# Nonadiabatic Breaking of Topological Pumping

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We study Thouless pumping out of the adiabatic limit. Our findings show that despite its topological nature, this phenomenon is not generically robust to nonadiabatic effects. Indeed, we find that the Floquet diagonal ensemble value of the pumped charge shows a deviation from the topologically quantized limit which is quadratic in the driving frequency for a sudden switch on of the driving. This is reflected also in the charge pumped in a single period, which shows a nonanalytic behavior on top of an overall quadratic decrease. Exponentially small corrections are recovered only with a careful tailoring of the driving protocol. We also discuss thermal effects and the experimental feasibility of observing such a deviation.

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*Introduction.*—The quantization of the charge transported upon a cyclic adiabatic driving of a band insulating system, known as Thouless topological pumping, is a cornerstone of condensed matter physics [1], recently experimentally realized in systems of ultracold atoms in optical lattices [2,3]. It laid the foundations of the field of charge pumping in mesoscopic systems [4] and played a central role in the development of the modern theory of polarization [5,6]. Moreover, despite being a dynamical phenomenon, it is a conceptual key for understanding many equilibrium properties related to the topology of the bands in momentum space. Most famously, the quantization of the Hall conductance in the integer quantum Hall effect (IQHE), through Laughlin's argument [7,8], can be seen as a Thouless topological pump. The quantization of the transported charge due to quantum topological effects crucially differentiates Thouless pumping from related phenomena. For example, parametric pumping [9] can be of geometric origin [10], but is in general not characterized by a topological quantization. Furthermore, some types of parametric pumping, as ratchets [11] or pistonlike pumps [12]—which share some formal analogies with Thouless pumping—have a classical counterpart. On the contrary, quantum tunneling effects are essential in making the charge quantization in Thouless pumping insensitive to a fine tuning of the model parameters [13]. Having a topological nature, the quantization of the transported charge shows robustness to various factors, such as disorder or interactions [14]. Nonadiabatic effects are also believed to be unimportant—exponentially small in the driving frequency $\omega$ [15,16]—in analogy with the IQHE, where the Hall plateaus show corrections that are exponentially small in the longitudinal electric field [17]. Theoretically, this follows from the fact that the quantized Chern number expression for the Hall conductivity, usually obtained through a Kubo formula in linear response, is valid at all orders in perturbation theory [18,19].

In this Letter we study Thouless pumping out of the perfect adiabatic limit $\omega \to 0$. In order to do that, we perform a careful Floquet analysis of a closed, clean, noninteracting system—the driven Rice-Mele model—in the thermodynamic limit. By analyzing the charge pumped after many cycles when the system starts from the initial ground-state Slater determinant, we find that for a suddenly switched-on driving, the pumped charge shows a deviation from perfect quantization that is always *polynomial* in the driving frequency $\omega$, contradicting the expected topological robustness. This quadratic deviation is present also after a finite number of pumping cycles, even if apparently hidden under a highly oscillatory nonanalytic behavior [19] in $\omega$. An exponentially small deviation would be obtained only if one was able to prepare the system in a specific Floquet state, which can be approximately obtained only with a suitable switch-on of the driving. We also discuss the effects of a thermal initial state.

*Model and method.*—A paradigmatic model for Thouless pumping is the driven Rice-Mele (RM) [20] model:

$$\hat{H}_{\mathrm{RM}}(t) = -\sum_{j=1}^{N} (J_1(t)\hat{b}^\dagger{}_j\hat{a}_j + J_2(t)\hat{a}^\dagger{}_{j+1}\hat{b}_j + \mathrm{H.c.}) + \sum_{j=1}^{N} \Delta(t)(\hat{a}^\dagger{}_j\hat{a}_j - \hat{b}^\dagger{}_j\hat{b}_j). \quad (1)$$

 

Here $\hat{a}_j^\dagger$ and $\hat{b}_j^\dagger$ create a spinless fermion at cell $j$ in sublattice $A$ and $B$, respectively, and we assume a half-filling situation. This simple tight-binding model describes the physics of cold atom experiments in some regimes [2,3]. The instantaneous spectrum becomes gapless for $J_1 = J_2$ and $\Delta = 0$, and a quantized adiabatic pumping is realized when a closed path in the $(J_1 - J_2, \Delta)$ parameter space encloses such a degeneracy point [21]. In the following, we will parametrize $J_{\frac{1}{2}}(t) = J_0 \pm \delta_0 \cos[\varphi(t)]$, and $\Delta(t) = \Delta_0 \sin[\varphi(t)]$. By choosing $\varphi(t) = \omega t$ we realize a sudden switch on of the driving. [We will also discuss different choices of $\varphi(t)$.] We impose periodic boundary conditions (PBC), and use momentum $k$ in the Brillouin zone (BZ) $[-(\pi/a), (\pi/a))$ to reduce the dynamics to $N$ independent two-dimensional Schrödinger problems, which can be numerically integrated by a fourth-order Runge-Kutta method.

*Floquet theory of the Thouless pump.*—Given the time periodicity of the Hamiltonian in a Thouless pump, with period $\tau = 2\pi/\omega$, it is natural to employ a Floquet analysis [16,19,22–24]. Because of the discrete time-translation invariance, there exists a basis of solutions of the time-dependent Schrödinger equation, that are periodic up to a phase: the Floquet states $|\psi_\alpha(t)\rangle = e^{-(i/\hbar)\varepsilon_\alpha t}|\phi_\alpha(t)\rangle$ [25,26]. The $\tau$-periodic states $|\phi_\alpha(t)\rangle$ are the so-called Floquet modes and $\varepsilon_\alpha$ are the quasienergies: they are defined modulo an integer number of $\hbar\omega = 2\pi\hbar/\tau$; hence, it is possible to restrict them to the first Floquet Brillouin zone (FBZ) $[-\hbar\omega/2, \hbar\omega/2)$.

In a PBC ring geometry, the total current operator $\hat{J}(t)$ is obtained as a derivative of $\hat{H}(t)$ with respect to a flux $\Phi$ threading the ring, $\hat{J} = \partial_\kappa \hat{H}/\hbar$, where $\kappa = (2\pi/L)(\Phi/\Phi_0)$, $L$ is the length of the system, and $\Phi_0$ the flux quantum. As a consequence, the charge pumped in one period $\tau$ by a single Floquet state $|\psi_\alpha(t)\rangle$ is [16,19,22,23] $Q_\alpha(\tau) = (1/L)\int_0^\tau dt \langle\psi_\alpha(t)|\hat{J}(t)|\psi_\alpha(t)\rangle = (\tau/\hbar L)\partial_\kappa \varepsilon_\alpha$. For a translationally invariant system, each completely filled Floquet-Bloch band with (single-particle) quasienergy dispersion $\varepsilon_{\alpha,k}$ would contribute to the charge pumped (in the thermodynamic limit $L \to \infty$) as

$$Q_\alpha(\tau) = \frac{1}{\hbar\omega}\int_{-\frac{\pi}{a}}^{+\frac{\pi}{a}} dk \frac{\partial \varepsilon_{\alpha,k}}{\partial k}, \tag{2}$$

where we have replaced the $\kappa$ derivative with a $k$ derivative, since $\varepsilon_{\alpha,k}$ depends on $k + \kappa$. Thus, if $\varepsilon_{\alpha,k}$ wraps around the FBZ in a continuous way as a function of $k$, $Q_\alpha(\tau)$ is equivalent to the *winding number* of the band; i.e., the number $n$ of times $\varepsilon_{\alpha,k}$ goes around the FBZ, $\varepsilon_{\alpha,+(\pi/a)} - \varepsilon_{\alpha,-(\pi/a)} = n\hbar\omega$, and $Q_\alpha(\tau)$ is therefore quantized: $Q_\alpha(\tau) = n$. This is what happens in the extreme adiabatic limit $\omega \to 0$: if $|\Psi_\alpha(t)\rangle$ is a Slater determinant made up of the instantaneous Hamiltonian Bloch eigenstates $e^{ikx}u_{\alpha,k}(x,t)$ belonging to a filled band $E_{\alpha,k}(t)$, the adiabatic theorem guarantees that such a state returns onto itself after a period $\tau$, $|\Psi_\alpha(\tau)\rangle = e^{i\sum_k^{\mathrm{BZ}}(\gamma_{\alpha,k}-\theta_{\alpha,k})}|\Psi_\alpha(0)\rangle$, by acquiring a geometric (Berry) phase $\gamma_{\alpha,k} = \int_0^\tau dt i\langle u_{\alpha,k}|\partial_t u_{\alpha,k}\rangle$ and a dynamical one $\theta_{\alpha,k} = \int_0^\tau dt E_{\alpha,k}(t)/\hbar$. This in turn implies that $|\Psi_\alpha(t)\rangle$ is a Floquet state with quasienergy $\varepsilon^0_{\alpha,k} = \hbar(-\gamma_{\alpha,k} + \theta_{\alpha,k})/\tau$. Substituting in Eq. (2), only the geometric phase survives, leading to the Thouless' formula [1],

$$Q_\alpha(\tau) = \int_{-\frac{\pi}{a}}^{+\frac{\pi}{a}} \frac{dk}{2\pi}\int_0^\tau dt i(\langle\partial_k u_{\alpha,k}|\partial_t u_{\alpha,k}\rangle - \text{c.c.}), \tag{3}$$

identifying the pumped charge with a Chern number [19].

Let us see what happens away from the adiabatic limit $\omega \to 0$. We consider a lattice model with a finite number of bands, such as Eq. (1). The sum of the winding numbers of all bands will be zero, since the sum of Chern numbers of a finite-dimensional Hamiltonian must be zero [19]. This fact, as noticed in Ref. [19], implies that the quasienergy spectrum must contain some crossings if at least one quasienergy band has nonvanishing winding number. These crossings, however, are not stable [19]: according to Wigner and von Neumann [27], a true crossing requires, for the present case of a complex $2 \times 2$ unitary operator, the tuning of at least three real parameters, while the quasienergy spectrum depends only on two, $\tau$ and $k$. Hence one expects, *generically*, that crossings turn into avoided crossings with opening of gaps for any finite $\tau$—in the present case at the border of the FBZ—implying a deviation from perfect quantization of the pumped charge for the Floquet band under consideration.

To better understand this point, let us focus on the Floquet-Bloch band whose pumped charge is closest to the integer value of the adiabatic limit. This band can be constructed [16] by choosing, for each $k$, the Floquet mode with (period-averaged) lowest-energy expectation $|\phi_{\mathrm{LE},k}(t)\rangle$. In the left panel of Fig. 1 we show a typical quasienergy spectrum of the RM model: the bold line denotes the lowest-energy Floquet band. In the right panel we zoom in the region around an avoided crossing (solid line),comparing with the perfect crossing occurring for the adiabatic approximation $\varepsilon^0_{\alpha,k}$ (dashed line): the visible gap is exponentially small in $1/\omega$—as it happens for all the gaps that open at such avoided crossings [28]. This implies that the lowest-energy Floquet band does *not* wrap continuously around the FBZ. Accordingly, its pumped charge $Q_{\mathrm{LE}} = (\hbar\omega)^{-1}\int_{-(\pi/a)}^{+(\pi/a)} dk \partial_k \varepsilon_{\mathrm{LE},k}$ deviates from an integer by terms proportional to the sum of the gaps when $\omega > 0$. This deviation is, therefore, exponentially small in $1/\omega$ (a similar result was found in Ref. [16] for a different model); see Fig. 2(a). Summarizing, if we were able to prepare an initial state coinciding with the lowest-energy Floquet band, the deviation from perfect quantization would be exponentially small. Nevertheless, in any real situation, the

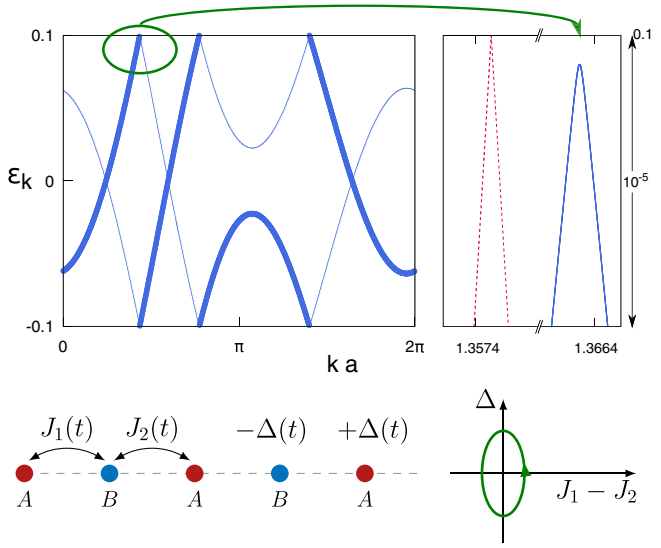


FIG. 1. Top left: quasienergy spectrum of the Rice-Mele model $\Delta_0 = 3J_0$, $\delta_0 = J_0$, $\omega = 0.2J_0/\hbar$. The thick band is the lowest-energy Floquet band $\varepsilon_{LE,k}$. Top right: (solid line) enlargement of the previous figure close to the upper border of the FBZ around $ka = 1.3664$; the dashed line denotes the quasienergies in the adiabatic limit $\varepsilon^0_{\alpha,k}$. Notice the gap of order $10^{-6}$. Bottom: A cartoon of the Rice-Mele model (left) and a path in parameter space.

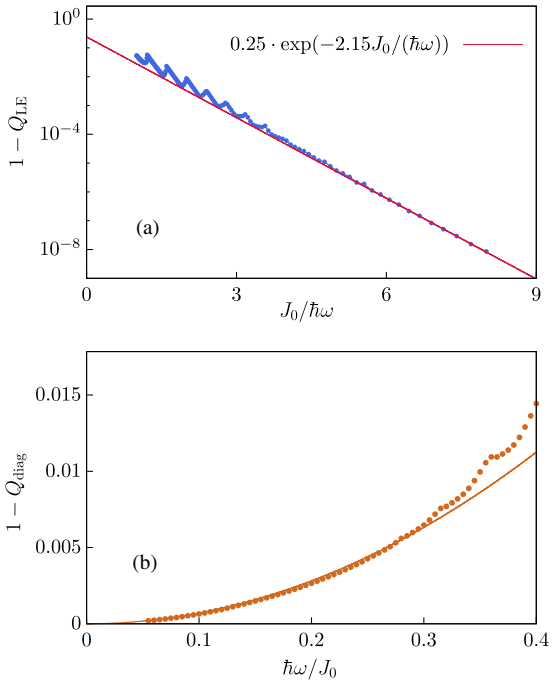


FIG. 2. (a) The deviation from 1 of the charge pumped by the lowest-energy Floquet band (proportional to the sum of gaps) as a function of $1/\hbar\omega$, with its exponential fit (red solid straight line). (b) Deviations from 1 of the diagonal pumped charge $Q_{\rm diag}$ in the RM model for a sudden switch on of the driving. The smooth curve $\frac{9}{128}(\hbar\omega/J_0)^2$ is obtained from Eq. (6). The model parameters are $\Delta_0 = 3J_0$, $\delta_0 = J_0$.

initial state $|\Psi(0)\rangle$ of the system is not a Floquet state: a more realistic starting point would be to assume that $|\Psi(0)\rangle$ is the *ground state* of the initial Hamiltonian $\hat{H}(0)$ before pumping is started. Whichever the initial state, any local observable attains, upon periodic driving and in the thermodynamic limit, a periodic steady state with the same periodicity as the driving [29]. This asymptotic regime is described by the Floquet diagonal density matrix [29,30]; in an integrable system this density matrix is not thermal, but is given by a generalized Gibbs ensemble. Let us denote by $Q(m\tau)$ the total charge pumped in the first $m$ periods starting from the initial ground state $|\Psi(0)\rangle$ of $\hat{H}(0)$. The *asymptotic* charge pumped in a single cycle, obtained from the infinite time limit, is given by the Floquet diagonal ensemble [31]:

$$Q_{\rm diag} \equiv \lim_{m\to\infty} \frac{Q(m\tau)}{m} = \frac{1}{\hbar\omega}\sum_\alpha \int_{-\frac{\pi}{a}}^{+\frac{\pi}{a}} dk n_{\alpha,k} \frac{\partial \varepsilon_{\alpha,k}}{\partial k}, \quad (4)$$

where $n_{\alpha,k} = \langle\Psi(0)|\hat{f}^\dagger{}_{\alpha,k}\hat{f}_{\alpha,k}|\Psi(0)\rangle$ is the initial ground-state occupation of the Floquet-Bloch $(\alpha, k)$ mode, with $\hat{f}^\dagger{}_{\alpha,k}|0\rangle = |\phi_{\alpha,k}(0)\rangle$. The occupations $n_{\alpha,k}$ can give rise to a stronger deviation from quantization than the gaps, as we are now showing.

*Results.*—In Fig. 2(b) we plot the diagonal pumped charge $Q_{\rm diag}$, calculated from Eq. (4), for the RM model (1) as a function of the driving frequency $\omega$, close to the adiabatic limit $\omega \to 0$, for the same parameters as Fig. 1.

The driving is suddenly switched on: $\varphi(t) = 0$ when $t < 0$ and $\varphi(t) = \omega t$ for $t \geq 0$, as realized in the experimental setting of Ref. [2]. The numerically determined points show a clear *quadratic* deviation with $\omega$ from the fully adiabatic integer value 1. We now show that this power-law deviation essentially originates from the Floquet bands occupations $n_{\alpha,k}$. To understand this point, consider the lowest-energy Floquet band $\varepsilon_{LE,k}$, and the associated occupations $n_{LE,k} = \langle\Psi(0)|\hat{f}^\dagger{}_{LE,k}\hat{f}_{LE,k}|\Psi(0)\rangle$. One can develop a perturbation theory in $\omega$ for the Floquet modes, along the lines of Ref. [33], to show that for our model

$$n_{LE,k} = 1 - \left|\frac{\hbar\omega\langle u_{1,k}(0)|\partial_s u_{0,k}(0)\rangle}{E_{1,k}(0) - E_{0,k}(0)}\right|^2 + \mathcal{O}(\omega^3). \quad (5)$$

Here, $s = t/\tau$ is a rescaled time, while $E_{\alpha,k}(t)$ and $|u_{\alpha,k}(t)\rangle$, with $\alpha = 0$, 1, are the energy and the periodic part of the two instantaneous Bloch eigenfunctions. The analytic calculation is simple:

$$n_{LE,k} = 1 - \frac{1}{64}\left(\frac{\hbar\omega\Delta_0}{J_0^2 + \delta_0^2 + (J_0^2 - \delta_0^2)\cos(ka)}\right)^2 + \cdots, \quad (6)$$

leading to quadratic corrections to $Q_{\rm diag}$. When $\delta_0 = J_0$, Eq. (6) predicts that $n_{LE,k}$ is $k$ independent and can be taken

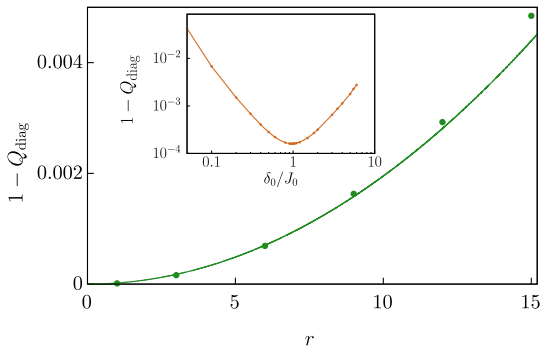


FIG. 3. Deviations from the integer value of the diagonal pumped charge $Q_{\rm diag}$ in the RM model versus the aspect ratio $r = \Delta_0/\delta_0$ of the driving ellipse for $\delta_0 = J_0$, for a sudden switch on of the driving with frequency $\omega = 0.05 J_0/\hbar$. The smooth curve is $\frac{1}{128}(\hbar\omega/J_0)^2 r^2$ and it was calculated with the first order perturbative calculation of the main text. In the inset, the deviation from 1 of $Q_{\rm diag}$ for a fixed $r = 3$ as a function of $\delta_0$: The minimum sits at $\delta_0 = J_0$.

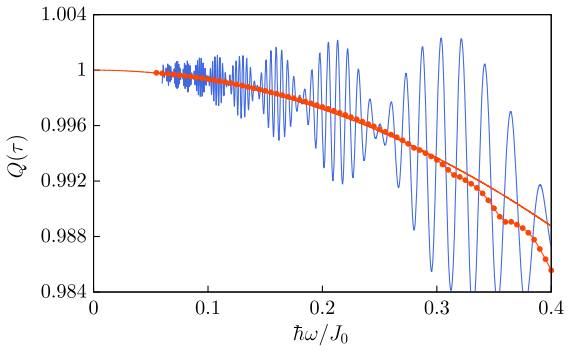


FIG. 4. The charge pumped after the first period, $Q(\tau)$, as a function of the frequency $\omega$, for the RM model with a suddenly switched on driving (smooth blue line). The red dotted line is the corresponding diagonal ensemble value $Q_{\rm diag}$, reported in Fig. 2(b). The model parameters are $\Delta_0 = 3J_0$, $\delta_0 = J_0$.

out of the integral in Eq. (4): we can calculate the charge deviation given by $\frac{1}{128}(\hbar\omega\Delta_0/J_0^2)^2$, which perfectly fits the numerical data points, as shown in Fig. 2(a) for $\Delta_0 = 3J_0$. It is apparent from Eq. (6) that the nonadiabatic corrections can be more or less pronounced, depending on the parameters of the driving ($\Delta_0$, $\delta_0$). Figure 3 illustrates how the deviation from quantization for a fixed value of frequency, $\omega = 0.05 J_0/\hbar$, depends on ($\Delta_0$, $\delta_0$). In the main plot, we fix the value $\delta_0 = J_0$ as before and we vary the dimensionless ratio $r = \Delta_0/\delta_0$. According to Eq. (6), the deviation increases with $r$ as $(\hbar^2\omega^2/128 J_0^2) r^2$. The agreement with the numerical data for this choice of $\omega$ is very good up to $r \lesssim 12$, where higher orders of the perturbation theory (5) become relevant. Conversely, in the inset of Fig. 3 we fix $r = \Delta_0/\delta_0 = 3$ and we consider the dependence on $\delta_0/J_0$: we see that the deviation shows a minimum around $\delta_0 = J_0$. Summarizing, the deviation should be more noticeable for paths in parameter space flattened on the $\Delta$ axis and far from $\delta_0 = J_0$. Note that a small $\delta_0/J_0$ corresponds to a weak pumping regime: quite surprisingly, this seems to imply a stronger nonadiabaticity. The possibility of controlling Hamiltonian parameters in ultracold atoms experiments makes the detection of these nonadiabatic effects likely feasible.

It is, however, possible to devise driving schemes that lead to a better filling of the lowest-energy Floquet band. The Floquet adiabatic theorem [34–37] suggests that a sufficiently smooth variation of the instantaneous driving frequency $\omega(t) = \dot{\varphi}(t)$ would lead to a much smaller deviation of the population $n_{LE,k}$, and hence of $Q_{\rm diag}$, from an integer value. This is what a detailed analysis of these issues, presented elsewhere [38], finds. Incidentally, a smoother switch on of the periodic driving is what the experimental realization of Ref. [[3]] adopts.

We now address the issue of nonadiabatic deviation for a *finite* number of pumping cycles. Diagonal expectation values are indeed attained after some transient and become exact only after an infinite number of pumping cycles. In Fig. 4 we plot the charge pumped after a single cycle, $Q(\tau)$, as a function of $\omega$: we see that $Q(\tau)$ exhibits remarkable beatinglike oscillations, on top of the overall quadratic decrease of $Q_{\rm diag}$, which become faster and faster as $\omega \to 0$. The theoretical prediction, according to a theorem of Ref. [19], is that the finite-time pumped charge must have an essential singularity in $\omega = 0$. The behavior that we find is indeed compatible with the presence of nonanalyticities, possibly of the kind of $\sin(c/\omega)$.

An alternative source of deviation from perfect quantization is finite temperature. In ultracold atom experiments, it is reasonable to consider the dynamics to be coherent even if the initial state is a thermal density matrix $\hat{\rho}_T$ at temperature $T$. The zero-temperature unitary evolution results of Eq. (4) get modified only through the replacement of the occupations $n_{\alpha,k}$ with thermal ones $n^T_{\alpha,k} = {\rm Tr}(\hat{\rho}_T \hat{f}^\dagger_{\alpha,k} \hat{f}_{\alpha,k})$. The final result is

$$n^T_{\alpha,k} = \tanh[-\beta E_{0,k}(0)] n_{\alpha,k} + \frac{e^{\beta E_{0,k}(0)}}{2\cosh[-\beta E_{0,k}(0)]}, \qquad (7)$$

where we used that $E_{0,k} = -E_{1,k}$ in the RM model. Thus, the $\omega^2$ behavior of the deviation is preserved, but can be hidden by thermal effects. They are exponentially small when the temperature $T$ is much smaller than the initial gap. For the specific choice used before, $\delta_0 = J_0$, thermal corrections only amount to multiplying the $T = 0$ result by a factor $\tanh[\beta E_{1,k}(0)]$, which turns out to be $k$ independent. In this case $E_{1,k}(0) = 2J_0$ and thermal effects start to compete with the nonadiabatic ones only when $T$ is of the order of the gap, $k_B T \approx J_0$.

*Conclusions.*—We have studied what happens to the quantization of the Thouless pumped charge out of the

perfect adiabatic limit. Within a Floquet framework, we have found that this transport phenomenon is in general not robust to nonadiabatic effects despite its topological nature. When the driving is switched on suddenly, $\phi(t) = \omega t$, or too fast [38], we see that the long-time asymptotic value of the pumped charge deviates from the quantized value in a polynomial fashion, i.e., quadratically in the driving frequency. This observation is, we believe, model independent, since it requires only that the initial state is the ground state (or any other eigenstate) of the initial Hamiltonian. The fact that a topologically robust property can be ruined by the occupation factors of the Floquet bands is in line with what was found in a resonantly driven graphene layer [39]. Our findings should be, in principle, observable in ultracold atoms experiments (for instance, with the methods used in Refs. [2,3]). Perspectives of future work include the study of the pumped charge in the prethermal regime of a nonintegrable system [28] and the analysis of disorder, especially in connection with the stabilization of charge pumping in a many-body localized system. Another important point will be understanding the switch on time scale marking the crossover between power-law and exponentially small deviations from quantized pumping.

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