Various topological Mott insulators and topological bulk charge pumping in strongly-interacting boson system in one-dimensional superlattice

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Abstract

In this paper, we study a one-dimensional boson system in a superlattice potential. This system is experimentally feasible by using ultracold atomic gases, and attracts much attention these days. It is expected that the system has a topological phase called a topological Mott insulator (TMI). We show that in strongly-interacting cases, the competition between the superlattice potential and the on-site interaction leads to various TMIs with a non-vanishing integer Chern number. Compared to the hard-core case, the soft-core boson system exhibits rich phase diagrams including various non-trivial TMIs. By using the exact diagonalization, we obtain detailed bulk-global phase diagrams including the TMIs with high Chern numbers and also various non-topological phases. We also show that in adiabatic experimental setups, the strongly-interacting bosonic TMIs exhibit the topological particle transfer, i.e., the topological charge pumping phenomenon, similarly to weakly-interacting systems. The various TMIs are characterized by topological charge pumping as it is closely related to the Chern number, and therefore the Chern number is to be observed in feasible experiments.

1. Introduction

In recent years, topological phase is one of the most interesting subjects in condensed matter physics. It is generally defined as a state characterized by a nontrivial topological number even though it has no local order parameters. Topological phase is expected to form even in one-dimensional (1D) system as suggested in the celebrated work by Thouless [1]. The topological phase in 1D system originates from geometrical similarity of the (1 + 1)D spacetime to 2D space, in which well-known topological states of matter, e.g., the integer quantum Hall (IQH) [2, 3] and fractional quantum Hall states [4, 5] form. Inspired by the important observation by Thouless [1], certain 1D models have been studied from the point of view of topological phase [6–9, 11, 12]. Also the experiments on cold atomic gases in an optical lattice have started to ‘quantum simulate’ such 1D systems [15]. As one of the recent remarkable successes in the experiments, we notice the realization of the topological Thouless pumping [16, 17]. The topological Thouless pumping is a phenomenon in which a spontaneous atomic transportation takes place by changing a Floquet parameter characterizing topological properties of the Hamiltonian. The experimental successes stimulate theoretical study of the topological phase of 1D cold atomic system in an optical lattice.

Motivated by these theoretical observations and experimental successes, we shall study the systems of strongly-interacting Bose gases on 1D superlattice in this work. In experiments, interactions between cold atoms can be controlled by using optical experimental techniques, e.g., Feshbach resonance [18, 19] and orbital Feshbach resonance [20]. The target system is described by the Bose–Hubbard model (BHM) with an applied modulate chemical potential term. Interestingly, the BHM with a modular chemical potential is expected to have non-trivial topological states [6–9, 11, 12] and it can be quantum simulated by the recent experiments [21].
Most of the previous studies have focused on the existence of non-trivial topological phases. Some numerical studies by using the density-matrix renormalization group method (DMRG) confirmed the existence of the non-trivial topological phase called topological Mott insulator (TMI) \[6, 7, 8\]. TMI is classified by a topological number such as the Chern number and it has a gap in the bulk but a gapless excitation in the (spacial as well as phase diagram) boundaries. A quantum Monte-Carlo simulation was also carried out to detect the topological phase \[10\]. However, the existence was verified only in a limited parameter regime, and detailed global phase diagrams are still lacking. In particular, strongly-correlated bosonic topological states with high Chern number in the bulk have not been clarified yet in a global parameter regime, nor it is understood well how the competition between the superlattice potential and the on-site repulsion determines the ground state of the system. Also, there is one important question, i.e., how the topological phases in the obtained phase diagrams are related with the topological charge pumping as bulk topological properties.

In this paper, we shall study the above problems in the strongly-interacting boson system by using the exact diagonalization \[22, 23\], and show explicitly relation between the equilibrium topological phases and the topological charge pumping in the adiabatic process by following \[24\]. From the relation, the global phase diagram plays a role of a guide for detecting various topological charge pumping in the experiments.

This paper is organized as follows. The target boson model in the 1D optical superlattice is explained in section 2. Section 3 studies the ground states of the system for the hard-core boson limit. We explain the single particle (SP) equation, which is related to the famous Harper equation in 2D electron lattice model in uniform magnetic fields, and we present the SP spectrum. We observe the ground states and their topological order by using the exact diagonalization. In section 4, we clarify the ground state properties of the soft-core boson system, where the on-site interaction plays an important role to determine the ground states and their topological properties. In particular, we shall show global phase diagrams of the Chern number. The phase diagrams include rich topological phases. In section 5, we discuss a relationship between the ground states obtained by the exact diagonalization and the dynamical topological charge pumping. We shall show that the Chern number of the many-body interacting ground-state is directly connected to the particle transfer performed in an adiabatic pumping cycle of superlattice. Section 6 is devoted for conclusion. Detailed calculations concerning to the Chern number and the topological charge pumping are given in appendices.

2. BHM on 1D superlattice

We consider a dilute Bose gas system in a superlattice, whose Hamiltonian is given as follows,

\[
H_{BH} = -\sum_i [e^{i\alpha \delta_i} a_i \dagger a_{i+1} + \text{h.c.}] + \frac{U}{2} \sum_i n_i (n_i - 1)
+ V_0 \sum_i \cos (2\pi \alpha i + \delta) n_i,
\]

where \( a_i (a_i \dagger) \) is the boson annihilation (creation) operator at superlattice sites \( i \), the density operator \( n_i = a_i \dagger a_i \), \( J \) is the hopping amplitude, \( U \) is the on-site repulsion. The superlattice is created in cold atom experiments by using two different standing-wave lasers as shown in figure 1. The parameter \( V_0 \) in \( H_{BH} \) (equation 1)) is related to the amplitude of the superlattice potential. The parameter \( \alpha \) is the superlattice period, which is a tunable parameter in experiments, and we call \( \alpha \) modulate parameter. On the other hand, \( \delta \) is the phase shift between the two standing-wave lasers. \( \theta \) is a twisted phase coming from the twisted boundary condition \[25, 26\] and \( L \) is the system size. In this paper, we consider the 1D system with the periodic boundary condition. From the view point of the topological state, adiabatic Floquet parameters of the present system are \( \theta \) and \( \delta \), i.e., the Hamiltonian \( H_{BH} \) (equation 1)) is invariant under the transformations of the adiabatic parameters such as \( \theta \rightarrow \theta + 2\pi \) and \( \delta \rightarrow \delta + 2\pi \), independently. From this fact, the adiabatic parameters span a 2D periodic parameter space, i.e., a torus \( T^2_0 \). In section 5, we shall study the topological charge pumping, which takes place by varying the parameter \( \delta \) as a function of time \( t \in [0, T] \) such as \( \delta(t) = 2\pi t/T \).

3. Phase diagrams of hard-core BHM

In this section, we shall consider the hard-core boson limit \( U \rightarrow \infty \), i.e., multiply occupied states are prohibited, and then we drop the on-site interaction term in \( H_{BH} \). In this limit, the system approaches to a non-interacting fermionic system. Under this condition, the SP spectrum of the model determines the ground state of the system. The previous studies \[6–8, 11\] showed that the SP spectrum of the present system is given by the solutions of the Harper equation, i.e., the Hofstadter butterfly \[27\], which describes the 2D lattice electron system in uniform magnetic fields. Interestingly, this correspondence can be understood by the consideration of

\[ \text{rigorously, the connection is achieved through the Jordan–Wigner transformation.} \]
the dimensional extension from spatial 1D system to spatial 2D system [28]. Actually, by substituting the SP wave function $|\Psi_n\rangle = \sum_i \psi_n, a_i^\dagger |0\rangle$ into $H_{BH}|\Psi\rangle = E|\Psi\rangle$ with the BHM Hamiltonian of equation (1), the SP equation is obtained as follows,

$$-iI(\psi_{i+1,n} + \psi_{i-1,n}) + V_0 \cos(2\pi a_i + \delta) \psi_{i,n} = E_n \psi_{i,n}. \tag{2}$$

Then, let us compare the above SP equation (2) with the Harper equation [27],

$$-t_x(\phi_{i+1,n} + \phi_{i-1,n}) - 2t_y \cos(2\pi f_i - k_y) \phi_{i,n} = E_n(k_y) \phi_{i,n},$$

where $t_{x(y)}$ is the hopping in the $x(y)$-direction and $f$ is the magnitude of the applied magnetic flux per plaquette. As shown in [28], the modulate parameter $\alpha$ and the phase shift $\delta$ in $H_{BH}$ correspond to $f$ and the $y$-component wave number $k_y$, respectively. Furthermore, there exists correspondence such as $t_x \leftrightarrow t_y = -2t_y \leftrightarrow V_0$. As a future work, it is interesting to study the above correspondence from a relativistic field-theoretical viewpoint [29].

From the SP equation of the BHM of equation (2), it is naturally expected that there exist a band insulator at specific filling factors (filling factor is an average particle number per site). As an example, figure 2(a) shows the energy spectrum $E_n$ obtained by solving equation (2) for the case of $\alpha = 1/3$, $\delta = 5\pi/3$ with various $V_0/J$. We observe that as increasing $V_0/J$, the SP spectrum splits into three bands, i.e., the spectrum has two band gaps, and each band has the $1/3$-filling. Then in the hard-core boson system with $\langle n \rangle = 1/3$, the first band is fully occupied, and a band insulating forms. Similarly for the system with $\langle n \rangle = 2/3$. (See later discussion and figures 2(c) and (d).) It is known that the band insulating ground state has non-trivial topological nature indicated by a non-vanishing integer Chern number [23].

For the present system, the Chern number is defined as follows on the 2D torus, $T^2_{\theta,\delta}$, of the adiabatic parameters ($\theta$, $\delta$),

$$C_N \equiv \frac{1}{2\pi} \int_{0}^{2\pi} \int_{0}^{2\pi} d\theta d\delta [\partial_\theta/\partial \theta + \delta (\partial_\theta/\partial \delta) - \partial_\delta/\partial \theta + \theta (\partial_\delta/\partial \theta)], \tag{3}$$

where $|\theta, \delta\rangle$ is the non-degenerate ground state depending on the adiabatic parameters $\theta$ and $\delta$.

In what follows, we focus on classifying the phase at vanishing temperature (i.e., the ground state) of the system. In the bosonic system described by the Hamiltonian $H_{BH}$ (equation (1)), three kinds of the ground states [6–8, 11] are expected to appear, i.e., superfluid (SF), trivial Mott insulator (MI), and TMI. In particular, the TMI is identified as the state with non-vanishing integer $C_N$ of equation (3) and without SF order. The TMI is regarded as an analogous state of the IQH states [2, 3].

We identify the TMI by using the exact diagonalization [22, 23, 30], which is an efficient method to study the bulk properties of the system. Figure 2 (b) exhibits our numerical results, i.e., the phase diagram in the $(\langle n \rangle - V_0/J)$-plane for the case of $J = 0.01$. For calculating the Chern number $C_N$, define by equation (3), we employed the methods proposed in [31] and used the discretized adiabatic parameter space with $N \times N$ mesh. (We took $N \geq 5$ as suggested in [6, 32].) As figure 2 (b) shows, the states at specific fillings have a non-vanishing Chern number while the others exhibit vanishing Chern number. The Chern number $C_N$ is quantized as $C_N = \pm 1$ at $\langle n \rangle = 1/3$ ($2/3$) in the finite-$V_0$ region. Here we note that even for fairly small values of $V_0/J$, a finite energy gap exists as seen from figure 2 (a), and this gap accompanies the non-vanishing $C_N$. For example, the TMI at $\langle n \rangle = 2/3$ with $C_N = -1$ forms for $V_0/J \geq 0.05$ at which the first-excited energy band.
appears. We also exhibit density snapshots for $V_{J10} = \alpha$ and $2/3$ in figures 2 (c) and (d). The ground states are non-degenerate and the (discrete) translational invariance is apparently broken there. This feature is different from that of the ordinary IQH state, in which the continuous translational invariance is preserved.

The results obtained in this work are in fairly good agreement with those of the previous studies using other numerical methods [6–8, 11].

4. Phase diagrams of soft-core BHM

In this section, we shall study the soft-core BHM on the superlattice. In the soft-core case, multiply occupied states are allowed at each site and therefore the on-site interaction plays an important role to determine the ground state of the system. In fact, it is expected that the competition between the on-site interaction, $U$, and the superlattice, $V_0$, leads to rich phase diagrams. That is, the TMIs with various Chern numbers form in the phase diagram in the $JUV_0$-plane. For the numerical methods, we employ the exact diagonalization as in the study on the hard-core case. In this section, we focus on the global phase diagrams for the cases $\alpha = 1/3$, $1/4$, and $1/5$.

To begin with, we obtained the phase diagrams in the $(J/U−V_0/U)$-plane with $\alpha = 1/3$. In figures 3(a)–(c), the phase diagrams of three cases are shown, where the particle filling is denoted by $\langle n \rangle$ as before.

Figure 3(a) for $\langle n \rangle = 1/3$ case shows that there are two phases, i.e., the SF, which is characterized by a finite value of the single particle density matrix (SPDM) [22], $\langle a_{j}^\dagger a_{j+L/3} \rangle > 0$ (\( \lfloor \cdot \rfloor \) is the floor function), and the TMI phase with $C_N = +1$. We determined the ground-state phase diagram as follows: if the ground state has a non-vanishing $C_N$, we regard the ground state as a TMI even though the SPDM has a finite value. That is, we regard the finite SPDM as a finite system-size effect in this case. (See later discussion.) On the other hand, if the ground state has a finite SPDM with $C_N = 0$, we regard the ground state as a SF state. Hereafter, we denote the TMI with the $C_N = \pm X \ (X = \text{positive integer})$ as TMI ($\pm X$).
As seen in figure 3(a), the SF phase forms for large $J/U$. The typical behaviors of the SPDM along the $V_0/U = 1$ line in figure 3(a) are shown in figure 4. The result exhibits the system size-dependence. On the other hand for the small $J/U$ regime, the system exists in the TMI ($+1$). Figure 5(a) shows the system size dependence of $C_N$ along the $V_0/U = 1$ line in figure 3(a). Interestingly, its system size dependence is much smaller than that of the SPDM. We also plot the ‘finite-size scaling’ of the critical point obtained by $C_N$ in figure 5(b). The result indicates that the critical point is almost independent of the system size. From the data, we can conclude that the Chern number $C_N$ is a good order parameter for identifying phase boundaries of the system. Similar numerical result concerning to the system size dependence of Chern number was reported in [13], though the target model is a spin model. In addition, we measured the energy gap $\Delta E$ between the ground state and the first excited state.

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4 In our exact diagonalization, the energy gap $\Delta E$ can be obtained from a tridiagonal matrix with the optimal size of the dimension from the Lanczos algorithm.
along the $V_0/U = 1$ line in figure 3(a). The result is shown in figure 6(a). There, gapless excitation in SF cannot be clearly seen due to the finite-size effect in the small system.

Next, we consider the $n = 2/3$ case for $\alpha = 1/3$. As shown in figure 3(b), we obtain the rich phase diagram. As far as we know, this phase diagram is one of new findings in this work. There are four phases, i.e., the SF phase exists for large $J/U$, and interestingly the TMIs with $C_N = 1$, $1$, $N = 1$ and $+2$ appear in the small $J/U$ regime. In particular, the TMI with $C_N = +2$ is an interesting phase, where the system permits the double occupancy at each site as shown in figure 7(a) since $V_0 > U$, and then the system essentially behaves as a two-species boson system. Each species of boson fully-occupies the lowest band in the SP spectrum in figure 2(a), therefore, $C_N = 1 + 1 = +2$. 

Figure 5. Behavior of the Chern number for $V_0/U = 1$, $\alpha = 1/3$ and $|n| = 1/3$ in figure 3. (a) System-size dependence of the Chern number $C_N$. (b) Finite-size scaling for transition point indicated by the Chern-number $C_N$. The location of the phase transition has a very small system-size dependence. The dotted line is for a guide for eyes.

Figure 6. (a) Energy gap $\Delta E$ for the TMI(+1)-SF phase transition on the $V_0/U = 1$ line. $\Delta E$ is getting small and the system approaches to gapless ground state, i.e., SF as $J/U$ increases. However, due to a finite-size effect, the gap does not close even in the SF. (b) $\Delta E$ for the $J/U = 0.01$ line in figure 3(b), $\alpha = 1/3$, $|n| = 2/3$. The value of $\Delta E$ tends to close on the critical points of the topological phase transition. (c) Plots of the Berry curvature for the points $V_0/U = 0.3$, 1.0 and 1.8 on the parameter space in (b). The mesh size $N = 10$. 

![Figure 5](image1.png)

![Figure 6](image2.png)
Figure 7. (a) Large $V_0/\ U$ case: the system permits double or higher occupancy. (b) Small $V_0/\ U$ case, bosons tend to exhibit the hard-core nature.

On the other hand for the case $V_0 < U$, since the on-site interaction is dominant, the multiple occupancy does not appear. Bosons behave like fermions as shown in figure 7(b). This situation leads to full-occupancy up to the second-lowest band of the SP spectrum. Thus, the TMI state exhibits $C_N = -1$. Similar discussion was given in [7]. Furthermore, we found that the TMI phase with $C_N = +1$ forms as an intermediate state between the two TMIs with $C_N = -1$ and $+2$. We consider that in this state with $C_N = +1$, the multiply-occupied sites appear in addition to the fully-occupied lowest band of the SP spectrum.

Here, we mention the possibility of the coexistence of the SF and TMI (non-vanishing $C_N$). In our simulation, the SPDM certainly exhibits a small but finite value in the TMIs near the SF regime. For example, as one of the possible regime of the coexistence, we indicate the area such as $0.1 \lesssim J/U \lesssim 0.5$ and $0.5 \lesssim V_0/\ U \lesssim 0.7$ in figure 3(b) by the dotted ellipse. There, a part of bosonic atoms form the TMI(+1) and the others may Bose condensate i.e., SF. However, due to the finite-size effect, the present calculation of the small system cannot reveal the precise behavior of the SPDM. This problem will be studied in more detail in the near future.

It is interesting to measure the energy gap $\Delta E$ along the lines in the parameter space, on which a phase transition between two different TMIs takes place. As a typical example, we plot the energy gap $\Delta E$ as a function of $V_0/\ U$ along the $J/U = 0.01$ line in the phase diagram in figure 3(b). The result is shown in figure 6(b). For calculation of $\Delta E$, we chose the minimums of $\Delta E$ in the adiabatic-parameter space $T_{3\alpha}$. We find that the gap $\Delta E$ apparently closes at two transition points between the TMI(−1) and TMI(+1) and between the TMI(+1) and TMI(+2). The result was independent of the size of the tridiagonal matrix of the Lanczos algorithm. Our numerical study obviously captures the level-crossing of the lowest and first-excited states. This level-crossing induces the change of the topological number of the ground state $C_N$.

For the $J/U = 0.01$ line in the phase diagram in figure 3(b), we show typical distributions of the Berry curvature, i.e., the integrand of equation (3). See figure 6(c). Its integral over $T_{3\alpha}$ gives the non-vanishing integer Chern number. From the data, the Berry curvature generated from the gauge field $i(\delta \partial_\mu)\theta (\mu = \theta, \delta)$ has no topological defect (quantized vortex), but it measures the density of the magnetic flux penetrating the surface of the 2D torus $T_{3\alpha}$. Then, non-vanishing Chern number indicates the existence of a hiding monopole that exists in the interior of the torus $T_{3\alpha}$. In other words, one can define a 3D gauge field induced by $i(\delta \partial_\mu)\theta (\mu = \theta, \delta)$ in the interior of the torus, which corresponds to the magnetic monopole.

Let us see how the phase diagram changes as the filling factor $\langle n \rangle$ increases further. Figure 3(c) shows the phase diagram for the filling $\langle n \rangle = 1$ and $\alpha = 1/3$. Here, we have a richer phase diagram than the lower filling cases in figures 3(a) and (b). In the phase diagram figure 3(c), the TMIs with the larger integer $C_N$ form for the large $V_0/\ U$ and small $J/U$ regime. In figure 3(c), the highest value of $C_N$ is +3. This value corresponds to the total particle number in the unit cell, i.e., three particle. In general, for $\alpha = 1/q$ and $\langle n \rangle = K/q$ where $K$ and $q$ are co-prime integers, the possible highest value of $C_N$ is expected to equal the total particle number $K$ in the unit cell.

5 A similar result is obtained in [31].
cannot be described by the SP equation of equation \((n) = 0\) and \(J/U = 0.01\). The results indicate the existence of two types of non-trivial TMI. We call the first one stable TMI (STMI) phase, in which \(C_N\) is robust for the change of the value of \(V_0/U\) as shown in figure 10(b). On the other hand, we call the second one random Chern number TMI (RTMI) phase, in which \(C_N\) takes various integer values as shown in figure 10(c). As seen from figure 10(b), the STMI phases when the filling-factor \((n)\) and the modulate parameter \(\alpha\) are tuned to produce the band-insulator regime, and the Chern number is determined as in the previous discussion based on the intuitive picture shown in figure 7. On the other hand, the RTMI forms when the parameters \((n)\) and \(\alpha\) are not located at the band insulator of the SP spectrum, and the interplay of the on-site repulsion and superlattice plays an essential role there. As far as we know, the phase diagram in figure 10(a) is one of new findings in this work.

To study detailed properties of the RTMI, we measured the energy gap \(\Delta E\) for the cases \((n) = 4/9, 5/9, 7/9\) and \(8/9\). The obtained results are shown in figure 10(d). It is obvious that the energy gaps are small for most of the

![Phase Diagrams](image)

**Figure 8.** Phase diagrams for soft-core case with \(\alpha = 1/4\). (a) \((n) = 1/2\) and \(L = 12\). (b) \((n) = 3/4\) and \(L = 8\). (c) \((n) = 1\) and \(L = 4\).
values of $V_0/U$. This indicates that the RTMI ground states are very close to the first-excited state. Then, the level-crossing frequently occurs as $V_0/U$ varies and states with various Chern number $C_N$ appear as the ground state.

5. Topological charge pumping and Chern number

In section 4, we clarified the ground-state phase diagram of $C_N$. Here we expect that each TMI with different $C_N$ exhibits different transport properties when one varies the cyclic pumping parameter $\delta$ adiabatically, e.g., as $\delta(t) = 2\pi t/T$ ($t \in [0, T]$), where $T$ is the period of one pumping cycle. Such a charge pumping phenomenon was studied both theoretically [1, 24, 33–35] and experimentally [16, 17, 36] for similar models to the present one. In this section, we shall show a connection between the Chern number $C_N$ (equation (3)) and the particle transfer.

To begin with, we introduce a current operator,

$$\hat{J} = \hbar^{-1} \partial_\theta H_{\text{BH}} = \frac{1}{\hbar L} \left[i e^{-i\theta/L} \sum_i a_i^\dagger a_{i+1} + \text{h.c.} \right].$$  \hspace{1cm} (4)

From the current operator $\hat{J}$, the current density $\delta I(t)$ at time $t$ can be directly calculated [24]. By using the genuine ground state denoted by $|\Psi(t)\rangle$, which satisfies the Schrödinger equation $i\hbar \partial_\theta |\Psi(t)\rangle = H_{\text{BH}} |\Psi(t)\rangle$ and an adiabatic instantaneous ground state denoted by $|\psi_0(t)\rangle$, the current density $\delta I(t)$ is expressed as

$$\delta I(t) = \langle \Psi(t) | \hat{J} | \psi_0(t) \rangle - \langle \psi_0(t) | \hat{J} | \psi_0(t) \rangle.$$  \hspace{1cm} (5)

Here, we assume that the many-body interacting system has a finite energy gap and introduce energy spectrum $E_n(t)$, where the corresponding eigenstate is the instantaneous normalized eigenfunctions $|\psi_n(t)\rangle$ satisfying $H_{\text{BH}} |\psi_n(t)\rangle = E_n(t) |\psi_n(t)\rangle$. For $n = 0$, the eigenfunction is nothing but the adiabatic instantaneous ground state. Then, the genuine ground state $|\Psi(t)\rangle$ is approximately expanded in terms of the states $|\psi_n(t)\rangle$ as [1]

$$|\Psi(t)\rangle = e^{-\frac{i}{\hbar} \int E_n(t) dt'} \left[ |\psi_0(t)\rangle + i\hbar \sum_{j=0}^{n-1} \frac{\langle \psi_j(t) | \partial_\theta | \psi_0(t) \rangle}{E_j(t) - E_0(t)} |\psi_j(t)\rangle \right].$$  \hspace{1cm} (6)

The derivation of equation (6) is given in appendix A. By substituting the expansion equation (6) into the current density $\delta I(t)$, equation (5), and by using the relation,
we obtain the following equation (the detailed calculation from equation (5) to (7) is given in appendix B),

$$\langle \psi_0(t) | \partial_t H_{\text{BH}} | \psi_j(t) \rangle = - [E_j(t) - E_0(t)] \langle \partial_t \psi_0(t) | \psi_j(t) \rangle,$$

we obtain the following equation (the detailed calculation from equation (5) to (7) is given in appendix B),

$$\delta I(t) \approx -i \langle \partial_t \psi_0(t) | \partial_t \psi_0(t) \rangle + i \langle \partial_t \psi_0(t) | \partial_t \psi_0(t) \rangle,$$

where we have assumed

$$\langle \langle \psi_0(t) | \partial_t | \psi_0(t) \rangle \rangle \ll E_j(t) - E_0(t).$$

We are interested in the current density $\delta I(t)$ averaged over $\theta \in [0, 2\pi]$ [26],

$$\langle \delta I(t) \rangle = \frac{1}{2\pi} \int_0^{2\pi} d\theta \ \delta I(t).$$

Then, we obtain the total particle transfer $\Delta Q$ for one pumping cycle $T$ as follows,

$$\Delta Q = \int_0^T dt \ \langle \delta I(t) \rangle = \frac{1}{2\pi} \int_0^T dt \int_0^{2\pi} d\theta \ \delta I(t).$$

By introducing the Berry connection $A_\mu$ ($\mu = 0, t$) by $i \langle \psi_0(t) | \partial_\mu | \psi_0(t) \rangle = A_\mu$, $\Delta Q$ is expressed as

$$\Delta Q \approx \frac{1}{2\pi} \int_0^{2\pi} d\theta \int_0^T dt \ [ \partial_t A_\theta - \partial_\theta A_t ],$$

Finally, by changing variables from $t$ to $\delta$, $\Delta Q$ is expressed as

$$\Delta Q \approx \frac{1}{2\pi} \int_0^{2\pi} d\theta \int_0^{2\pi} d\delta \ [ \partial_\delta A_\theta - \partial_\theta A_\delta ],$$

where $A_\delta \equiv i \langle \psi_0(t) | \partial_\delta | \psi_0(t) \rangle$. From the final expression of $\Delta Q$ in equation (11), the total particle transfer $\Delta Q$ obviously corresponds to the Chern number $C_N$ of equation (3), i.e.,
The above relation can be regarded as the interacting many-body version of the similar relation in the SP picture obtained by using a single Wannier state and the Bloch wave function \[ \psi(x) \], which is applicable for a non-interacting SP system.

Here, we note that the data shown in figure 6 directly show the time evolution of \( \delta(t) \) because \( \delta(t) = 2\pi t / T \). \( \delta(t) \) corresponds to the number of the transfer particle to a nearest-neighbor unit cell. The time evolution of \( \delta(t) \) originates from the form of the superlattice potential depending on the parameter \( \delta \). As one of typical example of the behavior of \( \delta(t) \), we focus on the TMI \((-1)\) state in the left panel in figure 6(c). We consider that the superlattice potential can be described as \( V_S(x) = -V_l \cos(2\pi x) + V_i \cos(2\pi ax + \delta) \) \[16, 17\], where the first term is the standard optical lattice potential with amplitude \( V_l \) and the second term is another lattice potential with amplitude \( V_i \) as shown in figure 1. We set a typical ratio \( V_i/V_l = 2 \) \[17\]. In figure 11, we show \( V_S(x) \) with \( \delta = 3\pi/5, \; 8\pi/5 \) and the corresponding particle density at \( \theta = 0 \) denoted by \( n_i(\theta = 0) \) in two nearest-neighbor unit cells. From the data, transfer property (hopping tendency) can be intuitively understood. In figure 11(a), the particle density of the two lattice sites between the nearest-neighbor unit cells is almost unity. Then, particle is hard to hop between the nearest-neighbor unit cells due to strong \( U \) and the particle current is suppressed. The result directly appears as the small value of the Berry curvature at \( \delta \sim 3\pi/5 \) in the left panel in figure 6(c). On the other hand in figure 11(b), the particle density of the two lattice sites between the nearest-neighbor unit cells are much less than unity and particle is easy to hop between the nearest-neighbor unit cells. The condition leads to significant particle current. The tendency clearly appears in figure 6(c). The value of the Berry curvature near \( \delta \sim 8\pi/5 \) is negatively large, i.e., the current to a left nearest-neighbor unit cell is large. The total amount of the negative current corresponds to the Chern number \( \mathcal{C}_N = -1 \).

In fact, the current density is determined by the wave functions of the genuine and instantaneous ground states, but we think that the above observation sheds light on the intuitive understanding of the relation between the charge pumping and the Berry connection for the interacting Bose particle cases. Here, we should mention the study on the system with edges in \[24\]. There, focusing on the bulk edge-correspondence in topological charge pumping, (for related experiments on cold atoms, see \[38, 39\]) it was shown that the Berry connection in the temporal gauge is directly related to the shift of the center of mass of the system, and the charge pumping is derived by that Berry connection. For the present system without edges, we think that there exists a direct relation between the Berry connection and the charge pumping. This problem is under study, and we hope that the results will be published in the near future.

Equation (12) shows that TMIs exhibit various amounts of the charge transfer in the topological charge pumping depending on the value of the Chern number \( \mathcal{C}_N \). Therefore, the obtained phase diagrams of \( \mathcal{C}_N \) in section 4 can be a guide for detecting new properties of topological charge pumping in the strongly-correlated bosonic systems in experiments on ultracold atoms.

6. Conclusion

In this paper we studied the strongly-interacting boson systems in superlattice potential, which are feasible in 1D optical superlattice system of ultracold atoms. The SP properties of the system are described by the Harper equation, and the system exhibits the band insulator in the hard-core boson limit. The band insulator has a non-trivial Chern number, and it was calculated by obtaining many-body wave functions with varying two adiabatic parameters in \( T^2_{\text{opt}} \). For the hard-core boson case with using the exact diagonalization, we first verified the locations of the band insulator corresponding to the TMI state, which is characterized by a non-vanishing Chern.
number. Then, we studied the soft-core boson case. There, the competition (interplay) between the superlattice amplitude $V_0$ and on-site interaction $U$ plays an important role. As a result, we observed the various TMIs with different integer Chern numbers. For the modulate parameter $\alpha = 1/3$, $1/4$ and $1/5$, we clarified the global phase diagrams of the Chern number by using the exact diagonalization. The numerical results obtained for different system sizes show that the behaviors of the Chern number are almost independent of the system size. Therefore, the obtained phase diagrams in the present study captures the essential properties of the system. Interestingly, these obtained phase diagrams exhibit a very rich phase structure including various TMIs with large Chern numbers. From the obtained results, we see that the TMI with a high Chern number tends to form when the superlattice amplitude $V_0$ is getting large. We conclude that this behavior originates from the higher occupancy of bosons per lattice site. Furthermore, we clarified particle-filling dependence of the ground state for $\alpha = 1/3$ by studying the $(\langle n \rangle - V_0 / U)$-phase diagram. We found that there are two types of non-trivial TMI, i.e., the RTMI and the STMI. The results concerning to the STMI are in fairly good agreement with the DMRG result for a similar model in [7], while the existence of the RTMI with the interesting behavior of the Chern number is one of new findings of the present work. We also found that level-crossing frequently occurs in the parameter region of the RTMI.

In section 5, we studied the relationship between the particle transfer and the Chern number of many-body wave functions. We conclude that in order to detect the various TMIs in real experiments, the charge pumping measurement by adiabatic time-evolution of the parameter $\delta$ [16, 17] is useful. To measure the TMIs in real experiments, the Streda formula [40] is expected to be useful as pointed out in [6].

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Appendix A. Derivation of equation (6)

We give the detailed derivation of equation (6) [37]. In adiabatic time evolution, the genuine ground ground state $|\Psi(t)\rangle$ can be expanded by using the instantaneous bases $|\psi_j(t)\rangle$, which satisfy $H_{BH}(t)|\psi_j(t)\rangle = E_j(t)|\psi_j(t)\rangle$, i.e.,

$$|\Psi(t)\rangle = c_0(t)e^{-\frac{i}{\hbar}\int_{t_0}^{t} E_0(t')dt'}|\psi_0(t)\rangle + \sum_{j \neq 0} c_j(t)e^{-\frac{i}{\hbar}\int_{t_0}^{t} E_j(t')dt'}|\psi_j(t)\rangle,$$

where $c_0(t)$ and $c_j(t)$ are time-dependent expansion coefficients. Since the genuine ground state $|\Psi(t)\rangle$ satisfies the Shrödinger equation $H_{BH}(t)|\Psi(t)\rangle = i\hbar \partial_t |\Psi(t)\rangle$ and adiabatic setup allows us to approximate $c_0(t) \approx 1$, $\partial_t c_0(t) \approx 0$ and $|c_j(t)| \ll 1$ ($j \neq 0$) along time evolution, we can show that the $j$th coefficient $c_j(t)$ satisfies the following time differential equation,

$$\partial_t c_j(t) \approx -e^{\frac{i}{\hbar}\int_{t_0}^{t} (E_j(t') - E_0(t'))dt'} \langle \psi_j(t)|\partial_t|\psi_0(t)\rangle.$$

Then, the adiabatic solution to equation (A.2) in $O([\langle \psi_j(t)|\partial_t|\psi_0(t)\rangle]/[E_j(t) - E_0(t)])$ is obtained as [37],

$$c_j(t) \approx i\hbar e^{\frac{i}{\hbar}\int_{t_0}^{t} (E_j(t') - E_0(t'))dt'} \langle \psi_j(t)|\partial_t|\psi_0(t)\rangle / E_j(t) - E_0(t).$$

By substituting the coefficients in equation (A.3) into (A.1) we obtain the adiabatic expansion equation (6) in section 5.

Appendix B. Derivation of equation (7)

We give the detailed calculation from equations (5) to (7). By substituting equation (6) into (5), the current $\delta I$ is expressed as,
where the term $\langle \psi_0(t) | \hat{H}_{\text{eff}} | \psi_0(t) \rangle$ was canceled. Here we drop the last term in equation (B.1) since we assume the energy gap between the ground state and the excited states, $E_f(t) - E_0(t)$, is large enough. Then we notice the following equations,

$$
\langle \psi_0(t) | \hat{H}_{\text{eff}} | \psi_0(t) \rangle = -[E_f(t) - E_0(t)] \langle \partial_t \psi_0(t) | \psi_0(t) \rangle,
$$

$$
\langle \psi_f(t) | \hat{H}_{\text{eff}} | \psi_0(t) \rangle = [E_f(t) - E_0(t)] \langle \psi_f(t) | \partial_t \psi_0(t) \rangle.
$$

The above equations are obtained from $\partial_t \langle \psi_0(t) | \psi_0(t) \rangle = 0$ and $\partial_0 \langle \psi_f(t) | \psi_0(t) \rangle = 0$. Then substituting the above equations in equation (B.1) and using the complete relation of the state bases $\sum \langle \psi_j(t) | \psi_j(t) \rangle = 1$, the current $\delta I(t)$ is expressed as

$$
\delta I(t) \approx -i \langle \partial_0 \psi_0(t) | \partial_0 \psi(t) \rangle + i \langle \partial_0 \psi_0(t) | \partial_0 \psi(t) \rangle. \tag{B.2}
$$

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