the phase diagrams for both cases are also plotted. To cross check the validity of our analytical method, we also calculate the phase boundaries of spin-1 Bose–Hubbard systems in triangular and square lattices and compare them with previous results [28, 47], an excellent agreement is found. In section 5, as an example, the momentum distribution function of anti-ferromagnetic case with the filling factor $n = 3$ is calculated analytically, the corresponding time-of-flight pictures are plotted. Section 6 is devoted to summary.

2. The model

A system of spin-1 bosons trapped in a honeycomb optical lattice can be portrayed by the Hamiltonian [1, 6, 7, 34]

$$
\hat{H} = \sum_\alpha \int \! d^3r \psi_\alpha^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2 \nabla^2}{2M} + V(\mathbf{r}) - \mu \right] \psi_\alpha(\mathbf{r}) \\
+ \frac{c_0}{2} \sum_{\alpha, \beta} \int \! d^3r \psi_\alpha^\dagger(\mathbf{r}) \psi_\beta(\mathbf{r}) \hat{\psi}_\alpha^\dagger(\mathbf{r}) \hat{\psi}_\beta(\mathbf{r}) \\
+ \frac{c_2}{2} \sum_{\alpha, \beta, \gamma, \delta} \int \! d^3r \psi_\alpha^\dagger(\mathbf{r}) \psi_\beta(\mathbf{r}) F_{\alpha \beta \gamma \delta} \psi_\gamma(\mathbf{r}) \psi_\delta^\dagger(\mathbf{r}),
$$

where $\hat{\psi}_\alpha(\mathbf{r})$ and $\psi_\beta^\dagger(\mathbf{r})$ are the field operators for a spin-1 boson in hyperfine states ($F = 1, m_F = \alpha$) with $\alpha = -1, 0, 1$. $M$ is the mass of atom, $\mu$ is the chemical potential, $V(\mathbf{r})$ represents the optical lattice potential and $\mathbf{F}$ is the vector of the three spin-1 generators of the rotation group

$$
F^x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad F^y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad F^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix},
$$

The coefficients $c_0$ and $c_2$ are defined as

$$
c_0 = \frac{4\pi\hbar^2(a_0 + 2a_2)}{3M}, \quad c_2 = \frac{4\pi\hbar^2(a_2 - a_0)}{3M},
$$

with $a_0$ and $a_2$ being the $s$-wave scattering lengths in singlet and quintet spin channels respectively. To investigate the ground state properties of the spinor Bose system as well as its quantum phase transitions, a convenient way is to artificially introduce a spin symmetry breaking term from the start and set it back to zero at the end of calculations. Thus, an additional Zeeman term $-\eta \sum_{\alpha, \beta} \int d^3r \hat{\psi}_\alpha^\dagger(\mathbf{r}) F_{\alpha \beta} \hat{\psi}_\beta(\mathbf{r})$ with infinitesimal external magnetic field $\eta$ has to be included in the Hamiltonian (1).

Due to the modulation of the optical lattice and the independence of the lattice potential on the spin of bosons, at extremely low temperature, the field operators $\hat{\psi}_\alpha(\mathbf{r})$ and $\hat{\psi}_\alpha^\dagger(\mathbf{r})$ can be expanded on the basis of spin-independent, orthonormal Wannier functions $w(\mathbf{r} - \mathbf{r}_i)$ of the lowest band [35, 36] as

$$
\hat{\psi}_\alpha(\mathbf{r}) = \sum_i \hat{a}_{i\alpha} w(\mathbf{r} - \mathbf{r}_i), \quad \hat{\psi}_\alpha^\dagger(\mathbf{r}) = \sum_i \hat{a}_{i\alpha}^\dagger w^*(\mathbf{r} - \mathbf{r}_i),
$$

where $\hat{a}_{i\alpha}^\dagger (\hat{a}_{i\alpha})$ is the bosonic creation (annihilation) operator on site $i$ with $m_F = \alpha$. In the tight-binding limit, the Hamiltonian of the system (1) reduces to the extended Bose–Hubbard model for spin-1 lattice bosons [6, 7, 23, 34, 37]

$$
\hat{H} = -J \sum_{\langle i, j \rangle} \hat{a}_{i\alpha}^\dagger \hat{a}_{j\alpha} + \sum_i \left[ \frac{1}{2} U_0 n_i (n_i - 1) \\
+ \frac{1}{2} U_2 (S_i^z - 2n_i) - \mu n_i - \eta S_i^z \right],
$$

where the nearest-neighbor hopping parameter is

$$
J = -\int d^3r \left[ \frac{\hbar^2}{2M} \nabla^2 + V(\mathbf{r}) \right] w(\mathbf{r} - \mathbf{r}_i),
$$

and the interactions $U_{0,2}$ are

$$
U_{0,2} = c_{0,2} \int d^3r |w(\mathbf{r} - \mathbf{r}_i)|^4.
$$

Note that $\langle i, j \rangle$ in (5) represents a nearest-neighbor pair of sites and $\hat{n}_i = \sum_{\alpha} \hat{a}_{i\alpha}^\dagger \hat{a}_{i\alpha}$ is the particle number operator on site-$i$. The spin operators $S_i^\mu = \sum_{\alpha, \beta} \hat{a}_{i\alpha}^\dagger F_{\alpha \beta} \hat{a}_{i\beta}$ fulfill the commutation relation $[\hat{S}_j^\mu, \hat{S}_j^\nu] = i \hbar \epsilon_{\mu \nu \lambda} \hat{S}_j^\lambda$. The spinor Hamiltonian $H$ can be written as

$$
H = \sum_\alpha \int \! d^3r \psi_\alpha^\dagger(\mathbf{r}) \left[ -\frac{\hbar^2 \nabla^2}{2M} + V(\mathbf{r}) - \mu \right] \psi_\alpha(\mathbf{r}) \\
+ \frac{c_0}{2} \sum_{\alpha, \beta} \int \! d^3r \psi_\alpha^\dagger(\mathbf{r}) \psi_\beta(\mathbf{r}) \hat{\psi}_\alpha^\dagger(\mathbf{r}) \hat{\psi}_\beta(\mathbf{r}) \\
+ \frac{c_2}{2} \sum_{\alpha, \beta, \gamma, \delta} \int \! d^3r \psi_\alpha^\dagger(\mathbf{r}) \psi_\beta(\mathbf{r}) F_{\alpha \beta \gamma \delta} \psi_\gamma(\mathbf{r}) \psi_\delta^\dagger(\mathbf{r}).
$$
As we can see from equation (5), the Hamiltonian consists of two parts, the hopping term
\[ \hat{H}_t = -J \sum_\alpha \sum_{\langle i,j \rangle} \hat{a}_{i,\alpha}^\dagger \hat{a}_{j,\alpha} \]  
and the diagonal one
\[ \hat{H}_0 = \sum_i \left[ \frac{1}{2} U_d \hat{n}_i(\hat{n}_i - 1) + \frac{1}{2} U_d (\hat{S}_i^2 - 2 \hat{n}_i) - \mu \hat{n}_i - \eta \hat{S}_i^z \right]. \]  

Due to their uncommutativity, the subtle balance between these two parts will give rise to a rich phase structure of the system. It has been shown that under Bogoliubov approximation, treating interactions approximately is unable to reveal the quantum phase transitions in Bose–Hubbard systems [38]. In order to address such a phase transition problem, the hopping term (8) will be treated as a perturbation in the following [30, 32, 33].

To investigate the quantum phase transitions in the system, the localized ground states at \( J = 0 \) need to be clarified at first. As shown in the expression of \( \hat{H}_0 \) (9), the competition among different parameters \( U_0, U_2, \mu \) and \( \eta \) will give the ground state different faces. These localized states are just the common eigenstates of \( \hat{S}_i^z, \hat{S}_i^x \) and \( \hat{n}_i \), which are denoted as \( |S_i, m_i; n_i\rangle \) with \( m_i = -S_i, -S_i + 1, \cdots, S_i - 1, S_i \). \( S_i \) represents total spin and \( n_i \) is the particle number on site \( i \). Thus we have the following eigenfunctions
\[ \hat{S}_i^z |S_i, m_i; n_i\rangle = S_i (S_i + 1) |S_i, m_i; n_i\rangle, \]  
\[ \hat{S}_i^x |S_i, m_i; n_i\rangle = m_i |S_i, m_i; n_i\rangle, \]  
\[ \hat{n}_i |S_i, m_i; n_i\rangle = n_i |S_i, m_i; n_i\rangle. \]  

Combining equations (10)–(12) with (9) we have the eigenenergies of the local Hamiltonian \( \hat{H}_0 \)
\[ \hat{H}_0 |S, m; n\rangle = E_{S, m, n} |S, m; n\rangle, \]  
\[ E_{S, m, n} = \frac{1}{2} U_d (n - 1) + \frac{1}{2} U_d (S(S + 1) - 2n) - \mu n - \eta m \]  
where \( N_S \) is the total number of the lattice sites.

In the case of anti-ferromagnetic interaction (\( U_2 > 0 \)), to minimize the ground state energy, equation (13) tells us that \( S \) must take the minimum value. Therefore the ground state is \( |0, 0; n\rangle \) when \( n \) is even and \( |1, 1; n\rangle \) for odd \( n \). The constraint on the chemical potential \( \mu \) for different filling factor can be determined as follows. For even filling factor \( n \), the eigenenergies have to satisfy the relations \( E_{0,0,n} \leq E_{1,1,n+1} \), and \( E_{0,0,n} \leq E_{1,1,n-1} \). This leads to \( (n-1)U_0 - 2U_2 + 2 \eta \leq \mu \leq nU_0 - 2 \eta \). Similarly, we have \( (n-1)U_0 - 2U_2 + 2 \eta \leq \mu \leq nU_0 - 2U_2 + 2 \eta \) for odd filling factor \( n \).

As for ferromagnetic interaction with \( U_2 < 0 \), to minimize the energy, the ground state of the system has to be the state of \( |n, n; n\rangle \). Hence the constraint on chemical potential for different filling factor becomes \( (n-1)(U_0 + U_2) - \eta \leq \mu \leq n(U_0 + U_2) - \eta \).

With the configurations of the localized states in hand, we can now tune on the hopping parameter \( J \) gradually. It can be imagined that the localized states will be softened by quantum fluctuations and be transformed into some delocalized states while \( J \) goes beyond some critical value, and thus a quantum phase transition is expected.

### 3. Cumulants expansion of the Green’s function

As is well known, for second-order phase transition, the one-particle Green’s function of the system diverges at the critical point [39, 40]. Meanwhile, the Green’s function can reveal the momentum distribution of the system, which has a direct connection with the time-of-flight measurements [13, 41–43] in real experiments. Based on these facts, in order to investigate the quantum phase transition of the spinor boson optical lattice systems as well as the corresponding time-of-flight absorption pictures, we are going to calculate the one-particle Green’s function of the system, which is defined as

\[ G(\tau', j', \alpha'|\tau, j, \alpha) = \left\langle \hat{T}_\tau [\hat{\beta}^\dagger_{j', \alpha'}(\tau')\hat{\beta}_{j, \alpha}(\tau)] \right\rangle. \]  

Here \( \tau \) is imaginary time, \( \langle \cdot \rangle \) denotes the statistical average with respect to the full Hamiltonian (5), and \( \hat{T} \) is the imaginary time ordering operator.

Since the hopping part \( (8) \) and the diagonal one \( (9) \) does not commute with each other, the exact eigenstates of the full Hamiltonian can hardly be determined. Thus we calculate the one-particle Green’s function \( (14) \) by treating the hopping term as perturbation in Dirac representation, i.e.

\[ G(\tau', j', \alpha'|\tau, j, \alpha) = \frac{\text{Tr}[e^{-\beta \hat{H}_0}\hat{T}_\tau [\hat{\beta}^\dagger_{j', \alpha'}(\tau')\hat{\beta}_{j, \alpha}(\tau)]]}{\text{Tr}[e^{-\beta \hat{H}_0}]} \]  

with \( \hat{A}(\tau) = \exp(\hat{H}_0\tau)\hat{A}\exp(-\hat{H}_0\tau) \) and the time evolution operator \( \hat{U}(\beta, 0) = \hat{T} \int_0^\beta d\tau \sum_{j, \alpha} \hat{\beta}_{j, \alpha}(\tau)\hat{\beta}^\dagger_{j, \alpha}(0) \) (setting \( h = 1 \) [44]). Using the expansion of \( \hat{U}(\beta, 0) \), it is easy to find that the perturbative expansion of the Green’s function consists of terms like

\[ \frac{1}{n!} \sum_{\vec{a}_{j_1} \cdots \vec{a}_{j_n}} \sum_{\alpha_1 \cdots \alpha_n} J_{j_1 \cdots j_n} \int_0^\beta d\tau \cdots \int_0^\beta d\tau_\alpha \left\langle \hat{T}_\tau [\hat{\beta}^\dagger_{j_1, \alpha_1}(\tau')\hat{\beta}_{j_1, \alpha_1}(\tau) \cdots \hat{\beta}^\dagger_{j_n, \alpha_n}(\tau')\hat{\beta}_{j_n, \alpha_n}(\tau)] \right\rangle_0. \]  

with \( \langle \cdot \rangle_0 \) denoting the average with respect to \( \hat{H}_0 \). We set \( J_{ij} = J \) if \( i \) and \( j \) are the nearest neighbors of each other, otherwise \( J_{ij} = 0 \).

Now, the problem of calculating the one-particle Green’s function with respect to the full ground state is reduced to the calculation of the \( n \)-particle Green function with respect to the unperturbed state which is defined as

\[ G_n^{(0)}(\tau'_1, j'_1, \alpha'_1; \cdots; \tau'_n, j'_n, \alpha'_n) = \left\langle \hat{T}_\tau [\hat{\beta}^\dagger_{j'_1, \alpha'_1}(\tau'_1)\hat{\beta}_{j_1, \alpha_1}(\tau_1) \cdots \hat{\beta}^\dagger_{j'_n, \alpha'_n}(\tau'_n)\hat{\beta}_{j_n, \alpha_n}(\tau_n)] \right\rangle_0. \]
It turns out that the calculation of $G_n^{(0)}$ can be further simplified by means of the so-called cumulant expansions [31]. Since the eigenstates of the unperturbed part $\hat{H}_0$ is local, each annihilation (creation) operator in the expression of $G_n^{(0)}$ has to be paired with a creation (annihilation) operator on the same site with the same quantum numbers. Therefore, $G_n^{(0)}$ can be decomposed in terms of the cumulants $C_m^{(0)}(\tau_1, \alpha_1; \cdots; \tau_m, \alpha_m)$ in which all the operators are at the same lattice site [31, 32, 45]. In this case the decomposition of $G_n^{(0)}$ is straightforward. As an example, we decompose the one-particle and two-particle Green’s functions in terms of the cumulants as

$$G_1^{(0)}(\tau_1, \alpha_1; \eta, \alpha_1) = \delta_{\eta\alpha_1} \sum_{i} C_1^{(0)}(\tau_1, \alpha_1; \eta, \alpha_1)$$

and

$$C_2^{(0)}(\tau_1, \alpha_1; \tau_2, \alpha_2; \eta, \alpha_1; \tau_2, \alpha_2) = C_2^{(0)}(\tau_1, \alpha_1; \tau_2, \alpha_2) + C_1^{(0)}(\tau_1, \alpha_1; \eta, \alpha_1) C_1^{(0)}(\tau_2, \alpha_2; \tau_2, \alpha_2)$$

In order to simplify the discussion, the $m$th order cumulant can be represented as an arrow-line diagram composed of $m$ incoming arrow lines (representing the creation operators) and $m$ outgoing arrow lines (representing the annihilation operators) at the same lattice site. For example, the first order and the second order cumulants can be represented diagrammatically as $C_1^{(0)}(\tau_1, \alpha_1; \eta, \alpha_1)$ and $C_2^{(0)}(\tau_1, \alpha_1; \tau_2, \alpha_2; \eta, \alpha_1; \tau_2, \alpha_2)$ respectively. Correspondingly, the hopping parameter $J_{ij}$ between nearest neighbor sites is also sketched as $J_{ij} = \sum_{\alpha} \delta_{\alpha}$. Thus, with the help of cumulants expansion, $G(\tau', j', \alpha'; \tau, j, \alpha)$ can be easily expressed diagrammatically [31]. When the cancellation effect of the numerator and the denominator in equation (15) is taken into account, it is found that the one-particle Green’s function $\tilde{G}_{1\alpha}(\omega_m, k)$ only consists of connected diagrams [31, 32]. From the above diagrammatic representation, it is not difficult to recognize that diagrams which only consists of the first order cumulants are line diagrams, while the higher order cumulants together with hoppings will form loops in corresponding diagrams.

In principle, the one-particle Green’s function (15) may be accurately calculated out by counting all the possible diagrams. However, in practice one can only calculate the Green’s function perturbatively by selecting a specific group of diagrams. Actually, this selection is very subtle. On one hand, the Green’s function should diverge at the phase boundaries of second-order phase transition. This property can not be fulfilled by just counting finite orders of perturbation parameter $J/U_0$. On the other hand, $J/U_0$ is no longer a small quantity near the phase boundaries. Hence, we re-group the diagrams based on the number of loops rather than on the order of $J$. This is the so-called resummed Green’s function technique [32, 33]. At present we only take line diagrams into account, as the diagram containing $n$ loops will be smaller than the corresponding line diagram at least by factor of $1/d^n$ with $d$ being the dimension of the system. This choice is going to be accurate in the limit $d \rightarrow \infty$. In this sense, our choice of the re-summed Green’s function may be looked upon as a type of mean-field approximation. Nevertheless, from the above discussion, we argue that in principle the re-summed Green’s function method can go beyond mean field by including loop diagrams constituted by higher order cumulants and related hoppings.

Since the honeycomb lattice is a non-Bravais one, we need to divide the honeycomb lattice into two sublattices, denoted by sublattice $A$ and sublattice $B$ respectively [30]. In this case, the hopping amplitude from sublattice $A$ to sublattice $B$ $J_{AB}$ and the hopping from sublattice $B$ to sublattice $A$ $J_{BA}$ can be expressed in momentum space as

$$J_{AB}(k) = \int \frac{d^2k}{(2\pi)^2} \frac{\exp(-ik, a) + 2\exp(-i\kappa, a)}{2} \cos \left(\frac{\sqrt{3}}{2}k, a\right)$$

$$J_{BA}(k) = \int \frac{d^2k}{(2\pi)^2} \frac{\exp(-ik, a) + 2\exp(-i\kappa, a)}{2} \cos \left(\frac{\sqrt{3}}{2}k, a\right)$$

Here the conservation of angular momentum has already been taken into account, i.e. $\alpha' = \alpha$ and $\omega_m = \omega'$. In this work, the Green’s function is expressed as

$$\tilde{G}_{1\alpha}(\omega_m, k) = \sum_{l=0}^{4\infty} \left( C_{1\alpha}^{(0)} + C_{1\alpha}^{(1)} \right) \left[ C_{1\alpha}^{(0)} C_{1\alpha}^{(1)} J_{AB}(k) J_{BA}(k) \right]^l$$

Note that since the cumulants are local quantities on each lattice site and there is no bias on these two sublattices in our system, to this end the cumulants on different sublattices will make the same contribution, i.e. $C_{1\alpha}^{(0)} = C_{1\alpha}^{(1)}$.
After having constructed the above Green’s function (23), our task turns to calculate the first-order cumulants. According to the definition (18), we have to calculate $(S, m, n)\hat{a}^\dagger_\alpha(t')\hat{a}_{\beta}(t)\langle S, m, n \rangle$ and $(S, m, n)\hat{a}_{\alpha}(t)\hat{a}_{\beta}(t')\langle S, m, n \rangle$. To do this, we first check how the creation and annihilation operators act on the eigenstate $(S, m, n)$ of $H_0$. Since the creation operator $\hat{a}^\dagger_\alpha(\hat{a}_\alpha)$ creates a spin-1 particle with its spin orientation specified by $\alpha$, we can easily have
\[
\hat{a}^\dagger_\alpha|S, m; n\rangle = M_{\alpha S mn}|S + 1, m + \alpha; n + 1\rangle + N_\alpha S mn|S - 1, m + \alpha; n + 1\rangle, \quad (24)
\]
\[
\hat{a}_\alpha|S, m; n\rangle = O_{\alpha S mn}|S + 1, m - \alpha; n - 1\rangle + P_{\alpha S mn}|S - 1, m - \alpha; n - 1\rangle, \quad (25)
\]
where $M_{\alpha S mn}$, $N_\alpha S mn$, $O_{\alpha S mn}$ and $P_{\alpha S mn}$ are superposition parameters, and their detail expressions are presented in the appendix. Combining equations (17), (18), (24) and (25), we obtain the following explicit expression of the first order cumulant in Matsubara space
\[
C^{(0)}(\omega_n) = \frac{1}{Z(0)} \sum_{s=0}^{\infty} \sum_{\beta=0}^{\infty} \sum_{\alpha=0}^{\infty} \sum_{\alpha'=0}^{\infty} e^{-\beta E_{n_\alpha n_{\alpha'}}} \left[ M_{\alpha S mn}^2 \right]_{\omega_n + E_{S+1,m+\alpha,n+1} - E_{S,m,n}} + N_\alpha S mn^2 \omega_n + E_{S+1,m+\alpha,n+1} - E_{S,m,n} - 1 O_{\alpha S mn}^2 \omega_n + E_{S,m,n} - E_{S+1,m+\alpha,n+1} - 1 P_{\alpha S mn}^2 \omega_n + E_{S,m,n} - E_{S+1,m+\alpha,n+1} - 1 \right]. \quad (26)
\]
At zero-temperature limit, the above expression reduces to
\[
C^{(0)}(\omega_n) = \frac{M_{\alpha S mn}^2}{\omega_n + E_{S+1,m+\alpha,n+1} - E_{S,m,n}} + \frac{N_\alpha S mn^2}{\omega_n + E_{S+1,m+\alpha,n+1} - E_{S,m,n}} + \frac{O_{\alpha S mn}^2}{\omega_n + E_{S,m,n} - E_{S+1,m+\alpha,n+1}} + \frac{P_{\alpha S mn}^2}{\omega_n + E_{S,m,n} - E_{S+1,m+\alpha,n+1} + 1}. \quad (27)
\]

4. Phase boundaries of spin-1 Bose systems on honeycomb optical lattices

For ferromagnetic interaction, both theoretical analysis [21] and quantum Monte Carlo results [28] indicate that the superfluid-Mott insulator phase transitions are always of second order. However, for antiferromagnetic interaction, the situation becomes complicated. The mean field analysis [21, 46] as well as some numerical results [22, 28] has shown that the phase transition can only be of second order for sufficiently strong $U_2$. Specifically, in the square lattice the first-order phase transition appears when $0.05U_0 < U_2 < 0.15U_0$ [28], while the second-order one happens when $U_2 \geq 0.32U_0$ for $n = 2$ and $U_2 \geq 0.014U_0$ for $n = 3$ [22]. In the present work, we will concentrate on the cases with strong $U_2$ so that a second-order phase transition can occur.

By summarizing the geometric sequences in equation (23) we get
\[
\tilde{G}_{1\alpha}(\omega_n, (k)) = \frac{2C^{(0)}_{1\alpha} + [C^{(0)}_{1\alpha}]^2 (J_{AB}(k) + J_{BS}(k))}{1 - [C^{(0)}_{1\alpha}]^2 J_{AB}(k)J_{BS}(k)}. \quad (28)
\]
The divergence of the Green function (28) at the phase transition point [39] requires that
\[
1 - [C^{(0)}_{1\alpha}]^2 J_{AB}(k)J_{BS}(k) = 0. \quad (29)
\]
Solving the above quadratic equation (29) and plugging in the cumulant result (27), finally we obtain the following phase boundary equation
\[
\frac{1}{z^2J_{c,\alpha}} = \frac{M_{\alpha S mn}^2}{E_{S+1,m+\alpha,n+1} - E_{S,m,n}} + \frac{N_\alpha S mn^2}{E_{S+1,m+\alpha,n+1} - E_{S,m,n}} - \frac{O_{\alpha S mn}^2}{E_{S,m,n} - E_{S+1,m+\alpha,n+1}} + \frac{P_{\alpha S mn}^2}{E_{S,m,n} - E_{S+1,m+\alpha,n+1} - 1} \right)^2, \quad (30)
\]
where $z$ is the coordination number and we have taken $\omega_n = 0, k = 0$ due to the fact that the phase transitions are governed by long-wavelength fluctuations [39, 40]. In the following, we are going to discuss the phase boundaries case by case.

Let us first consider an anti-ferromagnetic system with even filling factor. In this case the unperturbed ground state is [00n], i.e. $S = 0$ and $m = 0$ in the above equation (30). With the help of the recursion relations of the superposition parameters, it is easy to find that $N_{0,0,0} = 0$, $O_{0,0,0} = 0$, $|M_{0,0,0}|^2 = (n + 3)/3$ and $|O_{0,0,0}|^2 = n/3$. Together with $E_{1,\alpha,\alpha+1} = E_{0,0,n} = nU_0 - \mu - \eta\alpha$, $E_{0,0,n} - E_{1,\alpha,\alpha+1} = (n - 1)U_0 - 2U_2 - \mu - \eta\alpha$ and the limit of vanishing external field $\eta = 0$, we get the following phase boundary equation of the Mott state MI(0,n) with even filling factor $n$
\[
\frac{J_{c,\alpha}}{U_0} = \frac{1}{z} \frac{1}{\sqrt{2 + \frac{n + 3}{n + 2 + \mu}}}, \quad (31)
\]
with $U_2 = U_2/U_0$ and $\tilde{\mu} = \mu/U_0$.

The situation for odd filling cases is a little bit complicated, where the unperturbed ground state is three-fold degenerated when the external field is absent. Hence, after taking the limit $\eta \to 0$ in equation (30), we have to evaluate the following equation for all possible $\alpha$ and $m$
\[
z^2J_{c,\alpha,m,0,\pm 1} = \frac{1}{E_{S+1,m+\alpha,n+1} - E_{S,m,n}} + \frac{1}{E_{S+1,m+\alpha,n+1} - E_{S,m,n} - 1} \right]^2, \quad (32)
\]
The minimum $J_{c,\alpha,m,0,\pm 1}$ gives the phase boundaries of MI(1, $n$) (where $n$ is odd number) lope, i.e.
\[
J_c = \min_{\alpha,m} \left| J_{c,\alpha,m,0,\pm 1} \right|. \quad (33)
\]
With the matrix elements of creation and annihilation operators in hand, detailed calculation shows that $J_{c,\alpha,m,0,\pm 1}$ minimize at $\alpha = 0$ and $m = 0$. Thus the corresponding phase boundary can be expressed as
with the help of the one-particle Green function, it can be rewritten as \( e^{2|\langle 0,2|\hat{G}_{\alpha}\hat{A}_{\alpha}(0)\rangle|} \) respectively \([48, 49]\). By making use of (4) and the Fourier transform of the operators \( \hat{a}_{\alpha} = 1/\sqrt{N_\alpha} \sum_k \hat{a}_{\alpha,k} e^{-ikr} \), \( \hat{a}_{\alpha} = 1/\sqrt{N_\alpha} \sum_k \hat{a}_{\alpha,k} e^{-ikr} \), the momentum distribution function can be expressed as

\[
\begin{align*}
J_c &= \frac{1}{U_0} \left[ \sum_{\alpha} N_{\alpha,nn} - 1 + \frac{n+1}{n+1} - 1 \frac{n}{(n-1)(n+1)} \right].
\end{align*}
\]

The phase diagram of a fermionic system in a honeycomb lattice with \( U_2/U_0 = -0.1 \) is plotted in figure 2 (left). The phase boundary separates the Mott insulator states \(|n,n\rangle\) from superfluid phase. Our analytical result for ferromagnetic cases is also cross checked by being applied to square lattice system. The corresponding result is plotted in figure 2 (right) together with numerical result obtained via the diagonalized mean field approach \([28]\), and a good agreement is also found.

5. Time-of-flight pictures

Different from quantum phase diagram, time-of-flight absorption spectra \([5, 13]\) reveals the momentum distribution properties of a ultracold optical lattice system and can be detected directly in experiment. To offer a direct comparisons with possible experimental observations, as an example, we investigate the time-of-flight picture of spinor-1 Bose gases in a honeycomb optical lattice in antiferromagnetic cases. This can be realized by trapping ultracold \( ^{23}\text{Na} \) \([3]\) atoms in optical lattices, with the scattering lengths for different channels being \( a_0 \approx 50a_B \) and \( a_2 \approx 56a_B \) respectively \([48, 49]\) (\( a_B \) being the Bohr radius).

As is known, the momentum distribution function of the system is \([33, 36]\)

\[
\begin{align*}
\int d\mathbf{r} \int d\mathbf{r}' e^{ik(r-r')} \langle \psi_\alpha(\mathbf{r}) \psi_{\alpha}(\mathbf{r}') \rangle.
\end{align*}
\]

By making use of (4) and the Fourier transform of the operators \( \hat{a}_{\alpha}^{\dagger} = 1/\sqrt{N_\alpha} \sum_k \hat{a}_{\alpha,k} e^{-ikr} \), \( \hat{a}_{\alpha} = 1/\sqrt{N_\alpha} \sum_k \hat{a}_{\alpha,k} e^{-ikr} \), the momentum distribution function can be expressed as

\[
\begin{align*}
n_{\alpha}(\mathbf{k}) = N_\alpha |w(\mathbf{k})|^2 \langle \hat{a}_{\alpha,k}^{\dagger} \hat{a}_{\alpha,k} \rangle,
\end{align*}
\]

Since we have approximated \( \hat{G}_{\alpha}(\tau|0,\mathbf{k}) \) with \( \hat{G}_{\alpha}(\tau',\mathbf{k}) \), now the problem of calculating the density distribution \((39)\) is transformed to calculate the corresponding Green’s function.
\[ \tilde{G}_{1x}(r', k), \] which can be obtained via the following inverse Fourier transformation of (23)

\[ \tilde{G}_{1x}(r', k) = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega \tilde{G}_{1x}(\omega, m) e^{-i\omega r'}. \] (40)

According to equation (23), one needs to determine the explicit form of \( J \) and \( U_0, \gamma \) first. Experimentally, a honeycomb optical lattice can be created [29] by three laser beams with wavelength \( \lambda \approx 830 \text{ nm} \) intersecting with angles of \( 2\pi/3 \), leading to the lattice constant \( a = 2\lambda/3\sqrt{3} \). The optical trapping potential of the lattice is

\[
V(r) = -2V_0\left[ 3 - \cos\left( -\frac{\sqrt{3}\pi x}{\lambda} + \frac{3\pi y}{\lambda} \right) + \cos\left( \frac{\sqrt{3}\pi x}{\lambda} + \frac{3\pi y}{\lambda} \right) + \cos\left( \frac{2\sqrt{3}\pi x}{\lambda} \right) \right],
\] (41)

Under the harmonic approximation, the potential \( V(r) \) can be expanded around the minimal point \( (\frac{\lambda}{6\sqrt{3}}, \frac{\lambda}{6}) \) as

\[
V(r) = V_0\left[ -9 + \frac{4\pi^2}{3\lambda^2} \left( x + \frac{\lambda}{6\sqrt{3}} \right)^2 + \frac{4\pi^2}{3\lambda^2} \left( y - \frac{\lambda}{6} \right)^2 \right],
\] (42)

and the corresponding Wannier function takes the form

\[
w(r - r_i) = \frac{64V_0}{81} \left( \frac{\pi}{a^2} \right)^{\frac{1}{2}} \left( \frac{\pi}{a^2} \right)^{\frac{1}{2}} \exp\left[ \frac{\pi^2}{2} \frac{64V_0}{81} (x - x_i)^2 + (y - y_i)^2 \right],
\] (43)

with \( V_0 = V_0/E_R \) being the dimensionless lattice depth in unit of the recoil energy \( E_R = \hbar^2k^2/2M \). By substituting equations (42) and (43) into equation (6), we then have

\[
J = E_0\left[ \pi^2 + 18/3 V_0 - \frac{3}{2} V_0^{\frac{1}{2}} + 2V_0 \exp\left( -\frac{1}{2\sqrt{V_0}} \right) \exp\left( -\frac{2\pi^2\sqrt{V_0}}{9} \right) \right]
\] (44)

To create a 2D system in real experiment, people first create a 3D stacked optical lattice system and then set trapping potential in z-direction extremely stronger than that in x- and y-direction. In this case the influence of the third direction can be avoided and the system shows two-dimensional properties [29]. Plugging (43) into equation (7), and taking \( V_\epsilon = 60E_R \) (which would be deep enough in practice), we have

\[
U_0 = \frac{4\sqrt{6}}{9} a_0 + \frac{2a_0}{a} \sqrt{\pi V_0(60)^2}E_R,
\] (45)

and

\[
U_2 = \frac{4\sqrt{6}}{9} a_2 - \frac{a_0}{a} \sqrt{\pi V_0(60)^2}E_R.
\] (46)

According to the preceding discussion, while increasing the hopping amplitude or equivalently decreasing the lattice depth in experiment, in an antiferromagnetic system the component with \( \alpha = 0 \) and \( m = 0 \) will go from Mott insulating phase to superfluid state first. Therefore, in this paper we will concentrate on the case with \( \alpha = 0 \) and \( m = 0 \) for antiferromagnetic system. Without causing misleading, the index of \( \alpha \) will be dropped in abbreviation in the following.

For anti-ferromagnetic interaction, from equations (45) and (46), it is not difficult to verify that \( U_2 \approx 0.04U_0 \) for \( ^{23}\text{Na} \). In order to keep the system to stay in the region of second order phase transition, according to [22], we will keep the occupation number \( n = 3 \) in the following calculation.

For the time-of-flight processes released from the ground state \( |1, n\rangle \), the explicit form of the cumulant is

\[
\frac{C_1^{(n)}(\omega_m)}{C_1^{(0)}(\omega_m)} = \frac{4[4n - 4 - (4n + 11)U_2 - 5\mu + 5i\omega_m]}{15(n + U_2 - \mu + i\omega_m)(n - 1 - 3U_2 - \mu + i\omega_m)} + \frac{-2n - 1 + (2n + 4)U_2 + \mu - i\omega_m}{3(n - 2U_2 - \mu + i\omega_m)(n - 1 - \mu + i\omega_m)},
\] (47)
Substituting (47) into (23), it leads to

$$\tilde{G}(\tau, k) = \frac{2U_0}{2\pi} \sum_{l=0}^{+\infty} [J_{AB}(k)J_{BA}(k)]^l \times \int_{-\infty}^{+\infty} d\omega_m \left[ c^{\dagger}_{\alpha l}(\omega_m) \right]^{2l+1} e^{-i\omega_m \tau} \times \frac{U_0}{2\pi} \sum_{m=0}^{+\infty} (J_{AB}(k) + J_{BA}(k))(J_{AB}(k)J_{BA}(k))^{-m} \times \int_{-\infty}^{+\infty} d\omega_m \left[ c^{\dagger}_{\alpha 1}(\omega_m) \right]^{2m+2} e^{-i\omega_m \tau}. \quad (48)$$

With the help of the residue theorem and general Leibniz rule, the above equation (48) can be calculated out analytically, yet very tediously. Combining the momentum distribution function (39) with (20), (21), (43), (44), (45), in figure 3 we plot the time-of-flight absorption pictures of the system released from state $|1,3\rangle$ for different lattice depth $V_0$.

From the figures we see clearly that in both cases the momentum distribution $n_{\alpha}(k)$ exhibits sharp peaks at the reciprocal lattice sites of the honeycomb lattice for sufficiently shallow lattice depth, this reflects the coherence of the condensate, indicating that the system is in a superfluid state. For deeper lattice depth, the heights of the peaks decay and the widths of the peaks broaden. The sharp peaks disappear entirely for sufficient deep lattice depth, which is the case in Mott insulating phase. The graphs in figure 3 qualitatively show that the system undergoes a phase transition as the optical lattice potential varies, which is in agreement with our calculation of the phase diagram shown in figure 1.

6. Summary

In this work, by treating the hopping parameter in the spinor Bose–Hubbard model as a perturbation, with the help of cumulant and the re-summing technique, we have calculated the one-particle Green’s function of a spin-1 Bose system in a honeycomb optical lattice analytically. By use of the re-summed Green’s function, we determined the quantum phase diagrams of the system in bothferromagnetic cases and anti-ferromagnetic cases. We found that in anti-ferromagnetic cases the Mott insulating states with even filling factor are more robust against the hopping parameter than cases with odd filling factor. This is in agreement with results via different approaches [28, 47]. It should be pointed out that although the lowest order re-summed Green’s function is a sort of mean-field treatment, it is shown in section 3 that the developed method here is ready to go beyond mean field by adding loop diagrams which consists of higher order cumulants. Moreover, according to equation (26), it is also straightforward to investigate the finite temperature properties of the system via the re-summed Green’s function.

The momentum distribution function of the system, measured directly in experiment via time-of-flight technique by changing the depth of the optical lattice trapping potential, can also be exposed by the Green’s function. We therefore have also calculated analytically the time-of-flight absorption pictures of the honeycomb optical lattice spin-1 Bose system in anti-ferromagnetic cases. It is clearly shown that the time-of-flight absorption pictures dramatically change when crossing the phase boundaries by changing the depth of the optical lattice trapping potential. Our results may serve as a reference object for further studies.

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Appendix. The matrix elements of creation and annihilation operators

From preceding discussion, we know that

$$\hat{a}_\alpha^\dagger|S,m;n\rangle = M_{S\alpha mn}|S+1,m+\alpha;n+1\rangle + N_{S\alpha mn}|S-1,m+\alpha;n+1\rangle, \quad (A.1)$$

and

$$\hat{a}_\alpha|S,m;n\rangle = O_{S\alpha mn}|S-1,m-\alpha;n-1\rangle + P_{S\alpha mn}|S-1,m-\alpha;n-1\rangle. \quad (A.2)$$

In fact, the state of $|S,S;n\rangle$ can be rewritten as $|S,S;n\rangle = \frac{1}{\sqrt{f(Q,S)}}(\hat{a}^\dagger)^S(\hat{\Theta}^\dagger)^Q|0\rangle$ with $\hat{\Theta}^\dagger = (\hat{a}^\dagger)^S - 2\hat{a}_\alpha^\dagger\hat{a}^\dagger_{-\alpha}$, $n = 2Q + S$, and $f(Q,S) = S!\frac{2Q(2Q + 2S + 1)!}{(Q + S)!^2}$. With these in hand, by making use of the commutation relations among $\hat{a}_\alpha$ and spin operators, after a laborious yet straightforward calculation, we have the matrix elements of creation and annihilation operators...
and the following recursion relations

\[ M_{iS_{m-1}n} = \frac{S(S+1) - m(m-1)}{(S+1)(S+2) - m(m+1)} M_{iS_{m}n} + \frac{2}{(S+1)(S+2) - m(m+1)} M_{iS_{m+1}n}, \]

\[ M_{iS_{m}n} = \frac{S(S+1) - m(m+1)}{(S+1)(S+2) - m(m+1)} M_{iS_{m+1}n} + \frac{2}{(S+1)(S+2) - m(m+1)} M_{iS_{m+2}n}, \]

\[ M_{iS_{m+1}n} = \frac{S(S+1) - m(m+1)}{(S+1)(S+2) - m(m+1)} M_{iS_{m+2}n} + \frac{2}{(S+1)(S+2) - m(m+1)} M_{iS_{m+3}n}, \]

\[ N_{iS_{m-1}n} = \frac{S(S+1) - (m+1)(m-2)}{(S+1)(S+2) - (m+1)(m+2)} N_{iS_{m}n}, \]

\[ N_{iS_{m}n} = \frac{S(S+1) - m(m+1)}{(S+1)(S+2) - m(m+1)} N_{iS_{m+1}n} + \frac{2}{(S+1)(S+2) - m(m+1)} N_{iS_{m+2}n}, \]

\[ N_{iS_{m+1}n} = \frac{S(S+1) - (m+1)(m+2)}{(S+1)(S+2) - (m+1)(m+2)} N_{iS_{m+2}n}, \]

\[ O_{iS_{m-1}n} = \frac{S(S+1) - m(m-1)}{(S+1)(S+2) - (m+1)(m-1)} O_{iS_{m}n+1}, \]

\[ O_{iS_{m}n+1} = \frac{S(S+1) - m(m+1)}{(S+1)(S+2) - m(m+1)} O_{iS_{m+1}n+1} + \frac{2}{(S+1)(S+2) - m(m+1)} O_{iS_{m+2}n+1}, \]

\[ O_{iS_{m+1}n} = \frac{S(S+1) - m(m+1)}{(S+1)(S+2) - m(m+1)} O_{iS_{m+2}n} + \frac{2}{(S+1)(S+2) - m(m+1)} O_{iS_{m+3}n+1}, \]

\[ |P_{iS_{m}n}|^2 = \sum_{\alpha} |O_{\alpha S_{m}n}|^2, \]

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