Time-of-flight images of the Mott insulators in the Hofstadter-Bose-Hubbard model

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We analyze the momentum distribution function and its artificial-gauge-field dependence for the Mott insulator phases of the Hofstadter-Bose-Hubbard model. By benchmarking the results of the random-phase approximation (RPA) approach against those of the strong-coupling expansion (SCE) for the Landau and symmetric gauges, we find pronounced corrections to the former results in two dimensions.

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Introduction: The momentum distribution function $n(k)$ of atoms, which is defined as the Fourier transform of the one-body density matrix, can be directly measured in cold-atom systems by time-of-flight absorption imaging of freely expanding gas [1,2]. Since these systems are extremely dilute, the atom-atom interactions are negligible during such an expansion, and the position of atoms at time $\tau$ are strongly correlated with their velocity distribution at the moment of release from the trap, i.e., $r = \hbar k \tau / m$ with $\hbar$ the Planck constant and $m$ the atomic mass. Therefore, the $n(k)$ of atoms has not only been the easiest observable to measure but also been routinely used for probing distinct phases of matter in atomic systems.

In addition, followed by the recent advances in creating artificial gauge fields in atomic systems [4,5], there has been growing interest in first the realization of the Hofstadter-type lattice Hamiltonians and then the detection of the resultant many-body phases [3,4,10]. For instance, the MIT group has in their latest preprint measured the $n(k)$ of atoms in the superfluid (SF) phase [10], revealing both the reduced symmetry of their specific gauge field and the resultant degeneracy of the ground state [11]. There is no doubt that such a capacity to tune strong gauge fields together with strong interactions paves ultimately for creating and observing uncharted many-body phases and transitions in between, one of the immediate candidates of which is the renowned SF-MI transition [1,2].

Motivated by these recent works, in this Brief Report, we study $n(k)$ of atoms for the MI phases of the Hofstadter-Bose-Hubbard model on a square lattice. For this purpose, we compare the results of RPA and SCE approaches for the Landau and symmetric gauges, and find substantial corrections to the former results depending strongly on the specified gauge.

Hamiltonian and Phase Diagram: These results are obtained for the following Hamiltonian

$$H = -\sum_{ij} t_{ij} c_i^\dagger c_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i,$$

where the hopping parameter $t_{ij} = t e^{i\theta_{ij}}$ connects nearest-neighbor sites with phase factor $\theta_{ij}$ taking the gauge fields into account, $c_i^\dagger (c_i)$ creates (annihilates) a boson on site $i$, the boson-boson interaction is on-site and repulsive $U \geq 0$, $\hat{n}_i = c_i^\dagger c_i$ is the number operator, and $\mu \geq 0$ is the chemical potential. In this paper, we compare the results of the usual (A) no-gauge limit, where $\theta_{ij} = 0$ for all hoppings; with those of (B) Landau gauge, where $\theta_{ij} = 2\pi \phi u$ for $(u,v)$ to $(u,v+1)$ and 0 for $(u,v)$ to $(u+1,v)$ hoppings; (C) symmetric gauge, where $\theta_{ij} = \pi \phi u$ for $(u,v)$ to $(u,v+1)$ and $-\pi \phi v$ for $(u,v)$ to $(u+1,v)$ hoppings; and (D) MIT gauge [10], where $\theta_{ij} = 2\pi \phi (u+v)$ for $(u,v)$ to $(u,v+1)$ and 0 for $(u,v)$ to $(u+1,v)$ hoppings. Here, $(u,v)$ corresponds to the Cartesian coordinates of site $i$, and $\theta_{ij}$ are chosen such that the magnetic flux $\phi = p/q$ is the same for all gauges, with $p$ and $q$ are co-prime numbers with $p \leq q$.

In the atomic ($t = 0$) limit, since $H$ commutes with $\hat{n}_i$, the thermal average $n_i = \langle \hat{n}_i \rangle$ is such that the ground-state energy is minimised for a given $\mu$, leading to a uniform occupation $(n_i = n)$ of bosons thanks to the translational invariance of $H$. When $U = 0$ and $\mu = 0$, the spectrum of $H$ corresponds to the celebrated Hofstadter butterfly [12,13]. It is also very well-known that the range of $\mu$ about which the ground state is a MI with an integer occupation $n$ decreases as a function of increasing $t/U$, and depending on $n$ and $\phi$, the MIs disappear at a critical value of $t/U$, beyond which the system becomes a SF [14]. For instance, the qualitative phase diagram of $H$ can be obtained within the mean-field approximation, e.g., the decoupling or variational Gutzwiller techniques, leading to [15,16]

$$\frac{1}{e^{\phi q}} = \frac{n+1}{U n - \mu} - \frac{n}{U (n-1) - \mu}$$

at zero temperature for the MI-SF phase transition boundary, where $n \geq 0$ is an integer number. Here, $e^{\phi q}$ is the minimal eigenvalue of the hopping matrix $\sum_{ij} (-t_{ij}) f_j = e^{\phi q} f_i$ and it corresponds to the maximal single-particle kinetic energy of the Hofstadter butterfly, e.g., $e^0 = 4t$ when $\phi = 0$. Since the effects of $\theta_{ij}$ enter Eq. (2) through its dependence on $e^{\phi q}$, the mean-field phase boundary is clearly independent of the gauge, which is simply because only the position in the magnetic Brillouin zone but not the value of $e^{\phi q}$ depends on the gauge. However, this is not the case for the SF properties which are gauge dependent within the mean-field approaches.

In Fig. 1, we show the ground-state phase diagram as a function of $\mu$, $\phi = p/q$ and $4t$, which is obtained by solving Eq. (2) together with the Harper’s equation. Both the symmetry around $p/q = 1/2$ and the intriguing structure of the MI-SF phase transition boundary are due to the dependence of $e^{\phi q}$ on $\phi$ [12,13]. In addition, the incompressible (compressible) MI (SF) phase grows (shrinks) when $\phi$ increases from 0, a consequence of which is due to the localizing effects of magnetic flux on particles, and all of these results are
responds to the exact

We emphasize that while the result of the RPA approach corre-
gives zero magnetic flux, the results of the SCE approach

proaches:

has nothing to do with our

since it depends on the particular optical lattice potential and

M

where

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of atoms corresponds to the Fourier transform of the

where

FIG. 1. (Color online) The ground-state phase diagram is shown as a

in agreement with earlier findings[14–16]. Having introduced

the model Hamiltonian and reviewed its phase diagram, next

we are ready to discuss the momentum distribution of bosons

Momentum Distribution: As discussed in the Introduction,

the \( n(k) \) of atoms corresponds to the Fourier transform of the

one-body density matrix, and it is given by [17–20]

\[
\begin{align*}
n(k) &= \frac{|w(k)|^2}{M} \sum_{jj'} \langle c_j^+, c_{j'} \rangle e^{i \mathbf{k} \cdot (\mathbf{r}_{j'} - \mathbf{r}_j)},
\end{align*}
\]

(3)

where \( M \) is the number of sites and \( \mathbf{r}_i = (u\alpha, v\alpha) \) is the

position of site \( i \) with \( \alpha \) the lattice spacing. In the following, we

set the Fourier transform of the Wannier function \( w(k) \) to 1,

since it depends on the particular optical lattice potential and

has nothing to do with our \( H \).

In this paper, we calculate \( n(k) \) for the MIs using two

approaches: (I) RPA [18, 19] and (II) SCE in \( t/U \) [17, 18].

We emphasize that while the result of the RPA approach

corresponds to the exact \( n(k) \) only in the limit of infinite dimen-
sions and zero magnetic flux, the results of the SCE approach

are exact in two dimensions for the specified gauges up to the

given order in \( t/U \).

\( (I) \) Random-Phase Approximation: In the RPA

approach [18, 19], since the thermal averages of products of

operators are replaced by the product of their thermal averages,

the fluctuations are not fully taken into account. After a

lengthy but straightforward algebra, one finds

\[
\begin{align*}
n^{pq}_{\text{RPA}}(k) &= \frac{1}{2q} \sum_{\ell=0}^{q-1} \frac{\epsilon_{\ell}^{pq}(k) + \tilde{U}}{\sqrt{[\epsilon_{\ell}^{pq}(k)]^2 + 2U \epsilon_{\ell}^{pq}(k) + U^2}} - \frac{1}{2} (4)
\end{align*}
\]

for a MI with \( n \) bosons per site at zero temperature, where

\( \tilde{U} = U(2n + 1) \) and \( \epsilon_{\ell}^{pq}(k) \) is the energy dispersion of a

single particle in the \( \ell \)th Hofstadter band. While the set of \( \epsilon_{\ell}^{pq}(k) \)

values depends only on \( \phi \) and lattice geometry, their

corresponding positions in the 1st magnetic Brillouin zone,

and therefore \( n(k) \), are gauge dependent [19, 20]. For in-

stance, \( n(k) \) exhibits \( q \) peaks as a function of \( k \), and only

the number \( q \) but not the positions are controlled by \( \phi \). Note

that \( \epsilon_{\ell}^{pq} \equiv \max \{ \epsilon_{\ell}^{pq}(k) \} \) in Eq. (2) which is also a gauge-

independent quantity as remarked above. In particular, when

\( \phi = 0 \), a \( d \)-dimensional hypercubic lattice gives rise to a single

band with dispersion \( \epsilon^0(k) = -2t \sum_a \cos(k_a) \) and it is

already established that \( n^0_{\text{RPA}}(k) \) becomes exact as \( d \rightarrow \infty \)

while keeping \( dt \) fixed [17, 18].

To compare Eq. (4) with our exact results of the SCE

approach derived below, let us expand \( n^{pq}_{\text{RPA}}(k) \) in a power series

up to 3rd order in \( t/U \), leading to

\[
\begin{align*}
n^{pq}_{\text{RPA}}(k) &= n - \frac{2n(n+1)}{qU} \sum_{\ell=0}^{q-1} \epsilon_{\ell}^{pq}(k) \\
&\quad + \frac{3n(n+1)(2n+1)}{qU^2} \sum_{\ell=0}^{q-1} \left[ \epsilon_{\ell}^{pq}(k) \right]^2 \\
&\quad - \frac{4n(n+1)(5n^2+5n+1)}{qU^3} \sum_{\ell=0}^{q-1} \left[ \epsilon_{\ell}^{pq}(k) \right]^3. (5)
\end{align*}
\]

For a given \( \phi \), the sums over Hofstadter bands can be easily

evaluated for a given gauge by noting \( \sum_{\ell=0}^{q-1} \left[ \epsilon_{\ell}^{pq}(k) \right]^s =

\text{Trace}\{[T^{pq}(k)]^s\} \), where \( T^{pq}(k) \) describes the kinetic energy of a

single particle in the 1st magnetic Brillouin zone. For instance,

\( T^{pq}(k) \) is a \( q \times q \) matrix in the Landau gauge [12, 13],

leading to
Equations (6, 9) clearly show that the first $k$ dependence of $n^{pq}_{RPA}(k)$ arises at the 6th order in $t/U$. More importantly, we note that Eqs. (6, 9) are symmetric in $k_x$ and $k_y$ even though the spatial symmetry between $x$ and $y$ directions is explicitly broken by the Landau gauge. Note also that Eq. (6) coincides with that of the $\phi = 0$ result since $\epsilon^q_{ij}(k)$ is a periodic function of $\phi$ with a period of $1$. Unlike the $\phi = 0$ case for which the RPA approach captures the essential features of $n^0(k)$ even in finite dimensions [17, 18], next we use the SCE approach and show that the corrections to $n^{pq}_{RPA}(k)$ are quite dramatic in the presence of gauge fields in two dimensions.

(II) Strong-Coupling Expansion: In the SCE approach [17, 18], we need the wave function of MI as a function of $t$, which is achieved here by using a many-body perturbation theory in the kinetic energy term up to 3rd order in $t/U$. After a very lengthy and tedious algebra, one finds

$$n^{11}_{RPA}(k) = n + \frac{4n(n+1)}{(U/t)} [\cos(k_x a) + \cos(k_y a)] + \frac{12n(n+1)(2n+1)}{(U/t)^2} [\cos(k_x a) + \cos(k_y a)]^2$$

$$+ \frac{32n(n+1)(5n^2 + 5n + 1)}{(U/t)^3} [\cos(k_x a) + \cos(k_y a)]^3,$$

(6)

$$n^{12}_{RPA}(k) = n + \frac{6n(n+1)(2n+1)}{(U/t)^2} [\cos(2k_x a) + \cos(2k_y a) + 2] + O(t/U)^4,$$

(7)

$$n^{pq}_{RPA}(k) = n + \frac{12n(n+1)(2n+1)}{(U/t)^2} \left[ \cos(k_x a) + \cos(3k_y a) \right],$$

(8)

$$n^{pq>3}_{RPA}(k) = n + \frac{12n(n+1)(2n+1)}{(U/t)^2} + O(t/U)^4.$$

(9)

for a square lattice with nearest-neighbor hopping at zero temperature. We note in Eq. (10) that the 2 terms that are explicitly proportional to $t^2$ are finite-$d$ corrections, including the 2nd term in the 2nd line and the 4th line, as they vanish in the $d \to \infty$ limit while keeping $dt$ fixed. Since Eq. (10) is derived exactly using a generic hopping matrix $t_{ij}$, we are ready to benchmark it against the results of the RPA approach for a number of specified gauges.

(II-A) No-Gauge Limit: Setting $\theta_{ij} = 0$ for all hoppings in Eq. (10), we obtain

$$n^0(k) = n - \frac{2n(n+1)}{U} \epsilon^0(k)$$

$$+ \frac{3n(n+1)(2n+1)}{U^2} \left[ [\epsilon^0(k)]^2 - 4t^2 \right]$$

$$- \frac{4n(n+1)(5n^2 + 5n + 1)}{U^3} [\epsilon^0(k)]^3$$

$$+ \frac{n(n+1)(131n^2 + 131n + 26)}{U^3} t^2 \epsilon^0(k),$$

(11)

where $\epsilon^0(k) = -2t \cos(k_x a) - 2t \cos(k_y a)$ is the usual dispersion relation for a square lattice. Since the two terms that are explicitly proportional to $t^2$ are finite-$d$ corrections, they are not captured by the result of the RPA approach that is given in Eq. (6).

(II-B) Landau Gauge: On the other hand, setting $\theta_{ij} = 2\pi \delta_{ij}$ for $(u, v)$ to $(u, v + 1)$ and 0 for $(u, v)$ to $(u + 1, v)$ hoppings in Eq. (10), we obtain
Note that Eq. (12) exactly coincides with Eq. (11) since $\phi = 1$ and 0 are equivalent in this gauge. We also note that, unlike the results of the RPA approach that are given in Eqs. (6-9), these exact results are not symmetric in $k_x$ and $k_y$, showing that it is only the first $k_y$ dependence that arises at the $q$th order in $t/U$. In addition, on top of the RPA contributions, Eqs. (12-15) contain various other terms, showing that the finite-$d$ corrections are quite substantial in the presence of gauge fields in two dimensions [21]. Thus, one of our main conclusions in this paper is that the mismatch between the results of RPA and SCE approaches grows so dramatically as $q$ increases from 1 that the former approach fails to reproduce any of the exact terms up to 3rd order in $t/U$ for $q > 3$.

**II-C** Symmetric Gauge: Similarly, setting $\theta_{ij} = \pi \phi u$ for $(u, v)$ to $(u, v + 1)$ and $-\pi \phi v$ for $(u, v)$ to $(u + 1, v)$ hoppings in Eq. (10), we obtain

$$n^1_k(k) = n + \frac{4n(n + 1)}{(U/t)} \{ \cos(k_{x}a) + \cos(k_{y}a) \} + \frac{12n(n + 1)(2n + 1)}{(U/t)^2} \{ [\cos(k_{x}a) + \cos(k_{y}a)]^2 - 1 \}$$

$$+ \frac{32n(n + 1)(5n^2 + 5n + 1)}{(U/t)^3} \{ \cos(k_{x}a) + \cos(k_{y}a) \}^3 - \frac{2n(n + 1)(131n^2 + 131n + 26)}{(U/t)^3} \cos(k_{x}a) + \cos(k_{y}a),$$

$$n^{2}(k) = n + \frac{4n(n + 1)}{(U/t)} \cos(k_{x}a) + \frac{6n(n + 1)(2n + 1)}{(U/t)^2} \{ \cos(2k_{x}a) + \cos(2k_{y}a) \}$$

$$+ \frac{32n(n + 1)(5n^2 + 5n + 1)}{(U/t)^3} \cos(k_{x}a) \cos^2(k_{y}a) + \cos^2(k_{y}a) \} - \frac{2n(n + 1)(131n^2 + 131n + 26)}{(U/t)^3} \cos(k_{x}a),$$

$$n^{3}(k) = n + \frac{4n(n + 1)}{(U/t)} \cos(k_{x}a) + \frac{6n(n + 1)(2n + 1)}{(U/t)^2} \cos(2k_{x}a)$$

$$+ \frac{8n(n + 1)(5n^2 + 5n + 1)}{(U/t)^3} \{ \cos(3k_{x}a) + \cos(3k_{y}a) + 6 \cos(k_{x}a) \} - \frac{2n(n + 1)(131n^2 + 131n + 26)}{(U/t)^3} \cos(k_{x}a),$$

$$n^{p,q>3}(k) = n + \frac{4n(n + 1)}{(U/t)} \cos(k_{x}a) + \frac{6n(n + 1)(2n + 1)}{(U/t)^2} \cos(2k_{x}a)$$

$$+ \frac{8n(n + 1)(5n^2 + 5n + 1)}{(U/t)^3} \{ \cos(3k_{x}a) + \cos(3k_{y}a) + 6 \cos(k_{x}a) \} - \frac{2n(n + 1)(131n^2 + 131n + 26)}{(U/t)^3} \cos(k_{x}a).$$

Note that Eq. (16) does not reproduce Eq. (11) since $\phi = 1$ and 0 are not equivalent in this gauge. We also note that, unlike the results of the SCE approach for the Landau gauge that are given in Eqs. (12-15), here the $k$ dependence is not only symmetric in $k_x$ and $k_y$, thanks to the spatial symmetry between $x$ and $y$ directions, but also the first $k$ dependence arises at the $2q$th order in $t/U$. In addition, the $k$-independent $2n$ order term in Eq. (16) is a finite-$d$ correction to the result of the RPA approach in this gauge. Therefore, $n^{p,q}(k)$ becomes more and more featureless function of $k$ as $q$ increases from 1, especially deep in the MI's when $t/U$ is very small.

**II-D** MIT Gauge: Lastly, setting $\theta_{ij} = 2\pi \phi (u + v)$ for $(u, v)$ to $(u, v + 1)$ and 0 for $(u, v)$ to $(u + 1, v)$ hoppings in Eq. (10) leads exactly to Eqs. (12-15), and therefore, the MIT [10] and Landau gauges have exactly the same $n(k)$.

**Conclusions:** To summarize, we studied the expansion images of atoms for the MI phases of the Hofstadter-Bose-Hubbard model on a square lattice. In particular, we explicitly calculated the momentum distribution function for the Landau and symmetric gauges with both RPA and SCE approaches, and found marked corrections to the former results depending strongly on the specified gauge.

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