Charge density wave and charge pump of interacting fermions in circularly shaken hexagonal optical lattices

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We analyze strong correlation effects and topological properties of interacting fermions with a Falicov-Kimball type interaction in circularly shaken hexagonal optical lattices, which can be effectively described by the Haldane-Falicov-Kimball model, using the real-space Floquet dynamical mean-field theory (DMFT). The Haldane model, a paradigmatic model of the Chern insulator, is experimentally relevant, because it has been realized using circularly shaken hexagonal optical lattices. We show that in the presence of staggering a charge density wave emerges, which is affected by interactions and resonant tunneling. We demonstrate that interactions smear out the edge states by introducing a finite life time of quasiparticles. Even though a general method for calculating the topological invariant of a nonequilibrium steady state is lacking, we extract the topological invariant using a Laughlin charge pump set-up. We find and attribute to the dissipations into the bath connected to every lattice site, which is intrinsic to real-space Floquet DMFT methods, that the pumped charge is not an integer even for the non-interacting case at very low reservoir temperatures. Furthermore, using the rate equation based on the Floquet-Born-Markov approximation, we calculate the charge pump from the rate equations for the non-interacting case to identify the role of the spectral properties of the bath. Starting from this approach we propose an experimental protocol for measuring quantized charge pumping.

I. INTRODUCTION

Time periodically driven ultracold atoms in optical lattices are a versatile and powerful platform to simulate models with non-trivial topological properties [1, 2]. Two paradigmatic models, the Hofstadter model and the Haldane model have been realized with Raman laser assisted tunneling [3–5] and circularly shaken hexagonal lattices [6–8], respectively. Different techniques have been developed in setups with ultracold atoms in optical lattices to detect topological properties. Using a drift measurement, the topology of the lowest band of the Hofstadter model was determined [5]. By measuring the shift of atom clouds in a one-dimensional superlattice, the Thouless charge pump was realized in bosonic [9, 10] and fermionic [11] systems. A two-dimensional version of the topological charge pump was demonstrated by mapping a four-dimensional quantum Hall system to a two-dimensional square superlattice using dimensional reduction [12]. Using the topographic technique that was first proposed in Ref. [13], the Berry curvature of the Haldane model was mapped out in momentum space [7]. Also, dynamical vortices due to quenching into the Floquet Hamiltonian were observed [8], which are a nonequilibrium signature of topology. The trajectories of the dynamical vortices in momentum space were used to determine the linking number [14], which can be directly related to the Chern number of the Hamiltonian after a quench [15].

Introducing two-particle interactions into a time-periodically driven system is a highly non-trivial problem from the point of view of both experiment and theory. In experiments one needs to overcome the problem of heating. It was shown that an interacting time-periodically driven closed system will heat up to a trivial state with infinite temperature [16, 17], with only a few exceptions like many-body localized systems [18, 19], integrable systems [20] and the prethermalization plateau [21, 22]. Multi-photon interband heating has been observed in a shaken 1D optical lattice [23]. Resonant tunneling, which happens when interactions are integer multiples of the driving frequency and magnetic correlations have been measured for strongly correlated fermions in hexagonal optical lattices with periodic driving in one direction [24]. Floquet evaporative cooling was shown to reduce heating for interacting bosons in a one-dimensional optical lattice [25]. However, there are no artificial gauge fields in these setups. Further efforts are needed to go into the interacting regime and realize an interacting system with artificial gauge fields. Theoretically, in the high-frequency limit, where the time periodically driven system is supposed to be in a prethermalized regime [21], the system can be described by an effective Hamiltonian in high-frequency approximation [26–28]. With interactions turned on, the interacting Haldane model can be studied with the static mean-field approximation [29, 30] and exact diagonalization [31]. The possible drawback of the effective Hamiltonian approach is that it cannot describe the non-equilibrium properties of the system. In the strongly correlated regime, one can obtain the effective
low-energy Hamiltonian in the limit of large interaction using a high-frequency expansion, which is equivalent to a Schrieffer-Wolff transformation [32]. With it one can qualitatively analyze the properties of near-resonant and resonant tunneling. However, to solve the low energy effective Hamiltonian is still a very non-trivial many-body problem. Numerical tools such as quantum Monte-Carlo and density matrix renormalization method need to be adopted to solve it.

Based on the experimental progress [7, 8, 14], we investigate non-equilibrium steady states (NESS) of fermions with Falicov-Kimball type interactions in a circularly shaken hexagonal optical lattice in a non-perturbative way using the method of real-space Floquet dynamical mean field theory (DMFT) [33–37], which can deal with driving, interactions and dissipation on equal footing. We study the strong correlation effects and topological properties of the system. We investigate the charge density wave (CDW) induced by the staggered potential as a function of increasing interactions. To study topological properties, we use a Laughlin charge pump setup [38], where a flux is inserted in the direction of the axis of a cylinder geometry. We observe how the edge states are smeared out by interactions. Furthermore, we calculate the charge pump due to insertion of flux quanta for different interactions. The dissipation into the bath makes the pumped charge non-integer. In addition, we study the role of dissipation for the non-interacting case in the presence of a heat bath using rate equations based on the Floquet-Born-Markov approximation. We start from an initial state which is close to equilibrium, and ramp up the flux adiabatically to calculate the pumped charge. By comparison with the equilibrium case we believe our procedure is experimentally practical.

We include a bath in all our calculations. While the bath prevents serious heating of the driven system, it causes dissipation which smears the integer charge pump, at least within our theoretical approaches for dealing with the bath. Whether it is possible to recover the integer charge pump by bath engineering will be a future direction.

The manuscript is organized as follows. In Sec. II, we present the model and methods used in our calculations. We outline the real-space Floquet DMFT method for the interacting and driven system, and the rate equation for the non-interacting case. In Sec. III, we present our results on the charge density wave and charge pump for the interacting system. For the non-interacting case, we show calculations from rate equations. We conclude in Sec. IV.

II. MODEL AND METHODS

A. The model

We start with a model for fermions in circularly shaken hexagonal optical lattices which can describe the experimental setups described in Refs. [7, 8, 14, 39]

\[ H_0 = -J \sum_{\langle ll' \rangle} c_{l}^\dagger c_{l'} + \sum_{l} \epsilon_l c_{l} + \alpha (\Omega + \Delta) \sum_{l} \lambda_l n_l, \]

(1)

where \( l \) and \( l' \) label lattice sites, and \( n_l = c_{l}^\dagger c_{l} \). \( \Omega \) is the driving frequency and \( \Delta \) is the detuning between the driving frequency and the AB-offset in the static lattice. \( \lambda_{A(B)} = 0(1) \) for A and B sites in the unit-cell. \( \alpha = \pm 1 \) which is the sign of the staggered potential.

By comparison with the equilibrium case we believe our Hamiltonian in second-order high-frequency approximation has been shown to be a Haldane-type Hamiltonian [14]. We then transform the Hamiltonian (4) to the Floquet space with \( c_l = \sum_{m=-\infty}^{\infty} e^{-i\Omega t} c_{l,m} \), so

\[ \hat{H}_0^{m_1 m_2} = -J \sum_{\langle ll' \rangle} J_{m_2 - m_1 - \epsilon_{l'} \xi_{l'}} \left( \frac{K}{\Omega} \right) e^{-i \Phi_{l'}^{m_1 m_2}} c_{l,m}^\dagger c_{l', m_2} \]

(5)

where \( \Phi_{l'}^{m_1 m_2} = (m_2 - m_1 - \epsilon_{l'} \xi_{l'}) \pi \xi_{l'} \). \( \epsilon_{l'} \xi_{l'} = \lambda_l - \lambda_l \). \( J_{m_2 - m_1 - \epsilon_{l'} \xi_{l'}} \left( \frac{K}{\Omega} \right) \) is the Bessel function of the order \( m_2 - m_1 - \epsilon_{l'} \xi_{l'} \). \( m_1 \) and \( m_2 \) are Floquet indices.

We consider a Falicov-Kimball interaction, where the mobile atoms interact with localized atoms:

\[ H_{\text{int}} = U \sum_{l} c_{l}^\dagger f_{l}^\dagger f_{l}. \]

(6)

\( U \) is the interaction strength. \( f_{l} (f_{l}^\dagger) \) is the annihilation (creation) operator for localized atoms.

B. Real-space Floquet DMFT

We outline the real-space Floquet DMFT method that we adopt to deal with the Falicov-Kimball interaction [33,
It is a method to study the NESS in an inhomogeneous system. To reach the NESS, every lattice site is coupled to a bath. We use a free-fermion bath in our implementation [37, 42]. The full Green’s function of the lattice system satisfies Dyson’s equation,

\[
\left(G^{-1}\right)_{ll',mn}(\omega) = \left(G_0^{-1}\right)_{ll',mn}(\omega) - \Sigma_{bath,lmn}(\omega) \delta_{ll'} - \Sigma_{bath,lmn}(\omega) \delta_{ll'}
\]

where every part is defined on the Keldysh contour [43] and in Floquet space

\[
\hat{G}(\omega) = \left(\begin{array}{c} G^R & G^K \\ 0 & G^A \end{array}\right) (\omega) .
\]

\(\omega \in [-\frac{\Omega}{2}, \frac{\Omega}{2}]\) is in the first Brillouin zone of \(\Omega\). For the non-interacting part we have

\[
G_{0{ll',mn}}(\omega) = (\omega + n\Omega + i0^+) \delta_{mn} \delta_{ll'} - \hat{H}_{0{l'l'mn}},
\]

and \(G_0^R(\omega) = G_0^{R\dagger}(\omega)\), as well as \((G_0^{-1}(\omega))^K = 0\) [37, 42]. \(\Sigma_{bath,lmn}(\omega)\) is the correction to the self-energy on site \(l\) due to dissipation to the bath

\[
\Sigma_{bath,lmn}(\omega) = \left( i\Gamma \delta_{mn} - 2i\Gamma F_n(\omega) \delta_{mn} - i\Gamma \delta_{mn} \right),
\]

assuming that the density of states (DOS) of the bath is constant. \(\Gamma\) is a phenomenological dissipation rate to the bath, and \(F_n(\omega) = \tanh \frac{\omega + n\Omega}{2\kappa}\) where \(T\) is the temperature of the bath [37]. \(\Sigma_{lmn}(\omega)\) is the lattice self-energy due to two-particle interactions and is obtained from the impurity solver for every lattice site \(l\):

\[
G_l(\omega) = w_0 G_{0,l}(\omega) + w_1 \left[ G_{0,l}^{-1}(\omega) - U \right]^{-1}
\]

where \(w_1\) is the probability of one site being occupied by immobile atoms and \(w_0 = 1 - w_1\). In the following, we focus on the case of half filling, for which \(w_1 = \frac{1}{2}\) and \(w_0 = \frac{1}{2}\). The self-consistent loop is closed by

\[
G_{0,lmn}(\omega) = G_{l}^{-1}(\omega) + \Sigma_l(\omega).
\]

Here, the total Hamiltonian reads

\[
H(t) = \hat{H}_0(t) + \sqrt{T} \sum_\alpha \kappa_\alpha (b_\alpha + b_\alpha) + \sum_\alpha \omega_\alpha b_\alpha^\dagger b_\alpha,
\]

where the bath is modeled by a collection of harmonic oscillators \(b_\alpha\), corresponding frequencies \(\omega_\alpha\) and dimensionless coupling constants \(\kappa_\alpha\), and some system coupling operator \(v\). Note that we have separated the strength \(\sqrt{T}\) of the system–bath coupling from the coefficients \(\kappa_\alpha\). It turns out that the magnitude of the dissipation rate is given essentially by \(\Gamma\).

In the weak system–bath coupling limit, \(\Gamma \to 0\), we may perform the usual Born-Markov [44] and the full rotating wave approximation [45–47] in which we average over the long relaxation time scales \(\propto 1/\Gamma\) (rather than just one period of the driving). For a single fermion, \(N = 1\), one then finds that the reduced system density matrix is asymptotically diagonal in the Floquet states \([a(t)]\), i.e., \(g(t) = \sum_a p_a(t) [a(t)]\langle a(t)\rangle\), and the asymptotic dynamics is governed by a Pauli rate equation,

\[
\partial_t p_a(t) = \sum_b \left[ R_{ab} p_b(t) - R_{ba} p_a(t) \right] ,
\]

that describes the transfer between populations \(p_a(t)\) of the Floquet states. This happens at a rate

\[
R_{ab} = 2\pi T \sum_{m \in \mathbb{N}} |v_{ab}^{(m)}|^2 g(\varepsilon_a - \varepsilon_b - m\Omega),
\]

involving the quasienergy \(\varepsilon_a\) of Floquet state \(a\) and the \(m\)-th component of the Fourier transform of the coupling,

\[
v_{ab}^{(m)} = \frac{1}{T} \int_0^T dt \langle a(t) | v | b(t) \rangle e^{im\Omega t}.
\]

It also enters the bath-correlation function \(g\) that reads for the phonon bath

\[
g(E) = \left\{ \begin{array}{ll} J(E) n_B(E), & E > 0, \\ J(-E)(1 + n_B(-E)), & E < 0, \end{array} \right.
\]

with the occupation function \(n_B(E) = 1/(e^{E/T} - 1)\) and the spectral density of the bath \(J(E) = \sum_\alpha \kappa_\alpha^2 \delta(E - \omega_\alpha)\), for \(E \geq 0\). Typical baths with a continuum of modes \(\alpha\) obey

\[
J(E) \propto E^{d_\alpha} e^{-E/E_c},
\]

where the exponent \(d\) controls the low-frequency behaviour of \(J(E)\). Here \(d = 1\) denotes the ohmic case and \(d < 1\) (\(d > 1\)) is sub-(super-)ohmic. The high-frequency cutoff parameter \(E_c\) basically is set by the correlation time \(\tau_B \propto 1/E_c\) of the bath [44]. In order to be consistent with the Markov approximation, this time \(\tau_B\) must be small when compared to the typical time scale of relaxation \(\tau_R \propto 1/T\), which is always valid in the weak coupling limit \(\Gamma \to 0\) that we aim at.

The non-interacting Fermi gas may be considered in the same framework, however, one has to additionally
implement quantum statistics. This leads to the many particle version of the Pauli rate equation [48],
\[
\partial_t \langle n_a \rangle = \sum_b R_{ab}(1 - \langle n_a \rangle)\langle n_b \rangle - R_{ba}(1 - \langle n_b \rangle)\langle n_a \rangle,
\]
where \( \langle n_a \rangle \) is the mean occupation of the Floquet state \( a \) and where we have applied the mean field approximation \( \langle n_a n_b \rangle \approx \langle n_a \rangle \langle n_b \rangle \) discussed in Ref. [49]. The nonequilibrium steady state is found by solving for steady occupations, \( \partial_t \langle n_a \rangle = 0 \).

III. RESULTS AND DISCUSSIONS

A. Charge density wave

In this section, we focus on the effects of interactions and resonant tunneling on the charge density wave (CDW) induced by the staggered potential. We consider a two-dimensional hexagonal optical lattice with 9 \times 9 unit cells and periodic boundary conditions in both \( x \) and \( y \) directions. The charge densities are different on \( A \) and \( B \) sites, with the definition of the charge density on site \( A \) (\( B \)) \( N^c_i = \frac{1}{2\pi} \int_{-\Omega/2}^{\Omega/2} d\omega \sum_n G^<_{nn,i} \langle \omega \rangle \), where \( i = A \) (\( B \)), \( n \) is the Floquet index for the Floquet Green’s function \( G^<_{A(B)}(\omega) \) on site \( A \) (\( B \)), and \( G^<_{nn,i}(\omega) = \frac{1}{2}(G^K_{nn,i}(\omega) - G^R_{nn,i}(\omega) + G^A_{nn,i}(\omega)) \). Because of the periodic boundary conditions, there are only two different sites in the hexagonal optical lattice. Our study is different from those in Ref. [50–52], where the CDW order parameter is defined as \( \Delta_{\text{CDW}} = N^f_A - N^f_B \) because a finite density difference of localized \( f \)-atoms is needed to spontaneously break the symmetry between sublattice sites \( A \) and \( B \). However, in our case of the real space implementation of DMFT calculations, we choose \( \omega_1 = \frac{1}{2} \) for all sites. We nevertheless have a CDW also for \( \Delta = 0 \). Namely, for an integer \( \omega \), i.e., in the presence of the staggered potential \( \alpha \Omega \sum \lambda_i n_i \), will cause an effective energy offset between \( A \) and \( B \) sites (appearing in the second-order high-frequency expansion of the effective Hamiltonian [14]). It results from virtual second-order processes where a particle tunnels from an \( A \) (\( B \)) site to a neighboring \( B \) (\( A \)) site and back. In Fig. 1, we show a comparison calculation to prove this. We can see a perfect symmetry of the spectral functions for both \( A \) and \( B \) sites for the case without staggered potential, in contrast to a broken symmetry for the case when the staggered potential is present.

There is a rich relation between charge density and interactions. We show the charge density \( N^c_{A(B)} \) with increasing interactions in Fig. 2. (i) When \( U = 0 \), the detuning \( \Delta \) is the factor that affects occupation of \( A \) and \( B \) sites, and one can tune the occupations by changing \( \Delta \). (ii) We next discuss the case where \( 0 < U \leq 3 \). The repulsive interaction \( U \) counteracts the effect of \( \Delta \), and the density difference is reduced. In this region, the resonant tunneling is suppressed because the bandwidth is smaller than the driving frequency. We show the spectral functions for \( U = 3 \) in the lower panel of Fig. 1, and we observe that the band width is approximately \( \Omega \). The bandwidth is smaller than \( \Omega \) for a smaller \( U \). (iii) When \( U \geq 3 \), resonant tunneling plays an important role. We define \( N^+_{B(A)} = \frac{1}{2\pi} \int_{-\Omega/2}^{\Omega/2} d\omega \sum_{n,\omega+n\Omega \geq 0} \text{Im} G^<_{nn,B(A)}(\omega) \), which corresponds to the fraction of atoms occupying the upper Mott band. The reason for these excitations is the resonant tunneling induced by the hopping \( \langle F | e^{i\theta_n(t)} c^_B c^_A | I \rangle \) between \( A \) and \( B \) sites in the correlated regime. If there were no such resonant tunneling, the fraction of atoms on \( A \) site would be estimated as \( N_A - N^+_A + N^+_B \), and similarly for \( B \) site it would be \( N_B - N^+_A - N^+_B \). If the estimation were accurate, we would have \( N_A - N^+_A + N^+_B \approx N_B + N^+_A - N^+_B \approx 0.5 \) for interactions \( U \geq 3 \). As shown by blue and red dots in Fig. 2, we note that both \( N_A - N^+_A + N^+_B \) and \( N_B + N^+_A - N^+_B \) are close

![Figure 1: Spectral functions](image-url)
neighbor hopping is effectively generated by lattice shak-
tations. This is also evidence for that the next-nearest
the number of atoms on A and B sites, but create exci-
B-A-B), to
N
(iii) There is some deviation from 0.5 for
tunneling by calculating
One can then estimate the contribution of the resonant
tunneling between A and B sites is the main contribu-
tions from A (B) sites. Generally,
\[ N_A^+ - N_A^+ + N_B^+ \]
\[ N_B^+ - N_B^+ + N_A^+ \]. It shows that there are high-order
\( \int_{2\Omega/\omega} \sum_{n,\omega+n\Omega>0} \text{Im} G_{nn}(\omega) \) is
shown. It is corresponding to the effect of resonant tun-
\( \Omega \) is due to one-photon resonant tunneling when \( U = \Omega \). Other
parameters are the same as in Fig. 2.

Figure 2: Charge density wave (CDW) versus interactions
\( U \) for a two-dimensional hexagonal optical lattice with \( 9 \times 9 \)
unit cells and periodic boundary conditions in both \( x \) and \( y \)
directions. Bath parameters are \( \Gamma = T = 0.05 \). \( N_A(B) \) is
shown in Fig. 3.

to 0.5 when \( U \geq 3 \). This demonstrates that the resonant
tunneling between A and B sites is the main contribution
to the difference between the atom densities on A and B
sites when \( U \) is relatively large. This shows the charac-
teristic difference between the NESS and an equilibrium
state. On the other hand, it offers a way to estimate the
resonant tunneling. Suppose it is possible to measure
the charge density \( N_A \) and \( N_B \) for different interactions.
One can then estimate the contribution of the resonant
tunneling by calculating \( N_A - 0.5 \) or \( 0.5 - N_B \) for \( U \geq 3 \).
(\( N_A^+ - N_A^+ + N_B^+ \)
and \( N_B^+ - N_B^+ + N_A^+ \). It shows that there are high-order
\( \int_{2\Omega/\omega} \sum_{n,\omega+n\Omega>0} \text{Im} G_{nn}(\omega) \) is
shown. It is corresponding to the effect of resonant tun-
\( \Omega \) is due to one-photon resonant tunneling when \( U = \Omega \). Other
parameters are the same as in Fig. 2.

Figure 3: Charge density with positive frequency induced by
resonant tunneling, plotted versus interactions \( U \). The peak
is due to one-photon resonant tunneling when \( U = \Omega \). Other
parameters are the same as in Fig. 2.

We have a short comment regarding the case in the
upper panel of Fig. 1. When the staggered potential is
absent, there are still resonant tunnelings. However, they
are the same for A and B sites, in contrast to the case
with staggered potentials.

In Fig. 3, the charge density with positive frequency
\( (N_{A(B)}^+ = \frac{1}{2\pi} \int_{\Omega/2}^{\Omega/2} d\omega \sum_{n,\omega+n\Omega>0} \text{Im} G_{nn}(\omega) \) ) is
shown. It is corresponding to the effect of resonant tun-
ner [53]. The peak is at \( U = \Omega = 7 \), where the one-
photon resonant tunneling is dominant. As we have dis-
cussed above, the contribution \( N_A^+ (N_B^+) \) is due to the
direct hopping from B (A) sites, plus higher-order con-
tributions from A (B) sites. Generally, \( N_A^+ > N_B^+ \), and
atoms prefer to hop to A sites due to the higher staggered
potential on B sites.
B. Edge states

In this section, we present topological properties of a circularly shaken hexagonal optical lattice. We investigate edge states in a cylinder geometry of a hexagonal optical lattice, with a flux $\Phi$ insertion (Fig. 4) [54–56]. This is the setup in the Laughlin gedanken experiment [38]. The insertion of flux is equivalent to a twisted boundary condition in the direction with periodic boundary condition [57, 58]. It is a general setup with the potential to be generalized to disordered cases [58].

With insertion of one flux quantum, we demonstrate the change of topological properties of the system. Edge states are hallmarks of nontrivial topological properties. Using real-space Floquet DMFT, we study the interplay between interactions and edge states. We show the spectral functions in Fig. 5. For finite detuning $\Delta$, the cylinder geometry can host edge states when $U = 0$. With increasing interactions, the edge states as a function of the inserted flux $\Phi$ are smeared out as can be seen in Fig. 5. This corresponds to a finite lifetime of quasiparticles. The sharp spectral peak of a quasiparticle is gradually expanded due to increasing interactions. When $U = 3$, we see a simple Mott gap. We observe three different phases: Chern insulator with edge states present, pseudogap metallic phase with gap closed, and Mott insulator with gap open again. According to the effective Hamiltonian [14], the ratio between the next-nearest neighbor hopping $t_2$ and nearest neighbor hopping $t_1$ is $|t_2/t_1| = 0.1$ with $|t_1| = 0.5$. The pseudogap metallic phase exists approximately when $U \approx 2$. This is consistent with DMFT calculations in Ref. [52] for the Haldane-Falicov-Kimball model. The difference is that here we are considering a non-equilibrium driven system connected to a bath. The largest interaction $U = 3$ we have shown is much smaller than driving frequency $\Omega = 7$. It can therefore be expected that resonant tunneling is greatly suppressed. The dissipation rate $\Gamma$ into the bath has effects on the spectral functions especially for small $U$. It introduces an $i\Gamma$ correction to the self-energy and this term is equivalent to an interaction effect.

Figure 4: A cylinder geometry of a circularly shaken hexagonal optical lattice with a flux $\Phi$ insertion. This is the setup in the Laughlin gedanken experiment [38]. The zigzag boundary condition is used in the calculation.

Figure 5: Spectral functions versus the flux $\Phi$ for different interactions. It shows interaction effects on edge states in a cylinder geometry of $3 \times 10$ unit cells with 3 unit cells in the direction with a periodic boundary condition. Other parameters are $\Omega = 7$, $\alpha = 1.28$, and $\Delta = -0.35$. Bath parameters are $\Gamma = 0.005$ and $T = 0.01$. $\omega'$ indicates a general frequency which can be outside the first Brillouin zone of $\Omega$.

C. Charge pump

A second topological quantity which can be investigated in Laughlin’s setup is the charge pump, which is closely related to edge states. For an equilibrium system, when well-defined edge states are present in the cylinder geometry of a hexagonal optical lattice, a change of one flux quantum will induce an integer number of atoms to transfer from one edge of the cylinder to the other [38]. The number of transferred atoms depends on the number of edge states. An integer charge pump is a signature of non-trivial topological phase. Following Ref. [54], we define the charge pump with insertion of flux $\Phi$ as

$$Q_\Phi = Q_{\Phi,R} - Q_{\Phi,L}$$

(20)

which is the charge density difference between two halves of the cylinder (see Fig. 6: left and right of the cylinder). $Q_{\alpha,\Phi} = \frac{1}{2\pi} \int_{-\Omega/2}^{\Omega/2} d\omega \sum_{i,\alpha,nn} \text{Im} G_{i,\Phi,nn}^\alpha (\omega)$ with $\alpha = R, L$, and Floquet index $n$. $\text{Im} G_{i,\Phi,nn}^\alpha (\omega) = \frac{1}{2\pi} \text{Im} \sum_{n} G_{i,\Phi,nn}^{R/A} (\omega)$, $G_{i,\Phi,nn}^{R/A} (\omega)$, and $G_{i,\Phi,nn}^{\text{loc}} (\omega)$, where $i$ is the site index in the left or right half. The flux is implemented according to Ref. [56]. Using the sum rule $\frac{1}{2\pi} \int_{-\Omega/2}^{\Omega/2} d\omega \sum_n G_{i,\Phi,nn}^{R/A} = 1$, we have

$$Q_\Phi = \int_{-\Omega/2}^{\Omega/2} d\omega \sum_n \frac{1}{2\pi} \text{Im} \left[ G_{i,\Phi,nn}^K (\omega) - G_{\text{loc},\Phi,nn}^K (\omega) \right].$$

(21)
Figure 6: The charge pump with insertion of a flux $\Phi$ is defined as charge density difference $Q_\Phi = Q_{R,\Phi} - Q_{L,\Phi}$ between the two halves of the cylinder, as indicated by different background colors. When there are well-defined edge states, they are expected to be present in the left or the right half.

1. An isolated equilibrium system

We show that $Q$ can indeed be a topological invariant to distinguish non-trivial and trivial topological phases for an non-interacting equilibrium state. For this case, no bath is needed for energy dissipation. We can determine the Keldysh Green’s function using the fluctuation-dissipation theorem \cite{43}: 

$$G^K(\omega) = \tanh \frac{\beta_0 \omega}{2} (G^R(\omega) - G^A(\omega))$$

where $\beta_0 = \frac{1}{k_B T_0}$ with $T_0$ the equilibrium temperature of the system. We choose $T_0$ as a very small number close to 0. The charge pump can be calculated as:

$$Q_\Phi = -\frac{1}{\pi} \operatorname{Im} \int_{-\Omega/2}^{\Omega/2} d\omega \sum_n f(\omega + n\Omega) \times \operatorname{Im} [G^R_{R,\Phi,nn}(\omega) - G^R_{L,\Phi,nn}(\omega)] .$$

(22)

$Q_\Phi$ can be calculated directly or using the technique of the contour integral. In Fig. 7, we show the charge pump versus flux insertion $\Phi$ for topologically non-trivial and trivial cases. In the upper panel of Fig. 7, we observe a sharp jump of the charge density difference $Q$ at the point $\Phi$, where two edge states intersect each other. It means that one atom is transferred from one edge of the cylinder to the other. In contrast, in the topologically trivial case, we only observe a smooth change in the charge density. Therefore, $Q_\Phi$ can serve as a topological invariant for distinguishing topologically non-trivial and trivial cases.

2. System coupled to a free fermion bath

We present the charge pump $Q$ for a NESS obtained from the real-space Floquet DMFT in Fig. 8. Corresponding to edge states in Fig. 5, we show that there is a jump in the charge pump in Fig. 8. However, the jump is not an integer even for very small interactions. With increasing interactions, the jump becomes very smooth. We explain why the jump is not integer even for $U = 0$. It does not contradict to what we show in Fig. 7. In real-space Floquet DMFT, there is a bath coupled to every lattice site. With the approximation of constant DOS of the bath, the dissipation into the bath introduces a finite self-energy to the system. This is equivalent to an interaction effect. In fact, it is this effective interaction which destroys the integer charge pump when $U = 0$. When the system couples to the environment (the bath) and becomes open, the unavoidable dissipation plays a role in the topological properties. Even though the dissipation is rather small, the interaction effect induced by it can be pronounced because the effective hopping is heavily dressed by the driving.

3. System coupled to a heat bath

To further identify the role of dissipation to the bath in the charge pump for a non-interacting system, we here study the NESS that forms when the driven system at
half filling is coupled to an ohmic heat bath, using the rate equations.

Similar to the fermionic reservoir, we couple one heat bath at temperature $T$ to every site of the lattice. This is mediated by a coupling operator $v_{\ell}(t) = c^\dagger_\ell c_\ell$ for a given site $\ell$. Note that we assume this form of the coupling for the direct frame. However, if we transform the coupling to the co-moving frame, it still obeys the same form since the unitary rotation $U$ commutes with the coupling $c^\dagger_\ell c_\ell$.

From Eq. (15) one then infers rates $R_{ab}^{(l)}$ that result from coupling this site $l$ to the heat bath. The total rates for coupling the system globally to an external heat bath result from the incoherent sum of all of these processes, implying $R_{ab} = \sum_l R_{ab}^{(l)}$.

With these rates we solve the kinetic equation (19) for the NESS. Just to remind the reader, the resulting state is the long-time steady state that results when the system is under a constant driving and weakly coupled to the bath, meaning that the coupling constant is small when compared to all quasi-energy splittings in the system, $\sqrt{\Delta} \ll (\varepsilon_k - \varepsilon_q)$, for $k \neq q$.

We observe that for frequencies $\Omega$ which are large when compared to the bandwidth, the distributions $\langle n_a \rangle$ that we observe in the NESS are still close to thermal distributions with an effective temperature $T_{\text{eff}}$, cf. the examples in Fig. 9(a) and (b). This effective temperature is obtained by fitting the closest thermal distribution to the occupations such that $\langle n_a \rangle \approx 1/(e^{(\varepsilon_a - \mu)/T_{\text{eff}}} + 1)$, and therefore assuming what was called a “Floquet-Gibbs” state in the literature [59]. Note that in Fig. 9, the temperature of the bath is $T = 0.001 J$, but still, due to the driving, in the long-time limit the system heats up to quite high temperatures that are on the order of $T_{\text{eff}} \approx 0.1 J$ as shown in Fig. 9(c) and (d) for a heat bath with ohmic spectral density and no spectral cutoff, $J(E) \propto E$. Interestingly, in this frequency regime, the effective temperature of the steady state seems to depend only on the relative strength $K/\Omega$ of the driving. Note that this is in contrast to the analytic formula that was presented in Ref. [60], where in addition to the $K/\Omega$ dependence they find a term that scales as $1/\Omega^d$ (where $d$ is the exponent of the spectral density). In our calculations we also observe that $T_{\text{eff}}$ is practically independent of the size of the lattice.

Even by further decreasing the temperature $T$ of the bath, we are not able to reach lower effective temperatures $T_{\text{eff}}$. We checked this by comparing to the NESS for a hypothetic $T = 0$ bath, where there are no bath occupations $n_R = 0$, so that there is only spontaneous emission. These relatively large effective temperatures are detrimental for the observation of quantized charge pumping, since they correspond to a significant occupation of the “upper” Floquet band.

Note that this heating is due to the population transfer between Floquet states that is induced due to the presence of the driving.
ence of the coupling to the higher Floquet sidebands. As was pointed out in the literature [60–62], this heating can be suppressed by engineering the bath such that the spectral density $J(E)$ at large quasi-energy differences becomes smaller. For example if we suppose the bath is sub-ohmic with $J(E) \propto E^{0.5}$, as shown in Fig. 10(a), then at large frequencies $\Omega$ we find that heating is suppressed, leading to lower effective temperatures $T_{\text{eff}}$ in the NESS. Similar suppression of heating is found in Fig. 10(b) for an ohmic bath, but with a finite cutoff $E_c = 5J$ in the spectral density $J(E) \propto E \exp(-E/E_c)$. Note that it has been argued in the literature that in the limit $\Omega \gg E_c$ resonances are suppressed and one can expects an effectively thermalized “Floquet-Gibbs” state [59]. Such a finite frequency cutoff is the manifestation of bath correlation times $\tau_R \propto 1/E_c$ that are on the order of the time scales of the system dynamics $\tau_S \propto 1/J$. Note that such finite correlation times are tunable e.g. in the case where the bath is a weakly interacting Bose-Einstein condensate in a trap. There, excitations are nicely described by Bogoliubov quasiparticles (phonons) and the bath correlation times can be controlled by the trap frequency [63, 64]. Also, sympathetic cooling of fermions in Bose-Einstein condensates is a well established experimental technique, however there, typically a relatively strong coupling $\Gamma$ is favorable, while here we target weak couplings.

If we now use a NESS that was prepared in presence of such a heat bath, one again may ask whether one can observe the underlying topological nature of the model. Similar to the DMFT calculations in presence of the fermionic reservoir, in Fig. 11(a) we show the charge difference $Q_\Phi$ of the right and lefthand side of the system in the NESS that was prepared for a given value of the flux $\Phi$. However, even though for these parameters the model is topological and the effective temperatures are relatively low, especially in the case with a finite cutoff in the spectral density (green line), we do not see a pronounced peak in the charge difference.

In order to overcome this problem, we propose a different strategy to probe topology in the model. Namely, in Fig. 11(a) it is assumed that the ramp time $\tau$ is big when compared to the relaxation times $\tau_R$, i.e. we follow the system adiabatically in the thermodynamic sense. Here, since we are in the weak coupling regime where $\tau_R$ is large, we propose to perform a ramp on a much shorter time scale $\tau \ll \tau_R$, such that during the ramp one may neglect the action of the bath. However, this ramp should still be slow when compared to system time scales $\tau_s \ll \tau$, which one might call adiabatic in the closed system (without the presence of the bath). The solid lines in Fig. 11(b) show the charge transport that one observes in such a procedure, where we start with a NESS that is prepared without the presence of an external field, $\Phi_{\text{NESS}} = 0$. There, the values are quite high, for the ohmic bath with a cutoff. The density difference between two halve of the cylinder $Q_\Phi$ is up to about 1.4 (green line), corresponding to 0.7 of a charge is transported, which is very close to the quantized value that we expect for such a ramp.
if we assume a $T = 0$ population of the quasi-energies (dashed line).

### D. Experimental relevance

We discuss the possibilities to observe the physical quantities we have explored in an experiment. To detect the CDW, one can measure the local densities on A and B sites either in situ in a quantum gas microscope, after time of flight via adiabatic band mapping techniques, or via the double occupancy [65]. For the charge pump, one needs to compare the local particle density between two parts of the cylinder geometry. The extra flux, in fact, relaxes the requirement to have a periodic boundary condition in one direction. For a hexagonal lattice which is finite in both directions, if it is possible to connect the sites at the ends of one direction with a complex long-range hopping, we can realize this cylinder geometry with a flux. This might be easier using a synthetic dimension [66]. A second possible way is discussed in Ref. [67]. It proposes to use Laguerre-Gauss beams to create a cylinder optical lattice. Another possibility is to engineer a ring shaped system with the central hole pierced by a tunable magnetic flux, as it can be realized using the scheme proposed in Ref. [68]. For the charge pump measurement, as we have shown for the non-interacting case with rate equations, there is the possibility to couple the system weakly to a low-temperature heat bath to prepare the system in a state close to equilibrium. Bath engineering can be used to reach sufficiently low effective temperatures in the NESS. Then, the flux can be adiabatically ramped up to have a pronounced charge pump.

We have a comment on the bath. To study NESS in a driven system, it is necessary to connect the system to a bath to dissipate the extra energy. Most setups for cold atoms in optical lattices are isolated systems, but they can be in the prethermal regime when the driving frequency is sufficiently large. We may expect that the NESS in our setup may share some similarities for an isolated system in the prethermal regime [69].

### IV. CONCLUSION

In conclusion, we have studied the charge density wave and charge pump of fermions with Falicov-Kimball interactions in a circularly shaken hexagonal optical lattice. We show that the charge density wave is induced by the staggered potential and is dramatically changed because of resonant tunneling. We also show interaction effects on the topological properties. An increase of the Falicov-Kimball interaction tends to smear out the edge states, and finally makes the system enter the Mott insulator phase.

Furthermore, we study non-equilibrium steady states in a Laughlin charge pump setup which is coupled to either a fermionic reservoir or a heat bath. In the interacting case, we show that the charge pump is not integer for insertion of one flux quantum. Also for the non-interacting case, we find that it is not integer due to dissipation into a bath. We confirm this by detailed calculations via rate equations based on the Floquet-Born-Markov approximation. Moreover, we explored possibilities to lower the effective temperature characterizing the NESS of the driven system by engineering the spectral properties of the bath. Our calculations suggest that in theory one can indeed use the presence of a bath to cool down the system, e.g. after a quench where in the closed system typically there are excitations in the upper band, and also to some extent one can overcome the heating that is inherent in the interacting Floquet system. We propose an experimentally feasible procedure to ramp up the flux for the measurement of the charge pump.

In the future, the approaches developed here can also be applied to the Haldane-Hubbard model, where both spin states are mobile, and which is naturally realized with cold atoms in optical lattices.

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