Interaction-induced polarons and topological defects in a topological Mott insulator

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Introduction.—First proposed by R. Feynman in the 80s [1], quantum simulators are now a reality. These versatile platforms allow for the simulation of complex quantum many-body systems in a clean and highly controllable environment [2]. In particular, cold atoms in optical lattices, with the dramatic advances in atomic, molecular, and optical physics, are highly suitable quantum simulators of many-particle or spin systems with controlled interactions [3]. There, the study of topological insulators with quantum simulators has become a subject of intense research within the last decade [4, 5]. These exotic materials constitute a new paradigm of quantum matter [6]: they are characterized by a global order parameter, an integer called topological invariant, and present topologically protected surface currents. The quantum simulation of such phases typically relies on the generation of artificial gauge fields through Floquet engineering [7–10], or synthetic dimensions [11–13].

However, it has been shown recently that it is also possible to induce topology directly from interactions, hence giving rise to a spontaneous symmetry breaking (SSB) topological phase [14]. For example, interactions of the same order of magnitude between nearest neighbors (NN) and next-to-nearest neighbors (NNN) give rise to the celebrated topological Mott insulator (TMI) [15, 16], an anomalous quantum Hall (QAH) phase [17], in diverse geometries, such as hexagonal, Lieb, checkerboard, and Kagomé lattices [15, 18–26]. To observe these phases, control over the ratio of interaction strengths is crucial, and cold atoms constitute a prime candidate to simulate such phases in experiment [18, 19].

In this work, we explore the exotic nature of self-consistent solutions, such as polarons and topological defects, above the TMI. Remarkably, these solutions appear thanks to the interplay of the global topological order and the SSB local order parameter, and are thus absent in gauge-induced topological insulators. In a SSB lattice material, particle number deviations from the commensurate filling can favor static solutions breaking the translational symmetry [27–29]. These solutions, which can also be created in a dynamical way [30–35], can take the form of small perturbations, or topological defects in the local order parameter. In the TMI phase, we are interested in studying the impact of these inhomogeneities on the global topology of the system, and vice versa. In order to shed light onto this question, we abandon the usual assumption of spatially homogeneous TMI phases [15, 18–26] and report two type of solutions: (i) self-induced polarons on top of the topological background, and (ii) domain walls between regions from a different sector of the SSB phase. Interestingly, these lead to opposite topological invariants in the same material, and topologically protected chiral edge states at the domain boundaries.
We start by quantitatively studying the mean-field phase diagram of a checkerboard lattice of spinless fermions with NN and NNN interactions at half filling. We study the ground state around half filling in the QAH phase, with an unrestricted Hartree-Fock ansatz. At low particle doping, we observe the existence of a self-trapped polaron and study its effect both on the topological background and on the SSB local order parameter. We also analyze the accuracy of the mean-field description, and study the interaction between two polarons. For higher fillings, we report the appearance of topological defects in the form of domain walls separating the two sectors of the SSB phase at half filling, and inspect the topological chiral edge states on top of them. Finally, we discuss prospects of realizing such phases with cold Rydberg-dressed atoms in optical lattices.

Model.—We consider a Hamiltonian of spinless fermions on a checkerboard lattice, depicted in Fig. 1(a),

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{int}},$$

where $\hat{H}_0$ is the quadratic part, and $\hat{H}_{\text{int}}$ contains the interactions. On the one hand, the quadratic part of the fermionic Hamiltonian reads \cite{20, 21}

$$\hat{H}_0 = -t \sum_{\langle ij \rangle} (\hat{c}_{i,A}^{\dagger} \hat{c}_{j,B} + \text{H.c.}) + \sum_i \sum_{\alpha=A,B} \sum_{\mu=x,y} (J^\alpha_{i\mu,A,B} \hat{c}_{i\alpha}^{\dagger} \hat{c}_{i+2\mu,\alpha} + \text{H.c.}),$$

where $t$ stands for the NN hopping amplitude between sites $A$ and $B$ and $J^\alpha_{i\mu}$ is the NNN hopping amplitude, with $\mu = x, y$ and $\alpha = A, B$. In the remainder of the manuscript, we set $t = 1$, and $J^A_x = J^B_x = 0.5$ and $J^A_y = J^B_y = -0.5$, which generates a $\pi$-flux on each sublattice. Such Hamiltonian has two bands with a quadratic band touching at half-filling. On the other hand, the interaction part of the Hamiltonian reads

$$\hat{H}_{\text{int}} = V_1 \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j + V_2 \sum_{\langle ij \rangle} \hat{n}_i \hat{n}_j$$

and has NN and NNN density-density repulsive interactions. Such Hamiltonian has a rich phase diagram in terms of $V_1/t$ and $V_2/t$ already at the mean-field level, as will be discussed below.

Phase diagram at half-filling.—We treat the interaction Hamiltonian with a standard Hartree-Fock decoupling, respecting the Wick’s theorem,

$$\hat{n}_i \hat{n}_j \simeq -\xi_{ij} \hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\beta} - \xi_{ij} \hat{c}_{j\beta}^{\dagger} \hat{c}_{i\alpha} + \xi_{ij} |^2 + \langle \hat{n}_i \rangle \hat{n}_j + \langle \hat{n}_j \rangle \hat{n}_i - \langle \hat{n}_i \rangle \langle \hat{n}_j \rangle,$$

with $\xi_{ij} = \langle \hat{c}_{i\alpha}^{\dagger} \hat{c}_{j\beta} \rangle$. The Hartree-Fock values $\xi_{ij}$ and $\bar{n}_i \equiv \langle \hat{n}_i \rangle$ are found by solving the self-consistent equations at zero temperature. We also work with a 4-site unit-cell translationally invariant ansatz [see Fig. 1(b)], which we will refer to as the restricted Hartree-Fock (RHF) ansatz in the remainder of the text (see Supp. Mat.). The phase diagram \cite{20, 21}, presented in Fig. 1(b), has three insulating phases, each of them with an order parameter that captures a broken symmetry: (i) the site nematic insulating phase characterized by $\rho_n \equiv |\bar{n}_{A_1} + \bar{n}_{A_2} - \bar{n}_{B_1} - \bar{n}_{B_2}|$, (ii) the stripe insulating phase, with $\rho_s \equiv |\bar{n}_{A_1} - \bar{n}_{A_2} + \bar{n}_{B_1} - \bar{n}_{B_2}|$, and (iii) a QAH phase, with time-reversal symmetry breaking (TRSB) due to interaction-induced closed loops of imaginary NN hopping $\xi_{QAH} \equiv |\text{Im}(\xi_{A_1B_1} + \xi_{B_1A_2} + \xi_{A_2B_2} + \xi_{B_2A_1})|/4$.

In order to characterize the topology of the QAH phase, we obtain its RHF band structure, which shows two lower filled bands separated from the two upper bands by an energy gap $\Delta_{QAH} = 8V_1 \xi_{QAH}$. We compute the total Chern number $\nu$ of the filled bands and find $\nu = \pm 1$ (see Supp. Mat.). The two possible values of $\nu$ account for the two-fold ground state degeneracy in the interaction-induced QAH phase, i.e., the closed current loops can flow in two opposite directions, and the system reaches one of the two symmetry-breaking sectors through a spontaneous TRSB mechanism [see Fig. 1(b)].

Polaron.—We now focus on the system at low particle doping $\delta$, starting for the case of one extra particle ($\delta = 1$). In the non-interacting rigid band picture, the bulk of the system would lose its insulating character and become metallic, as the particle would occupy the first single-particle state above the gap. In order to analyze the interacting system, hereafter we fix the

FIG. 2. Self-induced polaron for $\delta = 1$. (a) Energies ($E$) of the single-particle states $\lambda$ in the gap region for the RHF (diamonds) and UHF (dots) ansatz. Here the dashed line indicates the chemical potential of the UHF solution, $\mu_{UHF}$, and green and red colors are used for occupied and empty states, respectively. (b) Density profile. (c) Imaginary hopping between NN, $\text{Im} \xi_{i, i+x, \pm y}$. (d) Local Chern number.
value of the interactions to $V_1/t = 2.5$ and $V_2/t = 1.5$. We first study the solution of the RHF ansatz, shown in Fig. 2(a). The self-consistent band structure (diamonds) exhibits only a slight deformation of the bands due to interactions and, indeed, we observe the occupation of a single-particle state above the gap. However, there is also the possibility of lowering the energy by creating states inside the gap, which need to be localized in a finite region of the lattice. In order to capture the latter type of solutions, we go one step further and work without the requirement of spatial translational invariance of the Hartree-Fock parameters $(\xi_{ij}, \bar{n}_i)$, known as the unrestricted Hartree-Fock (UHF) ansatz [36, 37], on a $24 \times 24$ unit cell lattice. The results are shown in Fig. 2(a): instead of populating the upper band of the half-filled state, the UHF bands are deformed in order to accommodate the extra particle, with the appearance of states inside the insulating gap, and a decrease of the energy $\Delta E_{\text{UHF}} \equiv \langle H \rangle_{\text{UHF}} - \langle H \rangle_{\text{RHF}} = -0.12t$. These mid-gap states are localized in a finite region of the lattice, leading to a self-induced polaron solution, as can be seen in the density profile of Fig. 2(b). This solution bears some similarities with an impurity interacting with a topological background [38]. However, here this solution appears due to the presence of a self-induced impurity generated by the same interactions that generate the topology and within the same fermionic species.

The appearance of self-trapped polarons and other localized excitations has been extensively studied using the UHF method [27–29] for non-topological phases. We here show that the topological character of the material leads to very interesting physics. On the one hand, Fig. 2(c) shows that, in the polaron region, there is a large reduction of the order parameter $\xi_{QAH}$ accompanied by a change of the SSB sector in the inner region (see Supp. Mat. for details). Notice that this behavior of the local order parameter is similar to the one exhibited by the antiferromagnetic polaron observed in the 2D Hubbard model in Ref. [27]. On the other hand, and despite the lack of translational invariance, one can characterize the topology of the system in real space, by means of the local Chern number $C$ [39–41]. As shown in Fig. 2(d), this quantity is not quantized at all inside the polaron, however, it stabilizes to $C = +1$ further away from the latter. We emphasize that, as in the half-filling case, the sign of $C$ depends on the ground state symmetry breaking sector. Notice also that these local fluctuations of $C$, which are caused by a spontaneous breaking of translational symmetry, are reminiscent of those induced by quenched disorder in a gauge-induced Chern insulator [42].

Configuration Interaction analysis.—We use the Configuration Interaction (CI) method [29, 43, 44] to analyze the stability of the localized polaron solution within the UHF ansatz. In a nutshell, in the CI method, one lowers the UHF energy by hybridizing several UHF solutions in order to restore some of the lattice symmetries spontaneously broken in each UHF solution. In particular, we use the CI method to restore the translational invariance of the polaron solution in checkerboard lattices with up to 162 sites (see Supp. Mat. for details). Our analysis yields a polaron band that supports the validity of our UHF treatment: the minimum energy of the band is similar to the UHF energy (with a reduction of approximately $\approx 0.1\%$), and this energy corresponds to a plateau of degenerate states in a region of the band of size $|\Delta k|$. The latter is compatible with a polaron extended over a finite lattice region with radius $l_p \simeq 1/|\Delta k|$, as observed in the UHF solution.

Two polarons.—We now focus on two extra particles ($\delta = 2$). In this case, we find two types of self-consistent solutions. The lowest energy solution presents a density accumulation in a single region of the lattice, giving rise to a composite state of two polarons [see Fig. 3(a)]. The inner region of this bipolaron, slightly larger than the one corresponding to the single polaron, also exhibits a change in the SSB sector (see Supp. Mat.). The other type of solutions corresponds to two spatially non-overlapping polarons [see Fig. 3(b)]. The latter are metastable solutions with a higher energy than the composite state, which indicates that there is an attractive interaction between polarons. However, if the doping mechanism deposits the extra particles in different regions of the lattice, the timescale to reach the lowest energy solution might become very large, and these metastable solutions are likely to be detectable. In order to characterize the formation of these metastable solutions, we choose for the initial UHF values those of a spatial superposition of two polarons of the type of the previous section, and vary their initial separation. Figure 3(c) shows the final distance between the two polarons $d_{p-p}$.

![Figure 3](image_url)
as a function of their initial separation \( \delta_{p-p} \). Considering the self-consistent UHF algorithm as some virtual dynamics for the Hartree-Fock parameters, we observe that there is a collapse radius \( \delta_{p-p} \simeq 12 \) in the initial separation, below which the two polarons interact until the stabilization of the lowest energy composite solution with \( \delta_{p-p} \simeq 9 \). At larger initial separations, the system stabilizes the non-overlapping solution, with a forbidden range \( \delta_{p-p} \in (12, 25] \), showing that metastable solutions avoid residual overlaps.

**Ring-shaped domain walls.**—Even at higher particle doping, we find that the system retains its bulk insulating character: it is energetically favorable to create several mid-gap localized states instead of populating the upper band, as can be seen in Fig. 4(a) for \( \delta = 8 \). Taking as a reference the polaron solutions, the attractive interaction between them leads to a ground state whose inner region is in the other SSB sector (see Supp. Mat.). For a sufficiently large value of \( \delta \), this eventually leads to the formation of a domain wall between two extended regions with half-filling occupation that are in the QAH phase, as can be seen in Fig. 4(b). Interestingly, the inversion of the TRSB order parameter across the domain wall leads to the two opposite values of the local Chern number \( \mathcal{C} = \pm 1 \) depicted in Fig. 4(b). Notice here the role of the interacting nature of the system, leading to a SSB: the coexistence of topologically opposite phases would not occur if the Chern insulator was induced by an homogeneous external gauge field, that would define the global topology sector of the system. Furthermore, the change of the local Chern number \( |\Delta \mathcal{C}| = 2 \) between the two regions gives rise to topologically protected edge states with a fixed chirality in the ring. This is exactly what we observe in the ground state currents shown in Figs. 4(c)-(d), which are carried by mid-gap states. We also verified (see Supp. Mat.) that the solution with \( \mathcal{C} = -1 \) in the inner part of the rig and \( \mathcal{C} = 1 \) in the outer part has the same energy and presents edge states with opposite chirality.

**Linear domain walls.**—For \( \delta = 8 \), we also find a metastable self-consistent solution, in which the system develops two domain walls (see Fig. 5). The extra density is deposited in these linear structures, as depicted in Fig. 5(b). As in the previous case, the domain walls separate two regions with a reversed TRSB order parameter, leading to two opposite values of the local Chern number, as can be seen in Fig. 5(c). The main difference, however, is that here the change in the local Chern number \( |\Delta \mathcal{C}| = 2 \) occurs in each of the two disconnected domain walls, leading to pairs of degenerare chiral edge states (one at each domain wall) with opposite chiralities, as shown in Figs. 5(a)-(d).

**Quantum simulation with Rydberg atoms in an optical lattice.**—Cold atoms in optical lattices provide a prime candidate platform to implement the interacting fermionic Hamiltonian (1) and observe the interaction-induced polarons and topological defects in a highly controllable experimental setup: Laser-coupling between different sublattices (c.f. Fig. 1), similar to the approach taken in Ref. [45], allows one to control hopping dynamics as described by (2). Optically trapped and laser-excited Rydberg atoms have become a versatile platform...
for quantum simulation of many-body physics [46, 47]. Weak off-resonant laser-dressing of ground state atoms
with Rydberg-states, as demonstrated e.g. in Ref. [48] allows one to induce effective NN and NNN interactions,
with associated energy scale $V_2$ of a similar magnitude as $V_1$ [18, 19], and both compatible with the kinetic
energy scales of (2). Detrimental incoherent processes, such as dephasing and radiative decay from metastable
Rydberg states are small for suitably chosen laser and atomic parameters [49] and occur at time scales larger
than those associated to the effective couplings of Hamiltonian (3) governing the coherent system dynamics. In
addition, techniques specifically adapted to the detection of topological order such as time-of-flight [45, 50], trans-
port [8, 51] or interband transition [9, 52] measurements, are suitable to spatially resolve the predicted interaction-
induced polarons and topological defects.

Finally, a quantum simulator of this system could be quenched into the QAHE phase [see Fig.1(b)] to study the quantum phase transition dynamics of such a correlated 2D system. In particular, the rate of creation of the static defects reported in this work can be characterized with the quantum Kibble-Zurek mechanism [30–34]. While this mechanism has been recently observed with cold Rydberg atoms for an Ising-type (non-topological) transition [35], it would be very interesting to extend this experiment to a SSB topological transition.

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SI. BAND STRUCTURE OF THE BARE HAMILTONIAN

In order to take advantage of the quadratic and translational invariance of the free Hamiltonian $\hat{H}_0$ (see Eq. (1) of the main text), we write it in terms of the $k$-space fermionic operators, defined as
\[
c_{k,\alpha} = \frac{1}{\sqrt{L}} \sum_j e^{i j \alpha k} c_{j,\alpha}, \quad \alpha = A, B. \tag{S1}
\]
Here the total number of two-site unit cells is given by $L = L_x \times L_y$, and we have $k = (k_x, k_y)$ with $k_x \in [0, \pi)$, $\Delta k_x = \pi/L_x$, and similarly for $k_y$. Importantly, $j$ is a tuple of indices $j \equiv (j_x, j_y)$ specifying the position of each unit cell in the 2D lattice. Moreover, notice that $j$ refers only to the unit cell, while the index $j_\alpha$ appearing in the exponent refers to the physical position of the fermionic operator. Therefore, for A sites, $j$ and $j_A$ coincide, whereas for B sites $j_B = j + (1, 1)$. In $k$-space, $H_0$ reads
\[
\hat{H}_0 = \sum_k \hat{\Psi}_k^\dagger H_0^k \hat{\Psi}_k, \tag{S2}
\]
with the definitions
\[
\hat{\Psi}_k = (\hat{c}_{k,A}, \hat{c}_{k,B})^T, \quad H_{0,01}^k = H_{0,10}^k = -4t \cos k_x \cos k_y, \quad H_{0,00}^k = -2 \left[ J_x^A \cos(2k_x) + J_y^A \cos(2k_y) \right], \quad H_{0,11}^k = -2 \left[ J_x^B \cos(2k_x) + J_y^B \cos(2k_y) \right]. \tag{S3}
\]
Now, Eq. (S2) can be brought into diagonal form
\[
\hat{H}_0 = \sum_k \hat{\Phi}_k^\dagger H_D^k \hat{\Phi}_k, \tag{S4}
\]
where
\[
\hat{\Phi}_k = (\hat{\Phi}_{k,0}, \hat{\Phi}_{k,1})^T, \quad H_D^k = \begin{pmatrix} E_{k,-} & 0 \\ 0 & E_{k,+} \end{pmatrix}. \tag{S5}
\]
Notice that for each $k$ we have two energies corresponding to the two bands of the lattice. Here we give the analytical form of these energy eigenvalues
\[
E_{k,\pm} = \pm \sqrt{\left[ T_x \cos(2k_x) + T_y \cos(2k_y) \right]^2 + 16t^2 \cos^2 k_x \cos^2 k_y}, \tag{S6}
\]
where we have defined $T_\mu(\Delta_\mu) = J_\mu^A + (-) J_\mu^B$. With the choice of parameters used in the main text, we have $t = 1$, $T_\mu = 0$ and $\Delta_x = 1 = -\Delta_y$, leading to
\[
E_{k,\pm} = \pm \sqrt{\left[ \cos(2k_x) - \cos(2k_y) \right]^2 + 16 \cos^2 k_x \cos^2 k_y}. \tag{S7}
\]
III. HARTREE-FOCK BAND STRUCTURE OF THE INTERACTING HAMILTONIAN (4-SITES UNIT CELL ANSATZ)

We extend $H_0$ by including density interactions between different sites as follows

$$\hat{H} = \hat{H}_0 + V_1 \sum_{\langle ij \rangle} \hat{n}_{i,A} \hat{n}_{j,B} + V_2 \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j. \quad (S8)$$

We take a Hartree-Fock (HF) approach to solve it by means of a self-consistent iterative algorithm at a given filling and zero temperature. We use the following decomposition that respects Wick’s Theorem

$$\hat{n}_i \hat{n}_j \simeq -\xi_{ij} \hat{c}_i^\dagger \hat{c}_i - \xi_{ij} \hat{c}_j^\dagger \hat{c}_j + |\xi_{ij}|^2 + (\hat{n}_i) \hat{n}_j + (\hat{n}_j) \hat{n}_i - (\hat{n}_i) (\hat{n}_j). \quad (S9)$$

with $\xi_{ij} = \langle \hat{c}_i^\dagger \hat{c}_j \rangle$. We now transform the interaction terms to momentum space, assuming a 4-sites unit-cell ansatz (see Fig. S1). In order to allow for loops of imaginary hopping between NNs, we furthermore impose $\langle \hat{c}_{1,Bi}^\dagger \hat{c}_{i,A_1} \rangle = \langle \hat{c}_{1,B1}^\dagger \hat{c}_{1-e_2,A_1} \rangle$, $\langle \hat{c}_{2,B2}^\dagger \hat{c}_{2,A_1} \rangle = \langle \hat{c}_{1-e_1,A_2} \hat{c}_{1,B1} \rangle$, and $\langle \hat{c}_{i,A_2} \hat{c}_{i,B_2} \rangle = \langle \hat{c}_{1-e_2,A_2} \hat{c}_{2,B_2} \rangle$. We also restrict the mean field to real $\xi_{N NN}$. We get to the following form for the Hamiltonian (S8)

$$\hat{H} = E_0 + \sum_k \hat{\Psi}_k^T H_k^V \hat{\Psi}_k, \quad (S10)$$

with

$$\hat{\Psi}_k = (\hat{c}_{k,A_1}^\dagger, \hat{c}_{k,B_1}^\dagger, \hat{c}_{k,B_2}^\dagger, \hat{c}_{k,A_2}^\dagger)^T,$$

$$H_{k,00}^V = 2V_1 (\bar{n}_{B_1} + \bar{n}_{B_2}) + 4V_2 \bar{n}_{A_2}, \quad H_{k,11}^V = 2V_1 (\bar{n}_{A_1} + \bar{n}_{A_2}) + 4V_2 \bar{n}_{B_2},$$

$$H_{k,22}^V = 2V_1 (\bar{n}_{A_1} + \bar{n}_{A_2}) + 4V_2 \bar{n}_{B_1}, \quad H_{k,00}^V = 2V_1 (\bar{n}_{B_1} + \bar{n}_{B_2}) + 4V_2 \bar{n}_{A_1},$$

$$H_{k,01}^V = -2(t + V_1 \xi_{A_1}^A) \cos(k_2) - 2iV_1 \xi_{A_1}^A \cos(k_2),$$

$$H_{k,02}^V = -2(t + V_1 \xi_{A_2}^B) \cos(k_1) - 2iV_1 \xi_{A_2}^B \cos(k_1),$$

$$H_{k,03}^V = 2(J_x^A - V_2 \xi_{B_1}^A) \cos(k_1 + k_2) + 2(J_y^A - V_2 \xi_{B_1}^A) \cos(k_1 - k_2),$$

$$H_{k,12}^V = 2(J_x^B - V_2 \xi_{B_2}^B) \cos(k_1 + k_2) + 2(J_y^B - V_2 \xi_{B_2}^B) \cos(k_1 - k_2),$$

$$H_{k,13}^V = -2(t + V_1 \xi_{A_1}^B) \cos(k_1) - 2iV_1 \xi_{A_1}^B \cos(k_1),$$

$$H_{k,23}^V = -2(t + V_1 \xi_{A_2}^A) \cos(k_2) - 2iV_1 \xi_{A_2}^A \cos(k_2),$$

$$\frac{E_0}{L_4} = 2V_1 \left[ |\xi_{A_1,B_1}|^2 + |\xi_{B_1,A_2}|^2 + |\xi_{B_1,B_2}|^2 - (\bar{n}_{A_1} + \bar{n}_{A_2})(\bar{n}_{B_1} + \bar{n}_{B_2}) \right] +$$

$$+ 2V_2 \left[ (\xi_{B_1,A_1}^y)^2 + (\xi_{B_1,B_2}^y)^2 + (\xi_{A_1,A_2}^y)^2 + (\xi_{B_1,B_2}^y)^2 + 2(\bar{n}_{A_1} \bar{n}_{A_2} + \bar{n}_{B_1} \bar{n}_{B_2}) \right],$$

$$k_1, k_2 \in [0, \pi).$$

Notice that, in this 4-sites unit-cell ansatz, the reciprocal space components $(k_1, k_2)$ are rotated by 45° with respect to the $(k_x, k_y)$ components of the previous Sec. III.

SIII. HARTREE-FOCK BAND STRUCTURE OF THE INTERACTING HAMILTONIAN (2-SITE UNIT CELL ANSATZ)

As the quantum anomalous Hall phase can be captured in a simplified ansatz of a 2-site unit cell (sites A and B in Fig. 1a of the main text), here we show the quasi-analytical band structure that can be derived from it. We also start from the interacting Hamiltonian

$$\hat{H} = \hat{H}_0 + V_1 \sum_{\langle ij \rangle} \hat{n}_{i,A} \hat{n}_{j,B} + V_2 \sum_{\langle i,j \rangle} \hat{n}_i \hat{n}_j. \quad (S12)$$

As in the previous case, we take a Hartree-Fock (HF) approach. We now transform the interaction terms to Fourier space, assuming $\langle \hat{c}_{i,B}^\dagger \hat{c}_{i,A} \rangle = |\xi_{BA}| e^{i\theta}$. The phase $\theta$ fulfills the constraint

$$\langle \hat{c}_{i,B}^\dagger \hat{c}_{i,A} \rangle = \langle \hat{c}_{i,B}^\dagger \hat{c}_{i+\epsilon_x,A} \rangle^* = \langle \hat{c}_{i,B}^\dagger \hat{c}_{i-\epsilon_y,A} \rangle^* = \langle \hat{c}_{i,B}^\dagger \hat{c}_{i+\epsilon_x-\epsilon_y,A} \rangle.$$  

(S13)
We also set to real \( \xi_{Ax/y} \) and \( \xi_{Bx/y} \). We get to the following form for the Hamiltonian (S12)
\[
\hat{H} = E_0 + \sum_{k} \hat{\Psi}_k^* H_V^k \hat{\Psi}_k, 
\]
with
\[
\hat{\Psi}_k = (\hat{c}_{k,A}, \hat{c}_{k,B})^T,
\]
\[
H_{V,00}^k = -2 \left[(J_A^x + V_2 \xi_{Ax}) \cos(2k_x) + (J_A^y + V_2 \xi_{Ay}) \cos(2k_y)\right] + 4(V_1 \bar{n}_B + V_2 \bar{n}_A),
\]
\[
H_{V,11}^k = -2 \left[(J_B^x + V_2 \xi_{Bx}) \cos(2k_x) + (J_B^y + V_2 \xi_{By}) \cos(2k_y)\right] + 4(V_1 \bar{n}_A + V_2 \bar{n}_B),
\]
\[
E_0 = 4V_1 \left(\xi_{BA}^2 - \bar{n}_A \bar{n}_B\right) + V_2 (\xi_{Ax}^2 + \xi_{Ay}^2 + \xi_{Bx}^2 + \xi_{By}^2 - 2 \bar{n}_A^2 - 2 \bar{n}_B^2),
\]
\(k_x, k_y \in [0, \pi]\).

To analytically diagonalize the Hamiltonian (S14), we write it in terms of Pauli matrices as
\[
\hat{\Psi}_k^\dagger \left((\alpha_k \mathbb{1} + \beta_k \sigma_z + \gamma_k \sigma_x + \lambda_k \sigma_y) \right) \hat{\Psi}_k \equiv \hat{\Psi}_k^\dagger \left(\alpha_k \mathbb{1} + \vec{n}_k \cdot \vec{\sigma}\right) \hat{\Psi}_k, 
\]
\(\vec{n}_k/|\vec{n}_k| = (\sin \theta \cos \phi, \sin \theta \sin \phi, \cos \theta)^T, (\sin \theta \geq 0)\)
\[
\alpha_k = -[T_x \cos(2k_x) + T_y \cos(2k_y)] + 2(V_1 + V_2)n, \quad \beta_k = -[\Delta_x \cos(2k_x) + \Delta_y \cos(2k_y)] - 2(V_1 - V_2)\rho,
\]
\[
\gamma_k = -4(t + V_1 \xi_{BA}^R) \cos(k_x) \cos(k_y), \quad \lambda_k = -4V_1 \xi_{BA} \sin(k_x) \sin(k_y),
\]
\[
T_\mu = J_\mu^A + J_\mu^B + V_2(\xi_{A\mu} - \xi_{B\mu}), \quad \Delta_\mu = J_\mu^A - J_\mu^B + V_2(\xi_{A\mu} - \xi_{B\mu}), \quad n = \bar{n}_A + \bar{n}_B, \quad \rho = \bar{n}_A - \bar{n}_B.
\]

We have the following energies and ground-state eigenvector
\[
E_{k,\pm} = \alpha_k \pm |\vec{n}_k|, \quad \vec{v}_{k,-} = \left(e^{-i\phi_k/2} \sin \theta_k/2, -e^{i\phi_k/2} \cos \theta_k/2\right)^T
\]
\(\text{(S18)}\). Now we can compute the expectation values in the ground state (we use the notation \(\vec{v} \equiv \vec{v}_{k,-}\))
\[
\rho = \frac{1}{L} \sum_k |\vec{v}_{00}|^2 - |\vec{v}_{11}|^2 = -\frac{1}{L} \sum_k \cos(\theta_k) = -\frac{1}{L} \sum_k \beta_k/|\vec{n}_k|,
\]
\[
\xi_{BA}^{R} = \frac{1}{2L} \sum_k \cos(k_x) \cos(k_y) \sin(\theta_k) \cos(\phi_k) = \frac{1}{2L} \sum_k \cos(k_x) \cos(k_y) \gamma_k/|\vec{n}_k|,
\]
\[
\xi_{BA}^{I} = \frac{1}{2L} \sum_k \cos(k_x) \cos(k_y) \sin(\theta_k) \sin(\phi_k) = \frac{1}{2L} \sum_k \cos(k_x) \cos(k_y) \lambda_k/|\vec{n}_k|,
\]
\(\text{(S19)}\)
\[
\xi_{Ax(y)} = \frac{1}{L} \sum_k \cos(2k_{x(y)}) |\vec{v}_{00}|^2, \quad \xi_{Bx(y)} = \frac{1}{L} \sum_k \cos(2k_{x(y)}) |\vec{v}_{11}|^2,
\]
\(\text{FIG. S1. Schematic of the 4 unit cell ansatz in the checkerboard lattice.}\)
and the value of the free energy
\[ F/L = 4V_1 \left[ (\xi_{BA}^R)^2 + (\xi_{BA}^I)^2 + \frac{1}{4} (\rho^2 - 1) \right] + V_2 \left[ \xi_{Ax}^2 + \xi_{Ay}^2 + \xi_{Bx}^2 + \xi_{By}^2 - (1 + \rho^2) \right] + \frac{1}{L} \sum_k (\alpha_k - |\bar{n}_k|), \] (S20)
which can be brought into the equivalent form
\[ \tilde{F}/L = 2V_1 \left[ (\xi_{BA}^R)^2 + (\xi_{BA}^I)^2 + \rho^2/4 \right] + V_2 \left[ \xi_{Ax}^2 + \xi_{Ay}^2 + \xi_{Bx}^2 + \xi_{By}^2 - \rho^2 \right] + \frac{1}{L} \sum_k (\alpha_k - |\bar{n}_k|). \] (S21)

**SIV. CHERN NUMBER FORMULA OF THE LOWER BAND IN THE 2-SITES ANSATZ**

We can write the Chern number of the checkerboard lattice as
\[ \nu = \frac{\pi}{2L} \sum_k \bar{n}_k \cdot \left( \frac{\partial \bar{n}_k}{\partial k_x} \times \frac{\partial \bar{n}_k}{\partial k_y} \right), \] (S22)
where \( \bar{n}_k \) is given in Eq. (S16). It is useful to define \( \bar{v}_k = (\gamma_k, \lambda_k, \beta_k) \), such that \( \bar{n}_k = \bar{v}_k/|\bar{v}_k| \). Then
\[ \frac{\partial \bar{n}_k}{\partial k_\mu} = \frac{1}{|\bar{v}_k|} \frac{\partial \bar{v}_k}{\partial k_\mu} - \frac{1}{|\bar{v}_k|^3} \left( \bar{v}_k \cdot \frac{\partial \bar{v}_k}{\partial k_\mu} \right) \bar{v}_k. \] (S23)
The expressions are the following
\[ \frac{\partial \bar{v}_k}{\partial k_x} = \left[ 4(t + V_1 \xi_{BA}^R) \sin(k_x) \cos(k_y), -4V_1 \xi_{BA}^I \cos(k_x) \sin(k_y), 2\Delta_x \sin(2k_x) \right], \]
\[ \frac{\partial \bar{v}_k}{\partial k_y} = \left[ 4(t + V_1 \xi_{BA}^R) \sin(k_y) \cos(k_x), -4V_1 \xi_{BA}^I \cos(k_y) \sin(k_x), -2\Delta_x \sin(2k_y) \right]. \] (S24)
Notice that to apply this formula we first have to determine the Hartree-Fock parameters \( \xi \)'s and \( \rho \).

**SV. CALCULATION OF THE LOCAL CHERN NUMBER**

We follow the procedure introduced in [S1] and used in [S2] to compute the real space Chern number for a non-homogeneous system. We first define the projectors onto the occupied and unoccupied single-particle states of the unrestricted Hartree-Fock Hamiltonian
\[ P = \sum_{i \in \text{occ}} |\Phi_i\rangle \langle \Phi_i|, \quad \hat{Q} = \mathbb{1} - \hat{P}. \] (S25)
We also define the operators
\[ \hat{r}_P = \hat{P} \hat{r} \hat{Q} = (\hat{x}_P, \hat{y}_P), \quad \hat{r}_Q = \hat{Q} \hat{r} \hat{P} = (\hat{x}_Q, \hat{y}_Q). \] (S26)
These operators are quasi-local, in the sense that \( \langle i | \hat{r}_{P,Q} | j \rangle \sim \exp (-\kappa_{P,Q} ||i - j||) \). Now, we define the local Chern marker as
\[ \mathcal{C}(i) = -4\pi \text{Im} \left[ \sum_j \langle i | \hat{x}_Q | j \rangle \langle j | \hat{y}_P | i \rangle \right] \] (S27)
with
\[ \langle i | \hat{x}_Q | j \rangle = \sum_l Q(i, l) x_l P(l, j), \quad \langle j | \hat{y}_P | i \rangle = \sum_l P(j, l) y_l Q(l, i). \] (S28)
Finally, to compute the Chern number $C$, one has to perform the spatial average of the local Chern marker (S27)

$$C = \frac{1}{A_{\text{disk}}} \sum_{i \in \text{disk}} \mathbf{c}(i),$$

(S29)

where the disk is the set of points inside a circle of a certain radius, considered to lie inside the bulk of the lattice, where edge effects do not play a role, and $A_{\text{disk}}$ is the area of this disk. In this work, we always set the radius to $r = a/\sqrt{2}$, where $a$ is the distance between NN.

SVI. BEHAVIOR OF THE TRSB LOCAL ORDER PARAMETER

Here we analyze the behavior of the imaginary part of the hopping between nearest neighbors $\xi_{\text{NN}}^I$ (i.e., the local order parameter of the spontaneous time-reversal symmetry breaking) in the different inhomogeneous solutions discussed in the main text. Figures S2(a)-(c) show its value in the lattice for the polaron, bipolaron, and ring solutions. We observe the non-zero value of this quantity in the bulk, with different signs indicating the closed current loops characteristic of the quantum Anomalous Hall phase. We also observe a large reduction of the absolute value of $\xi_{\text{NN}}^I$ in the polaron, bipolaron and ring regions, coinciding with the region where there is a deviation of the half-filling occupation. To analyze the evolution of $\xi_{\text{NN}}^I$ through the inhomogeneities, in Fig. S2(d) we plot $\xi_{\text{NN}}^I$ in a zig-zag line connecting NN, indicated in Figs. S2(a)-(c). Figure S2(d) then shows the transition from the polaron solution to the ring solution in terms of the SSB: inside the polaron there is change of the SSB sector due to the change in the sign of $\xi_{\text{NN}}^I$. However the inner region is too small to develop a well-defined domain of the SSB phase. In the bipolaron case the behavior is similar, with a slight widening of the curve. In the ring solution, however, we observe a full inversion of $\xi_{\text{NN}}^I$ in the inner region, leading to two domains belonging to the different sectors of the SSB phase.

![Image](https://via.placeholder.com/150)

FIG. S2. Local order parameter of the spontaneous time-reversal symmetry breaking $\xi_{\text{NN}}^I$ for different unrestricted Hartree-Fock solutions. (a) Polaron solution obtained for one extra particle ($\delta = 1$). (b) Bipolaron solution for $\delta = 2$. (c) Ring domain wall solution for $\delta = 8$. (d) Plot of $\xi_{\text{NN}}^I$ along the horizontal cut depicted in (a)-(c). This quantity reveals the inversion of the SSB sector inside the inhomogeneities.

SVII. SPONTANEOUS SYMMETRY BREAKING SECTORS OF THE RING SOLUTION

As explained in the main text, the spontaneous TRSB in the quantum anomalous Hall phase has two symmetry sectors at half-filling, which lead to two ground states with opposite Chern numbers. In the case of inhomogeneous topological phases, such as the ring domain solution presented in the main text, a first thing to notice is that they are highly degenerate as they spontaneously break the translational symmetry of the lattice. Moreover, we can also find a degenerate solution in which the local TRSB sectors are reversed. Figure S3 shows the comparison between these two degenerate ring solutions that are connected by an inversion of the local TRSB sectors. As can be seen in Figs. S3(a1)-(b1), the change in the TRSB sectors does not affect the density profile of the solution. However, we can observe in Figs. S3(a2)-(b2) that the values of the local Chern number $\mathcal{C}$ are reversed in the inner and outer regions of the ring. The latter leads to opposite chiralities of the edge states inside the ring [see Figs. S3(a3)-(b3)-(a4)-(b4)].
FIG. S3. Comparison between two degenerate UHF solutions corresponding to ring domain walls (a) and (b). (a1)-(b1) Density profiles, identical for the two solutions. (a2)-(b2) Local Chern number, which shows opposite SSB (topological) sectors for each solution. (a3)-(b3) Current in the $x$ direction. (a4)-(b4) Current in the $y$ direction. The currents reveal that the chirality of the ring edge states on each solution is reversed with respect to the other, due to the change in the values of the inner (outer) local Chern number.

SVIII. EXPRESSION OF THE CURRENT OPERATOR

To compute the current operator we use the continuity equation for the fermion density at each lattice site:

$$ \frac{d}{dt} \left\langle \hat{c}_i^\dagger \hat{c}_i \right\rangle = i \left\langle \left[ H, \hat{c}_i^\dagger \hat{c}_i \right] \right\rangle. $$

(S30)

Now, the non-diagonal terms of $H$ can be written as

$$ \sum_{m,n} \left( t_{m,n} \hat{c}_m^\dagger \hat{c}_n + \text{h.c.} \right), $$

(S31)

leading to

$$ \frac{d}{dt} \left\langle \hat{c}_i^\dagger \hat{c}_i \right\rangle = i \sum_{m,n} \left( t_{m,n} \left\langle \left[ \hat{c}_m^\dagger \hat{c}_n, \hat{c}_i^\dagger \hat{c}_i \right] \right\rangle - \text{h.c.} \right) = -2 \text{Im} \left( t_{m,n} \left\langle \left[ \hat{c}_m^\dagger \hat{c}_n, \hat{c}_i^\dagger \hat{c}_i \right] \right\rangle \right). $$

(S32)

Expanding the commutator in terms of anticommutators we easily find:

$$ t_{m,n} \left[ \hat{c}_m^\dagger \hat{c}_n, \hat{c}_i^\dagger \hat{c}_i \right] = t_{m,n} \left( \hat{c}_m^\dagger \hat{c}_i \delta_{n,i} - \hat{c}_i^\dagger \hat{c}_m \delta_{m,i} \right) = t_{m,n} \left( \hat{c}_m^\dagger \hat{c}_i \delta_{n,i} - \hat{c}_i^\dagger \hat{c}_m \delta_{m,i} \right) = t_{i+b,i+b} \hat{c}_i^\dagger \hat{c}_i - t_{i,i-b} \hat{c}_i^\dagger \hat{c}_i - b, $$

(S33)

where $b$ gives the bond direction, which can be $x+y$ and $x-y$ for nearest-neighbors, and $2x$ or $2y$ for next-to-nearest-neighbors. Introducing this into the continuity equation we get to:
\[
\frac{d}{dt} \langle \hat{c}_i^\dagger \hat{c}_i \rangle = -2 \text{Im} \left( t_{i+b,i} \hat{c}_{i+b}^\dagger \hat{c}_i - t_{i,i-b} \hat{c}_i^\dagger \hat{c}_{i-b} \right). \tag{S34}
\]
At this point, we identify the outgoing current in the \( b \) direction as \( \mathcal{J}_b^{\rightarrow} = 2 \text{Im} \left( t_{i+b,i} \hat{c}_{i+b}^\dagger \hat{c}_i \right) \) and the ingoing as \( \mathcal{J}_b^{\leftarrow} = 2 \text{Im} \left( t_{i,i-b} \hat{c}_i^\dagger \hat{c}_{i-b} \right) \), so that we can write the continuity equation simply as
\[
\frac{d}{dt} \langle \hat{c}_i^\dagger \hat{c}_i \rangle = \sum_b \mathcal{J}_b^{\rightarrow} - \sum_b \mathcal{J}_b^{\leftarrow}. \tag{S35}
\]
Now, we notice that in our model the Hartree-Fock correction to \( t_{m,n} \) does not affect the current, and therefore we should use the bare hopping elements \( t_{m,n} \).

\[
\mathcal{J}_b^{\rightarrow} = 2 \text{Im} \left( \left( t_{i+b,i}^0 - V_b \langle \hat{c}_{i+b} \rangle \right) \langle \hat{c}_{i+b}^\dagger \hat{c}_i \rangle \right) = 2 \text{Im} \left( t_{i+b,i}^0 \langle \hat{c}_{i+b}^\dagger \hat{c}_i \rangle - V_b \langle \hat{c}_{i+b} \rangle \langle \hat{c}_{i+b} \rangle \right) = 2 \text{Im} \ t_{i+b,i}^0 \langle \hat{c}_{i+b}^\dagger \hat{c}_i \rangle. \tag{S36}
\]
In the topological homogeneous phase, we have closed loops with non-zero \( \mathcal{J}_{ij} \) for nearest-neighbors sites, and \( \mathcal{J}_{ij} = 0 \) for next-to-nearest-neighbors (sites belonging to the same sublattice). In the case of domain walls separating two regions with opposite Chern number, we expect the appearance of chiral currents. We will therefore look for non-zero values of \( \mathcal{J}_{ij}^{A(B)} \) in these areas, to identify such currents.

**SIX. CONFIGURATION-INTERACTION**

Here we use the Configuration Interaction (CI) method [S3–S6] to analyze the stability of the UHF solutions presented in the main text. In the CI method, one first obtains a set \( \{ \Phi_j(N) \} \) of UHF solutions with low energy and a fixed number of particles \( N \). In the many-body basis, each of the solutions is given by the Slater determinant (SD) of the occupied single-particle UHF states. Then, one uses the variational ansatz
\[
\Psi(N) = \sum_j \alpha_j \Phi_j(N), \tag{S37}
\]
to minimize the energy of the system. Notice that the many-body wave-functions \( \{ \Phi_j(N) \} \) are not orthogonal. The overlap matrix between two SDs is given by [S3]
\[
S_{ij} \equiv \langle \Phi_i | \Phi_j \rangle = \begin{vmatrix} \langle \phi_1^i | \phi_1^j \rangle & \ldots & \langle \phi_1^i | \phi_N^j \rangle \\ \vdots & \ddots & \vdots \\ \langle \phi_N^i | \phi_1^j \rangle & \ldots & \langle \phi_N^i | \phi_N^j \rangle \end{vmatrix}. \tag{S38}
\]
The biggest numerical cost of the CI method is to compute the matrix elements \( H_{ij} = \langle \Phi_i | H | \Phi_j \rangle \) of the Hamiltonian (??). We first split it in the kinetic energy term \( T \) and the interaction term \( C \):
\[
H = T + C. \tag{S39}
\]
The matrix elements corresponding to \( T \), which are quadratic in fermionic operators, are then given by
\[
T_{ij} = \begin{vmatrix} \langle \phi_1^i | T | \phi_1^j \rangle & \ldots & \langle \phi_1^i | \phi_N^j \rangle \\ \vdots & \ddots & \vdots \\ \langle \phi_N^i | T | \phi_1^j \rangle & \ldots & \langle \phi_N^i | \phi_N^j \rangle \end{vmatrix} + \ldots + \begin{vmatrix} \langle \phi_1^i | \phi_1^j \rangle & \ldots & \langle \phi_1^i | \phi_N^j \rangle \\ \langle \phi_N^i | \phi_1^j \rangle & \ldots & \langle \phi_N^i | \phi_N^j \rangle \end{vmatrix}. \tag{S40}
\]
On the other hand, \( C \) contains two-body terms of the form \( n_k n_l \), whose matrix elements read
\[
\langle \Phi_i | n_k n_l | \Phi_j \rangle = \begin{vmatrix} \langle \phi_1^i | n_k | \phi_1^j \rangle & \ldots & \langle \phi_1^i | n_l | \phi_1^j \rangle \\ \vdots & \ddots & \vdots \\ \langle \phi_N^i | n_k | \phi_1^j \rangle & \ldots & \langle \phi_N^i | n_l | \phi_1^j \rangle \end{vmatrix} + \text{permutations}. \tag{S41}
\]
Once $H$ is computed, it has to be diagonalized, taking into account that we are working in a non-orthogonal basis. That is, we want to find the energies $\varepsilon$ and eigenvectors $\vec{\alpha}$ satisfying

$$ (H - \varepsilon S)\vec{\alpha} = 0 \quad \text{(S42)} $$

To find the energies of the system in this non-orthogonal basis we proceed as follows:

1. Diagonalize $S$, as $\sigma = D^\dagger SD$. Notice that $\sigma \geq 0$ due to the fact that $S$ is an overlap matrix. A zero eigenvalue indicates that one of the $\Phi_j$ is a linear combination of the others, and should be removed from the set.

2. Construct $A_{ij} = D_{ij} / \sqrt{\sigma}$. This means that $A^\dagger SA = I$.

3. By defining $A\vec{\alpha} \equiv \vec{c}$, and $\tilde{H} \equiv A^\dagger HA$, the eigenvalue problem has the standard form $(\tilde{H} - \varepsilon)\vec{c} = 0$.

### A. Polaron band in the QAH phase

The CI method can be used to restore the translational invariance of the system, which is spontaneously broken in the unrestricted Hartree-Fock method. To do so, we take one Hartree-Fock solution and perform all possible unit-cell translations. Notice that the SDs obtained through this procedure have the same energy. Then, one finds the band structure of the single-particle excitation $E(k)$ by diagonalizing $H$ in this non-orthogonal basis of translated states.

![CI spectrum for three different lattice sizes](image1)

![CI band structure](image2)

**FIG. S4.** Results of the CI method applied to the extended polaron obtained in the UHF ansatz ($\delta = 1$), and with the same hopping and interaction parameters as in the main text. (a) CI spectrum for three different lattice sizes. The unrestricted (restricted) Hartree-Fock energies are indicated as solid black (dashed red) lines. For each lattice size, the zero of energy is set as the CI ground state energy. (b) CI band structure.

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