Topological charge pumping of bound bosonic pairs

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(Received 14 October 2019; revised manuscript received 2 May 2020; accepted 4 May 2020; published 26 May 2020)

Experiments with bosonic atoms in optical superlattices allow for the interesting possibility to study the adiabatic quantized pumping of bosonic atoms in the presence of interactions. We investigate this exotic phenomenon for bound bosonic pairs in the paradigmatic Su-Schrieffer-Heeger model where the ground state exhibits topological properties due to dimerized hoppings. We show that at unit filling there exist crossovers and phase transitions to bond-order phases of paired bosons known as the pair-bond-order phase for attractive interactions. The pair-bond-order phase is found to exhibit effective topological properties such as the presence of polarized paired edge states. This is further analyzed by studying the emergence and breakdown of the Thouless charge pumping of bound bosonic pairs by a parametric extension to the famous Rice-Mele model. Finally, we discuss how the pumping of paired bosons or different regimes of breakdown of charge pumping can be probed by state-of-the-art experiments, for example, with repulsively bound bosons.

DOI: 10.1103/PhysRevA.101.053630

I. INTRODUCTION

Composite particles often exhibit fundamentally different properties, e.g., charge or exchange statistics, from the ones of their constituents, which may strongly influence the properties of many-body states of these composite objects. A paradigmatic example of this is the composite fermion picture of fractional quantum Hall states [1,2]. In particular, these phases have triggered a paramount interest in topological phases of matter influencing the field of condensed-matter physics, material sciences, and quantum computation [3]. Recently, much effort has been put forth to realize such interesting physics in ultracold quantum gases experiments [4–7]. Many topological quantum phases have been studied extensively in the context of noninteracting fermionic systems in their ground state. In recent years important progress has been made to extend these concepts to interacting fermions [8,9] and bosons [10], dynamical fields [11–13], finite temperatures, nonequilibrium, and mixed states [14–16]. In this paper we explore the nontrivial topological properties of bosonic composite pairs, for example, the bound bosonic pairs which may be directly accessible in state-of-the-art quantum gas experiments.

One of the simplest one-dimensional models which possesses nontrivial topological features is the Su-Schrieffer-Heeger (SSH) model [17] which has been extensively studied in the context of fermionic and bosonic systems [8–10,18–24]. These topological phases in the SSH model are characterized by the existence of polarized edge states which may be probed by the presence of adiabatic transport or pumping of a quantized topological charge. This concept was first introduced by Thouless [25] and may be studied by the generalization of the SSH to the Rice-Mele (RM) model [26]. Recently, with the observation of charge pumping in cold-atom experiments [4–7], the fate of Thouless pumping in interacting systems, such as the interacting fermionic or bosonic RM model, has attracted a great deal of interest [27–33].

In this paper we investigate theoretically the topological features and Thouless pumping for the bosonic pairs in the context of a generalized RM model given by (compare Fig. 1)

$$H_{\text{RM}} = -\sum_i [t - (-1)^i \delta \cos(2\tau)] a_i^\dagger a_{i+1} + \text{H.c.}$$

$$+ \frac{\delta \Delta}{2} \sin(2\tau) \sum_i (-1)^i n_i + H_{\text{int}},$$

with $a_i$ and $a_i^\dagger$ the bosonic annihilation and creation operators on site $i$, respectively, and $n_i = a_i^\dagger a_i$ the number operator. Here $\tau$ is a cyclic parameter which will be utilized for the pumping protocol. On-site interactions $H_{\text{int}} = \sum_i \Delta n_i$ are characterized by the term $U$. Note that the RM model reduces, for $\tau = 0$ and $\pi/2$, to the SSH model.

$$H_{\text{SSH}} = -t \sum_i [1 + \delta (-1)^i] a_i^\dagger a_{i+1} + \text{H.c.} + H_{\text{int}}$$

with staggered hopping rates $t_1$ and $t_2$ from odd and even sites, respectively ($t = \frac{t_1 + t_2}{2}$ and $\delta t = \frac{t_2 - t_1}{2}$). We exploit this scenario to first draw insight into the phase transitions of the bosonic pairs in the SSH model and then analyze the charge pumping of composite pairs in the RM model in one dimension. As we want to study the case of bound bosonic pairs, we impose a three-body constraint, i.e., $(a_i^\dagger)^3 = 0$, in order to stabilize the system against collapse due to the attractive on-site interactions. In the rest of the paper we typically choose parameters in units of $t = 1$.

The limit of strong attractive interactions $-U \gg t$ at unit filling is dual to the hard-core boson limit $U \to \infty$ with renormalized hopping coefficients $t_i^{\text{eff}} = t_i^2/|U|$ and half filling. As effective on-site pairs are formed, one can define the
finite on-site two-body interactions. We show that the phase diagram and the topological properties of paired bosons are possible for \( \tau = 0 \) and \( \tau = \pi / 2 \). The cases of \( \tau = \pi / 4 \) and \( \tau = 3 \pi / 4 \) depict a staggered potential with \( \delta \Delta = \Delta_+ - \Delta_- \).

corresponding operator \( c_j^\dagger = (a_j^\dagger)^2 \) and hence the paired boson model can be mapped to the free-fermion model

\[
H_f = -t \sum_j [1 + \delta t (-1)^j] c_j c_{j+1} + \text{H.c.} \quad (3)
\]

As this model exhibits well-defined nontrivial topological properties at half filling, we can expect to find similar properties of the paired-boson model in the limit \( -U \gg t \) at unit filling. In the following we analyze the ground-state phase diagram and the topological properties of paired bosons for finite on-site two-body interactions. We show that the system of bound bosonic pairs, even though not protected by symmetry, exhibits remarkable effective topological features such as edge states and pair pumping in a region of attractive finite \( U > -\infty \), which is adiabatically connected to a region with trivial effective topology. We discuss how some features of this phenomenology could be observed without implementation of a three-body hard-core constraint in cold-atom quantum gases.

The paper is organized as follows. After a discussion of the ground-state bulk physics of the model (2) in Sec. II at unit filling, we describe the edge state and effective topological properties in Sec. III and pair pumping in the Rice-Mele model in Sec. IV. We discuss possible experimental realizations in Sec. V and summarize in Sec. VI.

II. BULK PROPERTIES AT UNIT FILLING

In the SSH model, two types of hopping dimerization are possible for \( \tau = 0 \) and \( \pi / 2 \) (Fig. 1) corresponding to \( t_1 < t_2 \) and \( t_1 > t_2 \), which exhibit identical bulk properties. At half filling, the single-particle spectrum is gapless for any imbalance in hopping between the unit cells \( t_1 \neq t_2 \) [17]. In the limit of large interactions \( U \to \infty \), the bosons are hard core in nature and in this limit the model (2), after a Jordan-Wigner transformation to free fermions \( c_j^{(1)} \), can be considered as the topological SSH model as mentioned before. Hence, one gets a bond-order phase of bosons at half filling, i.e., \( n = N / L = 1 / 2 \) particles per lattice site as a result of natural dimerization due to the Peierls instability. The presence of chiral symmetry in the model leads to the emergence of gapless topological edge states for \( t_1 < t_2 \) which are characterized by a nontrivial winding number (or Zak phase) [19,20,34]. This paradigmatic example of bulk-boundary correspondence can be extended to the case of soft-core bosons at half filling [10].

The detailed ground-state bulk properties of the three-body constrained bosonic SSH model in a grand canonical ensemble are discussed in Ref. [35]. Here we will summarize the phases and phase transitions of the model focusing on the phase diagram at unit filling of \( n = N / L = 1 \) particles per lattice site. The case of \( \delta t = 0 \) of the model (2) is known to exhibit a Berezinskii-Kosterlitz-Thouless (BKT) type of phase transition from a gapless superfluid (SF) to a gapped Mott-insulator (MI) phase for strong repulsive interactions \( U > U_c > 0 \) (where \( U_c \) is the critical point for the SF-MI phase transition). For negative values of the interaction \( U < 0 \), the three-body constrained system exhibits an Ising-type phase transition to a SF phase of paired bosons called the pair superfluid (PSF) phase. In the limit of strong attractions \( -U \gg t \) the system is a stable ensemble of bosonic pairs (\( a_j^\dagger a_j^\dagger \)) [36] dual to the hard-core boson limit \( U \to \infty \) with renormalized hopping coefficients of bound pairs \( t_j^{\text{eff}} \equiv t_j / |U| \).

Before proceeding to the detailed numerical results, we will present the inference that can be obtained from analytical arguments. The properties of (constrained) bosons at unit filling can be best understood from field-theoretic arguments. In particular, the system of three-body constrained bosons can be understood as a spin-1 system, which itself can be described well by the triplet state of spin-1/2 states [37]. Spin-1 models with a staggered or dimerized exchange term have been studied before, e.g., in Refs. [38–40]. Here we will follow the bosonization scheme discussed, e.g., by Berg et al. in Ref. [41] and approximate the bosons by \( a_j^{(0)} \approx (a_j^{(0)} + a_j^{(1)})/\sqrt{2} \), with two different bosonic species \( a_{j,\alpha} \), \( \alpha = 0, 1 \). Within the standard bosonization dictionary [42], we introduce two sets of bosonic fields \( (\theta_0, \phi_0) \) and \( (\theta_1, \phi_1) \) corresponding to the density and phase fluctuations of \( a_{j,0} \). With Ref. [41], we obtain an effective decoupling of symmetric and antisymmetric combinations \( \phi_{\pm} = (\theta_0 \pm \theta_1) / 2 \) and \( \phi_{\pm} = \phi_0 \pm \phi_1 \), where \( \mathcal{H} \approx \mathcal{H}_+ + \mathcal{H}_- \) with

\[
\mathcal{H}_+ \sim v_+ \frac{\left( \partial_\theta \phi_+ \right)^2}{K_+} + K_+ (\partial_\phi \phi_+)^2 \quad + \quad g_1 \cos(2\phi_+) + \cdots
\]

\[
\mathcal{H}_- \sim \frac{v_-}{2} \left[ \left( \frac{\partial_\theta \phi_-}{K_-} \right)^2 + K_- (\partial_\phi \phi_-)^2 \right] + g_2 \cos(2\phi_-) + \cdots
\]

(4)

(5)

up to higher-order terms. In the weak-coupling limit with \( g_{1,2} \sim U, g_3 \sim t \), and phenomenological Luttinger-liquid parameters \( K_\pm \) and velocities \( v_{\pm} \), \( \mathcal{H}_- \) has the form of a double-sine-Gordon Hamiltonian [43]. For \( K_- > 1 / 2 \), the \( \cos(2\phi_-) \) term is relevant and will open up a gap in the antisymmetric sector. For strong attractive interactions \( U < 0 \), the system may enter a phase of paired bosons where the \( \phi_- \) field becomes gapped, which corresponds to the SF-PSF phase transition if the symmetric sector remains gapless. The \( g_1 \) term
may induce a transition to a gapped phase in the symmetric sector, which corresponds to the opening of the Mott gap and a SF-MI BKT-like transition. Note that a Haldane-insulator phase, as discussed in Ref. [41], will require a finite nearest-neighbor interaction between atoms and is also not consistent with the two-site unit cell of the SSH model. In this framework the SSH-model staggered tunneling term \((-\delta t)\) is a relevant term, it will here open up a gap also in the symmetric sector, introducing a phase transition to the pair-bond-order (PBO) phase. For strong \(\delta t\), \(\cos(\phi_{\pm})\) may directly open up a gap in the antisymmetric sector also at vanishing \(U\). Interestingly, both the \(\sin(\phi_{\pm})\) and \(\cos(2\phi_{\pm})\) terms stabilizing the PBO and the MI phases are compatible with the pinning of \(\phi_{\pm} \sim \pi/4\), and we may not expect any phase transition between the large-\(U\) MI state and the PBO state, but a smooth crossover between the two regimes.

Our numerical simulations are consistent with this qualitative bosonization analysis. The complete ground-state phase diagram of the bosonic constrained SSH model is shown in Fig. 2 as a function of the hopping ratios \(t_2/t_1\) as well as \(t_1/t_2\) and the interaction strengths \(U/t_1\) and \(U/t_2\), respectively. Ground-state properties of this system are analyzed using the density-matrix renormalization-group (DMRG) method. We consider typical system sizes up to 160 sites and retaining up to 800 density-matrix eigenstates. The phase diagram shows various quantum phases such as the gapped MI phase on the repulsive \(U\) regime and the PBO\(_0\) and PBO\(_{\infty}\) phases in the attractive regime, which will be discussed in more detail in the following. Apart from this there also exist the gapless SF and PSF phases. The black diamonds depict the phase transition to the SF phase and there exist smooth crossovers from the MI to the PBO phase denoted by the red dashed lines with pluses. The blue dotted line with crosses represents the emergence of edge states, as will be discussed below.

The gap to gapless phase transitions and crossovers of Fig. 2 are obtained by calculation of the momentum distribution function

\[
N(k) = \sum_{i,j} e^{i(k_j - k_i)_{ij}(a_ia_j^\dagger)}.
\]

Following Refs. [35,44,45], the maximum of the momentum distribution \(N(k)_{\text{max}}\) function is expected to scale as \(L^{3/4}\) with the finite system size at the BKT-type SF-MI transition. Figure 3 exemplifies this for the phase transition points at \(t_2/t_1 = 0.6\). We further compute the excitation gap of the single-particle \(G_1\) and two-particle sector \(G_2\) with

\[
G_m(L) = \left[ E_0(N + m, L) - 2E_0(N, L) + E_0(N - m, L) \right]/m.
\]

where \(E_0(N, L)\) is the ground-state energy of a system of \(N\) particles and \(L\) sites and \(m \in \{1, 2\}\). In order to verify the BKT character of the phase transitions we analyze the finite-size scaling of the energy gaps in the \(-U\) regime using the approach used in Refs. [46,47]. In the inset of Fig. 4(a) the rescaled single-particle energy gap \(G_1^* = G_1L[1 + 1/[\ln(L) + C]]\) for \(t_2/t_1 = 0.6\) exhibits the expected scaling close to the BKT transition point \((U_c = -2.9)\). This leads to a collapse of data points plotted against \(x_L = \ln(1 + \sqrt{U}/U_c)/u\), with fitting parameters \(C\), \(B\), and \(U_c\) [46,47].

For a strong staggered hopping \(\delta t\), as shown in Fig. 4(b), we do not observe any closing of the excitation gap \(G_{1,2}\) upon changing \(U\) from the PBO to the MI phase. We furthermore calculate the neutral excitation gap \(G_N(N, L) = E_1(N, L) - E_0(N, L)\) for strong \(\delta t\), as depicted in Fig. 4(c), which also remains finite. This shows that, interestingly, both phases remain adiabatically connected, as discussed already in Ref. [35]. In the inset of Fig. 4(b) we depict the fidelity...
susceptibility defined as
\[ \chi_{FS}(U) = \lim_{U' \to U} \frac{-2 \ln |\langle \psi_0(U) | \psi_0(U') \rangle|}{(U - U')^2}, \tag{9} \]

where $|\psi_0\rangle$ is the ground-state wave function. Here $\chi_{FS}/L$ exhibits a local maximum which stays finite as a function of the system size, consistent with the finite excitation gaps. The presence of a second local maximum may be attributed to an intermediate bond-ordered region [35], which we will not discuss further here. We may quantify the crossover points from the MI region to the PBO phase by a more detailed analysis of the excitation gap. As shown in Figs. 4(a) and 4(b), we observe a crossing between the single-particle gap $G_1$ (red dashed lines) and two-particle gap $G_2$ (blue solid lines) which indicates the crossover points. We show also the data for $L = 160$ along with the extrapolated data for $t_2 = 0.6$ [Fig. 4(a)] and $0.3$ [Fig. 4(b)]. The extrapolation is performed using the data for $L = 40, 80, 120,$ and 160. The arrow defines the crossover between MI-like and dimerized PBO states. The crossover position to a PBO region can also be seen in the bond-order structure factors [35].

Finally, in Fig. 5 we present numerical results for the phase transition to the PBO phase at large negative $U = -8t_1$. By fitting the bipartite von Neumann entanglement entropy $S_{vN}(j)$ to its conformal description [48]

\[ S_{vN} = \frac{c}{3} \ln \left[ \frac{L}{\pi} \sin \frac{\pi j}{L} \right] + g, \tag{10} \]

we obtain estimates of the central charge $c$ for several system sizes. Consistent with our bosonization analysis, the point $t_1 = t_2$ is critical and the central charge seems to converge to a value of $c = 1/2$ in the thermodynamic limit, as expected for a PSF phase. For a finite $\delta t > 0$, the central charge drops to $c = 0$ and the system enters the gapped PBO regime.

**III. TOPOLOGICAL PROPERTIES**

As argued above, for $U \to -\infty$, the model (2) is equivalent to a model of hard-core bosons or free fermions given in Eq. (3). At half filling, this exhibits nontrivial topological properties for $t_2 > t_1$, such as edge states. In the
following we discuss the fate of these features for finite interactions.

A. Edge states

In our numerical simulations, we observe the presence of polarized edges also at finite values of $U > -\infty$, in the region marked as the PBO$_x$ phase in Fig. 2. In Fig. 6 we sketch the edge density for a generalized RM model at $t_1/t_2 = 0.2$ for different values of $U$. In order to visualize the properties of the edges also for different values of $\tau$ clearly, we subtract the background average density $\bar{n}_j = \langle n_{L/2+j (j \mod 2)} \rangle$. The $\tau = 0$ curves show the edge densities of the corresponding SSH model. For smaller values of $U$ [Fig. 6(b)], the polarization vanishes abruptly and symmetric (Friedel-like) density oscillations are found at the boundaries of the system.

In order to quantify the edge properties in more detail, we calculate the polarization

$$P = \frac{1}{L} \sum_{j=0}^{L} \langle \psi | (i - i_0) n_j | \psi \rangle,$$

with $i_0 = (L - 1)/2$ and the ground state $|\psi\rangle$ of the model (1) or (2). We plot this quantity for different values of $t_1/t_2$ with respect to $U$ as shown in Fig. 7. In order to facilitate the numerical simulations, we add a small symmetry-breaking potential to the boundary sites, corresponding to the evolution of the RM model at a small value of $\delta \tau = 0.001$. Comparisons to results with a smaller $\delta \tau$ = 0.0001 and different system sizes indicate that our choice does not influence the physics of the system. Interestingly, we observe a sudden sharp transition between a region of $U < U_c$ with polarized edges and a polarization close to 0 = 1 and unpolarized systems with $P = 0$ for larger values of $U > U_c$.

In the phase diagram of Fig. 2 we depict the point of emergence of edge states $U_c$ as the blue dotted line with crosses. This transition line differs from the crossing position of two-particle and one-particle excitations (red dashed line in Fig. 2). The reason for this can be attributed to the bosonic enhancement which is energetically favorable to first delocalize a single doublon on the MI phase before the polarized edge states are formed [22].

B. Winding number

The concept of bulk-boundary correspondence states that the presence of topological edge states should be related to a nontrivial topological invariant of the bulk system. For the SSH model, this is the winding number [10] defined in the many-body context as

$$\omega = \int_0^{2\pi} d\theta \langle \psi(\theta) | \partial_\theta \psi(\theta) \rangle,$$

from the ground state $|\psi\rangle$ of the effective model with twisted boundary conditions $a_i \rightarrow e^{i\theta / L} a_i$. With this definition, we find that $\omega$ vanishes in all the gapped phases and in the SF phase it is accurately characterized by the winding number $\omega \neq 0$. However, we observe no distinction between the $t_1 < t_2$ and the $t_2 < t_1$ region as shown in Fig. 8(a).

To circumvent this we may identify $c_i \rightarrow (a_i^\dagger)^2$ and hence a single-fermion hopping corresponds to two-boson tunneling and will involve twice the phase. This simple argument explains why we observe $\omega = 0$ also for $t_2 < t_1$ as we are winding effectively twice around the parameter space. Hence, the winding number correctly describing the topological properties in this limit should be defined over half the period as

$$\omega_{1/2} = \int_0^{\pi} d\theta \langle \psi(\theta) | \partial_\theta \psi(\theta) \rangle.$$

FIG. 6. Polarized edge states for the RM model at (a) $U = -10$ and (b) $U = -2$ ($t_1 = 1$ and $t_2 = 0.2$) after subtracting the overall density modulation $\bar{n}_j = \langle n_{L/2+j (j \mod 2)} \rangle$ for clarity. The different curves are for $\tau = 0.0$ (blue dashed line with squares), 0.25$\pi$ (red solid line with pluses), and 0.5$\pi$ (green dotted line with crosses).

FIG. 7. Polarization $P$ for $t_1/t_2 = 0.1, 0.3,$ and 0.6 as a function of the interaction strength for $L = 160$ sites ($L = 80$ sites for light colored lines).

FIG. 8. Estimates of the winding numbers (a) $\omega$ and (b) $\omega_{1/2}$ from the small-system-size simulation ($L = 8$ sites, exact diagonalization) for the SSH model as a function of $U/t$ and $t_1/t_2$ as well as $t_2/t_1$. Black lines correspond to the lines of Fig. 2.
in analogy to a $Z_2$ index used for the description of, e.g., the quantum spin Hall effect [49]. In Fig. 8(b) we calculate $\omega_{1/2}$ for the full phase diagram for small system sizes and observe that, interestingly, $\omega_{1/2}$ stays remarkably close to a quantized value in all gapped regions. We also observe an extended region where $\omega_{1/2} = \pi$, which coincides roughly with the emergence of the edge states. We want to stress that $\omega_{1/2}$ is not protected by symmetry in the attractive boson model, but its robustness can be related to an effective chiral symmetry of the bound bosonic pairs. This is why the emerging topological properties without closing of many-body gap apparently seems to contradict the bulk-boundary correspondence. It allows us to discriminate between the $\text{PBO}_0$ and $\text{PBO}_\pi$ regions with nontrivial and trivial effective topologies $\omega_{1/2} = 0$ and $\omega_{1/2} = \pi$ and an abrupt jump between them.

IV. PAIR PUMPING IN THE RICE-MELE MODEL

We will now extend the discussion of the topological properties of the SSH model to the case of the RM model (1) which connects the $t_1 < t_2$ and the $t_2 < t_1$ region of the SSH model by a periodic process in the cyclic parameter $\tau$ realizing a Thouless charge pump. In the single-particle picture (i.e., for $U \rightarrow \infty$) the pumped charge can be related to a Chern number of the RM model (in momentum $k$ and $\tau$ space). Hence, here the pumped charge is quantized and directly linked to the nontrivial topology of the model if nonvanishing. In the following we will analyze how the topological feature of the attractive bosons at unit filling can give rise to a pumping of bosonic pairs and we will analyze the breakdown of the pair pumping upon approaching the crossover to the MI regime.

A. Phase diagram

As a starting point we may also obtain insight into the physics of the RM model at unit filling by means of the bosonization treatment discussed above. Analogously to Eq. (6), we may express the staggered potential as

$$\sim \Delta \cos(\phi_-) \cos(\phi_+) \tag{14}$$

For a pure staggered potential, we may hence expect a competition between the MI phase of dominant $\cos(2\phi_+)$ in the large-$U$ limit and the DW ordering $\cos(\phi_+)$ and observe a phase transition between both phases. For the case of the related spin-1 system with a staggered field $(-1)^y S_y^z$, this has been studied in detail in Refs. [50,51] and a Gaussian-type transition between the large-$U$ (which corresponds to the MI phase in the bosonic system) phase and the Néel ordered phase (corresponding to the density wave phase) has been observed.

The effect of both a staggered potential and staggered tunneling term as we will encounter during the pumping cycle can be expressed as a single cosine term

$$\sim \cos(\phi_-) \cos(\phi_+ + \varphi), \tag{15}$$

with $\varphi \sim \arctan(\delta t/\delta \Delta) \sim \tau$. The value of the pinned field $\phi_+$ will thus follow smoothly the variations of $\tau$. In a finite system, this will correspond to pumping of a charge. The competition with the MI term should lead again to an interesting crossover or transitions.

In Fig. 9(a) we sketch the phase diagram of the RM model in the $\tau-U$ plane according to our numerical simulations. For $\tau = \pi/4$ the system exhibits a gapless Gaussian transition point [50,51]. Note that, even though the excitation gap becomes small around the Gaussian transition point, we do not find any other gapless phases for the given parameters. We again mark the crossing between the $G_1$ and $G_2$ excitation gaps with a red dashed line.

B. Pair pumping

Following Ref. [30], we study the charge pumping for finite systems with open-boundary conditions by monitoring the polarization $P(\tau)$ of the model (1). The total transferred charge is given by

$$Q = \int_0^\tau d\tau \ \partial_\tau P(\tau) \tag{16}$$

and hence is directly linked to the presence of a polarized edge state for the SSH model. We plot the polarization over the pumping cycle in Fig. 10 for several values of the interactions. While for strong attractive interactions $U = -10t$ we observe a clear pumping of a charge $Q = 2$ corresponding to a bosonic pair, for $U > U_{p1} \approx -2.6$ (i.e., for the curves $U = -2, -1, 0$ and 4) we find zero pumped charge, i.e., $Q = 0$, corresponding to the abrupt vanishing of the polarized edge states discussed in the preceding section. Again, we cannot directly link the breakdown of the charge pumping to a gap closing in the pumping cycles as illustrated in the phase diagram in Fig. 9(a).

Interestingly, we can identify an intermediate pumping regime $U_{p1} < U < U_{p2}$, where the polarization during one cycle exhibits a discontinuous jump, as can be seen from the $U = -2$ curve in Fig. 10 around $\tau = 0.1 \pi$. The position and size of the jump are stable with the increase of system size (note that in Fig. 10 the lines contain more calculated data points than shown by the symbols). For $U \gtrsim -1.5$ the
discontinuity vanishes and the polarization becomes a smooth function of \( \tau \). We mark the jump positions of the intermediate breakdown regime of pumping in Fig. 9 by blue crosses.

As discussed by Hayward et al. [31], the charge pumping in the RM model may as well be visualized by the evolution of the entanglement spectrum \( \lambda_\mu \). In Fig. 11 we plot the largest eigenvalues \( \lambda_\mu \) of the reduced density matrix in the center of the system. Due to the total particle number conservation of the model, the eigenvalues may be labeled by \( \Delta N_\mu = N_\mu - N_0 \), where \( N_\mu \) corresponds to the number of eigenvalues \( \lambda_\mu \) and \( N_0 = N/2 \). As shown in Fig. 11(a), for strong attractive interaction \( U = -10 \)τ, the \( \Delta N_\mu = \pm 1 \) eigenstates dominate, leading to a nonzero pumped charge. With increasing \( U \), we observe a crossover to the MI regime where the \( \Delta N_\mu = 0 \) state has the largest contribution and no charge is pumped [Fig. 11(d)].

C. Different pumping cycles

As a topological feature charge pumping should be robust to smooth variations of the actual pumping protocol or periodic path chosen through the parameter space of the RM model. While so far we have discussed the case \( \delta \Delta = \delta t \), Fig. 9(b) shows the results of a similar analysis of more asymmetric pumping parameters \( \delta t = 0.9 \) and \( \delta \Delta = 2.0 \) in a phase diagram showing the pumping cycle as a function of \( U \). Indeed, again we observe pumping of bosonic pairs for strong attractions of \( U \to -\infty \). We observe however a different regime of breakdown of the pumping for \( U \gtrsim -3.5 \). Interestingly, the transition region of the breakdown of pumping gets extended and we observe sharp jumps of the polarization up to \( U \sim 4 \). The blue dotted line with crosses depicts the positions where we observe a sharp breakdown of charge pumping.

V. EXPERIMENTAL REALIZATION

While there has been active research on the bosonic systems with three-body hard-core constraint and attractive interactions [36,52–56], important features of the pair pumping and its breakdown can be studied with state-of-the-art bosonic quantum gas experiments without these properties. We discuss this scenario by considering a system of repulsively bound pairs in the following section.

A. Pumping of repulsively bound pairs

The pumping of attractive pairs can to some extent be simulated by repulsively bound particles: For a deep staggered potential, such as that shown in Fig. 9(b) \( (\delta t = 0.9 \) and \( \delta \Delta = 2.0) \), the ground state for \( \tau = \pi/4 \) with good accuracy is given by a Fock state of two bosons in every second lattice site. In a deep optical superlattice, this state can be accurately prepared [57] with unconstrained bosons with a small repulsive interaction \( U > 0 \). After initialization, we assume a quench to large repulsive interactions \( U_q \gg t, \delta t, \delta \Delta \) by means of a Feshbach resonance. These repulsively bound pairs as studied in Refs. [58,59] are stable due to energy conservation and propagate with a reduced hopping rate in a second-order tunneling process \( t_{\text{eff}} \sim 2t^2/U \). One may now try to perform a pumping cycle with these repulsively bound pairs which can simulate the physics of the attractively bound bosonic pairs. Note that the pumping process has to be slow compared to the effective tunneling rate but fast enough compared to the effective lifetime of the pairs.

In Fig. 12 we perform the time-dependent exact-diagonalization simulation of the pumping process after a quench of the interaction \( U \to U_q \) and compare it to the pumping of attractively bound pairs. Generally we choose a relatively fast evolution \( \tau = \tau / (\tau') = \pi / \tau' \), with the real time \( \tau' \). Interestingly, if we change the precise path through the phase space (path B as sketched in the inset of Fig. 12) the (partial) pumping cycle can be performed accurately as shown in Fig. 12. Instead of the elliptical path of Eq. (1) we choose...
a more rectangular contour (path B), connecting still the same intermediate points at $\tau \mod \pi/4$. On this path our real-time evolution is able to pump a repulsively bound pair, whereas on path A the evolution is too fast and the system evolves to an unpolarized state.

In Fig. 13(a) we study the pumping of repulsively and attractively bound pairs for various interaction strengths. The effective adiabatic condition may depend strongly on the precise path through the phase space chosen during the time of evolution. For the given examples, $U_q \gtrsim 20t$ is sufficient to pump one pair during the time evolution. Interestingly, we observe that slightly lower values of $U_q$ quickly lead to a completely distinct evolution without quantized pumped charges.

B. Pumping of soft-core bosons: Observation of the breakdown regime

The choice of more asymmetric pumping parameters, such as the ones in Fig. 9(b), shifts a large part of the region of breakdown of pumping [blue dotted line with crosses in Fig. 9(b)] to positive values of the interaction parameter $U \gtrsim t$. Here the three-body constrained system is to a good extent modeled by an unconstrained bosonic quantum gas, allowing for the experimental study of the interesting transition region without the three-body constraint. In Fig. 13(b) we compare cases of both constrained and unconstrained bosons for $U = 3t$. While both curves differ strongly, we observe also for the soft-core bosons the sudden kink in the pumped polarization for some values of $\tau = \tau_c < \pi$, which we could identify with the breakdown of pair pumping.

VI. CONCLUSION

In summary, we have investigated the ground-state phase diagram and topological properties of attractive bosons in the context of the SSH and RM models at unit filling. For strong attractive interactions the bosons pair up and dimerize to form the PBO phases, with different effective topological properties and winding numbers $\omega_{1/2} = 0$ and $\omega_{1/2} = \pi$, being linked to interesting edge states of paired bosons. Even though the effective topological properties of the bound pairs are not protected by symmetry, they remain remarkably robust across a wide range of parameters. Without closing a many-body gap, the system exhibits a crossover between regions with trivial and nontrivial effective topologies [60].

While aspects of the topological pumping of bosonic pairs could be reproduced with current setups of unconstrained bosons as we have shown, the flexibility to tune the interactions from attractive to repulsive regimes and the techniques to engineer third- and higher-order local interactions [36,52–55] and recent experimental observation [61] have broadened the scope of simulating the physics of many-body systems by several folds. With the existing state-of-the-art facilities, the current prediction can in principle be experimentally accessible in ultracold-atom experiments along the line of a recent experiment on Rydberg atoms in the SSH model [24].

ACKNOWLEDGMENTS

S.G. acknowledges important discussions with Thierry Giamarchi, Charles-E. Bardyn, Han-Ning Dai, and Zhen-Sheng Yuan as well as financial support from the Swiss National Science Foundation under Division II. T.M. acknowledges SERB (India) for the early career grant through Project No. ECR/2017/001069. The computational simulations were carried out using the Param-Ishan HPC facility at Indian Institute of Technology, Guwahati, India, and the Baobab cluster at University of Geneva.
