Topological transitions of interacting bosons in one-dimensional bi-chromatic optical lattices

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Ultra-cold atoms in 1D bi-chromatic lattices constitute a surprisingly simple system for the study of topological insulators. We show that topological phase transitions constitute a general feature of bosons in 1D bi-chromatic lattices, and that these transitions may occur both as a function of the superlattice strength and due to inter-site interactions. We discuss in addition the topological character of incommensurate density wave phases in quasi-periodic lattices.

**Introduction.** Topological insulators are many-body systems which are bulk-gapped, but present topologically protected gapless edge excitations\textsuperscript{1,2}. Prominent examples of topological insulators are provided by the integer quantum Hall effect (IQHE) of 2D electrons in a magnetic field\textsuperscript{3} and the quantum spin Hall effect in materials with strong spin-orbit coupling\textsuperscript{5}. Topological insulators have attracted a large deal of attention, not only because of their fundamental interest, but also for the possible applications of edge states for topological quantum computing and spintronics\textsuperscript{6,7}. Topological insulators of non-interacting fermions may be classified according to their symmetry properties\textsuperscript{8,9}.

Symmetry-protected topological (SPT) phases\textsuperscript{10} constitute a generalization of the idea of topological insulator to interacting bosons or fermions. SPT phases are bulk-gapped and possess robust edge modes as long as the relevant symmetry is not broken. These phases have been recently classified using group cohomology theory\textsuperscript{10}. Interacting topological insulators have attracted a large deal of attention\textsuperscript{11-13}. Special interest has been devoted in interacting systems to topological phase transitions, i.e. quantum phase transitions between phases of different topology\textsuperscript{14-19}.

Atoms in optical lattices (OLs) constitute an extraordinarily controllable environment for the investigation of many-body physics\textsuperscript{20,21}. In particular, the precise engineering of the lattice geometry and the inter-particle interactions, as well as the feasibility of inducing artificial magnetic fields for neutral atoms\textsuperscript{22}, have opened exciting perspectives for the realization of topological insulators with cold gases in OLs\textsuperscript{23-31}.

Interestingly, a recent experiment in photonic quasicrystals\textsuperscript{32} has shown that 1D quasicrystals may be assigned 2D Chern numbers, and present topologically protected edge states. Quasi-periodic 1D potentials may be also realized using incommensurate bi-chromatic OLs, a system recently investigated in the context of Anderson localization\textsuperscript{33}. Atoms in quasi-periodic OLs constitute hence a surprising simple scenario for topological insulators\textsuperscript{34-36}. Recently it has been shown that topological Mott-insulators may be realized at particular fractional fillings in Bose gases loaded in 1D commensurate bi-chromatic OLs\textsuperscript{37}.

In this Letter, we show that topological phase transitions constitute a general feature of bosons in 1D bi-chromatic OLs. These transitions result from the interplay between lattice geometry, interactions, and the bosonic nature of the particles. We show that topological transitions may occur both as a function of the strength of the secondary lattice, and as a function of inter-site interactions. We discuss in addition the topological character of the so-called incommensurate density wave phases in quasi-periodic bi-chromatic OLs.

**Model.** We consider a Bose gas loaded in the lowest band of a 1D OL of lattice spacing $\lambda$ with a superimposed lattice of spacing $\lambda/\beta$. The system is described by the Hamiltonian

$$H = -t \sum_{i} (b_{i}^{\dagger} b_{i+1} + H.c.) + \frac{U}{2} \sum_{i} n_{i} (n_{i} - 1) + \Delta \sum_{i} \cos(2\pi \beta i + \phi) n_{i},$$

(1)

where $b_{i}^{\dagger}$ and $b_{i}$ are the creation/annihilation operators for bosons at site $i$, $n_{i} = b_{i}^{\dagger} b_{i}$, $t$ is the hopping amplitude, $\phi$ is a tunable phase, $\Delta$ is the strength of the second lattice, and $U$ characterizes the on-site interactions. We determine the ground-state properties of the system, for both open and periodic boundary conditions (OBC and PBC), by means of the density matrix renormalization group (DMRG) method\textsuperscript{38}, assuming a maximal occupation $n_{\text{max}}$ that we increase until reaching convergence.

We are particularly interested in the topological properties of the ground-state phases, which we analyze by determining the Chern number for the many-body interacting system, following closely the procedure of Ref.\textsuperscript{39,40}. For a 2D insulator (on the $xy$ plane) the Chern number is defined as $C = \frac{1}{2\pi} \int \text{d} \theta_x \text{d} \theta_y F(\theta_x, \theta_y)$, where $\theta_x$ and $\theta_y$ are introduced as generalized twisted boundary conditions in $x$ and $y$ directions, respectively, and $F(\theta_x, \theta_y) = \text{Im} \left( \langle \partial_{\theta_x} \Psi^{\ast} | \partial_{\theta_y} \Psi \rangle - \langle \partial_{\theta_y} \Psi^{\ast} | \partial_{\theta_x} \Psi \rangle \right)$ is the Berry curvature\textsuperscript{41,42}, where $\Psi$ is the many-body ground-state wavefunction. We may proceed similarly for the case of the 1D superlattice, where the role of the twist angles $\theta_y$ and $\theta_x$ is, respectively, played by the superlattice phase $\phi \in [0,2\pi)$ and by a twist angle $\theta \in [0,2\pi)$ imposed by a twisted PBC, which we introduce by considering a tunneling $t e^{i\theta \phi}/L$, with $L$ the number of sites considered. In order to calculate the Chern number for a discrete set of $M$ values of the twist angles, we employ the method of Ref.\textsuperscript{43}, based on the evaluation for twisted PBC of the ground-state $\Psi_{\phi}$ corresponding to $\{\theta_i = 2\pi i/M, \phi_j = 2\pi j/M\}$, and on the calculation of the overlaps (fidelities) of the ground states for different $\theta_i, \phi_j$. 


**Quasi-periodic potential.** We start our discussion with the case of incommensurate lattices, which, while being interesting in itself, allow us to introduce some key concepts used in the rest of the Letter. We consider in particular the case of $\beta = (\sqrt{5} - 1)/2 \approx 0.618$. For a strong-enough second-lattice $(\Delta/t > 2)$ for non-interacting bosons the system experiences a transition from a superfluid (SF) phase to a gapless insulating phase known as Bose-glass (BG). Interestingly, for specific filling factors, in particular $(n) = \beta$ and $1 - \beta$, the system is for intermediate $U$ values a gapped insulator. This intermediate phase, placed between the SF and BG phases, is known as incommensurate charge-density wave (ICDW) \[43, 44\]. As shown below, ICDW phases present a non-trivial topological character.

An important insight on this topological character is obtained from the analysis of the chemical potential at a given total number of particles $N$, $\Delta E_N = E_{N+1} - E_N$. Figure 1 shows for the particular case of $L = 55$ sites \[45\] the results for $\Delta E_N$ for filling factors $0 \leq \langle n \rangle \leq 1$ as a function of $\phi$ for $U/t = 8$, $\Delta/t = 2$. Note that the structure of $\Delta E_N$ resembles the single-particle spectrum of a topological insulator \[11, 21\]. In particular, insulating phases (MI and ICDW) are characterized by a particle-hole gap $\Delta E_{p-h}(N) = \delta E_N - \delta E_{N-1}$. This gap is particularly clear for the ICDW phases with fillings $\langle n \rangle = 1 - \beta$ ($N = 21$) and $\beta$ ($N = 34$). Interestingly, whereas for PBC the ICDW phases remain gapped, for OBC the ICDW gap closes for some $\phi$, closely resembling the appearance of in-gap edge states in the single-particle spectrum of topological insulators. We illustrate the edge-like nature of the in-gap states of Fig. 1 for the case of $L = 55$ with OBC and $(n) \simeq \beta$ and $1 - \beta$. Figure 2 shows the difference in the density profile for $\phi_L$, slightly smaller than the value at which $\Delta E_{p-h}$ closes, and $\phi_R$, slightly larger than that value. Note that the change in the density profile is overwhelmingly concentrated at the boundaries.

The non-trivial topological character of the ICDW phases is confirmed by calculating the Chern number as mentioned above. We obtain in particular $C = -1$ for $(n) = 1 - \beta$ and $C = +1$ for $(n) = \beta$ (other ICDW phases are also topological, e.g. for $(n) = 2(1 - \beta)$ we obtain $C = -2$). This topological character is maintained as long as the system remains in the gapped ICDW phase. As both the SF and BG are non-topological, the edge states depend on the strength $\Delta$, becoming eventually delocalized when the ICDW gap closes at the SF-ICDW and ICDW-BG transitions.

The $(n) = 1$ case demands a separate discussion. Two different gapped phases are possible, a MI for $\Delta < U$ and a generalized ICDW (gICDW) for $\Delta > U$ up to the BG phase \[46\]. The gICDW is characterized by a density modulation at the beating quasi-period $1/(1 - \beta)$ that is absent in the MI. Although for PBC both phases present an excitation gap, the behavior under OBC is very different. Whereas for the MI $\Delta E_{p-h}$ never closes being $\phi$-independent (Fig. 1), for the gICDW it closes at two different $\phi$ values, which are exactly the one for $(n) = \beta$ and that for $(n) = 1 - \beta$. As for other ICDW phases, the closing of $\Delta E_{p-h}$ for OBC is linked to edge excitations. However, the Chern number of the gICDW phase is $C = 0$. The latter can be intuitively understood as follows. By comparing the density profile of the gICDW and the profiles for $(n) = \beta$ and $1 - \beta$, we find that the case $(n) = 1$ can be considered a superposition of two ICDW phases with $(n) = \beta$ and $(n) = 1 - \beta$ (note also the above mentioned $\phi$ values at which $\Delta E_{p-h}$ closes). Recall that these two phases are characterized, respectively, by $C = 1$ and $C = -1$, and hence the overall Chern number vanishes. Considering these sub-systems as a two-component boson system, we have the equivalent of pseudo-spin-1/2 bosons with counter-propagating edge states, reminiscent to the case recently discussed in the context of the IQHE for bosons \[13\].

**Topological phase transitions as a function of $\Delta/U$.** In our analysis of the quasi-periodic system we have observed that for growing $\Delta/U$ the system undergoes a transition between a non-topological phase (MI) and a phase with edge states (gICDW). We generalize this idea below to commensurate superlattices, showing that as a function of $\Delta/U$, a bo-

![FIG. 1: Chemical potential $\Delta E_N$ of a quasi-periodic model with OBC, for $L = 55$ sites, with $U/t = 8$ and $\Delta/t = 2$.](image1)

![FIG. 2: Difference in the density distribution for $\phi = \phi_L$ ($\phi_R$), slightly smaller (larger) than the $\phi$ value at which $\Delta E_{p-h}$ closes for OBC, $L = 55$, $U/t = 8$, $\Delta/t = 2$, and $(n) = \beta$ and $1 - \beta$.](image2)
son gas in a superlattice may experience transitions between phases of different topological properties. These transitions occur at a fixed overall filling factor, being a characteristic result of the bosonic nature of the particles.

We consider the particular case of a commensurate superlattice with $\beta = 1/3$. In the hard-core limit ($U \gg t, \Delta$), the MI with $\langle n \rangle = 1/3 (2/3)$ presents $C = -1 (+1)$ [37]. This result may be understood by mapping the bosonic system onto a free-fermion model, the topological properties being related to inter-gap edge states in the single-particle spectrum. The topological character of the MI is kept at finite $U$ [37]. However, we find that although the MI with $\langle n \rangle = 1/3$ presents $C = -1$ for any $\Delta/U$, the situation is crucially different for higher fillings $\langle n \rangle = p/3$, with integer $p > 1$.

Figure 3 shows the ground-state phases for $1 \leq p \leq 4$ for $U/t = 10$. For $\langle n \rangle = 2/3$, as expected from the hard-core results we find a Mott phase (MI1) with $C = 1$ for $\Delta/U < (\Delta/U)_{cr} \approx 0.6$. However for $\Delta/U > (\Delta/U)_{cr}$, we find another gapped Mott-like phase (MI2), but with Chern number $C = -2$. There is hence a topological transition at $(\Delta/U)_{cr}$. This transition is linked to the closing of the bulk gap $\Delta E_{ge}$ between the ground state and the first excited state, which occurs for $(\phi, \theta) = (\pi/3 + n\pi/3, \pi)$ with $n = 0, 1, 2$. The different nature of MI1 and MI2 is also evident from the inset of Fig. 4, which shows that with OBC $\Delta E_{p-h}$ closes only at a single $\phi$ value, whereas MI2 closes at two values (and hence has two associated edge-like excitations).

We stress that although the topological character, with $C = 1$, of the MI1 phase may be well understood from the hard-core limit, the topological phase transition into MI2 is a direct consequence of the bosonic nature of the particles. The phase transition is linked to the fact that for $\beta = 1/3$, $\langle n \rangle = 2/3 = 1 - \beta = 2\beta$. This observation is inconsequential for non-interacting fermions or hard-core bosons, but crucial for soft-core bosons. The physics behind the different topological phases may be illustrated for the case $\phi = \pi$. When $\Delta$ increases the single-particle spectrum is characterized by a lowest band and two upper bands, each one with 1/3 of the Bloch states. For large $\Delta \gg U$, only the lowest band is occupied. Due to the very narrow bandwidth (much smaller than $U$) of the lowest sub-band for $\Delta \gg U \gg t$, the Bose gas minimizes its energy by populating each available state of the lowest band twice, i.e. acting like a pseudo-spin-1/2 system. As a consequence, the system behaves as two copies of the hard-core $\langle n \rangle = 1/3$ case, and hence $C = -2$.

A similar reasoning may be applied for higher fillings, explaining the results of Fig. 3. In particular, whereas in the hard-core regime $\langle n \rangle = 1$ is a non-topological MI, for large $\Delta$, the system behaves as a triple copy of a $\langle n \rangle = 1/3$ MI, and as expected $C = -3$ is found. For $\langle n \rangle = 4/3 = 1 + \beta = 2(3\beta) = 4\beta$. We hence expect three possible topological phases depending on $\Delta/U$, which we indeed found in our numerics. At large $U$, we find a MI with $C = -1$, since the system behaves as a MI with 1/3 filling, i.e. $\langle n \rangle = 1 + \beta$. At intermediate $\Delta/U$ values, we observe a MI-like phase with $C = 2$, corresponding to two copies of a MI1 with 2/3 filling, i.e. $\langle n \rangle = 2(3\beta)$. Finally, for large $\Delta/U$ we find a phase with $C = -4$, corresponding to 4 copies of the MI phase at 1/3 filling, i.e. $\langle n \rangle = 4\beta$. Indeed the same arguments may be applied to bosons in superlattices with other commensurate values of $\beta$. Hence topological transitions for growing $\Delta/U$ are predicted to be a general feature of bosons in superlattices.

**Topological phase transitions due to inter-site interactions.** Although in current OL experiments only on-site interactions are relevant, inter-site interactions are expected to play a crucial role in future experiments with cold polar molecules, due to the long-range character of the electric dipole-dipole interaction [42-44]. We consider for simplicity only nearest-neighbor (NN) interactions, which result in an additional term $V \sum_i n_i n_{i+1}$ in Eq. (1). Inter-site interactions may drive as well topological phase transitions in superlattice bosons, as we illustrate below for $\beta = 1/3$ and $\langle n \rangle = 2/3$.

Figure 4 shows our results for the ground-state phases for $U/t = 10$. At small $V/U$ and $\Delta/U$ [50] we recover, as expected from the hard-core limit, the topological MI1 phase. For large $V/U$, the strong NN repulsion results in a doubly-degenerate ground state, characterized by a density modulation with a six-site periodicity [51]. E.g., for $\phi = 0$, each three-site elementary cell $j$ has two equal low sites (1,2) and an upper one (3), and may be characterized by the occupation $(n_{j,1}, n_{j,2}, n_{j,3})$. For $U, \Delta, V \gg t$, the ground state presents a distribution $(0, 2, 0)$ for even (odd) $j$ and $(1, 0, 1)$ for odd (even) $j$. Similar ground states are found for other $\phi$ values. Due to this modulation we denote this phase as density-wave (DW) phase. The DW phase is characterized by a Chern number $C = 2$ resulting from the sum of the Chern numbers ($C = 1$) of both degenerate states. Between the MI1 and DW phases we find the MI2 phase, with $C = -2$. The MI1-MI2 transition is marked, as mentioned above, by a vanishing bulk gap $\Delta E_{ge}$ for $(\phi, \theta) = (\pi/3 + n2\pi/3, \pi)$ with $n = 0, 1, 2$. These gapless points are characterized by the non-universal exponent $\alpha$ of the single-particle correlation function $\langle b^\dagger_i b_j \rangle \propto r^{-\alpha}$, which we have determined (Fig. 4) using
around a single discussted in Ref. [29]. Whereas MI1 presents marked edges of the phases in the presence of sharp boundaries. Sharp transitions (e.g. MI1-MI2) are the result of the bosonic nature of the particles, being absent in free fermions (or equivalently hard-core bosons). Topological transitions are hence a general feature of interacting bosons in both commensurate and incommensurate bi-chromatic lattices.

Conclusions. In this Letter we have shown that bosons in bi-chromatic OLs constitute a surprisingly simple scenario for the realization of topological phase transitions. We stress that, although the topological nature of some phases (e.g. MI1) may be understood from the hard-core case, being directly related to the lattice geometry and filling factor, the topological transitions (e.g. MI1-MI2) are the result of the bosonic nature of the particles, being absent in free fermions (or equivalently hard-core bosons). Topological transitions are hence a general feature of interacting bosons in both commensurate and incommensurate bi-chromatic lattices.

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