Exciton topology and condensation in a model quantum spin Hall insulator

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We study by a consistent mean-field scheme the role on the single- and two-particle properties of a local electron-electron repulsion, which also includes a symmetry-allowed dipolar component, in the Bernevig, Hughes and Zhang model of a quantum spin Hall insulator. We find that the interaction fosters the emergence of a new insulating and magnetoelectric phase, which breaks spontaneously inversion and time reversal symmetries, but not their product, and intrudes between the topological and non-topological insulators, so realising a path connecting the latter two that does not need to cross any gapless point.

The approach to this phase from both topological and non-topological sides is signalled by the softening of two exciton branches, related to each other by time-reversal, and possessing, in most cases, finite and opposite Chern numbers, thus allowing this phase being regarded as a condensate of topological excitons. We also discuss how those excitons, and especially their surface counterparts, may influence the physical observables at the surface layer.

I. INTRODUCTION

The physics of excitons in topological insulators has attracted considerable interest in the last decade, see, not as an exhaustive list, Refs. [1–8] recently renewed[9] by the evidence of a quantum spin Hall effect in two-dimensional transition metal dichalcogenides.[10,11]

More precisely, a consistent part of the research activity has focused into the possibility of an exciton condensation in thin samples of topological insulators[12–14] in much the spirit of what was proposed[15] and observed[16] in bilayer graphene.

In addition, the puzzling properties of the purported topological Kondo insulator SmB$_6$,[18]21 prompted interest in the excitons of such material[19] as partly responsible for its anomalous behaviour.

Even though evidences of excitons exist also in the three-dimensional topological insulator Bi$_2$Se$_3$, besides those in the still controversial SmB$_6$, a systematic study in model topological insulators is largely lacking.[22,23] Our aim here is to partly fill this gap. Specifically, we consider the prototypical model of a Quantum Spin Hall Insulator (QSHI) introduced by Bernevig, Hughes and Zhang,[24] and add a local interaction compatible with the symmetries, which, e.g., allow for a dipole-dipole term.

We deal with such an interaction in a conserving mean-field scheme. Namely, we assume the Hartree-Fock expression of the self-energy functional to compute the single-particle Green’s function. Next, we calculate the excitons by solving the Bethe-Salpeter equations for the response functions, using as irreducible vertex the functional derivative of the Hartree-Fock self-energy functional with respect to the Green’s function; what is often called random phase approximation plus exchange[25]

Our main result is that, starting from the non-interacting QSHI, branches of excitons that transform into each other under time reversal detach from the continuum of particle-hole excitations, and gradually soften upon increasing interaction strength. When the latter exceeds a critical value, those excitons become massless, and thus condense through a second order critical point, which coincides with that obtained directly through the Hartree-Fock calculation not forcing any symmetry. Such symmetry broken phase is still insulating, and displays magnetoelectric effects. Upon further increasing interaction, it eventually gives in to the non-topological symmetry invariant insulator via another second order transition.

None of those transitions is accompanied by any gap closing; therefore uncovering a path between the QSHI and the trivial insulator that does not cross any gapless point,[10,11] thanks to the interaction-driven spontaneous breakdown of time reversal symmetry.

We also find that, approaching the excitonic insulator from the QSHI, the excitons themselves may acquire a non trivial topology signalled by a non-zero Chern number, suggestive of the existence of chiral exciton edge modes. In addition, we have evidences that, in open boundary geometries, exciton condensation occurs at the surface earlier than in the bulk, which also foresees the existence of non-chiral surface excitons that go soft before the bulk ones.[23,24]

Our findings may have observable consequences that we discuss, some of which not in disagreement with existing experimental evidences.

This work is organised as follows. In section [II], we introduce the interacting model Hamiltonian, while the conserving Hartree-Fock approximation that we use to deal with interaction is discussed in sections [III] and [IV]. The results of the calculations are presented in section [V], specifically: in [VA] the Hartree-Fock phase diagram; in [VB] the excitons in the quantum spin Hall insulating phase; and, finally, in [VC] the magnetoelectric effect in the excitonic insulator. Section [VI] is devoted to concluding remarks.

II. THE MODEL HAMILTONIAN

We shall consider the model introduced by Bernevig, Hughes and Zhang, after them named BHZ model, to describe the QSHI phase in HgTe quantum well.[25] The
The BHZ model involves two spinful orbitals per unit cell, which transform like $s$-orbitals, $|s\sigma\rangle$, where $\sigma = \uparrow, \downarrow$ refers to the projection of the spin along the $z$-axis, and like the $J = 3/2, J_z = \pm 3/2$ spin-orbit coupled combinations of $p$-orbitals, i.e.,

$$|p_{+1\uparrow}\rangle \equiv |p\uparrow\rangle, \quad |p_{-1\downarrow}\rangle \equiv |p\downarrow\rangle \ .$$

We introduce two sets of Pauli matrices, $\sigma_a$ and $\tau_a$, $a = 0, \ldots, 3$, with $a = 0$ denoting the identity, which act, respectively, in the spin, $\uparrow$ and $\downarrow$, and orbital, $s$ and $p$, spaces.

With those definitions, the BHZ tight-binding Hamiltonian on a square lattice can be written as

$$\mathcal{H}_0 = \sum_{\mathbf{k}} \bar{\Psi}_\mathbf{k} \hat{H}_0(\mathbf{k}) \Psi_\mathbf{k} = \sum_{ij} \bar{\Psi}_i \hat{H}_0(\mathbf{R}_i - \mathbf{R}_j) \Psi_j \ ,$$

at density corresponding to two electrons per site, where

$$\bar{\Psi}_\mathbf{k} = \begin{pmatrix} s_{\mathbf{k}t} \\ s_{\mathbf{k}t}^* \\ p_{\mathbf{k}t} \\ p_{\mathbf{k}t}^* \end{pmatrix} , \quad \Psi_i = \begin{pmatrix} s_{i\uparrow} \\ s_{i\downarrow} \\ p_{i\uparrow} \\ p_{i\downarrow} \end{pmatrix} \ ,$$

are four component spinors in momentum, $\Psi_\mathbf{k}$, and real, $\bar{\Psi}_\mathbf{k}$, space, with $i$ labelling the unit cell at position $\mathbf{R}_i$. $\hat{H}_0(\mathbf{k})$ is the $4 \times 4$ matrix

$$\hat{H}_0(\mathbf{k}) = (M - \epsilon_\mathbf{k}) \sigma_0 \otimes \tau_3 - t' \epsilon_\mathbf{k} \sigma_0 \otimes \tau_0 + \lambda \sin k_x \sigma_3 \otimes \tau_1 - \lambda \sin k_y \sigma_0 \otimes \tau_2 ,$$

with $\mathbf{k} = (k_x, k_y)$ and $\epsilon_\mathbf{k} = (\cos k_x + \cos k_y)$, whose prefactor will be our unit of energy, while $\hat{H}_0(\mathbf{R}_i - \mathbf{R}_j)$ its Fourier transform in real space. Hereafter, we shall analyse the Hamiltonian (4) for $M > 0$, with $t' = 0.5$ and $\lambda = 0.3$ in our units.

The band structure can be easily calculated and yields two bands, each degenerate with respect to the spin label $\sigma$; a conduction and a valence band, with dispersion $\epsilon_c(\mathbf{k})$ and $\epsilon_v(\mathbf{k})$, respectively, which read

$$\epsilon_c(\mathbf{k}) = -t' \epsilon_\mathbf{k} + E_k \ , \quad \epsilon_v(\mathbf{k}) = -t' \epsilon_\mathbf{k} - E_k \ ,$$

where

$$E_k = \sqrt{(M - \epsilon_\mathbf{k})^2 + \lambda^2 \sin^2 k_x + \lambda^2 \sin^2 k_y} \ .$$

With our choice of parameters, these bands describe a direct gap semiconductor for any $M \neq 2$. At the high symmetry points in the Brillouin Zone (BZ), the bands have a defined orbital character, i.e., a defined parity under inversion. Specifically, at $\Gamma = (0,0)$,

$$\epsilon_c(\Gamma) = -2t' + |M - 2|, \quad \epsilon_v(\Gamma) = -2t' - |M - 2| ,$$

valence and conduction bands have, respectively, $s$ and $p$ orbital character if $M < 2$, and vice versa if $M > 2$. On the contrary, at the zone boundary points $\mathbf{M} = (\pi, \pi), \mathbf{X} = (\pi, 0)$, and $\mathbf{Y} = (0, \pi)$,

$$\epsilon_c(\mathbf{M}) = 2t' + (M + 2) , \quad \epsilon_v(\mathbf{M}) = 2t' - (M + 2) ,$$

$$\epsilon_c(\mathbf{X}) = \epsilon_c(\mathbf{Y}) = M , \quad \epsilon_v(\mathbf{X}) = \epsilon_v(\mathbf{Y}) = -M \ ,$$

the valence band is $p$ and the conduction one $s$ for any value of $M$. It follows that, if $M < 2$, there is an avoided band crossing, due to $\lambda \neq 0$, moving from $\Gamma$ towards the BZ boundary, while, if $M > 2$, each band has predominantly a single orbital character, $s$ the conduction band and $p$ the valence one, see Fig. 1. At $M = 2$ the gap closes at $\Gamma$, around which the dispersion becomes Dirac-like,

$$\epsilon_c(\mathbf{k}) \simeq +\lambda |\mathbf{k}| , \quad \epsilon_v(\mathbf{k}) \simeq -\lambda |\mathbf{k}| \ .$$

The transition between the two insulating phases is known to have topological character. We note that the Hamiltonian $\hat{H}_0(\mathbf{k})$ commutes with $\sigma_3$, i.e., is invariant under $U(1)$ spin rotations around the $z$-axis, as well as under inversion and time reversal, respectively represented by the operators

$$\mathcal{I} = \sigma_0 \otimes \tau_3 \mathbf{1} , \quad \mathcal{T} = (i\sigma_2 \otimes \tau_0) \mathbf{K} \ ,$$

where $\mathbf{I}: \mathbf{k} \rightarrow -\mathbf{k}$, and $\mathbf{K}$ is the complex conjugation operator. If $C_\sigma$ is the Chern number of the spin-$\sigma$ valence-band electrons, then invariance under both inversion and time reversal entails a vanishing $(C_\uparrow + C_\downarrow)$, which is proportional to the transverse charge-conductance, but a possibly non zero $(C_\uparrow - C_\downarrow)$, which would correspond to a finite transverse spin-conductance, thus the nontrivial topology of a QSH. Specifically, $(C_\uparrow - C_\downarrow) \neq 0$ occurs when $M < 2$ not surprisingly in view of the avoided band crossings. We emphasise that a robust topological invariant can be defined provided spin $U(1)$ symmetry is preserved.

So far we have discussed the main properties of the non-interacting Hamiltonian $\mathcal{H}_0$. However, physically, electrons unavoidably interact with each other. We shall therefore add to the non-interacting Hamiltonian $\mathcal{H}_0$ a local Coulomb interaction $U_{\text{int}}$, thus neglecting its long range tail, which includes, besides monopoles terms, also a dipole-dipole interaction $U_{\text{dip}}$, which is here allowed by symmetry. Specifically,

$$U_{\text{int}} = U + U_{\text{dip}} \ ,$$

FIG. 1. Band structure of the BHZ model in the topological, left panel, and trivial, right panel, regimes. Blue and red colours indicate, respectively, even ($s$ orbital character) and odd ($p$ orbital character) parity under inversion.
where

\[ U = \sum_i \left( U_s n_{i\sigma} n_{i\sigma} + U_p n_{i\sigma} n_{i\sigma} + V n_{i\sigma} n_{i\sigma} \right), \]  

(12)

includes monopole terms, while the dipole-dipole interaction, projected onto our basis of single-particle wavefunctions, reads

\[ U_{\text{dip}} = \frac{J}{2} \sum_i \left[ \left( \Psi_i^\dagger \sigma_0 \otimes \tau_j \Psi_i \right)^2 + \left( \Psi_i^\dagger \sigma_3 \otimes \tau_j \Psi_i \right)^2 \right]. \]  

(13)

All coupling constants, \( U_s, U_p, V \) and \( J \), are positive, \( n_{i\sigma} = s_{i\sigma}^\dagger s_{i\sigma} \) and \( n_{i\sigma} = p_{i\sigma}^\dagger p_{i\sigma} \). Hereafter, in order to reduce the number of independent parameters and thus simplify the analysis, we shall take \( U_s = U_p = U \). Moreover, the numerical solution will be carried out with the further simplification \( U = V \).

We end mentioning that a calculation similar to the one we are going to present has been already performed by Chen and Shindolov [23], though in the magnetised BHZ model, which includes just two orbitals, \( |s \uparrow \rangle \) and, differently from our time-reversal invariant case, see Eq. (1), the \( J = 3/2, J_z = +1/2 \) orbital \( |p_+ \downarrow \rangle \).

### III. HARTREE-FOCK APPROXIMATION

The simplest way to include the effects of a not too strong interaction is through the Hartree-Fock approximation (HF), which amounts to approximate the self-energy functional simply by the Hartree and Fock diagrams. For sake of simplicity, we shall introduce the HF approximation under the assumption of unbroken translational symmetry, so that the lattice total momentum is a good quantum number. Whenever needed, we will mention what changes when translational symmetry is broken.

Within the HF approximation, if

\[ \hat{G}_0(i\epsilon, \mathbf{k})^{-1} = i\epsilon - \hat{H}_0(\mathbf{k}), \]  

(14)

is the inverse of the non-interacting \( 4 \times 4 \) Green’s function matrix at momentum \( \mathbf{k} \) and in Matsubara frequencies, \( i\epsilon \), the interacting Green’s function is

\[ \hat{G}(i\epsilon, \mathbf{k})^{-1} = \hat{G}_0(i\epsilon, \mathbf{k})^{-1} - \hat{\Sigma}_{\text{HF}}[\hat{G}] , \]  

(15)

where, in the specific case under consideration, the self-energy within the HF approximation is functional of the local Green’s function

\[ \hat{\Sigma}_{\text{HF}}[\hat{G}(\mathbf{R}_i, \mathbf{R}_i)] = \sum_{\alpha, \alpha = 0}^3 \sigma_\alpha \otimes \tau_\alpha \Gamma_{\alpha \alpha}^0 \Delta_{\alpha \alpha}(\mathbf{R}_i), \]  

(16)

with

\[ \Delta_{\alpha \alpha}(\mathbf{R}_i) \equiv \sum_{\epsilon} e^{i\epsilon \theta^+} \text{Tr} \left( \hat{G}(i\epsilon, \mathbf{R}_i, \mathbf{R}_i) \sigma_\alpha \otimes \tau_\alpha \right) \]

\[ = \langle \Psi_i^\dagger \sigma_\alpha \otimes \tau_\alpha \Psi_i \rangle \equiv \langle \Omega_{\alpha \alpha}(\mathbf{R}_i) \rangle \in \mathbb{R} , \]  

(17)

which become independent of the site coordinates \( \mathbf{R}_i \) if translational symmetry holds, i.e., \( \Delta_{\alpha \alpha}(\mathbf{R}_i) \rightarrow \Delta_{\alpha \alpha}, \forall \mathbf{R}_i \). The Dyson equation [15], together with [16] and [17], yield a self-consistency condition that has to be solved. \( \Gamma_{\alpha \alpha}^0 \) are the irreducible scattering amplitudes in the HF approximation, and, through Eq. (11), their expressions can be readily derived:

\[ \Gamma_{00}^0 = \frac{U + 2V - 2J}{4} , \quad \Gamma_{03}^0 = \frac{U - 2V + 2J}{4} , \]  

\[ \Gamma_{01}^0 = \frac{-V - 4J}{4} , \quad \Gamma_{02}^0 = \frac{-V}{4} , \]  

\[ \Gamma_{10}^0 = \frac{U}{4} , \quad \Gamma_{00}^0 = \frac{U + 2J}{4} , \]  

\[ \Gamma_{11}^0 = \frac{-V + 4J}{4} , \quad \Gamma_{01}^0 = \frac{-V}{4} , \]  

\[ \Gamma_{12}^0 = \frac{-V - 2J}{4} , \quad \Gamma_{02}^0 = \frac{-V}{4} , \]  

\[ \Gamma_{13}^0 = \frac{U}{4} , \quad \Gamma_{03}^0 = \frac{U - 2J}{4} . \]  

(18)

We note that the scattering amplitudes posses the same \( U(1) \) symmetry of the non-interacting Hamiltonian, namely, \( \Gamma_{0a}^0 = \Gamma_{0a}^0 \neq \Gamma_{3a}^0, a = 0, \ldots, 3 \).

The expectation values \( \Delta_{00}(\mathbf{R}_i) = \langle n_{i\uparrow} + n_{i\downarrow} \rangle \) and \( \Delta_{03}(\mathbf{R}_i) = \langle n_{i\uparrow} - n_{i\downarrow} \rangle \), which measure the local density and orbital polarisation, respectively, are finite already in absence of interaction. In this case, the effects of the scattering amplitudes \( \Gamma_{00}^0 \) and \( \Gamma_{03}^0 \) treated within HF are, respectively, to shift the chemical potential, which we can discard since we work at fixed density, and renormalise upward the value of \( M \), thus enlarging the stability region of the non topological phase.

On the contrary, all other expectation values \( \Delta_{\alpha \alpha}(\mathbf{R}_i), (\alpha, \alpha) \neq (0, 0), (0, 3), \) break one or more symmetries of the non-interacting Hamiltonian, and therefore vanish identically in the non interacting case. They could become finite should interaction be strong enough to lead to spontaneous symmetry breaking. We expect this should primarily occur in those channels whose scattering amplitudes are the most negative ones, being \( \Delta_{00}(\mathbf{R}_i) \) real by definition. If \( V \approx U \), as we shall assume in the following numerical calculations, the dominant symmetry breaking channels are therefore those with \( (\alpha, \alpha) = (3, 0), (1, 1), (2, 1) \). We emphasise that the dipolar coupling constant \( J \) plays an important role in splitting the large degeneracies of the scattering amplitudes in [18] that exist at \( J = 0 \).

Specifically,

\[ \Delta_{30}(\mathbf{R}_i) = \langle \Psi_i^\dagger \sigma_3 \otimes \tau_0 \Psi_i \rangle = \sum_{l=s, p} \langle n_{il\uparrow} - n_{il\downarrow} \rangle , \]  

(19)
corresponds to a spontaneous spin polarisation along the $z$-axis, which breaks time reversal symmetry. We shall investigate two possible magnetic orders, $\Delta_{30}(\mathbf{R}) = \Delta_0 e^{iQ \cdot \mathbf{R}}$, with $Q = (0, 0)$ or $Q = (\pi, \pi)$, corresponding, respectively, to ferromagnetism or antiferromagnetism.

We point out that the latter implies a breakdown of translational symmetry, in which case the Green’s function is not anymore diagonal in $\mathbf{k}$, but depends on it as well as on $\mathbf{k} + \mathbf{Q}$, so it becomes an $8 \times 8$ matrix, and Eq. (15) must be modified accordingly.

On the contrary,

$$\Delta_{11}(\mathbf{R}) = \langle \Psi_1^\dagger \sigma_1 \otimes \tau_1 \Psi_1 \rangle$$

$$\Delta_{21}(\mathbf{R}) = \langle \Psi_1^\dagger \sigma_2 \otimes \tau_1 \Psi_1 \rangle$$

(20)

describe a spin-triplet exciton condensate polarised in the plane. Since the insulator has a direct gap, excitons condense at $Q = 0$, namely $\Delta_{a1}(\mathbf{R}) = \Delta_{a1}$, $\forall \mathbf{R}$ and $a = 1, 2$. Moreover, because $\Gamma_{11} = \Gamma_{21}$, if we write

$$\Delta_{11} = \Delta \cos \phi, \quad \Delta_{21} = \Delta \sin \phi,$$

(21)

we expect to find a solution with the same amplitude $\Delta$ for any value of $\phi$, which reflects the spin $U(1)$ symmetry. At any given $\phi$, such exciton condensation would break all Hamiltonian symmetries: spin $U(1)$, inversion and time reversal.

The emergence of an exciton condensate is therefore accompanied by a spontaneous spin $U(1)$ symmetry breaking. As previously mentioned, such breakdown prevents the existence of the strong topological invariant that characterises the QSHI phase. Specifically, since the $z$-component of the spin is not anymore a good quantum number, the counter propagating edge states of opposite spin are allowed to couple each other, which turns their crossing into an avoided one. The boundary thus becomes insulating, spoiling the topological transport properties of the QSHI.

We shall study this phenomenon performing an HF calculation in a ribbon geometry with open boundary conditions (OBC) along $x$, but periodic ones along $y$. Consequently, the non-interacting BHZ Hamiltonian loses translational invariance along the $x$-direction, while keeping it along $y$, so that the Green’s function becomes a $4N_x \times 4N_x$ matrix for each momentum $k_y$, with $N_x$ the number of sites along $x$. A further complication is that HF self-energy in Eq. (15) unavoidably depends on the $x$-coordinate of each site, which enlarges the number of self-consistency equations to be fulfilled. However, since those equations can be easily solved iteratively, we can still numerically afford ribbon widths, i.e., values of $N_x$, which provide physically sensible results with negligible size effects.

The OBC calculation gives access not only to the states that may form at the boundaries, but also, in the event of a spontaneous symmetry breaking, to the behaviour of the corresponding order parameter moving from the edges towards the bulk interior. In practice, we shall investigate such circumstance only in the region of Hamiltonian parameters where the dominant instability is towards the spin-triplet exciton condensation.

**IV. BETHE-SALPETER EQUATION**

If we start from the QSHI, $M < 2$, and adiabatically switch on the interaction $\hat{\Sigma}$, we expect that such phase will for a while survive because of the gap, till, for strong enough interaction, it will eventually give up to a different phase. We already mentioned that the first effect of interaction is to renormalises upwards $M$, thus pushing the topological insulator towards the transition into the non topological one. Beside that, a repulsive interaction can also bind across gap particle-hole excitations, i.e., create excitons. A direct way to reveal excitons is through the in-gap poles of linear response functions. Within the HF approximation for the self-energy functional, the linear response functions must be calculated solving the corresponding Bethe-Salpeter (BS) equations using the HF Green’s functions together with the irreducible scattering amplitudes in Eq. (18), which are actually the functional derivatives of $\Sigma_{HF}(G)$ with respect to $\hat{G}$.

If the interaction is indeed able to stabilise in-gap excitons, their binding energy must increase with increasing interaction strength. It is therefore well possible that the excitons touch zero energy at a critical interaction strength, which would signal an instability towards a different, possibly symmetry-variant phase. Consistency of our approximation requires that such instability should also appear in the unconstrained HF calculation as a transition from the topological insulator to another phase, especially if such transition were continuous. We shall check that is indeed the case.

With our notations, see Eqs. (17) and (18), a generic correlation function will be defined as

$$\chi_{\alpha a; \beta b}(\tau, \mathbf{R}) \equiv -\langle T_\tau \{ \hat{O}_{\alpha a}(\tau, \mathbf{R}) \hat{O}_{\beta b}(0, \mathbf{0}) \} \rangle,$$

(22)

where $T_\tau$ is the time-ordering operator, and the operators $\hat{O}_{\alpha a}(\mathbf{R}) = \Psi_1^\dagger \sigma_\alpha \otimes \tau_\alpha \Psi_1$ are evolved in imaginary time $\tau$. Spin $U(1)$ symmetry implies that the $z$-component of the total spin is conserved. It follows that the non zero correlation functions $\chi_{\alpha a; \beta b}$ have $a$ and $\beta$ either 0 and 3, corresponding to $S_z = 0$, or 1 and 2, satisfying

$$\chi_{1a; 1b}(\tau, \mathbf{R}) = \chi_{2a; 2b}(\tau, \mathbf{R}),$$

$$\chi_{1a; 2b}(\tau, \mathbf{R}) = -\chi_{2a; 1b}(\tau, \mathbf{R}),$$

(23)

whose combinations $\chi_{1a; 1b, \pm i 1a; 2b}$ describe the independent propagation of $S_z = \pm 1$ particle-hole excitations.
The Fourier transform $\chi_{aa;\beta\beta}(i\omega, \mathbf{q})$, in momentum and in Matsubara frequencies, are obtained through the solution of a set of BS equations

$$\chi_{aa;\beta\beta}(i\omega, \mathbf{q}) = \chi_{aa;\beta\beta}^{(0)}(i\omega, \mathbf{q}) + \sum_{\gamma c} \chi_{aa;\gamma c}^{(0)}(i\omega, \mathbf{q}) \Gamma_{ac}^{0} \chi_{\gamma c;\beta\beta}(i\omega, \mathbf{q}),$$

where

$$\chi_{aa;\beta\beta}^{(0)}(i\omega, \mathbf{q}) = \frac{1}{N} \sum_{\mathbf{k}} T \sum_{c} \text{Tr} \left[ \sigma_{\alpha} \otimes \tau_{a} \hat{G}(i\epsilon, \mathbf{k} + \mathbf{q}) \sigma_{\beta} \otimes \tau_{b} \hat{G}(i\epsilon, \mathbf{k}) \right].$$

In Eq. (25), $N$ is the number of sites, and $\hat{G}(i\epsilon, \mathbf{k})$ the HF Green’s function matrices.

We shall perform the above calculation at zero temperature without allowing in the HF calculation any symmetry breaking. With this assumption, the HF Green’s function reads

$$\hat{G}(i\epsilon, \mathbf{k}) = \frac{(i\epsilon + t_{\epsilon}'(\mathbf{k}) \sigma_{\alpha} \otimes \tau_{a} + \hat{H}_{HF}(\mathbf{k}))}{(i\epsilon - \epsilon_{c}(\mathbf{k}))},$$

where $\hat{H}_{HF}(\mathbf{k})$, $\epsilon_{c}(\mathbf{k})$ and $\epsilon_{v}(\mathbf{k})$ are those in equations (4) and (5), with $M$ in (4) and (5) replaced by an effective $M_{HF}$ determined through the self-consistency equation

$$M_{HF} = M - \frac{2 \Gamma_{03}^{0}}{N} \sum_{\mathbf{k}} \frac{M_{HF} - \epsilon_{c}(\mathbf{k})}{\epsilon_{c}(\mathbf{k})}.$$

For $V \simeq U$, $\Gamma_{03}^{0} < 0$ so that, since the sum over $\mathbf{k}$ is positive, $M_{HF} > M$, as anticipated.

In short notations, and after analytic continuation on the real axis from above, $i\omega \to \omega + i\eta$, with $\eta > 0$ infinitesimal, the physical response functions are obtained through the set of linear equations

$$\hat{\chi}(\omega, \mathbf{q}) = \left[ 1 - \hat{\chi}^{(0)}(\omega, \mathbf{q}) \hat{\chi}^{0} \right]^{-1} \hat{\chi}^{(0)}(\omega, \mathbf{q}).$$

The excitons are in-gap solutions $\omega_{i}(\mathbf{q})$, i.e.,

$$\omega_{i}(\mathbf{q}) < \omega_{\text{min}}(\mathbf{q}) \equiv \min_{\mathbf{k}} \left( \epsilon_{c}(\mathbf{k} + \mathbf{q}) - \epsilon_{v}(\mathbf{k}) \right),$$

of the equation

$$\det \left[ 1 - \hat{\chi}^{(0)}(\omega_{i}(\mathbf{q}), \mathbf{q}) \hat{\chi}^{0} \right] = 0,$$

and have either $z$-component of the spin $S_{z} = 0$, if they appear in the channels with $\alpha, \beta = 0, 3$, or $S_{z} = \pm 1$, in the channels with $\alpha, \beta = 1, 2$. For $\omega \simeq \omega_{i}(\mathbf{q})$, the response functions can be expanded in Laurent series

$$\hat{\chi}(\mathbf{q}, \omega) = \sum_{i} \frac{A_{i}(\mathbf{q})}{\omega - \omega_{i}(\mathbf{q}) + i\eta} |\psi_{i}(\mathbf{q}) \rangle \langle \psi_{i}(\mathbf{q})| + ...,$$

where $|\psi_{i}(\mathbf{q}) \rangle$ is the exciton wavefunction and $A_{i}(\mathbf{q})$ its spectral weight. This allows computing the exciton Chern number through the integral of the Berry curvature

$$C_{i} = \frac{1}{2\pi} \int d^{2}\mathbf{q} \Omega_{i}(\mathbf{q}),$$

$$\Omega_{i}(\mathbf{q}) = \text{Im} \left( \frac{\partial_{\psi_{i}}}{\partial_{\psi_{i}}} | \langle \psi_{i}(\mathbf{q}) | \partial_{\psi_{i}} \psi_{i}(\mathbf{q}) \rangle \right).$$

The curvature is even under inversion and odd under time reversal; if a system is invariant under both, the Chern number thus vanishes by symmetry.

We observe that all the excitons are invariant under inversion, but, while the $S_{z} = 0$ ones are also invariant under time reversal, the latter maps onto each other the $S_{z} = +1$ and $S_{z} = -1$ excitons. Accordingly, only the $S_{z} = \pm 1$ excitons can have non-zero Chern numbers, actually opposite for opposite $S_{z}$, while the $S_{z} = 0$ excitons are constrained to have trivial topology. We stress that such result, being based only upon symmetry considerations, remains valid for every inversion symmetric QSHI, and not only in the context of the interacting BHZ model. The exciton Chern number does not seem to be directly related to any quantised observable. Nonetheless, as pointed out in Refs. [20] and [21], a nonzero $C_{i}$ ensures the presence of chiral exciton modes localised at the edges of the sample, which may have direct experimental consequences.

V. RESULTS

In the preceding sections we have introduced a conserving mean-field scheme to consistently calculate both the phase diagram and the linear response functions. Now, we move to present the numerical results obtained by that method at zero temperature and with Hamiltonian parameters $t' = 0.5$, $\lambda = 0.3$, $V = U = U_{1} = U_{p}$ and $J = U/16$, see equations (4), (11), (12) and (13).

A. Hartree-Fock phase diagram

The HF phase diagram is shown in Fig. [2]. As we previously mentioned, the interaction effectively increases $M$, thus pushing the transition from the topological insulator (QSHI) to the non topological one (Band Insulator) to lower values of $M$ the larger $U$. This is precisely what happens for $M \gtrsim 1.1$: $U$ increases the effective $M_{HF}$, see eq. (27), until $M_{HF} = 2$. At this point the gap closes and, for still larger $U$, the QSHI turns into the trivial Band Insulator.

For very small $M \lesssim 0.2$, upon increasing $U$ the QSHI gives in to an antiferromagnetic insulator (AFM), characterised by finite order parameters $\Delta_{30}(R_{z}) = \Delta_{30} H_{Q \cdot R_{z}}$, see Eq. (19), with $Q = (\pi, \pi)$, thus magnetised along $z$. HF predicts such transition to be of first order, in accordance to more accurate dynamical mean field theory...
the symmetry variant phase happens to be continuous, at least within HF. As we mentioned, consistency of our approach implies that this transition must be accompanied by the softening of the excitons whose condensation signals the birth of the symmetry breaking. These excitons are those with \( S_z = \pm 1 \), and indeed get massless on both sides of the transition, see Fig. 3.

The HF numerical results in the ribbon geometry with OBC along \( x \) show that electron correlations get effectively enhanced near the boundaries, unsurprisingly because of the reduced coordination. Indeed, the order parameter is rather large at the edges, and, moving away from them, decays exponentially towards its bulk value, as expected in an insulator. Remarkably, even when the bulk is in the QSHI stability region, a finite symmetry breaking order parameter exponentially localised at the edges of the system, still it has a strong effect on the single-particle edge states: a gap opens between the two branches, preventing a genuine symmetry breaking, should all the same substantially affect the physics at the edges.

The mechanism that triggers exciton topology is similar to the band inversion in the single-particle case: a topological exciton is composed by particle-hole excitations that have different parity under inversion in different regions of the BZ. In our case study, four possible orbital channels \( \tau_a, a = 0, \ldots, 3 \), are allowed,

![FIG. 2. Hartree-Fock phase diagram at \( \lambda = 0.3, t' = 0.5, U_s = U_p = V = U \) and \( J = U/16 \). The topological insulator is denoted as QSHI, while the non topological one as Band Insulator. For small value of \( M \), antiferromagnetism (AFM) is stabilised upon increasing \( U \). For larger values of \( M \), \( U \) stabilises a symmetry broken phase with Exciton Condensate. The thick black line that separates the QSHI from the Band Insulator, as well as that at \( M = 0 \) extending from \( U = 0 \) to the AFM phase, indicate a gapless metallic phase. The transition between the Exciton Insulator and the QSHI or the Band Insulator is continuous, while the transition into the AFM insulator is first order.](image)

![FIG. 3. Order parameter \( \Delta \) of Eq. (21) (blue), lowest \( S_z = \pm 1 \) exciton energy at \( Q = 0 \) (green), and band gap (orange) along the path A to C in Fig. 2 (\( M = 1, U \in [1.25, 3.5] \)), i.e., from the topological to the trivial insulator crossing the exciton insulator. We note that the intermediate phase emerges exactly when the exciton becomes massless, as well as that the band gap never vanishes.](image)

![FIG. 4. Left panel: exciton condensation order parameter \( \Delta(x) \) in Eq. (21) as function of the \( x \)-coordinate in a ribbon geometry with \( N_x = 50 \) sites, calculated at point B in Fig. 2 (\( M = 1, U = 1.5 \)). Right panel: The ribbon band structure as function of the momentum \( k_y \). We note that, even though the condensate is exponentially localised at the edges of the system, still it has a strong effect on the single-particle edge states: a gap opens between the two branches, preventing topological spin transport.](image)

B. Excitons and their topological properties

More interesting is what happens for \( 0.2 \lesssim M \lesssim 1.1 \). Here, increasing the interaction \( U \) drives a transition into a phase characterised by the finite order parameter in Eq. (21), thus by a spontaneous symmetry breaking of all symmetries, spin \( U(1) \), time reversal and inversion. The breaking of time reversal allows the system moving from the QSHI to the Band Insulator without any gap closing, see Fig. 3. We note that the transition into
each possessing a well defined parity: $\tau_1$ and $\tau_2$ odd, while $\tau_0$ and $\tau_3$ even. In the non-topological insulator, the $S_z = \pm 1$ excitons have the same parity character at all inversion invariant $k$-points, $\Gamma, M, X$ and $Y$, and thus are topologically trivial. On the contrary, in the QSHI, the highly mixed bands entail that all channels have finite weight in the exciton, which may acquire non trivial topology when its symmetry under parity changes among the inversion invariant $k$-points, thus entailing one or more avoided crossings.

In Fig. 5 we show the Chern number of the lowest energy exciton branch with $S_z = -1$ calculated through Eq. (32) with $U_s = U_p = V = 1.5$ as function of $M$ and $J$ along the way from the QSHI to the symmetry broken phase where excitons condense. We observe that the dipole-dipole interaction $J$ favours not only the instability of the $S_z = \pm 1$ excitons, but also their non trivial topology, signalled by a non zero Chern number. In Fig. 6 we show for the two points A and B of Fig. 5 the dispersion of the $S_z = 0$ excitons. Since they are invariant under time reversal, we also indicate their symmetry, even (black dots) or odd (yellow dots), which correspond, respectively, to the spin singlet and spin triplet with $S_z = 0$ components of the exciton. Comparing Fig. 6 with 5 we note that the $S_z = 0$ excitons are far less bound than the $S_z = -1$ ones. However, it is conceivable that the inclusion of the long range part of the Coulomb interaction, especially its dipolar component, could increase the binding energy of the $S_z = 0$ excitons, even though we believe that the $S_z = \pm 1$ excitons will still be lower in energy.

Moving to the sample surface at point A we expect two phenomena to occur. First, chiral exciton edge modes should appear, and connect the two branches with opposite Chern numbers, in analogy with the single particle case, and as thoroughly discussed by the authors of Ref. 26 in the magnetised BHZ model. In addition, our previous results in the ribbon geometry, showing that the exciton condensate appears on the surface earlier than the bulk, suggest the existence of genuine surface excitons, more bound than their bulk counterparts, definitely in the $S_z = \pm 1$ channel, but possibly also in the $S_z = 0$ one. Both the chiral exciton edge modes as well as the surface excitons may potentially have important effects on the physical behaviour at the boundaries. First of all, since the most bound ones correspond to coherent $S_z = \pm 1$ particle-hole excitations, they may provide efficient decay channels for the single-particle edge modes, which
The magnetization, \( M \), susceptibility, and magnetoelectric tensors, respectively.

are counter propagating waves with opposite \( S_z = \pm 1/2 \). Experimental evidences of such phenomenon in the purported topological Kondo insulator SmB\(_6\) have been indeed observed\,[23,24] and previously attributed to scattering off bulk excitons\,[22]. This is well possible, but should be much less efficient than the scattering off surface exciton modes, which we propose as an alternative explanation. Furthermore, the presence of odd-parity excitons localised at the surface might have direct consequences on the surface optical activity, which could be worth investigating.

C. Exciton condensate and magnetoelectricity

Since the order parameter in the phase with exciton condensation breaks spin \( U(1) \) symmetry, inversion \( \mathcal{I} \) and time reversal \( \mathcal{T} \), but not \( \mathcal{T} \times \mathcal{I} \), it is eligible to display magnetoelectric effects, which can be experimentally detected.

The free energy density expanded up to second order in the external electric and magnetic fields, both assumed constant in space and time, can be written as

\[
F(E, B) = F_0 - \frac{1}{2} E \cdot \chi_e E - \frac{1}{2} B \cdot \chi B - E \cdot \hat{\alpha} B ,
\]

where \( \chi_e, \hat{\chi} \) and \( \hat{\alpha} \) are the electric polarisability, magnetic susceptibility, and magnetoelectric tensors, respectively. The magnetization, \( \mathbf{M} \), and polarization, \( \mathbf{P} \), are conjugates variables of the fields, namely

\[
\mathbf{M} = - \frac{\partial F}{\partial B} = \hat{\chi} \mathbf{B} + \hat{\alpha} \mathbf{E} ,
\]

\[
\mathbf{P} = - \frac{\partial F}{\partial E} = \hat{\chi} e \mathbf{E} + \hat{\alpha} \mathbf{B} .
\]

We observe that, since \( \mathbf{E} \) and \( \mathbf{B} \) have opposite properties under inversion and time reversal, a non-zero \( \hat{\alpha} \) is allowed only when both symmetries are broken, but not their product.

Since the exciton condensate Eq. (21) is spin-polarised in the \( x-y \) plane, with azimuthal angle \( \phi \), and involves dipole excitations \( s \leftrightarrow p_{\pm 1} \), see Eq. (1), we restrict our analysis to fields \( \mathbf{E} \) and \( \mathbf{B} \) that have only \( x \) and \( y \) components, which allows us discarding the electromagnetic coupling to the electron charge current. Consequently, the magnetoelectric tensor \( \hat{\alpha} \) of our interest will be a \( 2 \times 2 \) matrix with components \( \alpha_{ij} i, j = x, y \).

In the exciton condensed phase, which is insulating, the coupling to the planar electric field is via the polarisation density, namely, in proper units,

\[
\delta H_E = - \sum_i \Psi_i^\dagger \left( E_x \hat{d}_x + E_y \hat{d}_y \right) \Psi_i ,
\]

with dipole operators

\[
\hat{d}_x = \sigma_0 \otimes \tau_1 , \quad \hat{d}_y = \sigma_3 \otimes \tau_2 .
\]

Moreover, as the orbitals \( |s \sigma \rangle \) have physical total momentum \( J_z = L_z + S_z = \pm 1/2 \), while \( |p \sigma \rangle \) have \( J_z = \pm 3/2 \), the in-plane magnetic field only couples to the magnetic moment of the \( s \)-orbitals. Specifically,

\[
\delta H_B = - \sum_i \Psi_i^\dagger \left( B_x \hat{m}_x + B_y \hat{m}_y \right) \Psi_i ,
\]

where

\[
\hat{m}_x = \sigma_1 \otimes \frac{\tau_0 + \tau_3}{2} , \quad \hat{m}_y = \sigma_2 \otimes \frac{\tau_0 + \tau_3}{2} .
\]

Since we are interested in the effects of the external fields once the the symmetry has been broken, we performed a non self-consistent calculation with the HF self-energy calculated at \( \mathbf{E} = \mathbf{B} = 0 \). The finite magnetoelectric effect in the presence of the exciton condensate is indeed confirmed, see Fig. 8 where we show the components of \( \hat{\alpha} \) as function of the azimuthal angle \( \phi \) in Eq. (21), and which we find to behave as

\[
\hat{\alpha} = \alpha_0 \begin{pmatrix} -\cos \phi & -\sin \phi \\ -\sin \phi & \cos \phi \end{pmatrix} ,
\]

where \( \alpha_0 \) is proportional to the amplitude \( \Delta \) of the order parameter, see Eq. (21), and thus vanishes when the symmetry is restored.
In the prototype BHZ model of a quantum spin Hall mean-field scheme the role of a local electron repulsion also a dipolar one, which we find to play a rather important role.

In absence of interaction, the BHZ model displays, as function of a mass parameter \( M > 0 \), two insulating phases, one topological at \( M < M_c \), and another non-topological above \( M_c \), separated by a metal point with Dirac-like dispersion at \( M = M_c \). The primary effect of Coulomb interaction, namely the level repulsion between occupied and unoccupied states, pushes the critical \( M_c \) to lower values, thus enlarging the stability region of the non-topological insulator. Besides that, and for intermediate values of \( M \), our mean field results predict that interaction makes a new insulating phase to intrude between the topological and non-topological insulators, uncovering a path connecting the latter two that does not cross any metal point. In this phase, inversion symmetry and time reversal are spontaneously broken, though their product is not, implying the existence of magnetoelectric effects. The approach to this phase from both topological and non-topological sides is signalled by the softening of two exciton branches, related to each other by time-reversal and possessing, for \( M \lesssim 1 \) with the parameters of Fig. 2, finite and opposite Chern numbers. This phase can therefore be legitimately regarded as a condensate of topological excitons.

Since, starting from the quantum spin Hall insulator, the softening of those excitons and their eventual condensation occurs upon increasing the interaction, it is rather natural to expect those phenomena to be enhanced at the surface layers. Indeed, the mean field approach in a ribbon geometry predicts the surface instability to precede the bulk one. Even though a genuine exciton condensation at the surface layer might be prevented by quantum and thermal fluctuations, still it would sensibly affect the physics at the surface. The simplest consequence we may envisage is that the soft surface excitons would provide an efficient decay channel for the chiral single-particle edge modes, as indeed observed in the supposedly three-dimensional topological Kondo insulator SmB\(_6\)\[5,23\]. In addition, we cannot exclude important consequences on the transport properties and optical activity at the surface.

We believe that our results, though obtained by a mean field calculation and for a specific model topological insulator, catch sight of still not fully explored effects of electron electron interaction in topological insulators, which might be worth investigating experimentally, as well as theoretically in other models and, eventually, by means of more reliable tools\[39,40\].

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