

Quantum theory of fractional topological pumping of lattice solitons

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One of the hallmarks of topological systems is the robust quantization of particle transport. It is the origin of the integer-valued quantum Hall conductivity and a potential tool for quantum information technology. Recent experiments on topological pumps constructed by using arrays of photonic waveguides and described by the Andre-Aubry-Harper (AAH) model, have demonstrated both integer and fractional transport of lattice solitons. In these systems, a background medium mediates interactions between photons via a Kerr nonlinearity and leads to the formation of self-bound multi-photon states. Upon increasing the interaction strength a sequence of transitions was observed from a phase with integer transport in a pump cycle through different phases of fractional transport to a phase with no transport. We here present a quantum description of topological pumps of self-bound many-particle states in terms of an effective Hamiltonian of their center-of-mass (COM) motion, which allows to classify topological phases in terms of generalized symmetries. We identify a topological invariant, an effective single-particle Chern number, which fully governs the soliton transport. Increasing the interaction strength in the AAH model leads to a successive merging of COM bands, which is the origin of the observed sequence of topological phase transitions and also the potential breakdown of topological quantization for some interaction strength.

I. INTRODUCTION

Topological quantum systems have been intensively studied since the discovery of the quantum Hall effect [1]. One of the simplest examples for such systems is a Thouless pump [2], which displays a quantized particle transport in an insulating bulk state of a 1D lattice upon cyclic adiabatic changes of system parameters. The transport is governed by an integer topological invariant, equivalent to a Chern number. The quantization of transport not only applies to a fully filled fermion band, it is also observable in the center-of-mass motion of a single particle equally distributed over all momentum states (see e.g. [3] for a detailed overview.) A major problem in the single particle case is the fast dispersion of the wavefunction. A possible solution for this has been utilized in [4–6] using bound many-particle objects: lattice solitons. They show quantized transport in a topological pump while being almost nondispersive due to their large mass. The notion solitons is used here colloquially as the self-bound many-particle states may not fulfill all properties of true solitons [7–9]. In the experiments of [6], laser pulses have been injected into spatially modulated waveguide arrays simulating a time-dependent Aubry-André-Harper (AAH) Hamiltonian with a Kerr nonlinearity mediating interactions [10–12]. Increasing the light intensity, solitons form, for which integer transport in a full pump cycle was observed. Above a certain power threshold, all transport is halted. In subsequent work [13], an interaction controlled transition between phases with integer and *fractional* transport was demonstrated (see Fig.1).

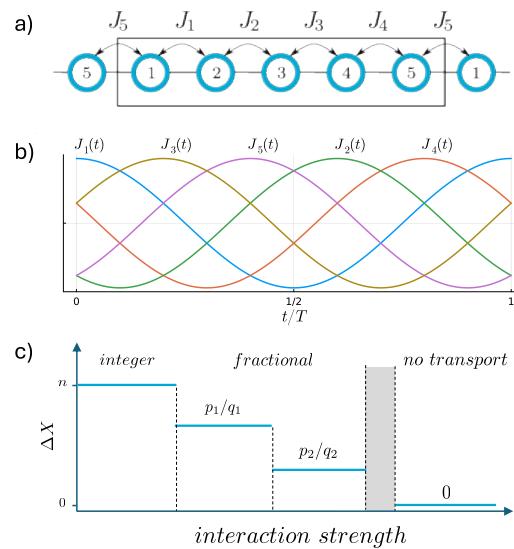


FIG. 1: (a) and (b) 1D Aubry-André-Harper model with modulated hopping rates $J_1(t)\dots J_5(t)$ and on-site interactions U . (c) Motion of center of mass of a soliton ΔX in a pump cycle. Upon increasing the interaction strength there are multiple transitions between phases of integer, fractional and eventually absent transport, in some cases intersected by a small interval of non-quantized transport (grey area).

These observations triggered an extended body of theoretical work [14–17] based on the discrete nonlinear Schrödinger equation (DNLSE) [18]. While the DNLSE accurately reproduces the observed shift in the COM, the underlying mean-field description fails to provide an explanation for the quantized transport and of the origin of the topological phase transitions. Using pertur-

bation theory it has been argued in [14, 19] that the transport is governed by the Chern number of the single-particle band from which the soliton bifurcates. However, already weak interactions destroy a uniform occupation of Bloch states, necessary for the one-to-one relation between particle transport and Chern-number of single-particle bands. Furthermore, as shown in Sec. II B, there is a gradually growing admixture of higher single-particle bands when the interaction is increased, and the perturbative arguments fails entirely in the fractional case. Finally, cases of anomalous nonlinear Thouless pumping were found [20], and in [21] it was predicted that multi-component solitons can show fractional transport, despite the fact that the single-particle bands are all topologically trivial. This shows that the topological transport of solitons cannot be traced back to topological properties of the underlying single-particle Hamiltonian. Most recently a fermionic model with repulsive interactions has been investigated [22] where fractional transport emerges from coupling of single-particle bands by repulsive interactions of fermions. We here unravel the origin of the quantized soliton transport and provide an explanation for the observed phase transitions by developing a fully quantum description of topological soliton pumps. To be specific, we consider the AAH model as generic example; the approach applies, however, to all systems with self-bound many-particle states. We show that the topological contribution to their transport can be described in terms of an effective single-particle Chern number, provided the soliton band is gapped from all extended (not self-bound) many-body states. Introducing an effective single-particle Hamiltonian for solitons we show that in the AAH model for increasing interaction strength different soliton bands merge at some parameter values of the pump cycle. At this point, the transport is governed by a Wilson loop, giving rise to different phases with fractionally quantized average transport. Increasing the interaction further eventually mixes all soliton bands, and since the total Wilson loop of all soliton COM bands must vanish, the topological transport breaks down [6, 23]. Finally, we show that in some intermediate interaction regimes the energetically highest of a set of crossing soliton bands may be degenerate with extended states. In such a case the transport is no longer (fractionally) quantized and may take arbitrary values, explaining the fluctuating transport numerically predicted in [15]. Since the effective Hamiltonian of solitons is a single-particle Hamiltonian, its symmetries under time-reversal, charge-conjugation and chiral transformation provide a full classification of possible topological phases according to Ref. [24, 25].

II. MODEL AND MEAN-FIELD APPROACH

A. Aubry-André-Harper-model

We consider a generic lattice model with attractive on-site interactions. Specifically, we investigate the bosonic tight-binding Hamiltonian

$$\begin{aligned} \mathcal{H}(t) &= \mathcal{H}_0(t) + \mathcal{H}_{\text{int}} & (1) \\ &= -\sum_l \left[(J_l(t)\hat{a}_l^\dagger\hat{a}_{l+1} + h.c.) + \epsilon_l(t)\hat{a}_l^\dagger\hat{a}_l + \frac{U}{2}\hat{n}_l(\hat{n}_l - 1) \right] \end{aligned}$$

where \mathcal{H}_0 describes the single-particle dynamics in the lattice and is periodic in time with period T , i.e. $\mathcal{H}_0(t) = \mathcal{H}_0(t+T)$. The corresponding hopping amplitudes J_l and on-site energies ϵ_l have a spatial period p , which defines the unit cell size. \mathcal{H}_{int} describes an (attractive) on-site interaction of strength $U > 0$, which will be parameterized as $U = U_0/N$ with N being the total number of particles. In order to understand the emergence of topological phase transitions observed in [6, 13] we consider specifically the 1D Aubry-André-Harper model [10, 11] with hopping amplitudes

$$J_l(t) = J \left(1 + \delta \cos \left(\Omega t + \frac{2\pi lk}{p} \right) \right), \quad (2)$$

with $0 < \delta < 1$, see Fig. 1. p , which we take as a prime number, whereas k controls the phase shift between the hopping amplitudes. All on-site potentials ϵ_l in Eq. (1) are chosen to be 0.

With periodic boundary conditions, the Hamiltonian is translational invariant, i.e. $\hat{T}\mathcal{H}\hat{T}^{-1} = \mathcal{H}$, where \hat{T} is the translation operator by one unit cell, i.e. $\hat{T}\hat{a}_l\hat{T}^{-1} = \hat{a}_{l+p}$. As a consequence, the lattice momentum K of the center of mass (COM) is a conserved quantity.

Attractive interactions U lead to localized soliton states. These are states with a distribution of occupation numbers that decay with increasing distance to the center of mass with a localization length ξ , i.e. $\langle \hat{n}_{l+q}\hat{n}_l \rangle \sim \exp\{-|d|/\xi\}$ for $d \gg 1$. We call them *stable* if they have an energy gap to all extended states with the same K . On the quantum level, a minimum value U_c is required for a soliton to form, which tends to zero as $N \rightarrow \infty$ [26]. In a complex band structure multiple soliton solutions can exist, which for some parameter values may become degenerate. Furthermore, stable excited soliton solutions may not exist at all times, as they can become degenerate with extended states in some parts of the pump cycle. In this case we call these solitons partially stable.

B. Mean-field approach: Discrete nonlinear Schrödinger equation

In mean-field approximation the dynamics of solitons in a 1D lattice are described by the discrete nonlin-

ear Schrödinger equation. This equation can be obtained from a Gutzwiller coherent-state ansatz [27] for the many-body quantum state

$$|\psi\rangle = \prod_l |\phi_l\rangle, \quad \text{where} \quad \hat{a}_l |\phi_l\rangle = \phi_l |\phi_l\rangle.$$

For the AAH Hamiltonian, Eq. (1), it reads

$$i \frac{\partial}{\partial t} \phi_l = -J_l \phi_{l+1} - J_{l-1} \phi_{l-1} - \epsilon_l \phi_l - U |\phi_l|^2 \phi_l. \quad (3)$$

Numerical simulations of Eq. (3) have provided a good description of soliton energies and the observed soliton transport in parameter regimes where the soliton is stable. The semiclassical description, however, fails to explain the topological nature of the transport and the origin of topological phase transitions. In [14, 19] it was argued that for weak interactions the solitons can be represented in terms of the most localized Wannier states of only one single-particle Bloch band. The authors state that under this assumption the topological transport is described by the Chern number of the Bloch band the soliton bifurcates from.

In Fig. 2 we have plotted the integrated overlap of a soliton obtained from a self-consistent solution of Eq. (3) with the single particle Bloch wavefunctions for two lowest bands for the AAH model with phase offset $k = 2$ and unit cell size $p = 5$ as a function of interaction strength. The vertical spread of data points reflects different times in the pump cycle. One recognizes that while in the perturbative limit of very small absolute values of interaction strengths there is indeed a very large overlap with the lowest Bloch band, contributions from higher bands continuously grow with nonlinearity. In the regime of fractional transport, following the above argument, one would expect equal contributions from the lowest and the first excited band, which is clearly not the case. Moreover, if one calculates the overlap with the Bloch states in a momentum resolved way, one finds an inhomogeneous contribution from different lattice momenta, see [6]. Therefore, the resulting topological invariant is not just the average of the single-particle Chern-numbers.

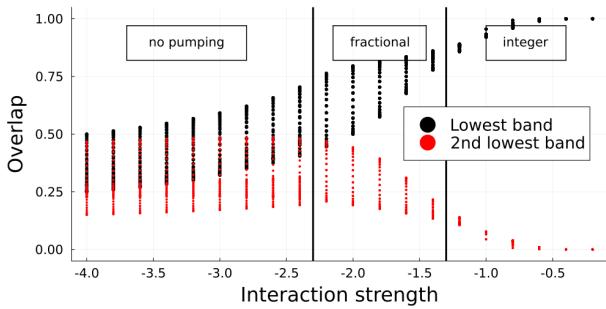


FIG. 2: Overlap of eigensolution of the DNLSE with single-particle Bloch bands for different interaction strength. Data points for the same interaction strength correspond to different times in the pumping cycle.

III. CENTER-OF-MASS TRANSPORT AND MANY-BODY CHERN NUMBER

Since the semi-classical approaches to describe the transport of lattice solitons were shown to be incomplete, we will here derive a quantum mechanical description. Specifically we are interested in the transport of the COM of a soliton when $\mathcal{H}_0(t)$ is adiabatically varied over a period T , where the translational invariance is not changed. The instantaneous eigenstates of $\mathcal{H}(t)$ can be classified in terms of the conserved COM momentum K and a band index μ , and will be denoted as $|E_\mu(K)\rangle$ with energy $E_\mu(K)$.

The time evolution of the center of mass position of the N particles, $\hat{X} = \sum_{j=1}^N \hat{x}_j/N$, is governed by the N -particle velocity operator $\partial_t \hat{X} = \hat{V} = -i[\hat{X}, \mathcal{H}] = -i[\hat{X}, \mathcal{H}_0]$, which can be conveniently expressed in terms of a momentum-shifted Hamiltonian $\mathcal{H}(q) = e^{-iq\hat{X}} \mathcal{H} e^{iq\hat{X}}$. I.e. $\hat{V} = \hat{V}(q)|_{q=0}$ with $\hat{V}(q) = e^{-iq\hat{X}} \hat{V} e^{iq\hat{X}} = \partial \mathcal{H}(q)/\partial q$.

$$\frac{d}{dt} \langle \hat{X} \rangle = \left\langle \hat{V}(q) \right\rangle_{q=0} = \left\langle \frac{\partial \mathcal{H}(q)}{\partial q} \right\rangle_{q=0}. \quad (4)$$

In the following we discuss the topological contributions to $d\langle \hat{X} \rangle/dt$ for degenerate and non-degenerate bands separately.

A. Non-degenerated soliton bands

Let us first consider a non-degenerate soliton band, i.e. for a given COM momentum K there is only one eigenstate for each energy value in the whole pump cycle. In order to calculate the transport of a soliton from a single non-degenerate band, one can follow the well-known arguments for the transport of a single particle [2, 28]. To account for the topological transport starting in an instantaneous eigenstate $|E_0(K, t)\rangle$ at time t , one has to take into account non-adiabatic corrections. As the modulation of the Hamiltonian does not affect the translational invariance, non-adiabatic transitions only couple to states with the same COM momentum. Non-degenerate time-dependent perturbation theory yields

$$|\Psi(K, t)\rangle = |E_0(K)\rangle + i \sum_{\alpha \neq 0} |E_\alpha(K)\rangle \frac{\langle E_\alpha(K) | \partial_t E_0(K) \rangle}{E_\alpha(K) - E_0(K)} \quad (5)$$

where we have suppressed the dependence on time for notational simplicity. We note that $|\partial_t E_0(K)\rangle$ is orthogonal to $|E_0(K)\rangle$ and that the second term in the above expression is small. Calculating the average velocity in

this states gives in lowest order of perturbation theory

$$\begin{aligned} \langle \hat{V}(q=0, t) \rangle &= \frac{\partial E_0(K)}{\partial K} + \\ &+ i \sum_{\alpha \neq 0} \left(\frac{\langle E_0 | \partial_q \mathcal{H}(q) |_{q=0} | E_\alpha \rangle \langle E_\alpha | \partial_t E_0 \rangle}{E_\alpha - E_0} - c.c. \right) \\ &= \frac{\partial E_0(K)}{\partial K} + i \left(\left\langle \left. \frac{\partial E_0}{\partial t} \right| \frac{\partial E_0}{\partial K} \right\rangle - c.c. \right). \end{aligned} \quad (6)$$

For the second step we used

$$\begin{aligned} 0 &= \partial_q \langle E_0 | \mathcal{H}(q) | E_\alpha \rangle \\ &= \langle E_0 | \partial_q \mathcal{H}(q) | E_\alpha \rangle + E_0 \langle E_0 | \partial_q E_\alpha \rangle + E_\alpha \langle \partial_q E_0 | E_\alpha \rangle \end{aligned} \quad (7)$$

as well as

$$0 = \partial_q \langle E_0 | E_\alpha \rangle = \langle E_0 | \partial_q E_\alpha \rangle + \langle \partial_q E_0 | E_\alpha \rangle. \quad (8)$$

The first term in expression Eq. (6) describes the dynamical contribution to the transport. If we consider an initial state that has equal probability in all COM momenta K in the Brillouin zone $\{-\pi, \pi\}$, the dynamical contribution vanishes. Then, the shift of the center of mass of the soliton in one period T is given by the second term integrated over all COM momenta K

$$\Delta \langle \hat{X} \rangle = i \int_0^T dt \int_{-\pi}^{\pi} \frac{dK}{2\pi} \left(\left\langle \left. \frac{\partial E_0}{\partial t} \right| \frac{\partial E_0}{\partial K} \right\rangle - c.c. \right) = C. \quad (9)$$

This is the effective single-particle Chern number of the soliton Bloch band. Note that we did not make any assumption about the many-body wavefunction other than its gapfulness. In particular, no assumption about its behavior in the *relative* coordinates of the particles was made. However, the assumption of gapfulness of the N -particle state with fixed COM momentum K requires in general that the N particles are bound to each other.

B. Degenerated soliton bands

In the degenerate case, i.e. if there are crossings of m bands at some points in time, we need to apply degenerate time-dependent perturbation theory to an m component vector $|\underline{\Psi}(K)\rangle = (|\Psi_0(K)\rangle, \dots, |\Psi_{m-1}(K)\rangle)^\top$ and can express the time-evolved state as [29]

$$\begin{aligned} |\underline{\Psi}(K, t)\rangle &= \mathcal{T} \exp \left\{ -i \int_0^t d\tau \mathbf{A}_K(\tau) \right\} |\underline{\Psi}(K, 0)\rangle \\ &+ \text{non-adiabatic terms}, \end{aligned} \quad (10)$$

where

$$\begin{aligned} \mathbf{A}_K(\tau) &= \\ &\begin{pmatrix} E_0 & -i\langle E_0 | \partial_t E_1 \rangle & -i\langle E_0 | \partial_t E_2 \rangle & \dots \\ -i\langle E_1 | \partial_t E_0 \rangle & E_1 & -i\langle E_1 | \partial_t E_2 \rangle & \dots \\ -i\langle E_2 | \partial_t E_0 \rangle & -i\langle E_2 | \partial_t E_1 \rangle & E_2 & \dots \\ \dots & \dots & \dots & \dots \end{pmatrix} \end{aligned} \quad (11)$$

is the Wilczek-Zee non-Abelian Berry phase, and non-adiabatic terms denotes the perturbative contributions due to non-adiabatic couplings to other, energetically separated states similar to the non-degenerate case. We note that since $\langle E_l | \partial_t E_m \rangle = (\langle E_l | \partial_t \mathcal{H} | E_m \rangle) / (E_m - E_l)$ (compare Eq. (7) and (8)), the eigenstates of the matrix \mathbf{A}_K coincide with the bare states $|E_0\rangle \dots |E_m\rangle$ far away from the crossing point in the adiabatic limit. At the crossing point the off-diagonal elements however diverge in general, which leads to a mixing.

Suppose the cyclic change of the Hamiltonian starts at a point where there is no degeneracy between COM bands and the system is prepared in one band, say $|E_0(K)\rangle$. Then, in the presence of isolated crossing points with other bands $|E_\alpha(K)\rangle$, a single cycle $t = 0 \rightarrow t = T$ will in general not return the initial state to itself, but multiple cycles are needed. Therefore, the topological transport is only integer quantized after multiple cycles, giving rise to a fractional average transport per cycle. In this case where there are crossings of soliton bands at some point in time, say of $|E_0(K, t)\rangle$ and $|E_1(K, t)\rangle$, the Chern number must be generalized to a Wilson loop

$$C_n = \frac{1}{2\pi} \int_0^T dt \partial_t \text{Im} \log \det \mathbf{P}(t) \quad (12)$$

where $\mathbf{P}(t) = \mathcal{T} \exp \left\{ -i \int_{\text{BZ}} dK \mathbf{B}_t(K) \right\}$, and

$$\mathbf{B}_t = \begin{pmatrix} E_0 & -i\langle E_0 | \partial_K E_1 \rangle \\ -i\langle E_1 | \partial_K E_0 \rangle & E_1 \end{pmatrix} \quad (13)$$

is the Wilczek-Zee non-Abelian Berry phase [29] for fixed time, here for $n = 2$ crossing bands. C_n is an integer and the *average* topological transport per cycle in the n bands is given by C_n/n .

The COM transport of a soliton is then *fractional*, provided it returns to its original band only after n periods. We will show that this is the case for the Aubry-André-Harper model of Ref. [13].

IV. CHERN NUMBER AND WILSON LOOP OF SOLITONS IN THE AAH MODEL

While the soliton band structure can be well approximated by a self-consistent solution of the DNLSE, the many-body eigenstates and the Chern number, Eq. (9), or the Wilson loop, Eq. (12), must be obtained from solving the many-body Schrödinger equation, which constitutes a substantial challenge for more than a few particles. To tackle this problem we introduce the following basis of states with a fixed K [30, 31]

$$|\Psi_\alpha(K)\rangle = \sum_{m=0}^{L-1} (e^{iK\hat{T}})^m |\Phi_\alpha(0; K)\rangle. \quad (14)$$

Here we assume a lattice with L unit cells, each containing p sites, and periodic boundary conditions. The states

$$|\Phi_\alpha(0; K)\rangle = \sum_{\{n_l\}}' c_\alpha[\{n_l\}; K] |\{n_l\}\rangle$$

describe the distribution of particles $n_l = \{n_{-pL/2+1} \dots n_{pL/2}\}$ around the lattice site $l = 0$ (conveniently chosen close to the center of mass of all particles), with coefficients $c_\alpha[\{n_l\}, K] = c_\alpha[n_{-pL/2+1} \dots n_{pL/2}; K]$ and $|\{n_l\}\rangle$ being a number state. We assume for simplicity that L is even. $\sum'_{\{n_l\}}$ denotes summation over all n_l 's for which $\sum_l n_l = N$. Translation by a unit cell gives $\hat{T}|\Phi_\alpha(0, K)\rangle = |\Phi_\alpha(p, K)\rangle$. (Note that in order to guarantee orthonormality, states $|n_{-\frac{pL}{2}+1}, \dots, n_{\frac{pL}{2}}\rangle$ must not be eigenstates of \hat{T} .) Now we can make use of the fact that for large attractive interactions the solitons have a small localization length ξ . Thus we can restrict ourselves to special cases: (i) two-site solitons where the basis states have at most two (neighboring) sites populated (i.e. $n_0, n_1 = N - n_0 \neq N$ in general) and (ii) three-site solitons where three adjacent lattice sites might be populated (i.e. $n_0, n_1, n_2 = N - (n_0 + n_1) \neq N$ in general). In the basis of COM-momenta K the many-body Hamiltonian (Eq. (1)) is block diagonal, i.e. the COM-momenta are decoupled. For the two-site solitons the block dimension is $p \cdot N$, for the three-site soliton it is $p \cdot N(N+1)/2$, which allows us to perform numerical simulations for tens to hundreds of particles. Due to the limitation to two-site or three-site solitons, some of the higher energy solutions are not true eigen-solutions, but are enforced by the boundary conditions. These states can be detected, however, by comparing two and three-site solutions and are not relevant in the low-energy regime, discussed here.

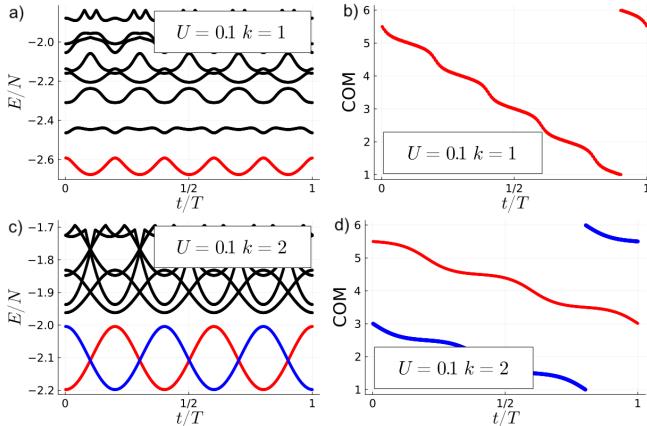


FIG. 3: Instantaneous soliton energies for 10 particles for attractive interaction $U = 0.1$ with phase-offset $k = 1$ in (a) and with phase-offset $k = 2$ in (c), and unit-cell size $p = 5$. The corresponding COM-movements in a pump cycle of the red and blue marked energies are shown in (b) and (d). The solutions are obtained with the three-site soliton ansatz.

In Fig. 3 we have plotted the energies of the soliton bands for the AAH model, Eq. (1), and the COM transport, for $N = 10$ particles with unit cell size $p = 5$ and $U = 0.1$ for phase offsets $k = 1$ and $k = 2$. In the first

case (Fig. 3 a, b) there is a single lowest-energy soliton band with many-body Chern number, Eq. (9), $C = 1$ and integer transport. In the second case (Fig. 3 c, d) two bands cross with a non-trivial Wilson loop, Eq. (12), $C_2 = 1$ giving rise to fractional transport of $1/2$.

V. TOPOLOGICAL PHASE TRANSITIONS

In the following we provide an explanation for the transitions between phases with integer, fractional and vanishing transport observed in the experiments. The COM dynamics of bound N -particle objects (solitons) can be described by an effective single-particle Hamiltonian with eigenstates $|E_\mu(K)\rangle$:

$$\mathcal{H}_{\text{eff}} = \sum_\mu \sum_K E_\mu(K) |E_\mu(K)\rangle \langle E_\mu(K)|. \quad (15)$$

Since such a model misses out the continuum of extended states, it is only adequate for stable soliton bands. Defining annihilation and creation operators for solitons centered at lattice site l as \hat{d}_l and \hat{d}_l^\dagger , respectively, the effective soliton Hamiltonian would read in coordinate space

$$\mathcal{H}_{\text{eff}}(t) = - \sum_l \left[(J_{l,\text{eff}}(t) \hat{d}_l^\dagger \hat{d}_{l+1} + \text{h.c.}) + \epsilon_{l,\text{eff}}(t) \hat{d}_l^\dagger \hat{d}_l \right]. \quad (16)$$

where the $J_{l,\text{eff}}$ are the effective hopping rates of the soliton and the $\epsilon_{l,\text{eff}}$ effective local energies. (Note that we here have assumed only nearest neighbor hopping.) All topological properties, including the topological classification according to the Altland-Zirnbauer scheme [24, 25], as well as all phase transitions of solitons are determined by this effective Hamilton. We will explicitly construct \mathcal{H}_{eff} for $N = 3$ particles in the strong interaction limit in Sec. VII. Here we will first discuss some of its general properties.

In the Aubry-Andre-Harper model, Eq. (1), any small attraction U_0 is sufficient to form a bound state (lattice soliton) with an energy band below the continuum of extended N -particle states, if N is large. Increasing the attractive interaction, the energy of these bands is lowered and the bands deform. Moreover, excited soliton bands can emerge. If the soliton bands have a non-trivial Chern number or Wilson loop, (fractional) quantized topological transport can be observed [6, 13].

The experiments in [6, 13] and DNLSE simulations showed that for very large but still finite values of the interaction, the topological transport stops altogether. This can be understood as follows: In the large U limit the localization length of all soliton solutions is reduced to a single lattice site. Thus the contribution of the local interaction to the energy, $UN(N-1)/2$, is the same for all soliton bands and the total number of stable soliton bands in this limit is equal to the number of single-particle bands. Using a perturbative ansatz one can show that moreover the contribution of the kinetic energy can

be disregarded as it scales as $\sim J(\frac{J}{U})^{N-1}$ (see Appendix and Ref. [32]). Thus the effective soliton Hamiltonian becomes approximately diagonal and is entirely determined by local energies $\epsilon_{l,\text{eff}}$, which for the AAH model result from virtual hopping processes of a single particle from the soliton site l to an empty neighboring site (and back) and are in second-order perturbation theory proportional to $\epsilon_l \sim (J_l^2(t) + J_{l+1}^2(t))/U$. As a consequence, all soliton bands cross at different points of the pump cycle and the topological transport is given by the total Wilson loop of all COM bands, which is always zero for general reasons.

The two limiting cases show that as U is increased, initially separated soliton bands must approach each other and eventually merge. As shown in Fig. 4, obtained from exact diagonalization (ED) simulations of a small system (30 lattice sites), they do so by forming Dirac-like cones which touch at a critical interaction U_c . In this case the Chern numbers of the lowest two soliton bands are no longer adequate topological invariants, but one has to consider the Wilson loop. The topological transport can then become fractional, provided the soliton solutions which started at $t = 0$ in energetically well separated bands flip bands at the Dirac-like points. We now show that this is indeed the case:

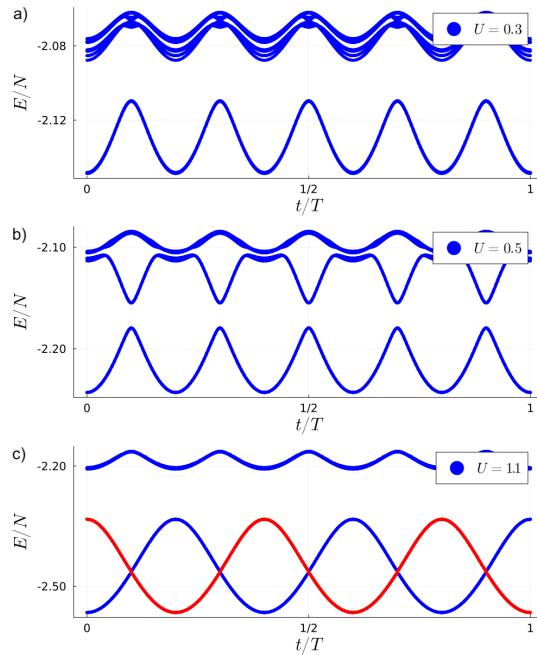


FIG. 4: Merging of soliton energies obtained from exact diagonalization with increasing interaction strength U for $N = 3$ particles and $p = 5$, $k = 2$. The number of unit cells is $L = 6$. A soliton originally prepared at $t = 0$ in one of the two bands will remain in this band if the changes are adiabatic and the soliton bands do not touch (Figs. a) and b)). Once the bands touch in Dirac-like cones, the solution switches bands at every crossing (red curve in Fig. c)). The width of the lines reflects the width of the soliton bands in K space.

When the two soliton bands touch, the adiabatic evolution is governed by a $U(2)$ transformation [29] (compare Eq. (10) in Sec. III B)

$$|\Psi(K, t)\rangle = \mathcal{T} \exp \left\{ -i \int_0^t d\tau \mathbf{A}_K(K, \tau) \right\} |\Psi(K, 0)\rangle \quad (17)$$

Close to the crossing points, which we assume to take place at $t = t_0$, the non-Abelian Berry phase \mathbf{A}_K takes on the form

$$\mathbf{A}_K = \begin{pmatrix} a|\tau| & \frac{ib}{\tau} \\ -\frac{ib}{\tau} & -a|\tau| \end{pmatrix}, \quad (18)$$

with $\tau = t - t_0$. Here, we assumed that apart from a common energy offset $E_0 = -E_1 = a|\tau|$, and thus $\langle E_0 | \partial_t \mathcal{H} | E_1 \rangle / (E_1 - E_0) \approx b/\tau$. Due to the diverging off-diagonal elements, the eigensolutions no longer follow the original bands but cross from one band to the other (see color code in Fig. 4 c)). Since p is a prime number, there is an odd number of crossing points in one period in the AAH model. Thus, two periods are required for a soliton to return to the band it started from. The shift in the COM position is then integer quantized only after two periods and the average transport per cycle is fractionally quantized.

VI. FAILURE OF TRANSPORT QUANTIZATION

Based on solutions of the mean-field DNLSE it was shown in Ref. [15] for the example of the Rice-Mele model [33–35] with local attractive interactions that the transition between quantized topological pumping of a soliton to zero pumping upon increasing the interaction strength may go through an intermediate regime of non-quantized transport. This transient failure of transport quantization, where $\langle \Delta \hat{X} \rangle$ strongly fluctuates, was attributed in [15] to a "self-crossing" of solutions of the semiclassical DNLSE. This phenomenon can be easily understood in the full quantum picture. For intermediate interactions, the excited soliton band is in some parts of the pump cycle degenerate with the continuum of extended states and thus unstable. If this band merges with the lower soliton band, the time evolution is no longer adiabatic and the transport is not quantized until the interaction is large enough such that also the excited band becomes fully gapped. In Fig. 5 we show the soliton bands in the Rice-Mele model with different values of the attractive onsite interaction U obtained from exact diagonalization simulations of a $N = 4$ soliton. Although only marginally visible due to finite size effects, Fig. 5b indicates the existence of a parameter range where the lowest soliton band merges with an unstable excited band leading to a fluctuating, non-quantized transport.

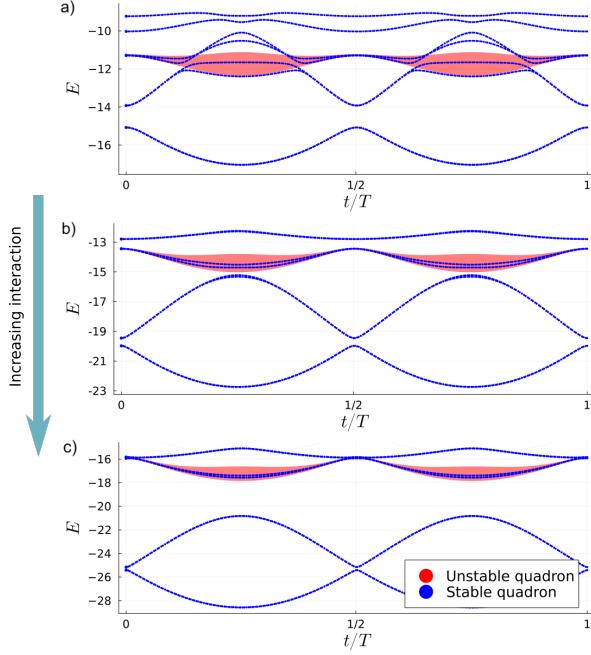


FIG. 5: Breakdown of transport quantization in the Rice-Mele model for intermediate values of onsite interactions. Shown are lowest energies for $N = 4$ bosons. a) $U = 2.0$: lowest soliton (quadron) band is gapped with Chern number $C = 1$ ($\langle \Delta \hat{X} \rangle = 1$). b) $U = 3.0$: lowest two bands merge but (except for finite-size effects) overlap with extended states (unstable quadron) where the transport is not quantized. c) $U = 4.0$ lowest two quadron bands merge with vanishing Wilson loop ($\langle \Delta \hat{X} \rangle = 0$).

VII. EFFECTIVE HAMILTONIAN: TRIPOLON MODEL

We can explicitly construct the effective soliton Hamiltonian in the strongly interacting limit where the non-interacting part of the Hamiltonian, Eq. (1), can be treated as a small perturbation and the solitons become maximally localized (i.e. with a localization length ξ smaller than the lattice spacing).

In this limit, the binding energy $\frac{U}{2}N(N-1)$ is equal for all soliton solutions and will be disregarded. Transport of the composite object occurs through collective hopping of particles, arising in N th order perturbation theory, which has a very small effective amplitude of $\sim J^N/U^{N-1}$ [32]. At the same time, virtual hopping processes of particles from the soliton site to a neighboring site and back give rise to local energy shifts with an amplitude proportional to $\sim J^2/U$. As shown in detail in the Appendix, this results in the effective energies and hopping amplitudes

$$\epsilon_{l,\text{eff}} = \frac{3}{2} \frac{J_{l-1}^2 + J_l^2}{U}, \quad J_{l,\text{eff}} = \frac{3}{2} \frac{J_l^3}{U^2} \quad (19)$$

for the triplon model (i.e. $N = 3$). (For effective Bloch Hamiltonians of bound doublons and their topological

features see also [36–38]).

$$\mathcal{H}_{\text{eff}}(t) = - \sum_l \left[(J_{l,\text{eff}}(t) \hat{d}_l^\dagger \hat{d}_{l+1} + h.c.) + \epsilon_{l,\text{eff}}(t) \hat{d}_l^\dagger \hat{d}_l \right]. \quad (20)$$

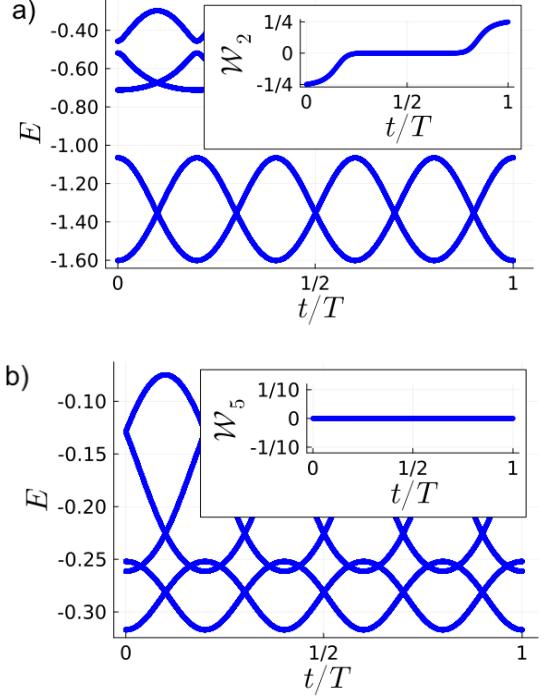


FIG. 6: Instantaneous soliton energies of the effective triplon model, Eq. (19), for attractive interaction $U = 5$ in (a), and $U = 20$ in (b), phase-offset $k = 2$ and unit-cell size $p = 5$. The insert shows the winding of $\mathcal{W} = \text{Im} \log \det \mathbf{P}(t)$, Eq. (12), determining the Wilson loop.

In Fig. 6 we have shown the soliton energies of the effective triplon model for two different interaction strengths for the AAH model along with the integrand of the Wilson-loop in Eq. (12) $\mathcal{W}_m = \text{Im} \log \det \mathbf{P}(t)$, where m is the number of crossing bands. One clearly sees that for increased interaction strength the bands merge. Eventually, all 5 bands cross and there is no winding of \mathcal{W}_5 , i.e. the total Wilson loop vanishes. Thus, despite the fact that the soliton mass is still finite, the topological transport vanishes exactly.

VIII. SUMMARY AND OUTLOOK

We developed a full quantum description of topological pumps of self-bound N -particle states, i.e. lattice solitons. The quantum description allowed us to identify and to explicitly calculate a topological invariant, i.e. an effective single-particle Chern-number or Wilson-loop explaining the emergence of integer and fractional transport in the full range of interaction strength, where

perturbative arguments [14, 19] fail. Transitions between phases of differently quantized topological transport observed in experiments [6, 13] as well as the possibility of parameter regimes without quantized transport were explained by coalescence of soliton bands and possible degeneracies with extended states. The concept can easily be extended to multi-component solitons [20, 21, 39], where, among other things, fractional transport was predicted despite the fact that all single-particle bands are topologically trivial. In the latter case interactions not only lead to the modification of topological properties, such as the transition from integer to fractional phases, but to the *emergence* of topology.

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APPENDIX

To derive an effective model for strongly localized composite particles, let us first look at the binding energy of such a maximally localized soliton in the AAH model (1) (i.e. a localization length ξ smaller than the lattice spacing) which has a binding energy given by

$$E_{\text{int},N} = \frac{U}{2} N(N-1) \quad (21)$$

whereas states with $N-1$ localized particles have an energy

$$E_{\text{int},N-1} = \frac{U}{2} (N-1)(N-2). \quad (22)$$

The energy difference $|E_{\text{int},N} - E_{\text{int},N-1}|$ is $U(N-1)$. So if U is sufficiently larger than the bose-enhanced hopping $\sqrt{N}J$, the energetically lowest states are localized solitons.

To derive an effective description of the maximally localized solitons, as proposed in Eq. (16), we have to identify the relevant processes, treating the particle hopping as perturbation. These processes have to be resonant between the degenerate groundstates of the interaction Hamiltonian \mathcal{H}_{int} [32]: For the effective potential, it is the virtual hopping of a single-particle occurring in second order perturbation theory

$$\sim \hat{a}_l^\dagger \hat{a}_{l+1} \hat{a}_{l+1}^\dagger \hat{a}_l |\Psi\rangle.$$

On the other hand, the effective hopping of the complete composite particle emerges only in N th order perturbation theory

$$\sim (\hat{a}_{l+1}^\dagger \hat{a}_l)^N |\Psi\rangle.$$

The amplitude for the virtual hopping scales as $\sim 1/U$, while the effective hopping goes with $\sim 1/U^{N-1}$.

The minimal particle number: Triplons – In the following we will explicitly calculate an effective Hamiltonian for the minimal possible particle number: the triplon. For a composite object consisting of only two particles, both processes (virtual and effective hopping) would have the same scaling $1/U$ and therefore the interaction has no qualitative influence on the system properties.

The effective potential is calculated directly within second order perturbation theory of the Hamiltonian and is given as

$$\epsilon_{l,\text{eff}} = \frac{3}{2} \frac{J_{l-1}^2 + J_l^2}{U}. \quad (23)$$

Calculating the effective triplon hopping in perturbation theory is possible but already requires good bookkeeping since it is a third order process.

Therefore, we will take a look at the local basis of two sites for three particles:

$$|30\rangle, |21\rangle, |12\rangle, |03\rangle.$$

The local Hamiltonian for these states can be written in matrix form:

$$\begin{pmatrix} -3U & -\sqrt{3}J_l & 0 & 0 \\ -\sqrt{3}J_l & -U & -2J_l & 0 \\ 0 & -2J_l & -U & -\sqrt{3}J_l \\ 0 & 0 & -\sqrt{3}J_l & -3U \end{pmatrix}.$$

Here we assume - without loss of generality - the left site is located at position l in our system. Diagonalizing this 4x4-matrix yields four eigenstates. The two low-energy eigenstates are (for sufficient large values of the interaction strength U):

$$|\psi_{\pm}\rangle \propto |30\rangle \pm |03\rangle.$$

The corresponding eigenenergies are:

$$E_{\pm} \propto \mp t - 2U - \sqrt{4t^2 \mp 2tU + U^2}.$$

In the effective Hamiltonian (compare Eq. (16)) the eigenenergies of $|\psi_{\pm}\rangle$ can be shown to be

$$\begin{aligned} E_{\text{eff},\pm} &= \mp J_{l,\text{eff}} + \text{const} \\ E_{\text{eff},+} - E_{\text{eff},-} &= -2J_{l,\text{eff}} \end{aligned}$$

Given these two relations we can Taylor expand the energy difference $E_+ - E_-$ for small values of the hopping amplitude and extract the effective hopping:

$$J_{l,\text{eff}} = -\frac{E_+ - E_-}{2} = \frac{3}{2} \frac{J_l^3}{U^2} + \mathcal{O}\left(\frac{J_l^5}{U^4}\right). \quad (24)$$

With both the virtual and the effective hopping Eqs. (23) and (24) we can calculate an effective single-particle Hamiltonian Eq. (16) reflecting the same physics as the full model in the strong interacting limit.

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