Fractionally quantized charge pumping in a one-dimensional superlattice

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A one-dimensional quantum charge pump transfers a quantized charge in each pumping cycle. This quantization is topologically robust being analogous to the quantum Hall effect. The charge transferred in a fraction of the pumping period is instead generally not quantized. We show, however, that with specific symmetries in parameter space constraining the pumping protocol, the charge transferred at well-defined fractions of the pumping period is quantized as integer fractions of the Chern number. We discuss the relevance of this fractionally quantized charge pumping for cold atomic gases in one-dimensional optical superlattices with closed as well as open geometries.

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Three decades ago, it was established that the quantized Hall conductance of the integer quantum Hall effect (QHE) [1] is a topologically invariant [2] classifying the ground state of the system. The recent discovery of topological insulators both in two-dimensional (2D) [3–4] and three-dimensional (3D) systems [5, 6] has enormously boosted the interest in topologically non-trivial states of matter. Apart from these presently much studied 2D and 3D states of matter, there is another quantum phenomenon of topological origin: the one-dimensional (1D) quantum charge pump. Thouless [7] has shown indeed that the amount of charge pumped in one cycle can be expressed in terms of the Chern invariant precisely as in the 2D QHE. The strict analogy among these two phenomena is also reflected in the profound relations among the 2D QHE Hamiltonian and the 1D Harper model and its off-diagonal variant [7–10].

To verify the topological nature of the charge pumped during a cycle, in a recent experiment the off-diagonal Harper model was implemented in a photonic waveguide array [11]. The periodic modulation of the on-site potential was produced by controlling inter-waveguide distances. By adiabatically varying the relative phase between the modulation and the underlying lattice, light was pumped across the sample, revealing the topological nature of the pumping. Other experiments which have reported the realization of the Harper Hamiltonian have instead used the interaction between cold atoms and lasers to create a system that exhibits Hofstadter excitations. As reported in Refs. [12, 13], rubidium atoms were loaded in an optical lattice and external lasers were used to coax the atoms into circular motion, analogous to the motion of electrons in a magnetic field.

These advances on the experimental side renewed the interest [11, 14, 15] in the theory of the quantum charge pump. In this paper we uncover an important property of quantum charge pumps with additional symmetries in the parameter space: at well-defined fractions of the pumping period the system transfers a fractionally quantized charge whose value is directly related to the Chern invariant of the system. As we show below, this is a consequence of the underlying symmetries of the gauge-invariant Berry curvature in parameter space.

We start illustrating this point and recalling that in a Bloch electron system the Chern number of an occupied electron band is proportional to the integral of the Berry curvature over the whole Brillouin zone [6, 10]. The Chern number is topologically invariant and is quantized as an integer number provided there is a full gap separating the set of j occupied bands and the first unoccupied band. Let us then consider the case where additional point or space group symmetries induce a partitioning of the Brillouin zone into subregions which are transformed one into the other under a certain group of symmetry transformations. More precisely, one can imagine a number q of simply-connected and non-overlapping subsets S_n which cover the whole Brillouin zone, as shown in Fig. 1(a) and such that the Bloch states |ψ(k)⟩ are equivalent up to a gauge transformation, i.e., |ψ(k′)⟩ = e^{iθ(k′)}|ψ(k)⟩ with k′ ∈ S_n and k ∈ S, since the Berry curvature is a gauge-invariant measurable quantity — it is defined as Ω(k) = [∇_k × A(k)] · z, where A(k) = −i⟨ψ(k)| ∂z/∂k|ψ(k)⟩ is the Berry connection — the total Chern number can be evaluated as a sum of integrals of the Berry curvature over each of the subsets.
chain at the time \(t\). The number of electrons transported across any section of the chain at the time \(t\), can be expressed as an integral over the Brillouin zone [7, 17].

If, as stated above, the symmetries of the Hamiltonian are robust against any perturbation preserving the parameter space, then it follows that the charge transferred, i.e., the number of electrons transported across any section of the Brillouin zone \([7, 17]\),

\[
Q(t) = \frac{i}{\pi} \sum_{i < j} \int_{\varphi(0)}^{\varphi(t)} d\varphi \int_{BZ} dk \Im \left\{ \frac{\partial \psi_i}{\partial \varphi} \frac{\partial \psi_j}{\partial k} \right\},
\]

where \(j\) is the total number of filled bands of the system and \(|\psi_i\rangle = \psi_i(k, \varphi) c^\dagger_i |0\rangle\) the \(ith\) band eigenstate, being \(c^\dagger_i\) the creation operator of the \(ith\) band acting on the ground state \(|0\rangle\). The second integral in Eq. (2) can be related to the Zak phase [18] of the system while the charge transferred can be written in terms of the variation of the charge polarization of the 1D system along the path \(\Delta \varphi = \varphi(t) - \varphi(0)\) (c.f. Appendices).

Since the underlying time-dependent Hamiltonian of the system is periodic both in the parameter \(\varphi\) and in the 1D momentum \(k\), it follows that, for an evolution over a full period \(T\), the parameter space corresponds to a torus and \(2\pi Q\) is nothing but the Berry phase over this closed manifold. However, the integral over the full torus can be seen as composed of \(q\) non-overlapping subsets, as shown in Fig. 1(a) in which the momentum \(k\) traces a circle while the parameter \(\varphi \in [\varphi(0), \varphi(T/q)]\). If, as stated above, the symmetries of the Hamiltonian in the parameter space mandate that all these integrals give an equal contribution then it follows that the charge transferred in the \(T/q\) fraction of the pumping period is \(Q(T/q) = C_j/q\). Hence the partitioning of the torus in parameter space combined with the symmetry of the Berry curvature leads to a well-defined physical response: a fractionally quantized pumped charge. This fractionalization is robust against any perturbation preserving the symmetries of the parameter space.

Next we show how such a situation can be achieved in a time-varying 1D superlattice generated by an external potential periodic in real space. Specifically, we consider a system of spinless particles at zero temperature confined in a 1D lattice, like the one in Fig. 1(b) subject to a weak external potential with period \(1/\alpha\) times the lattice parameter. The system is described by the tight binding Hamiltonian

\[
\mathcal{H} = \sum_k \Delta \varepsilon \cos (2\pi \alpha R_k + \varphi) c_k^\dagger c_k - \sum_{<i,j>} t c_i^\dagger c_j,
\]

where \(\Delta \varepsilon\) is the characteristic perturbation strength while \(\varphi\) is an arbitrary phase which we will assume to vary linearly in time. We note here that this Hamiltonian describes either spinless fermions [14] or hardcore bosons in 1D optical superlattices. In momentum space, the tight binding Hamiltonian [4] becomes

\[
\mathcal{H} = \sum_k -2t \cos k c_k^\dagger c_k + \Delta \varepsilon \frac{e^{i\varphi}}{2} c_k^\dagger e^{2\pi i k} c_k + \text{h.c.},
\]

which is not diagonal with respect to Bloch states, as the substrate periodicity couples states with momenta \(k' = k - 2\pi \alpha\).

The non-trivial topological properties of the model Hamiltonian [4] can be revealed by considering the external perturbation to be commensurate with the lattice, i.e., \(\alpha = p/q\) with \(p < q\) coprimes, leading to a superlattice with \(q\) atoms in the unit cell and a corresponding mini-Brillouin zone \(k \in [0, 2\pi/q]\). Fig. 2 shows the ensuing energy spectra obtained by diagonalizing Eq. (3) with the phase \(\varphi\) varying in the interval \([0, 2\pi]\), for rational values of the commensuration \(\alpha\) and different values of the substrate modulation intensity \(\Delta \varepsilon\). The energy spectrum in the case \(\Delta \varepsilon = 2t\) [Fig. 2(a)] coincides with the well known Hofstadter spectrum [19] of a 2D electron system on a square lattice subject to a uniform magnetic field oriented perpendicularly to the lattice plane. Similarly, the energy spectra obtained for \(\Delta \varepsilon \neq 2t\) [c.f. Figs. 2(a) and 2(b)] correspond to the Hofstadter spectra in the case of rectangular lattices. This result is an immediate consequence of the mapping [15] among the lattice version of the integer QHE problem and the 1D Hamiltonian [4]. Since any of the \(q - 1\) gaps of the Hofstadter butterfly
corresponds to a gapped state of the 1D system in the full torus spanned by \( k \) and \( \varphi \), one can identify the charge transferred of the 1D system with the Chern number \( C_j \) labeling the \( j \)th gap of the Hofstadter butterfly \(^{2}\) and given by the unique (nonzero) integer solution \(|C_j| < q/2\) of the Diophantine equation \(^{20}\) \( nq - pC_j = j \).

Having established the quantized particle transport in the time-varying 1D systems, we now proceed to reveal the symmetry of the Hamiltonian \(^{3}\), which leads to a fractionally quantized charge pumping. To do so, we introduce the translation operator \( T(n) \) which translates the whole system of \( n \) lattice sites, and the phase shift operator \( \Pi(\Delta \varphi) \) which transforms the phase of the time-varying perturbation as \( \varphi \rightarrow \varphi + \Delta \varphi \). It is possible to verify, by a direct substitution in the Hamiltonian \(^{3}\), that the system is invariant under the transformation \( T(-n)\Pi(2\pi a n)H = H \) and therefore \( T(n) = \Pi(2\pi a n) \), i.e., the translation of \( n \) lattice sites corresponds to a change in the modulation phase of \( \Delta \varphi = 2\pi a n \). If \( n, m \) are any of the integer solutions of the Diophantine equation \( np + mq = 1 \), one has that \( \Pi(2\pi a n) = \Pi(2\pi/q - 2\pi m) = \Pi(2\pi/q) \). Therefore, one can conclude that there exists an integer \( n \) such that \( \Pi(2\pi/q) = T(n) \), i.e., a change in the modulation phase \( \Delta \varphi = 2\pi/q \) is equivalent to a translation of the system of an integer number of lattice sites and thus the Hamiltonian \(^{1}\) is invariant up to a change of the modulation phase equal to \( 2\pi/q \). This is immediately manifested in Fig. 1(b) where the different configurations of the system for \( \varphi = 2\pi n/3 \) are all equivalent up to lattice translations.

Let us now consider the charge transferred for an adiabatic evolution \( \varphi \rightarrow \varphi + 2\pi/q \). As a consequence of the periodicity in parameter space, any such an evolution contributes equally to the integral in Eq. \( (2) \), for any initial modulation phase \( \varphi \). This implies that the total transferred charge over the cycle \( 2\pi \) is given by \( Q(2\pi) = qQ(2\pi/q) \). Hence, the charge transferred in any of the adiabatically gapped phases, described by an adiabatic evolution with \( \Delta \varphi = 2\pi/q \), is quantized in multiples of a fraction \( 1/q \) of the elementary charge

\[
Q \left( \frac{2\pi}{q} \right) = \frac{C_j}{q},
\]

which is the main result of this paper. More generally, for any path corresponding to a phase variation \( \Delta \varphi = 2\pi n/q \) with \( n \) integer, one has \( Q(2\pi n/q) = nC_j/q \). This result is confirmed by a direct calculation of Eq. \( (2) \), where the eigenstates have been obtained via exact diagonalization of the Hamiltonian \(^{4}\). Fig. 3(a) shows the calculated charge transferred as a function of the modulation phase variation \( \Delta \varphi \) for \( p/q = 1/3 \). While the charge transferred in any of the the adiabatically gapped phase \( j \) along the path \( \Delta \varphi = 2\pi \) is quantized as \( Q = C_j \), the charge transferred along \( \Delta \varphi = 2\pi/q \) is quantized as a fraction of the Chern number according to Eq. \( (5) \) independent of the initial phase. As we show in the Appendices, the fractionalization of the pumped charge is robust against perturbations preserving the symmetries of the parameter space. The fractional quantum pumping is also reflected in the shift of the local charge density \( \rho(r, \varphi) = \sum_{i\leq j} |\psi_i(r, \varphi)|^2 \), shown in Fig. 3(b), that has been calculated via exact diagonalization of the system Hamiltonian on the basis of maximally localized Wannier functions \( \phi_i(r) \propto \sum_k e^{i(\mathbf{k}\cdot\mathbf{R}_i - E_i)} u(r) \), with \( u(r) \) an arbitrary periodic function with the same period of the lattice. For each increment \( \Delta \varphi = 2\pi/3 \) we observe a shift of the local charge density of one lattice site, and of one superlattice unit cell for a full pumping cycle. We emphasize that the local charge densities are directly accessible in experiments by in situ measurement of the density distribution, or deduced from time-of-flight imaging \(^{21}\) in cold atoms systems.

In order to connect with experiments, we now show how the fractionally quantized charge pump is related with the shift of the center of charge in a 1D finite system. The center of charge of a system confined in the spatial
range \([0, L]\) is defined as
\[
\langle r(\varphi) \rangle = \frac{1}{N} \sum_{i \leq j} \int_{0}^{L} dr |\psi_{i}(r, \varphi)|^{2} r .
\]

Let us now consider the adiabatic evolution \(\varphi(0) \to \varphi(t)\) taking place in a finite time interval. If one multiplies \(r\) to both terms of the continuity equation \[14\], integrates over space and time, and assumes that the phase parameter is linear in time, one has
\[
N \int_{\varphi(0)}^{\varphi(t)} \frac{d\varphi}{d\varphi} = \int_{0}^{L} dr Q(r) - L \int_{\varphi(0)}^{\varphi(t)} d\varphi J(L, \varphi) ,
\]
where \(Q(r)\) is the pumped charge inside the system, while \(J(L, \varphi)\) is the current density at the edge \(L\). The first integral on the right side of the equation can be written in terms of the average pumped charge \(Q\), while we define the second integral as the edge charge \(\sigma\), i.e., the current at the edge \(L\) integrated over the time interval \([0, t]\). Therefore, along any adiabatic evolution \(\varphi(0) \to \varphi(t)\), the shift of the center of charge \(\Delta r = \langle r(\varphi(t)) \rangle - \langle r(\varphi(0)) \rangle\) is proportional to the sum of the pumped charge and of the edge charge
\[
\frac{N}{L} \Delta r = Q - \sigma .
\]

If the size of the system is large, one can assume that the bulk properties are not affected by finite size effects, and the pumped charge \(Q\) can be approximated with the pumped charge of an infinite system, as in Ref. \[14\].

Fig. 3(c) shows the shift of the center of charge \(\Delta r\) for a finite systems with \(p/q = 1/3, L = 300\) and at filling \(N/L = 1/3, 2/3\). Moreover, as one can see from Fig. 3(c) in the case \(p/q = 1/3\), at any \(\Delta \varphi = 2\pi n/3\), the calculated shift of the center of charge is well described by Eq. \((7)\) with the pumped charge given by Eq. \((5)\), under the assumption that the edge charge \(\sigma\) is quantized as multiples of the elementary charge at \(\Delta \varphi = 2\pi n/3\). Therefore, the quantization of the charge pumped in an infinite system as fractions of the Chern number corresponds to the quantization of the shift of the center of charge in a finite system.

We also point out that finite temperature effects do not interfere with the quantum pumping process for temperatures smaller than the energy gap. For a shallow optical lattice the quantum to thermal behavior is expected to occur at temperatures much larger than the recoil energy \(E_{R}\), and temperature of the order of \(0.1 E_{R}/k_B\) (tens of nK) can be easily achieved in current experiments with, e.g., \(^{40}\)K atoms.

In conclusion, we have shown that for a quantum pump, in presence of additional symmetries, the charge transferred at well-defined fractions of the pumping period is quantized as fractions of the Chern number. This quantization has a topological nature and could be achieved in current experiments with cold atoms in optical superlattices. Demonstration of a fractional quantization of charge could constitute an important step towards the comprehension of topological phases of matter.

**Appendices**

**Polarization in an infinite 1D system**

In this Appendix, we will show how in an infinite 1D system, the variation of the polarization equates the pumped charge during an adiabatic evolution. An obvious way to define the polarization in a 1D system is
\[
P(\varphi) = \frac{1}{L} \sum_{i \leq j} \int_{0}^{L} dr \rho_i(r, \varphi) r ,
\]
with \([0, L]\) the unit cell, and where \(\rho_i(r, \varphi)\) is the charge density of the \(i\)th of the \(j\) occupied bands. However, it can be shown that this definition is ill-defined \[22\], since in this way the polarization would depend on the choice of the unit cell. Following Refs. \[22\] \[23\] one can instead define the polarization in terms of the Zak phase \[18\] as
\[
P(\varphi) = -\frac{1}{2\pi} \sum_{i \leq j} \int_{BZ} dk A_{i,k}(k, \varphi) ,
\]
where \(A_{i,k}(k, \varphi) = -i \langle \psi(k)|\frac{\partial}{\partial k}|\psi(k)\rangle\) is the component \(k\) of the Berry connection of the \(i\)th band. The variation of the polarization along an adiabatic evolution \(\varphi(0) \to \varphi(t)\) is given by
\[
\Delta P = P[\varphi(t)] - P[\varphi(0)] = \int_{\varphi(0)}^{\varphi(t)} d\varphi \frac{\partial P(\varphi)}{\partial \varphi} ,
\]
which can be written using Eq. \((8)\) in terms of the Berry curvature \(\Omega_{i}(k, \varphi)\) as \[18\] \[23\]
\[
\Delta P = -\frac{1}{2\pi} \sum_{i \leq j} \int_{\varphi(0)}^{\varphi(t)} d\varphi \int_{BZ} dk \Omega_{i}(k, \varphi) ,
\]
with \(\Omega_{i}(k, \varphi) = \partial_{k} A_{\varphi,i}(k, \varphi) - \partial_{\varphi} A_{k,i}(k, \varphi)\), where \(A_{\varphi,i}(k, \varphi) = -i \langle \psi(k)|\frac{\partial}{\partial \varphi}|\psi(k, \varphi)\rangle\) and \(A_{k,i}(k, \varphi) = -i \langle \psi(k, \varphi)|\frac{\partial}{\partial k}|\psi(k, \varphi)\rangle\) are the two components of the Berry connection. We notice here \[23\] that both the polarization and its variations in Eqs. \((8)\) and \((9)\) are defined up to multiples of the elementary charge. By a comparison of Eq. \((9)\) with Eq. \((4)\) one can conclude that
\[
\Delta P \equiv Q \mod 1 ,
\]
in units of the elementary charge. Therefore, along any adiabatic evolution \(\varphi(0) \to \varphi(t)\), the variation of the polarization equates the charge pumped.


Hofstadter Hamiltonian in momentum space reads enough for electron spins to be completely aligned, the flux quantum. Assuming that the magnetic field is strong $j > i$ sign for $L$ with $n$ linear combination of states with momenta $k$ where $g$ has $t$ modulation phase variation $\Delta \phi$ for a finite 1D superlattice. In this Appendix, we will show that the Hamiltonian in Eq. (4) is equivalent to the Hamiltonian of the 1D system in Eq. (4) is periodic in momentum with period $2\pi \alpha$. This can be also inferred from the equivalence of the 1D superlattice and the 2D Hofstadter system. In the Hofstadter system, the uniform magnetic field perpendicular to the 2D lattice is described by a vector potential whose direction can be chosen, due to the gauge invariance, arbitrarily in the lattice plane. This gauge invariance implies that the two components of the momentum are equivalent upon rotations. Correspondingly, the Hamiltonian of the 1D system in Eq. (4) is self-dual [25] under the transformation $t \leftrightarrow -\Delta \varepsilon / 2$ and $k \leftrightarrow \varphi$. Hence, the periodicity of the Hamiltonian in the momentum $k$ implies the periodicity in the modulation phase $\varphi$ with the same period $2\pi / q$.

Robustness of the fractionally quantized charge pumping

The quantization of the charge pumped as fractions of the Chern number is robust against perturbations that preserves the symmetries of the parameter space. This is because the quantization mechanism relies merely on the partitioning of the parameter space in subsets which are equivalent up to a gauge transformation. In this Appendix we will show an example of such a perturbation, and discuss briefly how this perturbation preserves the quantization of the shift of the center of charge at fractions of the pumping cycle. We consider a perturbed Hamiltonian

$$\mathcal{H} = \mathcal{H} - \sum_{\langle i,j \rangle} t' c_i^\dagger c_j \, ,$$

where $\mathcal{H}$ is defined as in Eq. (3), and where the perturbation is in the form of a second-nearest neighbor interaction with strength $t'$. This perturbation preserves the translational symmetry and the periodicity of the parameter space of the system with respect to the modulation phase $\varphi$. If one takes $p/q = 1/3$, $\Delta \varepsilon = 2t$ and $t' \ll t$ the spectrum shows two gaps as in the unperturbed case.
while at $t' \simeq 0.5t$ the lowest energy gap closes and therefore the system is no longer topologically equivalent to the unperturbed one. Fig. 3(c) shows the shift of the center of charge in a finite 1D system for different strength of the second-nearest neighbor perturbation. By a comparison with Fig. 3(c), one can see that the quantization of the shift of the center of charge at $\Delta \varphi = 2\pi n/3$ as fractions of the Chern number is preserved in the case of small perturbations, i.e., for $t' = 0.2t$ [Fig. 3(a)] and $t' = 0.4t$ [Fig. 3(b)], but not for $t' = 0.6t$ [Fig. 3(c)]. Therefore, in this system, the quantization is robust against a small second-nearest neighbor perturbation, which preserves the symmetries of the parameter space and the topology of the energy spectrum.

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