Physica Scripta

Excitation spectrum and momentum distribution of the ionic Bose–Hubbard model

Hiroki Nishizawa
Department of Applied Physics, The University of Tokyo, Hongo, Tokyo 113-8656, Japan
E-mail: hiroki-nishizawa752@g.ecc.u-tokyo.ac.jp

Keywords: Bose–Hubbard, Green’s function, supersolid, momentum distribution

Abstract
We investigate the excitation spectrum and momentum distribution of the ionic Bose–Hubbard model by the standard basis operator method. We derive Green’s functions in the random phase approximation in Mott insulator, superfluid, charge density wave, and supersolid phases. The excitation spectrum has gapped modes and gapless Goldstone modes in the superfluid and supersolid phases. We show that the momentum distribution has a peak at the zone corner in the supersolid phase and the charge density wave phase close to the phase boundary. In addition, we demonstrate that the momentum distribution can be explained by the excitation spectrum and spectral weights of hole excitation modes.

1. Introduction

The Bose–Hubbard model (BHM) [1, 2] describes bosonic atoms in optical lattices. Since parameters of optical lattices can be tuned flexibly, the BHM is ideal for the investigation of many-body effects. This model undergoes the phase transition from a superfluid (SF) phase to a Mott insulator (MI) phase at the critical ratio of the onsite repulsion to the hopping amplitude [3–5]. These phases are characterized by the excitation spectrum. In the MI phase, all excitation modes are gapped. In contrast, in the SF phase, the spectrum consists of gapped and gapless Goldstone modes [6–14]. The momentum distribution, which can be measured by time-of-flight spectroscopy, is also an important indicator of the SF-MI phase transition. In the SF phase, the momentum distribution has a sharp peak at zero momentum, which indicates the existence of Bose–Einstein condensation and superfluidity [8, 14–18]. The excitation spectrum and momentum distribution provide important information about the phase of the BHM.

In addition to the MI and SF phase, there are solid-ordered phases: the phases with a periodic density modulation such as a charge density wave (CDW) and supersolid (SS) phase. The properties of solid-ordered phases have been discussed in studies of the extended Bose–Hubbard model [19–28]. Although there are a few studies on the excitation spectrum [21, 29] and the momentum distribution [30, 31], the nearest-neighbor repulsion makes it difficult to investigate generally these properties. Another way to form solid-ordered phases is to introduce the staggered potential. In contrast to the nearest-neighbor repulsion, the staggered potential causes a density modulation non-spontaneously. The BHM with the staggered potential is called the ionic Bose–Hubbard model (IBHM) [32, 33]. The IBHM is suitable for investigating solid-ordered phases, but few studies have been carried out on the IBHM. The excitation spectrum of the IBHM has been calculated by the spin-wave approximation in the hard-core limit [34]. However, only the half-filling case has been considered. Moreover, there is no theoretical study of the momentum distribution of the IBHM.

The purpose of this study is to investigate the excitation spectrum and momentum distribution of the IBHM on a square lattice by the standard basis operator (SBO) method. The SBO method has been applied to the BHM in both the MI and SF phases [6–8, 35]. We extend the SBO method to the IBHM on a bipartite square lattice, which has two sublattices due to a periodic density modulation. In section 2, we summarize the mean-field phase diagram of the IBHM. In section 3, we derive equations for Green’s functions by the SBO method in the random phase approximation. By solving the equations, we obtain the Green’s functions in the MI, SF, CDW, and SS
The momentum distribution can be understood by the excitation spectrum and spectral weights of hole excitations.

In section 5, we show that the momentum distribution has a peak at the zone corner in the SS phase and the CDW phase close to the CDW-SS phase transition. In addition, we demonstrate that the momentum distribution can be used by the excitation spectrum and spectral weights of hole excitations.

### 2. Mean-field phase diagram

In this section, we summarize the phase diagram of the ionic Bose–Hubbard model

\[
H = -t \sum_i \langle ij \rangle b_i^\dagger b_j + \text{H.c.} + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i - \Delta \sum_{i \in A} n_i + \Delta \sum_{i \in B} n_i, \tag{1}
\]

where \( b_i^\dagger \) and \( b_i \) are the boson creation and annihilation operators at site \( i \), \( n_i = b_i^\dagger b_i \) is the number operator, \( t \) is the hopping amplitude, \( \langle ij \rangle \) denotes the summation over the nearest-neighbor sites, \( U \) is the onsite repulsion, \( \mu \) is the chemical potential, and \( \Delta \) is the staggered potential on sublattices \( A \) and \( B \).

To study the phase diagram, we apply the mean-field approximation [22]. In this approximation, the hopping term is decoupled as \( b_i^\dagger b_j \simeq b_i \langle b_j \rangle + \langle b_i \rangle b_j - \langle b_i \rangle \langle b_j \rangle \). The mean-field Hamiltonian is

\[
H_{\text{MF}} = \sum_{i \in A} H_A + \sum_{i \in B} H_B + 2zt \phi_A \phi_B, \tag{2}
\]

\[
H_A = -zt \phi_A (b_i^\dagger + b_i) + \frac{U}{2} n_i(n_i - 1) - (\mu + \Delta) n_i, \tag{3}
\]

\[
H_B = -zt \phi_B (b_i^\dagger + b_i) + \frac{U}{2} n_i(n_i - 1) - (\mu - \Delta) n_i, \tag{4}
\]

where \( z \) is the lattice coordination number (\( z = 4 \) for a square lattice), \( \phi_A = \langle b_i \rangle_{i \in A} \) and \( \phi_B = \langle b_i \rangle_{i \in B} = \langle b_i^\dagger \rangle_{i \in B} \) are the expectation values of the annihilation operators on sublattices \( A \) and \( B \), respectively. Likewise, \( n_A = \langle n_i \rangle_{i \in A} \) and \( n_B = \langle n_i \rangle_{i \in B} \) are the expectation values of the number operators on sublattices \( A \) and \( B \), respectively. The expectation values are calculated numerically using the eigenstates of \( H_A \) and \( H_B \).

The phase diagrams of the ionic Bose–Hubbard model on a square lattice are shown in figure 1. Since the staggered potential \( \Delta \) induces a density modulation, the term 'supersolid' (SS) is used in a broad sense to include non-spontaneous translational symmetry breaking. The phase diagram for \( \Delta = 0 \) agrees with that for the standard Bose–Hubbard model. There are MI phases (\( \phi_A = \phi_B = 0 \), \( n_A = n_B \)) and the SF phase (\( \phi_A = \phi_B > 0 \)). For \( \Delta = 0.3 U \), CDW phases (\( \phi_A = \phi_B = 0 \), \( n_A = n_B \)) and the SS phase (\( \phi_A = \phi_B \)) exist. In the atomic limit (\( t = 0 \)), the expectation value \( n_i \) is given by the integer \( n \) that minimizes the energy \( E_n = Un(n - 1)/2 - (\mu + \Delta)n \). Thus, \( n_A = n \) for \( U(n - 1) - \Delta < \mu < Un - \Delta \). Likewise, \( n_B = n \) for \( U(n - 1) + \Delta < \mu < Un + \Delta \). Due to the staggered potential \( \Delta \neq 0 \), the ground state alternates between CDW and MI phases as \( \mu \) increases. When \( t \) increases, MI and CDW regions shrink, and the SS phase appears. This phase transition is second-order since the order parameters \( \phi_A \) and \( \phi_B \) become nonzero continuously.

![Figure 1. Phase diagrams of the ionic Bose–Hubbard model on a square lattice \((z = 4)\) at zero temperature by the mean-field approximation for (a) \( \Delta = 0 \) and (b) \( \Delta = 0.3 U \). The MI and CDW phases are labeled by \( (n_A, n_B) \), which represents the expectation values of number operators on sublattices \( A \) and \( B \).](image-url)
3. Green’s function

To calculate the momentum dependence of the excitation energy and distribution function, we derive Green’s functions by the standard basis operator method [6–8, 30, 35–37]. By considering fluctuations around the mean-field ground state, the Hamiltonian is rewritten as

\[ H = H_{\text{MF}} - t \sum_{\langle ij \rangle} (\delta b_i^\dagger \delta b_j + \text{H.c.}), \]

where the operators \( \delta b_i = b_i - \phi \) and \( \delta b_i = b_i - \phi \) represent the deviations from the mean-field Hamiltonian. By using the energy eigenstates \( |i, \alpha \rangle \) of the mean-field Hamiltonian at site \( i \) with eigenenergies \( E_{\alpha} \), equation (5) is rewritten as

\[ H = \sum_{\alpha} E_{\alpha} \hat{c}_{\alpha}^\dagger \hat{c}_{\alpha} + t \sum_{\langle \alpha \beta \rangle} (\hat{c}_{\alpha}^\dagger \hat{c}_{\beta} + \text{H.c.}), \]

where \( \hat{c}_{\alpha}^\dagger = |i, \alpha \rangle \langle i, \alpha | \) is the standard basis operator (SBO) [37], \( \delta \hat{c}_{\alpha}^\dagger = \hat{c}_{\alpha}^\dagger - (\hat{c}_{\alpha}^\dagger) \), \( \delta c_{\alpha} = (i, \alpha | b_i | i, \alpha' \rangle \), and \( c_{\alpha} = (j, \beta | b_j | j, \beta' \rangle \). In this formalism, the retarded Green’s function is given by

\[ G^R(t'' - t') = \sum_{\alpha \beta} \sum_{\beta' \alpha'} c_{\alpha}^\dagger c_{\beta} G_{\alpha \alpha', \beta \beta'}(t'' - t'), \]

where

\[ G_{\alpha \alpha', \beta \beta'}(t'' - t') = -i \Theta(t'' - t') \langle \hat{c}_{\alpha}^\dagger (t''), \hat{c}_{\beta} (t') \rangle. \]

The equation for the Green’s function in frequency space in the random phase approximation (RPA) [6–8, 30, 35, 36] is

\[ \left[ \omega - E_{\alpha} \right] G_{\alpha \alpha', \beta \beta'}^{\omega} = P_{\alpha \beta} \delta_{\alpha' \beta'} \delta_{\alpha \beta'} \delta^{\omega} - t P_{\alpha \beta} \sum_{\gamma \gamma'} T_{\alpha \gamma \beta}^{\omega} G_{\gamma' \gamma, \beta \beta'}^{\omega}(\omega), \]

where \( E_{\alpha} = E_{\alpha} - E_{\alpha}^{\text{MF}} = \sum_{\gamma \gamma'} T_{\alpha \gamma \beta}^{\omega} G_{\gamma' \gamma, \beta \beta'}^{\omega}(\omega) \), and \( P_{\alpha} \) is the occupation probability. This quantity is equal to unity when \( \alpha \) is the ground state, and it is zero when \( \alpha \) is another state at zero temperature. By solving equation (9), we obtain the Green’s function \( G_k(\omega) \), which is expressed by the mean-field local Green’s functions given by

\[ \left( \begin{array}{cc} F_d^k & F_s^k \\ F_d^k & F_s^k \end{array} \right) = \sum_{\alpha \alpha'} \frac{p_{\alpha \alpha'}}{\omega - E_{\alpha}^{\omega}} \left( \begin{array}{cc} c_{\alpha}^\dagger c_{\alpha'}^\dagger & c_{\alpha}^\dagger c_{\alpha'}^\dagger \\ d_{\alpha}^\dagger d_{\alpha'}^\dagger & d_{\alpha}^\dagger d_{\alpha'}^\dagger \end{array} \right). \]

We solve equation (9) and calculate the excitation spectrum and momentum distribution in the MI, SF, CDW, and SS phases. First, we consider Green’s functions for the staggered potential \( \Delta = 0 \). Then, we derive Green’s functions for \( \Delta \neq 0 \).

3.1. MI (\( \Delta = 0 \))

For \( \Delta = 0 \), sublattices \( A \) and \( B \) are equivalent. Thus, the Fourier transformation of the Green’s function in equation (7) is defined as

\[ G_{\omega} = \frac{1}{N} \sum_k G_k(\omega) e^{-i k (R_i - R_j)}, \]

\[ G_k(\omega) = \frac{1}{N} \sum_q G_{\omega} e^{i k (R_i - R_j)}, \]

where \( N \) is the number of lattice sites, and \( R_i \) are the lattice site positions. In momentum space, the equation for the Green’s function is

\[ G_k(\omega) = F_d + \epsilon_k F_d G_k(\omega), \]

where \( \epsilon_k = -2t \sum_{\gamma = x,y} \cos(k_i) \), and the lattice constant is set to unity. From equation (13), the Green’s function is

\[ G_k(\omega) = F_d/(1 - \epsilon_k F_d). \]

In the MI phase, \( G_k(\omega) \) is analytically obtained since \( F_d \) is given analytically. Considering that the ground state is the number state \( |n_i, n_j \rangle \) with \( E_{n_i} = \text{Un}_i(n_i - 1)/2 - \mu n_i \) and \( c_{n_i}^\dagger n_i = \sqrt{\text{Un}_i} n_i - 1 \), the mean-field Green’s function is
where \( E^p = E_{n+1} - E_n = U \mu + \mu \) and \( E^h = E_{n-1} - E_n = -U(n-1) + \mu \) are particle and hole excitation energies, respectively. By substituting equation (15) into equation (14), the Green’s function is

\[
G_k(\omega) = \frac{C^p(k)}{\omega - E^p(k)} - \frac{C^h(k)}{\omega + E^h(k)},
\]

where \( E^p(k) = E^p - [U - E^U(k) - \epsilon_k]/2, E^h(k) = E^h - [U - E^U(k) + \epsilon_k]/2, \)

\[
E^U(k) = \left( \epsilon_k^2 + 2(U(2n+1) + U^2), C^p(k) = [\epsilon_k + (2n+1)U + E^U(k)]/[2E^U(k)],\right. \text{ and}
\]

\[
C^h(k) = [\epsilon_k + (2n+1)U - E^U(k)]/[2E^U(k)]. \]

The spectral function is

\[
A(k, \omega) = -\frac{1}{\pi} \text{Im} G_k(\omega + i\delta^+),
\]

\[
= -C^p(k)\delta[\omega - E^p(k)] - C^h(k)\delta[\omega + E^h(k)],
\]

where \( C^p(k) \) is the spectral weight of the particle excitation, and \( C^h(k) \) is that of the hole excitation. The momentum distribution is

\[
n(k) = -\int_{-\infty}^\infty A(k, \omega) d\omega = C^h(k).
\]

### 3.2. SF

In the SF phase (\( \phi_A = \phi_B = 0, n_A = n_B \)), it is necessary to introduce the anomalous Green’s function [35] defined by

\[
H^\phi(t'' - t') = -i\Theta(t'' - t') \langle [b^\dagger_j(t''), b_j(t')] \rangle = \sum_{\alpha, \beta, \beta'} \sum_{ij} d^\alpha_i d^\beta_j G_{\alpha, \beta'}^\phi(t'' - t').
\]

The equations for the Green’s functions are

\[
G_k(\omega) = F_{dd} + \epsilon_k F_{dc} H_k(\omega) + \epsilon_k F_{dd} G_k(\omega),
\]

\[
H_k(\omega) = F_{dd} + \epsilon_k F_{dc} H_k(\omega) + \epsilon_k F_{dd} G_k(\omega).
\]

From these equations,

\[
G_k(\omega) = (F_{dd} - \epsilon_k F_{dc} F_{dc} + \epsilon_k F_{dc} F_{dd})/D_k,
\]

\[
H_k(\omega) = F_{dd}/D_k,
\]

where

\[
D_k = 1 - \epsilon_k F_{dc} - \epsilon_k F_{dc} + \epsilon_k^2 F_{dc} F_{dc} - \epsilon_k^2 F_{dc} F_{dd}.
\]

Equation (22) is the same as \( G_k(\omega) = \Pi_k(\omega)[1 - \epsilon_k \Pi_k(\omega)] \), where \( \Pi_k(\omega) = F_{dd} + \epsilon_k F_{dc} F_{dd}/(1 - \epsilon_k F_{dc})[7, 8, 35] \). In contrast to the MI phase, the mean-field Green’s functions can not be obtained analytically, so the Green’s function is obtained numerically. To obtain the excitation energies and spectral weights, we factor the numerator and denominator of the Green’s function and then cancel out common terms numerically. Consequently, the Green’s function is decomposed as

\[
G_k(\omega) = \sum_{\alpha} \frac{C^p_{\alpha}(k)}{\omega - E^p_{\alpha}(k)} - \sum_{\alpha} \frac{C^h_{\alpha}(k)}{\omega + E^h_{\alpha}(k)}.
\]

The number of the poles of the Green’s function is the same as that of the mean-field Green’s functions. When the mean-field Hamiltonian is diagonalized in the occupation number basis \( \{0\}, \{1\}, \ldots, \{n_{\text{max}}\} \), the number of the poles is \( 2n_{\text{max}} \) at zero temperature. The momentum distribution is

\[
n(k) = \sum_{\alpha} C^h_{\alpha}(k) + N\phi^2 \delta_{k, \Gamma},
\]

where \( \phi^2 = \phi_A^2 = \phi_B^2 \) is the condensate fraction, \( N\phi^2 \) is the contribution of the condensate, and \( \Gamma = (0, 0) \) is the zone center, where the excitation energy is zero.

### 3.3. CDW and MI (\( \Delta \neq 0 \))

For \( \Delta \neq 0 \), sublattices \( A \) and \( B \) are inequivalent and each consists of \( N/2 \) lattice sites. Therefore, the Fourier transformation of Green’s functions for sublattices is defined as

\[
G^{\text{AB}}_k(\omega) = \frac{2}{N} \sum_k G^{\text{AB}}_k(\omega) e^{-i\mathbf{R}_m - \mathbf{R}_n},
\]
where indices $m$ and $n$ label sublattices $A$ and $B$ [39]. The equations for the Green’s functions in momentum space are

\[ G_k^{m\alpha}(\omega) = F_{cd}^A + \epsilon_k F_{cd}^A G_k^{B\alpha}(\omega), \]

\[ G_k^{B\alpha}(\omega) = c_k F_{cd}^A G_k^{A\alpha}(\omega), \]

\[ G_k^{AB}(\omega) = F_{cd}^B + \epsilon_k F_{cd}^B G_k^{B\alpha}(\omega), \]

\[ G_k^{AB}(\omega) = c_k F_{cd}^A G_k^{A\alpha}(\omega). \]

From these equations, the Green’s functions are

\[ G_k^{A\alpha}(\omega) = F_{cd}^A/D_k, \]

\[ G_k^{B\alpha}(\omega) = G_k^{AB}(\omega) = c_k F_{cd}^A F_{cd}^B/D_k, \]

\[ G_k^{BB}(\omega) = F_{cd}^B/D_k, \]

where $D_k = 1 - \epsilon_k^2 F_{cd}^A F_{cd}^B$. These Green’s functions can be analytically expressed since $F_{cd}^A$ and $F_{cd}^B$ are given by

\[ F_{cd}^A = \frac{n_A + 1}{\omega - E_A^\alpha} - \frac{n_A}{\omega + E_A^\alpha}, \]

\[ F_{cd}^B = \frac{n_B + 1}{\omega - E_B^\alpha} - \frac{n_B}{\omega + E_B^\alpha}, \]

where $E_A^\alpha = U n_A - (\mu + \Delta)$, $E_A^\alpha = -U(n_A - 1) + (\mu + \Delta)$, $E_B^\alpha = U n_B - (\mu - \Delta)$, and $E_B^\alpha = -U(n_B - 1) + (\mu - \Delta)$. The Green’s function is

\[ G_k(\omega) = \frac{1}{N} \sum_{\alpha} G_k^{\alpha}(\omega) \bar{e}^{ik(R_A - R_k)} = \frac{1}{2} \sum_{mn} G_k^{mn}(\omega) \]

\[ = \frac{1}{2} \left[ G_k^{AA}(\omega) + G_k^{BB}(\omega) + G_k^{AB}(\omega) + G_k^{BB}(\omega) \right]. \]

The excitation energies are the poles of the Green’s function, which are the solutions of $D_k = 1 - \epsilon_k^2 F_{cd}^A F_{cd}^B = 0$. This is a quartic equation in $\omega$, so the poles are analytically obtained by Ferrari’s formula. Thus, the Green’s function is written as

\[ G_k(\omega) = \frac{C_A^k(\omega)}{\omega - E_A^\alpha(\omega)} + \frac{C_B^k(\omega)}{\omega - E_B^\alpha(\omega)} - \frac{C_A^k(\omega)}{\omega + E_A^\alpha(\omega)} - \frac{C_B^k(\omega)}{\omega + E_B^\alpha(\omega)}, \]

where the excitation energies and spectral weights can be analytically expressed, but the expressions are too long to write here. The momentum distribution is

\[ n(k) = -\int_{-\infty}^{0} A(k, \omega) d\omega = C_A^k(\omega) + C_B^k(\omega). \]

### 3.4. SS

We derive Green’s functions in the SS phase ($\phi_A \approx \phi_B, n_A \approx n_B$). The equations for the Green’s functions are

\[ G_k^{BB}(\omega) = F_{cd}^B + \epsilon_k F_{cd}^B G_k^{AB}(\omega), \]

\[ G_k^{AB}(\omega) = c_k F_{cd}^B G_k^{BB}(\omega), \]

\[ H_k^{BB}(\omega) = F_{cd}^B + \epsilon_k F_{cd}^B H_k^{AB}(\omega), \]

\[ H_k^{AB}(\omega) = c_k F_{cd}^B H_k^{BB}(\omega), \]

\[ G_k^{AA}(\omega) = F_{cd}^A + \epsilon_k F_{cd}^A G_k^{BB}(\omega), \]

\[ G_k^{BA}(\omega) = c_k F_{cd}^A G_k^{BB}(\omega), \]

\[ H_k^{AA}(\omega) = F_{cd}^A + \epsilon_k F_{cd}^A H_k^{BB}(\omega), \]

\[ H_k^{BA}(\omega) = c_k F_{cd}^A H_k^{BB}(\omega). \]

From equations (41)–(44), the Green’s functions are

\[ G_k^{BB}(\omega) = (F_{cd}^B - \epsilon_k^2 F_{cd}^B F_{cd}^B + \epsilon_k^2 F_{cd}^A F_{cd}^B) / D_k, \]
The excitation spectrum is given by the poles of the Green's function. Figure 2 shows the excitation spectrum of the ionic Bose–Hubbard model on a square lattice for $U = 1$. Positive and negative excitation energies are particle and hole excitation energies, respectively. The excitation energy calculated by the standard basis operator method agrees with the mean-field excitation energy at X, where the correction to the mean-field result is zero since $v_F = 0$ at X.

In the MI phase, the spectrum is gapped for all $\mathbf{k}$. The particle excitation energy increases along $\mathbf{X}$ to that at $\mathbf{M}$. The particle excitation energy at $\mathbf{X}$ is the same as that along $\mathbf{M}$ or $\mathbf{\Gamma}$. The MI-SF phase transition occurs when either $E_p^\mathbf{k}$ is the same as that along $\mathbf{M}$ to that at $\mathbf{\Gamma}$.

Thus, the peak at $\mathbf{M}$ is smaller than that at $\mathbf{\Gamma}$.

### 4. Excitation spectrum

The excitation spectrum is given by the poles of the Green's function. Figure 2 shows the excitation spectrum of the ionic Bose–Hubbard model on a square lattice for $U = 1$. Positive and negative excitation energies are particle and hole excitation energies, respectively. The excitation energy calculated by the standard basis operator method agrees with the mean-field excitation energy at X, where the correction to the mean-field result is zero since $v_F = 0$ at X.

In the MI phase, the spectrum is gapped for all $\mathbf{k}$. The particle excitation energy increases along $\mathbf{X}$ to that at $\mathbf{M}$. The particle excitation energy at $\mathbf{X}$ is the same as that along $\mathbf{M}$ or $\mathbf{\Gamma}$. The MI-SF phase transition occurs when either $E_p^\mathbf{k}$ is the same as that along $\mathbf{M}$ to that at $\mathbf{\Gamma}$.

Thus, the peak at $\mathbf{M}$ is smaller than that at $\mathbf{\Gamma}$.

### 4. Excitation spectrum

The excitation spectrum is given by the poles of the Green's function. Figure 2 shows the excitation spectrum of the ionic Bose–Hubbard model on a square lattice for $U = 1$. Positive and negative excitation energies are particle and hole excitation energies, respectively. The excitation energy calculated by the standard basis operator method agrees with the mean-field excitation energy at X, where the correction to the mean-field result is zero since $v_F = 0$ at X.

In the MI phase, the spectrum is gapped for all $\mathbf{k}$. The particle excitation energy increases along $\mathbf{X}$ to that at $\mathbf{M}$. The particle excitation energy at $\mathbf{X}$ is the same as that along $\mathbf{M}$ or $\mathbf{\Gamma}$. The MI-SF phase transition occurs when either $E_p^\mathbf{k}$ is the same as that along $\mathbf{M}$ to that at $\mathbf{\Gamma}$.

Thus, the peak at $\mathbf{M}$ is smaller than that at $\mathbf{\Gamma}$.

### 4. Excitation spectrum

The excitation spectrum is given by the poles of the Green's function. Figure 2 shows the excitation spectrum of the ionic Bose–Hubbard model on a square lattice for $U = 1$. Positive and negative excitation energies are particle and hole excitation energies, respectively. The excitation energy calculated by the standard basis operator method agrees with the mean-field excitation energy at X, where the correction to the mean-field result is zero since $v_F = 0$ at X.

In the MI phase, the spectrum is gapped for all $\mathbf{k}$. The particle excitation energy increases along $\mathbf{X}$ to that at $\mathbf{M}$. The particle excitation energy at $\mathbf{X}$ is the same as that along $\mathbf{M}$ or $\mathbf{\Gamma}$. The MI-SF phase transition occurs when either $E_p^\mathbf{k}$ is the same as that along $\mathbf{M}$ to that at $\mathbf{\Gamma}$.

Thus, the peak at $\mathbf{M}$ is smaller than that at $\mathbf{\Gamma}$.
5. Momentum distribution

The momentum distribution is given by the sum of the spectral weights of hole excitation modes. Figure 3 shows the momentum distribution of the ionic Bose–Hubbard model on a square lattice for \( U = 1 \). In the MI phase, the momentum distribution decreases along \( \Gamma - X - M \) because \( n(k) \) is a monotonically decreasing function of \( \epsilon_k \).

In the SF phase, the momentum distribution is given by the sum of the spectral weights of the gapless hole excitation mode and that of the gapped hole excitation mode. The momentum distribution at \( k = \Gamma \) is given by the contribution of the condensate. It is proportional to the number of lattice sites \( N \) and diverges in the thermodynamic limit \( (N \to \infty) \). The momentum distribution increases drastically and diverges when \( k \to \Gamma \). This infrared divergence comes from the gapless excitation modes. When the gapless particle and hole excitation energies are given by \( E_g^p(k) \) and \( E_g^h(k) \), the Green’s function is

\[
G_k(\omega) \propto \frac{1}{\omega - E_g^p(k)} \frac{1}{\omega + E_g^h(k)}.
\]

Thus, the spectral weight of the gapless hole excitation mode is

\[
C_g^h(k) = - \lim_{\omega \to E_g^p(k)} [\omega + E_g^h(k)] G_k(\omega) \propto \frac{1}{E_g^h(k) + E_g^p(k)} \propto \frac{1}{k}.
\]

Therefore, the momentum distribution diverges when \( k \to 0 \). This divergence is consistent with the analysis in the long wavelength limit [40, 41]. The spectral weight of the gapped hole excitation mode also contributes to the momentum distribution around \( \Gamma \), but that of the gapless hole excitation mode gives a major contribution.

In the CDW phase, in addition to a large peak at \( \Gamma \), there is a small peak at \( M \). This peak does not exist in the MI phase. The peak at \( M \) appears only close to the CDW-SS phase boundary. This behavior is similar to that of the extended Bose–Hubbard model [30]. The critical value \( t_m \) where \( n(k) \) at \( M \) becomes a local maximum is the value which satisfies \( dn(k = M)/dt = 0 \).

In the SS phase, in addition to \( \Gamma \), the momentum distribution diverges as \( k \to M \) since the excitation is gapless at \( M \). The peak at \( M \) indicates the coexistence of superfluid and solid order. A peak at \( M \) is also observed in the quantum Monte Carlo simulations of the extended Bose–Hubbard model [31]. The peak around \( M \) is narrower than that around \( \Gamma \). This reflects that the peak at \( M \) is smaller than that at \( \Gamma \). The spectral weight of the gapless hole excitation mode makes a great contribution to the momentum distribution around \( \Gamma \) and \( M \). Away

\[\text{Figure 2. Excitation spectrum of the ionic Bose–Hubbard model on a square lattice at zero temperature for (a) MI (\( \Delta = 0, t/U = 0.02, \mu/U = 0.4 \)), (b) SF (\( \Delta = 0, t/U = 0.05, \mu/U = 0.4 \)), (c) CDW (\( \Delta = 0.3, t/U = 0.05, \mu/U = 0.05 \)), and (d) SS (\( \Delta = 0.3, t/U = 0.05, \mu/U = 0.4 \)). We take \( U = 1 \) as the energy unit. The points \( \Gamma, X, \) and \( M \) are \((0, 0), (\pi, 0), \) and \((\pi, \pi)\), respectively. The solid lines are the excitation energies calculated by the standard basis operator method, and the dotted lines are the mean-field excitation energies. Different colors correspond to different excitation modes.}\]
from $\Gamma$ and M, the spectral weights of the gapped hole excitation modes give a major contribution. Thus, both gapless and gapped modes are important to understand the momentum distribution.

6. Conclusions

By the standard operator method, we have derived Green’s functions of the ionic Bose–Hubbard model in MI, SF, CDW, and SS phases. The excitation spectrum has gapped modes in all the phases and gapless Goldstone modes in the SF and SS phases. We have shown that the momentum distribution has a peak at $\Gamma$ in all the phases and a peak at M in the SS phase and the CDW phase close to the CDW-SS phase boundary. Furthermore, we have demonstrated that the momentum distribution can be described by the excitation spectrum and spectral weights of hole excitation modes. We have clarified the contribution of both gapless and gapped hole excitation modes to the momentum distribution in the SF and SS phases.

The SBO method developed in this study will be applied to other lattices and contribute to understanding of Bose–Hubbard models. Moreover, this study will give a new insight into the ionic Hubbard model, which is the fermionic version of the IBHM [42–44].

Acknowledgments

This work was supported by JST SPRING, Grant Number JPMJSP2108.

Data availability statement

No new data were created or analysed in this study.
Appendix. Contribution of the condensate

The Green’s function for bosons at zero temperature is

\[ G^{0}(\omega) = \sum_{\alpha} \left( \frac{\langle g|b_{\alpha}|g\rangle \langle \alpha|b_{\alpha}^\dagger|g\rangle}{\omega - E_{\alpha}} - \frac{\langle \alpha|b_{\alpha}^\dagger|g\rangle \langle g|b_{\alpha}|\alpha\rangle}{\omega + E_{\alpha}} \right), \]  

(A.1)

where \( |g\rangle \) is the ground state and \( E_{\alpha} \) is the excitation energy of the eigenstate \( |\alpha\rangle \). For \( \alpha = g, E_{\alpha} = 0 \), and the term in the brackets vanishes. Thus, the momentum distribution of the condensate, which is the ground state in the SF and SS phases, can not be calculated from the Green’s function. The contribution of the condensate is given by

\[ n_{c}(k) = \frac{1}{N} \sum_{\alpha} \langle g|b_{\alpha}|g\rangle \langle \alpha|b_{\alpha}^\dagger|g\rangle e^{ik(R_{\alpha} - R_{\alpha})}. \]  

(A.2)

In the SF phase, the excitation energy is zero at \( k = (0, 0) = \Gamma \), and \( n_{c}(k = \Gamma) = N \phi^{2} \), where \( \phi = \langle g|b_{\alpha}^\dagger|g\rangle = \langle g|b_{\alpha}|g\rangle \). In the SS phase, since sublattices A and B are inequivalent,

\[ n_{c}(k) = \frac{1}{N} \left[ \sum_{iA} \phi_{A}^{2} e^{ik(R_{iA} - R_{iA})} + \sum_{iB} \phi_{B}^{2} e^{ik(R_{iB} - R_{iB})} \right], \]  

(A.3)

where \( \phi_{m} = \langle g|b_{m}^\dagger|g\rangle = \langle g|b_{m}|g\rangle \). The excitation energy is zero at \( k = (0, 0) = \Gamma \) and \( k = (\pi, \pi) = M \). For \( k = (0, 0) \), \( e^{ik(R_{m} - R_{m})} = 1 \) for all sites, so

\[ n_{c}(k = \Gamma) = N [(\phi_{A} + \phi_{B})/2]^{2}. \]  

(A.4)

For \( k = (\pi, \pi) \), \( e^{ik(R_{m} - R_{m})} = 1 \) for \( m = n \), and \( e^{ik(R_{m} - R_{m})} = -1 \) for \( m \neq n \), so

\[ n_{c}(k = M) = N [(\phi_{A} - \phi_{B})/2]^{2}. \]  

(A.5)

ORCID iDs

Hiroki Nishizawa @ https://orcid.org/0000-0002-7020-7125

References

[1] Fisher M P, Weichman P B, Grinstein G and Fisher D S 1989 Boson localization and the superfluid-insulator transition Phys. Rev. B 40 546
[2] Jakob D, Bruder C, Cirac I L, Gardiner C W and Zoller P 1998 Cold bosonic atoms in optical lattices Phys. Rev. Lett. 81 3108
[3] Freericks J and Monien H 1994 Phase diagram of the boson-hubbard model EPL (Europhysics Letters) 26 545
[4] Van Oosten D, van der Straten P and Stooft H 2001 Quantum phases in an optical lattice Phys. Rev. A 63 053601 A
[5] Capogrosso-Sansone B, Prokof’Ev N and Svistunov B 2007 Phase diagram and thermodynamics of the three-dimensional boson-hubbard model Phys. Rev. B 75 134502 B
[6] Sheshadri K, Krishnamurthy H, Pandit R and Ramakrishnan T 1993 Superfluid and insulating phases in an interacting-boson model: mean-field theory and the rpa EPL (Europhysics Letters) 22 257
[7] Ohashi Y, Kitaura M and Matsumoto H 2006 Itinerant-localized dual character of a strongly correlated superfluid Bose gas in an optical lattice Phys. Rev. B 73 033617 A
[8] Menotti C and Trivedi N 2008 Spectral weight redistribution in strongly correlated bosons in optical lattices Phys. Rev. Lett. 100 053610 B
[9] Huber S D, Altman E, Büchler H P and Blatter G 2007 Dynamical properties of ultracold bosons in an optical lattice Phys. Rev. B 75 105106 B
[10] Kunitsky K V and Navez P 2011 Excitation dynamics in a lattice Bose gas within the time-dependent gutzwiler mean-field approach Phys. Rev. A 84 033607 A
[11] Dutta A, Trefzger C and Sengupta K 2012 Projection operator approach to the boson-hubbard model Phys. Rev. B 86 085140 B
[12] Di Liberto M, Recati A, Trivedi N, Carusotto I and Menotti C 2018 Particle-hole character of the higgs and goldstone modes in strongly interacting lattice bosons Phys. Rev. Lett. 120 073201
[13] Calef F, Capone M, Menotti C, Carusotto I and Recati A 2020 Quantum fluctuations beyond the gutzwiler approximation in the boson-hubbard model Physical Review Research 2 033276
[14] Sengupta K and Dupuis N 2005 Mott-insulator-to-superfluid transition in the boson-hubbard model: a strong-coupling approach Phys. Rev. B 71 033629 A
[15] Kato Y, Zhou Q, Kawashima N and Trivedi N 2008 Sharp peaks in the momentum distribution of bosons in optical lattices in the normal state Nat. Phys. 4 617–21
[16] Freericks J, Krishnamurthy H, Kato Y, Kawashima N and Trivedi N 2009 Strong-coupling expansion for the momentum distribution of the boson-hubbard model with benchmarking against exact numerical results Phys. Rev. B 79 053631 A
[17] Knap M, Arrigoni E and von der Linden W 2010 Spectral properties of strongly correlated bosons in two-dimensional optical lattices Phys. Rev. B 81 024301 B
[18] Fitzpatrick M R and Bennett M P 2018 Contour-time approach to the bose-hubbard model in the strong coupling regime: studying two-point spatio-temporal correlations at the hartree-fock-bogoliubov level Nucl. Phys. B 930 1–44
[19] Batrouni G, Scalletta R, Zimanyi G and Kampf A P 1995 Supersolids in the bose-hubbard hamiltonian Phys. Rev. Lett. 74 2527
[20] Sengupta P, Pryadko L P, Alet F, Troyer M and Schmid G 2005 Supersolids versus phase separation in two-dimensional lattice bosons Phys. Rev. Lett. 94 207202
[21] Kovrizhin D L, Pai G V and Sinha S 2005 Density wave and supersolid phases of correlated bosons in an optical lattice EPL (Europhysics Letters) 72 162
[22] Yamamoto K, Todo S and Miyashita S 2009 Successive phase transitions at finite temperatures toward the supersolid state in a three-dimensional extended bose-hubbard model Phys. Rev. B 79 094503
[23] Iskin M 2011 Route to supersolidity for the extended bose-hubbard model Phys. Rev. B 83 035106
[24] Kimura T 2011 Gutzwiller study of extended hubbard models with fixed boson densities Phys. Rev. B 84 064530
[25] Trefzger C, Menotti C, Capogrosso-Sansone B and Lewenstein M 2011 Ultracold dipolar gases in optical lattices J. Phys. B: At. Mol. Opt. Phys. A 44 193001
[26] Rossini D and Fazio R 2012 Phase diagram of the extended bose–hubbard model New J. Phys. 14 065012
[27] Ohgoe T, Suzuki T and Kawashima N 2012 Commensurate supersolid of three-dimensional lattice bosons Phys. Rev. Lett. 108 185302
[28] Dutta O, Gajda M, Hauke P, Lewenstein M, Lühmann D S, Malomed B A, Sowiński T and Zakrzewski J 2015 Non-standard hubbard models in optical lattices: a review Rep. Prog. Phys. 78 066001
[29] Grémel B and Batrouni G G 2016 Excitation and dynamics in the extended bose-hubbard model Phys. Rev. B 93 035108
[30] Iskin M and Freericks J 2009 Momentum distribution of the insulating phases of the extended bose-hubbard model Phys. Rev. B 80 064510
[31] Ohgoe T, Suzuki T and Kawashima N 2012 Ground-state phase diagram of the two-dimensional extended bose–hubbard model Phys. Rev. B 86 054520
[32] Guo H, Wen Y and Feng S 2009 Cold atoms on a two-dimensional square optical lattice with an alternating potential Phys. Rev. B 80 035101
[33] Sawhney A and Mueller E J 2021 Influence of sublattice bias on superfluid to mott insulator transitions Phys. Rev. B 103 064308
[34] Li X J and Wen Y C 2005 Gutzwiller study of extended hubbard models in optical lattices: a review Rep. Prog. Phys. 78 066001
[35] Sajna A, Polak T, Micnas R and Rożek P 2015 Ground-state and finite-temperature properties of correlated ultracold bosons on optical lattices Phys. Rev. A 92 013602
[36] Konabe S, Niki T and Nakamura M 2006 Laser probing of the single-particle energy gap of a boson gas in an optical lattice in the mott-insulator phase Phys. Rev. B 73 035121
[37] Haley S B and Erdős P 1972 Standard-basis operator method in the green’s-function technique of many-body systems with an application to ferромagnetism Phys. Rev. B 5 1106
[38] Zubarev D N 1960 Double-time Green functions in statistical physics Soviet Physics Uspekhi 3 320
[39] Frohlich P and Kuntz P J 2006 Many-body green’s function theory of heisenberg films Phys. Rep. 432 223–304
[40] Gavoret J and Nozières P 1964 Structure of the perturbation expansion for the boson liquid at zero temperature Ann. Phys. 28 349–99
[41] Griffin A et al 1993 Excitations in a Bose Condensed Liquid (Cambridge: Cambridge University Press)
[42] Garg A, Krishnamurthy H and Randeria M 2006 Can correlations drive a band insulator metallic? Phys. Rev. Lett. 97 046403
[43] Kanchchara S S and Dagotto E 2007 Correlated insulating phase suggests bond order between band and mott insulators in two dimensions Phys. Rev. Lett. 98 016402
[44] Bouadim K, Paris N, Hébert F, Batrouni G and Scalletta R 2007 Metallic phase in the two-dimensional ionic hubbard model Phys. Rev. B 76 085112