Topological Mott Insulator with Bosonic Edge Modes in 1D Fermionic Superlattices

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We investigate topological phase transitions driven by interaction and identify a novel topological Mott insulator state in one-dimensional fermionic optical superlattices through numerical density matrix renormalization group (DMRG) method. Remarkably, the low-energy edge excitations change from spin-1/2 fermionic single-particle modes to spin-1 bosonic collective modes across the phase transition. Due to spin-charge separation, the low-energy theory is governed by an effective spin superexchange model, whereas the charge degree of freedom is fully gapped out. Such topological Mott state can be characterized by a spin Chern number and gapless magnon modes protected by a finite spin gap. The proposed experimental setup is simple and may pave the way for the experimental observation of exotic topological Mott states.

Introduction.—The interplay between single-particle band topology and many-body interaction plays a crucial role in many important strongly-correlated phenomena in condensed matter physics. Unlike single-particle topological states [1, 2], interactions can induce remarkable physical phenomena such as fractionalization of emergent collective excitations and give rise to intriguing correlated states that exhibit non-trivial topological properties. Prominent examples are fractional quantum Hall effects [3, 4] where constituent particles are electrons but emergent quasiparticles only carry fractions of electron charge, and topological Mott insulator [5] with deconfined spinon excitations.

One-dimensional (1D) interacting systems, which are amenable to exact methods, provide fundamental insights for understanding strongly-correlated states. Due to the confined geometry, the low-energy excitations are collective and exhibit a peculiar fractionalization, spin-charge separation (SCS). A single-particle excitation is divided into two collective modes, which possess charge and spin degrees of freedom, respectively. In a topological Mott insulator, low-energy excitations lie in the spin sector, whereas charge excitations are frozen by strong interactions. The topological properties manifest themselves by the appearance of gapless modes at the boundary protected by the insulating bulk. In previous studies, these edge modes are composed of spinons [6, 7] carrying spin-1/2 and no charge. As spinful modes can also carry integer spin (like magnon, spin-1), two natural and important questions need to be addressed: i) Are there topological Mott insulator states hosting other types of spinful edge modes and how to characterize them? ii) Since SCS severely changes the low-energy excitations, what is the bulk-edge correspondence in a topological Mott insulator state?

In this paper, we address these two important questions by studying the Mott insulator states in a 1D fermionic optical superlattice. Ultracold atoms in optical lattices have provided unprecedented controllability to simulate strongly interacting systems. In particular, 1D optical superlattices open a new and simple avenue towards realizing exotic topological states [8–14] because of their exact correspondence with quantum Hall physics [15, 16] in an extended space. Here we scrutinize Mott transitions in 1D optical superlattices and identify a novel topological Mott insulator using the quasi-exact numerical density matrix renormalization group (DMRG). Such Mott phase transition from a band topological insulator to a topological Mott insulator is accompanied by bulk excitation gap closing, SCS, and the change of topological spin Chern number. The corresponding low-energy excitations change from single-particle spin-1/2 fermionic modes to collective spin-1 bosonic modes, in consistent with the spin Chern number change across the transition (i.e., bulk-edge correspondence). The low-energy physics is governed by an antiferromagnetic spin superexchange model due to SCS. Our proposed experimental setup involves fermions in a 1D triple-well superlattice and is simple to realize in experiments comparing to other complex lattice models or materials [5–7].

Single-particle physics.—We consider 1D Fermi gases with two internal states (labeled by $\sigma = \uparrow, \downarrow$) tightly confined in transverse directions [Fig. 1(a)]. Two counterpropagating laser beams (wavelength $\lambda$) form a main optical lattice $V_0(x) = V_0 \cos^2(k_0 x)$ with $k_0 = 2\pi/\lambda$. Two additional laser beams (wavelength $\lambda'$) incident at a tilt angle $\theta_0$ form a secondary weak lattice $V_2(x) = V_2 \cos^2(k_2 x + \varphi)$ with $k_2 = 2\pi \cos \theta_0 / \lambda'$ and relative phase $\varphi$ with respect to the main lattice. As illustrated in Fig. 1(b), the total potential $V(x) = V_0(x) + V_2(x)$ forms a superlattice, with its period determined by the ratio $q = k_0 / k_2 = \lambda' / \lambda \cos \theta_0$. Such optical superlattices have been experimentally realized by many groups [17–19].

When the potential depth $V_0$ is much larger than the recoil energy $E_r = h^2 k_0^2 / 2M$ ($M$ is the atomic mass), only the lowest Bloch band need be considered and the system can be well approximated [20–23] by the following
on the wave function, $F(\theta, \varphi) = \text{Im}(\langle \frac{\partial \Psi}{\partial \theta} | \frac{\partial \Psi}{\partial \varphi} \rangle - \langle \frac{\partial \Psi}{\partial \varphi} | \frac{\partial \Psi}{\partial \theta} \rangle)$ is the Berry curvature. $C = 1$ and $-1$ when the chemical potential lies in the first and second band gaps, respectively. According to bulk-edge correspondence, the Chern number is equal to the number of chiral edge states by adiabatically evolving $\varphi$, as long as the bulk gap remains finite in the whole process [24, 28–30].

**Topological Mott transition and SCS.**—Now we consider an interacting many-body system ($N_{\uparrow}, N_{\downarrow}$), composed of $N_{\uparrow}$ spin-up and $N_{\downarrow}$ spin-down atoms. Both total density $\rho = \sum_{j}(n_{j\uparrow} + n_{j\downarrow})/L$ and magnetization $m = \sum_{j}(n_{j\uparrow} - n_{j\downarrow})/L$ are conserved quantities. We denote the $n$-th lowest eigenenergy and corresponding wave function as $E_{n}(N_{\uparrow}, N_{\downarrow})$ and $\Psi_{n}(N_{\uparrow}, N_{\downarrow})$, respectively. $n = 0$ then refers to the many-body ground state. In the subsequent DMRG calculations, density-matrix eigenstates are kept dynamically to ensure the discarded weight less than $10^{-9}$. The maximum truncation error of the ground state energy is about $10^{-7}$ and in general $10 - 15$ sweeps are enough to reach the required precision.

We utilize three different bulk excitation gaps to characterize the low-energy modes: charge gap $\Delta_{c} = [E_{0}(N_{\uparrow} + 1, N_{\downarrow} + 1) + E_{0}(N_{\uparrow} - 1, N_{\downarrow} - 1) - 2E_{0}(N_{\uparrow}, N_{\downarrow})]/2$ with a fixed magnetization $m$, spin gap $\Delta_{s} = [E_{0}(N_{\uparrow} + 1, N_{\downarrow} - 1) + E_{0}(N_{\uparrow} - 1, N_{\downarrow} + 1) - 2E_{0}(N_{\uparrow}, N_{\downarrow})]/2$ with a fixed density $\rho$, and neutral gap $\Delta_{ne} = E_{1}(N_{\uparrow}, N_{\downarrow}) - E_{0}(N_{\uparrow}, N_{\downarrow})$. The neutral gap directly gives the lowest excitation energy of the many-body system ($N_{\uparrow}, N_{\downarrow}$).

We concentrate on the half-filling case with $\rho = 1$, $m = -1/3$. In the non-interacting limit, two-component fermionic atoms populate single-particle levels from low to high independently as sketched in Fig. 2(a). The spin-up atoms are filled up to the first band gap (denoted as $\delta_{1}$) and spin-down atoms to the second band gap (denoted as $\delta_{2}$). Because two band gaps are characterized by opposite Chern numbers $C = \pm 1$, the system is in a quantum spin Hall-like state with a spin Chern numbers $C_{s} = 2$ [31, 32] that is defined by Eq. (2) through choosing $\theta_{1} = -\theta_{1}$ for the twisted boundary condition. Here a single-particle excitation should overcome the band gaps and carry both charge and spin degree of freedom. The spin and charge gaps are equal, determined by: $\Delta_{c} = \Delta_{s} = (\delta_{1} + \delta_{2})/2$ because spin and charge modes are tightly bound together. $\Delta_{ne} = \min\{\delta_{1}, \delta_{2}\}$ in this case.

With increasing interaction, the spin and charge modes would exhibit totally different behaviors. Fig. 2(b) plots the three gaps with respect to $U$. Due to the repulsion between different components, the atoms prefer occupying higher levels. Starting from the same value, both $\Delta_{c}$ and $\Delta_{s}$ decrease first. $\Delta_{c}$ arrives its minimum at $U_{c} \approx 2.9$, where $\Delta_{ne}$ closes. $\Delta_{c}$ and $\Delta_{s}$ coincide with each other at $U < U_{c}$, revealing that spin and charge modes are coupled together. After the critical point, an obvious separation between spin and charge excitations happens. $\Delta_{c}$ grows rapidly (linearly) by further increasing $U$, whereas
Δs is suppressed (with 1/U). Note that none of the three excitation gaps can close for any U > Uc, and the system enters into a Mott insulator phase, with every lattice sites being populated at U → ∞. Since the low-energy excitation now possesses only spin degree of freedom, Δne coincides with Δs in this regime, as clearly demonstrated by our numerical results. To rule out the size effect, we do a finite-size scaling of different gaps after Mott transition. As shown in the inset of Fig. 2(b), Δs and Δne (Δne) both tend to finite values in thermodynamic limit, which is crucial for the protection of non-trivial topological properties.

The Mott transition at U = Uc is of first-order, with gap closing between ground and first excited states. Lattice translation symmetry forces E_n(φ) = E_n(φ + π/3) at ρ = 1, therefore there are six gap closing points φ_p = pπ/3 (0 ≤ p ≤ 5 is an integer) in the whole evolution period of φ ∈ [0, 2π]. Across the Mott transition, the spin Chern number changes six from C_s = 2 to C_s = −4, in consistent with simultaneous gap closing at six φ_p.

The Mott transition is accompanied with SCS. After the transition, the Hamiltonian can be represented by two distinct sectors H = H_c + H_s. While the charge sector H_c is fully gapped out due to the strong interaction, the low-energy physics is governed by an effective spin sector H_s. A second-order perturbation theory at large U leads to an antiferromagnetic spin superexchange Hamiltonian [33]

\[ H_s = \sum_j J \left[1 + \frac{(\mu_{j+1} - \mu_j)^2}{U^2}\right] S_j \cdot S_{j+1} \]  

with periodically modulated exchange couplings. Here S_j = c_j^T \sigma c_j/2 is the local spin operator at j-th site. J = 4t^2/U is the key energy scale of Mott physics. Δne (Δs) decreases by 1/U to the leading order. From the standard bosonization theory [34], m = −1/3 is a quantized magnetization plateau that is topologically protected [13]. All non-trivial properties can be understood from the above low-energy theory [33].

**Bulk-edge correspondence.**—The appearance of edge states is usually considered as a hallmark of topological properties. As SCS has severely changed the nature of low-energy excitations, bulk-edge correspondence of a topological Mott state is different. To this end, we study the low-energy spectrum under OBC and demonstrate the consequence of SCS. The charge distribution of a neutral excitation is n^ne = n_j[Ψ(N↑, N↓)] − n_j[Ψ(N↑, N↓)]. Here [Ψ] represents for taking expectation value on state Ψ and n_j = n_j↑ + n_j↓. Similarly, the spin distribution of a neutral excitation is S^ne = S^y_j[Ψ(N↑, N↓)] − S^y_j[Ψ(N↑, N↓)] with S^y_j = (n_j↑ − n_j↓)/2. For each end, the accumulated charge (spin) is n^ne(S^ne) = \sum_{j \leq \ell/2} n^ne(S^ne), and n^ne(S^ne) = \sum_{j > \ell/2} n^ne(S^ne), respectively.

Our results are summarized in Fig. 3. Before SCS, there exist gapless modes inside the neutral gap under OBC by advancing φ. While prohibited under PBC [Fig. 3(a)], the ground state and first excited state cross at φ = −π/3, 2π/3 under OBC as shown in Fig. 3(c), indicating these modes are localized end modes. The crossings are reminiscent of the level crossings of single-particle levels in Fig. 1(c). Fig. 3(e) plots the spatial distributions of spin and charge for one of the in-gap neutral excitations. It is clear that the excitation carries both spin and charge at two ends. Our numeric shows n^ne = 1, S^ne = −1/2 for the left end and vice versa for the right end, which is in agreement with the bulk spin Chern number C_s = 2 and validates the single-particle nature of these low-energy modes.
FIG. 4: (a) Magnon spectrum \( \Delta E_c(24, 48) \) and \( \Delta E_s(25, 47) \) at filling \( \rho = 1 \). The blue and magenta points are for PBC and OBC, respectively. (b) Charge spectrum \( \Delta E_c(24, 48) \) and \( \Delta E_s(23, 47) \) for magnetization \( m = -1/3 \). (c) Spatial distributions \( \Delta S_j \) for two in-gap magnon modes [labeled by “cross” in (a)]. (d) Spatial distributions \( \Delta n_j \) for the charge excitation at \( \varphi = 0 \). \( \mu = 1.2, U = 3.5 \). The double-headed arrows denote the spin and charge gaps.

After SCS, the low-energy spectrum is fully gapped under PBC [Fig. 3(b)] and gapless end modes still emerge as shown in Fig. 3(d). Note that the appearance of these modes is at different \( \varphi \)'s (\( \varphi = -5\pi/6, \pi/6 \)), which can be understood from the adiabatic continuity [33] of the effective spin Hamiltonian (3). \( n_{t, r}^c = 0 \), and \( S_{t, r}^c = \pm 1 \) for left and right ends (Fig. 3(f)). These two pairs of spin-1 edge modes are in consistent with bulk \( \mathcal{C}_s = -4 \).

Topological magnon excitation.—The spin-1 low-energy excitations after SCS indicates the existence of pure collective magnon edge excitations in the spin sector. Starting from the many-body ground state \( \Psi_0(N_{l, r}, N_j) \), the magnon spectrum is defined as \( \Delta E_c(N_l, N_j) = E_0(N_l - 1, N_j + 1) - E_0(N_l, N_j) \) by fixing the total density of the system, with spatial spin distribution \( \Delta S_j = S_j^c[\Psi_0(N_l - 1, N_j + 1)] - S_j^c[\Psi_0(N_l, N_j)] \) and no charge. Similarly, we define charge spectrum with fixed magnetization as \( \Delta E_s(N_l, N_j) = E_0(N_l + 1, N_j + 1) - E_0(N_l, N_j) \) and associated spatial distribution as \( \Delta n_j = n_j[\Psi_0(N_l + 1, N_j + 1)] - n_j[\Psi_0(N_l, N_j)] \).

In Fig. 4(a)(b), we show these two spectra after Mott transition, respectively. A magnon gap (\( \sim 2\Delta_s \)) separates the magnon bands under PBC, whereas in-gap modes under OBC cross at \( \varphi = -5\pi/6 \) and \( \pi/6 \) [Fig. 4(iii)], same as the neutral excitations in Fig. 3(d). The distributions of magnon excitations in two typical phases \( \varphi = -14\pi/15 \), \( \varphi = -11\pi/15 \) are shown in Fig. 4(c), which are well localized end modes. Once touching the bulk band, they merge into the bulk and reappear on the other end. The non-trivial magnon excitations are closely related to the quantized magnetization plateau [13] of our effective model (3). For the charge spectrum in Fig. 4(b), a charge gap (\( \sim 2\Delta_c \)) always exists regardless of boundary conditions. For any \( \varphi \), the charge excitations distribute on the whole lattice [Fig. 4(d)], revealing the triviality in the charge sector.

Discussion and summary.—Our mechanism of inducing topological Mott insulator states based on SCS is quite general. The topological Mott physics here can be extended to i) other period-\( q \) (including incommensurate case, i.e., the famous Aubry-André model [35]); ii) other fillings or magnetizations; iii) off-diagonal counterparts of model (1), i.e., triple-well lattices with period modulations on tunneling \( t \), instead of on-site energy \( \mu_j \). The emergence of topological Mott insulator states with various spin Chern numbers and spinful edge modes is expected from our low-energy theory.

The proposed topological Mott insulator state and associated low-energy excitations can be experimentally probed in ultracold atomic gases. In addition to the proposed scheme using two sets of optical lattices, the 1D fermionic superlattice can also be generated using the recently developed digital micromirror device [36, 37]. For fermionic \(^6\text{Li} \) atoms [38, 39], the wavelength of the laser beam is chosen as \( \lambda = 1064 \) nm, with the recoil energy \( E_r \approx 2\pi\hbar \times 29.4 \) kHz. At \( V_0/E_r = 5 \), \( \Delta \approx 2\pi\hbar \times 1.9 \) kHz. The neutral and spin gaps of the topological Mott insulator state is then \( \Delta_{ne} \approx 0.2t = 2\pi\hbar \times 390 \) Hz, which is large enough (compared to temperature) to protect the topological properties [39]. These excitation gaps may be measured using radio-frequency spectroscopy [40–42]. The edge magnon excitations in the spin sector can be generated using a two-photon Raman process and their spin distributions at each site can be measured by detecting atomic spin distributions of different many-body ground states using spin-resolved quantum gas microscope [43–48] in optical lattices.

In summary, we have studied topological Mott transitions accompanied by SCS in a simple 1D optical superlattices, with low-energy excitations changing from single-particle spin-1/2 modes to bosonic spin-1 collective modes at the boundary. A novel topological Mott insulator state, characterized by spin Chern number and gapless magnon excitations is identified. Our work may pave the way for the experimental observation of topological Mott insulator states in ultracold atomic gases.

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We give a simple derivation of the effective spin superexchange model (3) in the main text using the second-order perturbation theory. To this end, we split the Hamiltonian (1) into two parts $H = U n_{j\uparrow} n_{j\downarrow} + H_{\text{pert}}$, with $H_{\text{pert}} = \sum_{j,\sigma} [-t(c_{j\sigma}^c c_{j+1\sigma} + \text{h.c.}) + \mu_j n_{j\sigma}]$ as the perturbation term. For the half-filling case $\rho = 1$ and $U \gg t$, the local Hilbert space on sites $j$ and $j+1$ is spanned by the following four basis: $| \uparrow_j, \uparrow_{j+1} \rangle$, $| \uparrow_j, \downarrow_{j+1} \rangle$, $| \downarrow_j, \uparrow_{j+1} \rangle$, $| \downarrow_j, \downarrow_{j+1} \rangle$. The effective Hamiltonian can be represented in this basis as $H_s = \sum_j H_{j,j+1}$, with

$$H_{j,j+1} = \begin{pmatrix}
0 & -t U^2 + t^2 U - t U^2 & 0 & 0 \\
0 & -t U^2 + t^2 U - t U^2 & 0 & 0 \\
0 & 0 & -t U^2 + t^2 U - t U^2 & 0 \\
0 & 0 & 0 & -t U^2 + t^2 U - t U^2
\end{pmatrix}.
$$

Using spin-1/2 operator $S = (S_x, S_y, S_z)$, the above Hamiltonian can be further represented as

$$H_s = \sum_j \frac{4t^2 U}{U^2 - (\mu_{j+1} - \mu_j)^2} [S_j \cdot S_{j+1} - 1/4].
$$

By setting $J = \frac{4t^2 U}{U^2}$ and Taylor expanding the exchange coefficient by $1/U$ to the second term, we can get the effective spin superexchange model (3) after neglecting the constant term.

### Adiabatic continuity and topological properties

Now we demonstrate the topological properties of the spin superexchange model, which dictates the low-energy physics of the system. To be more intuitive and clear, we introduce an anisotropy parameter $g$ in $S_j^z S_{j+1}^z$ term:

$$H_s(g) = \sum_j \left[ J \left( \frac{\mu_{j+1} - \mu_j}{U^2} \right)^2 \right] \left( S_j^+ S_{j+1}^+ + S_j^- S_{j+1}^- + g S_j^z S_{j+1}^z \right).
$$

When $g = 1$, the above model recovers our low-energy Hamiltonian (3). $g = 0$ corresponds to an exactly solvable spin-XX chain by Jordan-Wigner transformation. We first show the non-trivial topology of $g = 0$ case and then demonstrate the adiabatic continuity in the whole region $g \geq 0$.

For $g = 0$, the Jordan-Wigner transformation (denote $S_k^\pm = S_k^x \pm i S_k^y$)

$$d_j^\uparrow = e^{i\pi \sum_{k=1}^{j-1} S_k^z} S_j^+ \cdot S_j^z, \quad d_j^\downarrow = e^{-i\pi \sum_{k=1}^{j-1} S_k^z} S_j^- \cdot S_j^z,$$

takes the model (6) to a spinless fermion model: $H_{J-W} = \sum_j J \left[ 1 + \frac{\mu_{j+1} - \mu_j}{U^2} \right] (d_j^\uparrow d_{j+1}^\downarrow + d_j^\downarrow d_{j+1}^\uparrow)$. The band structure is shown in Fig. 5(a). Due to the periodically modulated hopping of Jordan-Wigner fermions, the single-particle spectrum $\epsilon_{n}^{J-W}$ consists of three topological bands and gapless end modes inside the band gap with the evolution of phase $\varphi$ under OBC. Notice that different from the original single-particle band in Fig. 1, these end modes now cross at $\varphi = -5\pi/6$ and $\varphi = \pi/6$ (in consistent with the DMRG results in Fig. 3(b) and Fig. 4(a) in the main text) and represent for low-energy collective spinful modes.

To demonstrate the adiabatic continuity in the whole region $g \geq 0$, we plot the excitation gap (energy difference between the ground state and first excited state) of model (6) with respect to $g$ in Fig. 5(b). With increasing $g$ from Jordan-Wigner limit $g = 0$, the excitation gap increases. From the scaling behavior of the gap [Inset of Fig. 5(b)], we can see it tends to a finite value in thermodynamical limit at $g = 1$. The above adiabatic continuity reveals that our effective spin superexchange model $H_s$ has the same topological properties with that of Jordan-Wigner fermions.
FIG. 5: (a) Single-particle band of Jordan-Wigner fermions, $g = 0$. (b) Excitation gap with respect to $g$. The inset shows the finite size scaling at $g = 1$, $\phi = 0$. (c) The lowest two eigenenergies of model (6) under OBC (magenta circle) and PBC (blue square) with the evolution of $\phi$. $\mu^2/U^2 = 0.2$ for all figures.

Furthermore, we show the low-energy spectrum of the spin superexchange model (3) in Fig. 5(c). Although there always exist an excitation gap at any $\phi$ under PBC, the ground state and first excited state touch at $\phi = -5\pi/6$ and $\phi = \pi/6$ under OBC (in consistent with the DMRG results in Fig. 3(b) and Fig. 4(a) in the main text). As these crossings depend on boundary condition, the excitations around the touching points are well localized end modes [not shown]. For example, at $\phi = -9\pi/10$, our numeric gives accumulated spin distribution $\Delta S_z = 0.996$ on the left end and $\Delta S_z = -0.996$ on the right end. The integer spinful end modes are in consistent with those neutral excitations in the main text.