Quantized pumping and phase diagram topology of interacting bosons

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Interacting lattice bosons at integer filling can support two distinct insulating phases, which are separated by a critical point: the Mott insulator and the Haldane insulator\cite{1}. The critical point can be gapped out by breaking lattice inversion symmetry. Here, we show that encircling this critical point adiabatically pumps one boson across the system. When multiple chains are coupled, the two insulating phases are no longer sharply distinct, but the pumping property survives. This leads to strict constraints on the topology of the phase diagram of systems of quasi-one dimensional interacting bosons.

In the early 1980s, Thouless \cite{2} made the surprising observation that certain band insulators can sustain dissipationless and quantized charge transport by adiabatic pumping. The classic example of this effect is seen in a half filled tight binding chain with two sites per unit cell\cite{2}. As parameters of the hamiltonian are changed adiabatically along a closed loop around the single gapless point in the two parameter space, a unit charge is transported through the chain. This simple observation had interesting implications to other systems. For example, it was quickly realized \cite{3, 4}, that Laughlin’s original argument for the quantization of the Hall conductance may be formulated in the same mathematical terms as the pumping problem. In connection with more recent developments, the ideas of topological pumping through band insulators were precursors of the theoretical\cite{5–8} and subsequent experimental\cite{9, 10} discovery of topological band insulators. Indeed, the $\mathbb{Z}_2$ topological invariant associated with these systems can be reformulated in terms of adiabatic pumping \cite{11}.

Although quantized pumping has been discussed primarily in the context of non–interacting fermions, the concept is much more general. The pumped charge can be formulated in terms of a topological Chern number associated with parallel transport of the many-body wavefunction in Hilbert space\cite{3, 4}. In particular this formulation ensures robustness of the quantization to disorder and interaction and also enables direct extension of the concepts to spin pumping in spin-1/2 chains\cite{12}. All these extensions are adiabatically connected to the case of a band insulator, either directly or via a Jordan-Wigner transformation.

In this paper we show that a natural model of interacting lattice bosons at integer filling, which is not directly mappable to a band insulator, allows quantized transport through Mott insulating states by adiabatic pumping. The existence of non trivial loops in the gapped regions of parameter space defines a topological index, which may be associated with the gapless (superfluid) phases they surround. It also sets constraints on the structure of the phase diagram, or more precisely, on the topology of the gapless regions within it.

The basic model we consider is an extended Bose Hubbard model (EBHM), at integer filling, on coupled chains

\begin{equation}
H = \sum_{\alpha} \left[ H_{\alpha} + H_{\lambda,\alpha} + H_{\perp,\alpha} \right],
\end{equation}

FIG. 1: Phase diagram topology. (a) Phase diagram of a single chain. The parameter $g$ tunes across the Haldane (HI) to Mott (MI) insulator transition. These two phases are sharply defined only in presence of inversion symmetry ($\lambda = 0$). A closed adiabatic path which encircles the critical point (path A) entails pumping of a single boson across the insulator. (b) Schematic phase diagram of two coupled chains. The MI and HI phases can be adiabatically connected via the dashed path. However, since path 1 pumps one boson per chain, it cannot be collapsed adiabatically to a point without crossing the gapless region. Path 2 entails pumping of one boson per two chains.
where

\[
H_\alpha = \sum_j \left[ -t(b_{\alpha,j}^\dagger b_{\alpha,j+1} + H.c.) + \frac{U}{2} n_{\alpha,j}(n_{\alpha,j} + 1) \right] + V \sum_j n_{\alpha,j}n_{\alpha,j+1},
\]

(2)

is a single chain hamiltonian defined on chain \( \alpha \). \( b_{\alpha,j}^\dagger \) creates a boson at position \( j \) in chain \( \alpha \), and \( n_{\alpha,j} \equiv b_{\alpha,j}^\dagger b_{\alpha,j} \). The hamiltonian

\[
H_\lambda,\alpha = \lambda \sum_j \left[ n_{\alpha,j} b_{\alpha,j}^\dagger b_{\alpha,j+1} - n_{\alpha,j+1} b_{\alpha,j}^\dagger b_{\alpha,j} + H.c. \right],
\]

(3)

is a perturbation that breaks the bond-centered inversion symmetry of \( H_\alpha \). Finally,

\[
H_{\perp,\alpha} = \sum_j \left[ -t_{\perp}(b_{\alpha,j}^\dagger b_{\alpha+1,j} + H.c.) + V_\perp n_{\alpha,j}n_{\alpha+1,j} \right].
\]

(4)

denotes interchain coupling. The model (1) or related hamiltonians can be realized with ultracold dipolar molecules or atoms with optically induced dipole moments[13]. Crucial for our analysis is the presence of the perturbation \( \lambda \), which breaks the inversion symmetry of the chain. It will be naturally generated if the underlying optical potential is not symmetric under inversion. Such a lattice potential can be produced by two lasers, one of which has double the wavelength of the other. In one extreme limit this configuration gives rise to a lattice of double well potentials[14, 15], which indeed are not inversion symmetric in general.

A single chain – We have shown previously, that the EBHM on a single chain (Eq. 2) exhibits a quantum phase transition from a Mott insulating (MI) state to a novel gapped phase, which we termed a “Haldane insulator” (HI), upon increasing the nearest neighbor interaction[1]. Both phases are completely disordered in the sense that they do not break any symmetry of the Hamiltonian. The new state is analogous to the Haldane gapped state of spin-1 chains, and is characterized by a string order parameter, albeit in the boson density rather than the spin. It was later shown [16–19], that the distinction between the HI and MI phases is protected by lattice inversion symmetry. A perturbation, such as \( H_{\lambda,\alpha} \) above, which breaks the inversion symmetry about a bond, opens a gap at the HI–MI transition and allows adiabatic connection between the two gapped phases. Thus, in the two parameter space \((V, \lambda)\) the transition becomes an isolated critical point. We shall argue that an adiabatic passage around the critical point entails transport of a single boson through the chain.

To see this we turn to the long wavelength description of the extended Hubbard chain, with the inversion symmetry breaking perturbation \( \lambda \). Near to the HI–MI phase transition it is given by the following Sine-Gordon field theory[16]

\[
H_0 = \frac{u}{2\pi} \int dx \left[ K (\partial_x \theta)^2 + \frac{1}{K} (\partial_x \phi)^2 - g \cos(2\phi) - \lambda \sin(2\phi) \right],
\]

(5)

with the Luttinger parameter \( K \) in the regime \( 1/2 < K < 2 \). The parameter \( g \) is in general a complicated function of the microscopic interactions, \( g(U, V, t) > 0 \) in the MI, \( g < 0 \) in HI and vanishes on the critical line separating these two phases. A naive continuum limit gives the approximate dependence \( g \approx U/2 - V \) [16]. Here \( \partial_x \phi/\pi = \rho \) is the long-wavelength component of the boson density, \( \theta \) is its dual field satisfying \( [\partial_x \phi(x), \theta(x')] = i\pi \delta(x - x') \), and \( u \) is the sound velocity. Note that under inversion, \( \rho(x) \rightarrow -\rho(-x) \), therefore \( \phi(x) \rightarrow -\phi(-x) \), which makes it clear that the \( \lambda \) term is odd under inversion. The last two terms can be written compactly as \( \tilde{g} \cos(2\phi - \chi) \), where \( \tilde{g} = \sqrt{g^2 + \chi^2} \) and \( \chi = \arctan(\lambda/g) \). In the regime of interest \( K < 2 \), making the cosine term relevant. \( \cos(2n\phi) \) and \( \sin(2n\phi) \) with \( n > 1 \) may also appear in \( H_0 \), but we assume that these terms are irrelevant at the HI–MI critical point, \( (\lambda = 0, g = 0) \).

The critical point is entirely surrounded by a gapped state (see Fig. 1a) in which the field \( \phi \) is essentially locked to the value \( \chi/2 \). Therefore an adiabatic change of the system parameters, which takes it in a counter clockwise loop around the critical point incurs a continuous change of \( \phi(x) \) by \( \pi \) everywhere in space. By definition of the field, \( \phi(x) \) suffers a \( \pi \) shift every time a particle passes through \( x \). The last observation implies the transport of exactly one boson from left to right in a counter-clockwise loop. Another way to derive the quantization is to refermionize the field theory (5). The quantized charge can be computed directly for \( K = 1 \), which maps to free fermions [20]. It follows for other values of \( K \) by adiabatic continuity.

To enable continuous pumping, the chain must be connected to gapless reservoirs. This arises naturally in a realization using an optical lattice and a harmonic trap in which the incompressible phase will be flanked by superfluid wings. The adiabaticity condition needed to ensure quantized pumping is \( \dot{\chi} \ll \Delta \sim \Lambda(\tilde{g}/\Lambda)^{1/2(K-1)} \)[20], where \( \Delta \) is the gap along the cycle, \( \Lambda \), the ultraviolet cutoff of the continuum theory is of the order of the bandwidth \( 2t \).

The topological character of the pumped charge makes it robust to small perturbations of the hamiltonian[3]. In particular, for the case of many weakly coupled chains, driving all chains adiabatically along loop \( A \) still pumps one boson per chain. For arbitrary coupling between chains, we shall see that the quantization of the pumped charge imposes stringent constraints on the topology of the phase diagram in the enlarged parameter space. We demonstrate this below using the example of two coupled chains and then comment on generalizations to any
number of coupled chains.

Two coupled chains. The critical point at \((g, \lambda) = 0\) is unstable to weak tunnel coupling \(t_\perp\) between a pair of chains[16]. Using an RG analysis we have shown that the critical point expands to a gapless phase (Luttinger liquid) with radius \(t_\perp \sim 1\). Upon turning on \(t_\perp\), the critical point expands to a finite superfluid (SF) region, and the two gapped phases are not sharply distinct. For \(\lambda > 0\), the MI–HI critical point at \(t_\perp = 0\) becomes gapped. The gapless region shrinks upon increasing \(\lambda\), but does not disappear. The phase diagram has the same topology as in Fig. 1b.

How is the pumped charge associated with an adiabatic cycle around the critical point, affected by turning on the inter-chain coupling \(t_\perp\)? As long as the path encircles the gapless region from the outside, then it is adiabatically connected to the non-trivial pumping cycle around the HI–MI critical point of the decoupled chains. The topological Chern number cannot change and hence the pumped charge must remain quantized at one boson per chain upon encircling the gapless region. Below we address the evolution of the gapless region for increasing inter-chain coupling beyond weak-coupling.

To understand how the phase diagram evolves with stronger values of inter-chain coupling we should take into account another crucial fact. For two chains there is no sharp distinction between the HI and MI phases, even in the presence of inversion symmetry (\(\lambda = 0\))[18]. This means that the HI and MI phases of two decoupled chains can be connected adiabatically by a path in hamiltonian space going through a region with non zero inter-chain coupling. We demonstrate this explicitly using a Density Matrix Renormalization Group (DMRG) calculation of the following spin-1 ladder model:

\[
H_{\text{spin}} = \sum_{i,\alpha} \left[ V S^z_{\alpha,i} S^z_{\alpha,i+1} - t (S^+_{\alpha,i} S^-_{\alpha,i+1} + H.c.) + U (S^z_{\alpha,i})^2 \right. \\
+ \lambda (S^z_{\alpha,i} S^+_{\alpha,i} S^-_{\alpha,i+1} - S^z_{\alpha,i+1} S^+_{\alpha,i+1} S^-_{\alpha,i} + H.c.) \left. + \sum_{i} \left[ V_{\perp} S^z_{1,i} S^z_{2,i} - t_\perp (S^+_{1,i} S^-_{2,i} + H.c.) \right \right] 
\]

This model can be thought of as a truncation of the EBHM (1) to the space of the three lowest occupation states \(n_i = S^z_i + 1/2\). Crucially, the two models have the same low energy limit[16, 22].

Fig. 2 shows the phase diagram of the model (6), as a function of \(t_\perp\), \(g\), and \(U\), which is used to tune the MI–HI transition. \((U)\) is related to \(g\) in Eq. 5 by \(g \propto U - U_c\), where \(U_c\) is the location of the MI–HI transition.) We have fixed \(V = 2t\) and \(V_{\perp} = 2t_\perp\). The phase diagram was determined by measuring the spin gap, \(\Delta_s = E(S = 1) - E(S = 0)\), and extrapolating it to the thermodynamic limit. System sizes of up to \(L = 64 \times 2\) were used, keeping \(m = 200\) states.

We see in Fig. 2, that upon increasing the inter-chain coupling \(t_\perp\) and \(V_{\perp}\) the HI-MI critical point first expands to a gapless region as predicted by the weak coupling theory [16], but collapses at stronger coupling, allowing for an adiabatic connection between the HI and MI states.

The fact that the gapless region ends may at first seem contradictory to our previous assertion that an adiabatic loop around this region in the space \((g, \lambda)\) entails pumping of one boson per chain. If the gapless region ends, and the loop can be collapsed adiabatically to a trivial point in the gapped state with increasing inter-chain coupling, how can it sustain a non-trivial Chern number?

To avoid this contradiction, the gapless region must split into two branches in the \(\pm \lambda\) directions, which either extend indefinitely, or terminate discontinuously on a 1st order transition plane. With this topology, a loop surrounding the original critical point at \(t_\perp = 0\) cannot be collapsed adiabatically into a point. The numerically obtained phase diagram in Fig. 2 is consistent with these considerations: although the superfluid region in the \(\lambda = 0\) plane is finite, it has two branches which extend in the \(\pm \lambda\) directions. These branches do not terminate up to the largest values of \(\lambda\) we examined (in [20] we present results for higher \(\lambda\) values).

Given the topology of the gapless phase it is natural to ask what is the pumped charge associated with a path surrounding only one of the two branches at either positive or negative \(\lambda\) (path 2 in Fig. 1b). Such a path has no counterpart in the single chain system and it cannot be continuously deformed into a loop that surrounds an isolated critical point. Nevertheless, we argue that the Chern number associated with this path is determined by the topological character of the HI-MI critical point. A simple way to approach this problem...
is to note that two loops, each encircling one of the two branches, can be deformed into a single loop which encircles both branches. Such a loop corresponds to pumping of two bosons as discussed above. Therefore, by symmetry of the ±λ branches, each of the isolated loops entails pumping of one boson along the ladder, or half a boson per chain.

The distribution of quantized charge among different loops in parameter space can be succinctly represented in terms of a fictitious quantized magnetic flux running through gapless regions in the three dimensional parameter space. Two flux quanta, one for each chain, are inserted through the isolated HI-MI critical point in the t⊥ direction, and must split evenly between the two branches at ±λ. The quantized pumping therefore defines a topological index, the fictitious quantized-flux, that is associated with the gapless phases.

More than two chains – Without inter-chain coupling, N parallel chains are just N copies of the single chain problem, and so an adiabatic cycle around the critical point implies pumping of N bosons along the decoupled chains. As before, this charge cannot change suddenly with the introduction of inter-chain coupling t⊥. Hence, the extended parameter space the critical point at the origin t⊥ = 0 is a source of N quanta of the fictitious flux. The gapless phase at finite t⊥ may branch out, as in the case of two chains, while the fictitious flux running through all the branches must add up to exactly N.

There is another topological constraint on the branching of the gapless phase with increasing t⊥. From the construction of Ref. [18, 19], follows a sharp distinction between the Haldane insulator and the Mott insulator phase on any ladder with an odd number of chains. That is, without breaking inversion symmetry, 2N + 1 decoupled chains in the HI phase cannot be connected adiabatically to decoupled chains in the MI by an adiabatic path going through finite t⊥, in contrast to the two leg case considered above. Therefore in a ladder with odd number of legs the gapless phase must persist indefinitely on the plane with inversion symmetry, i.e λ = 0.

Conclusions – Topological properties of matter are usually associated with gapped regions of the phase diagram. Here, we have shown that in a model of interacting bosons, it is natural to associate a topological “flux” with the gapless (superfluid) regions, which is defined by the pumped charge upon encircling these regions adiabatically. This property can be argued to be more profound, in the sense that the gapped phases discussed here are only distinct from each other as long as certain symmetries (e.g. inversion symmetry) are preserved, while the topological flux associated with the gapless region is robust against arbitrary particle number conserving perturbations. This principle can be used to impose constraints on the topology of the phase diagram; for example, it implies that a gapless region which carries a non-zero topological flux cannot terminate.

Similarly, topological insulators in two and three dimensions are only well-defined as long as time-reversal symmetry is preserved. However, the gapless region separating the topologically trivial and non-trivial phase may carry a topological “flux”, which remains well-defined even when time-reversal symmetry is broken. That can hopefully shed new light on the nature of topological insulators.[23]

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Supplementary material for: Quantized pumping and phase diagram topology of interacting bosons

I. proof of quantized pumping by mapping to fermions

In the main text, starting from the Sine-Gordon field theory for the MI-HI transition,

\[ H_0 = \frac{u}{2\pi} \int dx \left[ K (\partial_x \theta)^2 + \frac{1}{K} (\partial_x \phi)^2 - g \cos(2\phi) - \lambda \sin(2\phi) \right] \]

(7)

where the Luttinger parameter satisfies \(1/2 < K < 2\), we argued that upon encircling the point \((g = 0, \lambda = 0)\) adiabatically, exactly one boson is transported across the system. The argument was based on semi-classical considerations. In this Supplementary Material, we derive this result by considering the special “Luther-Emery” point \(K = 1\) [24].

At this point the hamiltonian can be rewritten in terms of non-interacting fermions, which carry the same charge as the original bosons. The right/left moving fermions \(\psi^\pm\) are defined through the bosonization formula

\[ \psi^\pm = \frac{1}{\sqrt{2\pi a}} e^{i(\theta^\pm \phi)}, \]

(8)

where \(a\) is the microscopic cutoff of the theory. The fermionic hamiltonian is

\[ H_f = \int \frac{dk}{2\pi} \psi^\dagger (k) \left[ \hat{d}(k) \cdot \hat{\sigma} \right] \psi (k). \]

(9)

Here we have defined \(\psi (k)^\dagger \equiv \left[ \psi_\theta^\dagger (k), \psi_\phi^\dagger (k) \right], \hat{d}(k) \equiv (\lambda, g, uk),\) and \(\hat{\sigma}\) are Pauli matrices. This hamiltonian is identical to the low energy limit of the model given by Thouless in Ref. [2], describing spinless fermions on a one-dimensional lattice at half filling, with a hopping dimerization proportional to \(g\) and a staggered potential proportional to \(\lambda\). The pumped charge is obtained by computing the Chern number, which can be expressed as an integral over the Brillouin zone

\[ C_{\ell} = \int_{\ell} d\gamma dk \frac{1}{4\pi} \hat{d} \cdot \left( \frac{\partial \hat{d}}{\partial \gamma} \times \frac{\partial \hat{d}}{\partial k} \right) \]

(10)

where \(\hat{d} \equiv \hat{d}/|\hat{d}|\) and \(\gamma \in [-\pi, \pi]\) parametrizes the loop \(\ell = A, B\) (see Fig. 1a in the main text). The integral (10) measures the number of times the mapping \(\hat{d}(\gamma, k)\) covers the unit sphere, and hence it is quantized. Note that it is, in general, impossible to compute the Chern number from the continuum hamiltonian (9), since the latter is accurate only in a small range of momenta up to a cutoff \(\Lambda \sim \frac{1}{a}\), while the Chern number requires knowledge of the hamiltonian in the entire Brillouin zone.

In order to extract the Chern number from our low energy model, we subtract the Chern number of loop B which does not enclose the critical point from that of the nearby loop A which does enclose it. This procedure removes the sensitivity to momenta near \(A\). In Fig. 3 we show schematically \(\hat{d}(\gamma, k)\) for the two loops A and B. In order to obtain \(C_A - C_B\), we replace \(k \to -k\) for loop B (which changes the sign of the integrand in Eq. 10), and perform the integral over the combined \(k\) range for both \(C_A\) and \(C_B\). Note that the vector \(\hat{d}\) satisfied periodic boundary conditions at the ends of this region, and therefore \(C_A - C_B\) is guaranteed to be an integer. From the figure, and from the geometric interpretation of \(C_{A,B}\) as the area covered by \(\hat{d}(\gamma,k)\) on the unit sphere, one can see that \(C_A - C_B = 1\). Therefore, loop A corresponds to pumping of exactly one more charge than loop B. The fact that loop B is contractible to a point without ever closing a gap implies that \(C_B = 0\) and hence \(C_A = 1\).
FIG. 3: Direction of the unit vector $\hat{d}$ (see Eq. 9) as a function of momentum $k$ and the loop parameter $\gamma$. Left: loop A (shown in Fig. 1a in the main text), which encloses the critical point; right: loop B, which does not enclose the critical point.

The Chern number can be generalized to interacting systems by writing it in terms of the dependence of the many-body ground state on a phase twist $\varphi$ in the periodic boundary conditions[3]. From this construction, it is clear that the value of the quantized charge along the loop $A$ cannot change even when we move away from the free Fermion “Luther-Emery” point $K = 1$. We conclude that any path which can be deformed adiabatically to a cycle which encircles the MI–HI critical point in the $(g, \lambda)$ space entails pumping of a single boson across the system.

II. Adiabaticity condition for pumping

The adiabaticity condition required for quantization of the pumping can be obtained from adiabatic perturbation theory (see Ref. [25]). Given a time dependent Hamiltonian, we expand the evolving wave-function in the instantaneous eigenstates of $H(t)$

$$|\psi(t)\rangle = \sum_n a_n(t) |\phi_n(t)\rangle,$$

where $H(t) |\phi_n(t)\rangle = E_n(t) |\phi_n(t)\rangle$. It is then useful to define $a_n(t)$ through the gauge transformation $a_n(t) = \alpha_n(t) \exp(-i\Theta_n(t))$, where $\Theta_n(t) \equiv \int_0^t E_n(t') dt'$. Let us now assume that initially only the ground state is occupied such that $\alpha_n(0) = \delta_{n0}$. The rate of change of the excitation amplitudes is then

$$\dot{\alpha}_n = -\langle n | \partial_t | 0 \rangle e^{i\Theta_n(t)} = -\frac{\langle n | \partial_t H | 0 \rangle}{E_n(t) - E_0(t)} e^{i\Theta_n(t)}$$

We are interested in excitations above the gap, so that $E_n(t) - E_0(t) \approx \Delta$. In addition, $\partial_t H = g\chi \int dx \sin(2\phi + \chi(t))$. We shall denote by $C_{in}$ the time independent matrix element $\langle n | \int dx \sin(2\phi + \chi(t)) | 0 \rangle$. Plugging this into Eq.
(12) and integrating over time we have:

$$\alpha_n(t) = -\frac{C_{n00g}}{\Delta} \int_{t_0}^{t} dt' \hat{\chi} e^{i\Delta t'}$$

(13)

To compute this amplitude we should specify how the time dependence is turned on and off. Since we are interested in the adiabatic limit it is natural to do this in a smooth way. We take $\chi(t) = \pi \tanh(t/\tau)$.

**III. Phase diagram at higher values of $\lambda$**

In order to verify that the gapless superfluid region in the phase diagram (Fig. 2 in the main text) does not terminate, we have extended the calculation to larger $\lambda$ values. Fig. 4 shows the phase diagram of the effective spin model (Eq. 6 in the main text) with $V_\perp = 2t_\perp$, extended up to $\lambda = \pm 1$. Consistently with the charge pumping argument, we found that the superfluid “horns” extend in the $\pm \lambda$ direction and persist to the largest $\lambda$ we have examined. Further calculations show that the superfluid region extends to at least $\lambda = \pm 2$ (not shown). Ultimately, the superfluid region can either extend to $\lambda \rightarrow \pm \infty$, or collapse onto itself to form a donut-like shape.