I. INTRODUCTION

A topological insulator (TI) hosts gapless surface or edge states, while the bulk of the material has an insulating energy gap.\(^1\) In three-dimensional TIs, the gapless surface states are spin-polarized two-dimensional (2D) Dirac fermions, whereas 2D TIs contain one-dimensional (1D) helical edge states. The helical edge states appear in counterpropagating pairs, and the states with equal energy and opposite wave numbers, \(k\) and \(-k\), form a Kramers pair. Thus elastic scattering from one helical edge state (HES) to the other one within a pair cannot be induced by time-reversal invariant potentials, e.g., stemming from impurities.\(^5\) Therefore the transport through a 2D TI is to a large extent ballistic with a quantized conductance of \(e^2/h\) per pair of HESs. This highlights the central role of time-reversal symmetry in TIs.

Quantized conductance has recently been measured in micrometer-sized samples in HgTe quantum wells.\(^6\) -\(^11\) which to date is the most important experimental demonstration of a 2D TI. Evidence of edge state transport was found in both two-terminal\(^6\) and multiterminal\(^7\) devices. Moreover, clever experiments combining the metallic spin Hall effect and a 2D TI in a HgTe quantum well (QW) demonstrated the connection between the spin and the propagation direction.\(^10\) However, also deviations from perfect conductance have been observed in longer HgTe devices,\(^6\)\(^7\)\(^11\)\(^12\) which could stem from, e.g., inelastic scattering mechanisms.\(^13\)\(^14\)\(^15\)\(^16\)\(^17\) The effect of external magnetic fields have also been considered.\(^6\)\(^8\)\(^19\)\(^20\)\(^21\)\(^22\)\(^23\)\(^24\)\(^25\)\(^26\)\(^27\)\(^28\)\(^29\)\(^30\)\(^31\)\(^32\)\(^33\)\(^34\)\(^35\)\(^36\)\(^37\)\(^38\)\(^39\)\(^40\)\(^41\)\(^42\)\(^43\)\(^44\)\(^45\)\(^46\) The TI state in HgTe QWs was predicted by Bernevig, Hughes, and Zhang (BHZ)\(^25\) by using a simplified \(k\cdot p\) model containing states with \(S\)- and \(P\)-like symmetries, respectively. They found that beyond a critical thickness of the HgTe QW, the TI state would appear as confirmed experimentally.\(^6\)\(^7\)\(^8\)\(^9\)\(^10\) Furthermore, interesting experimental progress on 2D TI properties has also been achieved in InAs/GaSb QWs\(^26\)\(^27\)\(^28\) as proposed theoretically.\(^29\)

Hyperfine (HF) interactions between the electron and nuclear spins can play an important role in nanostructures—

![Hyperfine Coupling in the BHZ Basis](image)

FIG. 1. (Color online) Hyperfine coupling between the BHZ basis states \(|H+\rangle\), \(|E+\rangle\), \(|E−\rangle\), \(|H−\rangle\), which have the total angular momentum projections on the \(z\)-axis \(m_j\) as indicated. Every increase (decrease) of \(m_j\) in the electronic sector is accompanied by a decrease (increase) of a nuclear spin due to angular momentum conservation. Hyperfine interactions due to both \(S\)- and \(P\)-like states connect the two time-reversed blocks of the BHZ model (red full arrows). However, only hyperfine interactions due to \(P\)-like states connect states within a single time-reversed block (blue dashed arrows).
However, for \( P \)-like orbital states—such as the valence band in GaAs—the contact HF interaction is absent. Nevertheless, other anisotropic HF interactions are present for \( P \)-like states such as the dipole-dipole-like HF interaction,\(^{47-51} \) which can play a significant role, e.g., for the decoherence of a hole confined in a quantum dot.\(^ {47,48,51,52} \)

HF interactions and dynamical nuclear spin polarization have also been investigated in the context of integer quantum Hall systems.\(^ {53-60} \) Appendices A–E provide various details for the conductance change.\(^ {63-65} \) In the previous works,\(^ {61-65} \) the interactions within a 2D TI. Thus, the HF coupling constants to be about one order of magnitude lower for \( P \)-like states in GaAs.

As an illustrative example, we find the HF interactions for a 2D TI, namely that embedded fixed spins such as the nuclear spins in a 2D TI can polarize locally at the boundary due to a current through the HESs.\(^ {61} \) Interestingly, the details of the HF interactions depend on the spatial direction of the boundary at which the HESs are included in the sum.

The paper is structured as follows. First, the HF interactions and the BHZ model are outlined in Secs. II and III. Then the HF interactions within \( n \)-th nuclear spin components perpendicular to the propagation direction of the HESs. This kind of coupling is unusual compared to, e.g., an ordinary Heisenberg model. Interestingly, the details of the HF interactions depend on the spacial direction of the boundary at which the HESs propagate.

The paper is structured as follows. First, the HF interactions and the BHZ model are outlined in Secs. II and III. Then the HF interactions are found within the BHZ model for a HgTe QW. To this end, we take into account both the \( S \)- and \( P \)-like states of the HESs. Here, \( P \)-like states couple differently to the nuclear spins. We show that all the HF Hamiltonians couple the time-reversed blocks of the BHZ model. However, only HF interactions relevant for the localized spins are present.\(^ {61} \) However, combining localized spins and Rashba spin-orbit coupling in the 2D TI can produce a conductance change.\(^ {63-65} \) In the previous works,\(^ {61-65} \) the interaction between the fixed spins embedded into the 2D TI and the HESs were modeled phenomenologically. In contrast, here we pay special attention to the detailed forms of the HF interactions within a 2D TI.

In this paper, we find the different HF interactions within the BHZ model for a HgTe QW. To this end, we take into account both the \( S \)- and \( P \)-like states of the BHZ model, which couple differently to the nuclear spins. We show that all the HF Hamiltonians couple the time-reversed blocks of the BHZ model. However, only HF interactions relevant for the localized spins are present.\(^ {61} \) However, combining localized spins and Rashba spin-orbit coupling in the 2D TI can produce a conductance change.\(^ {63-65} \) In the previous works,\(^ {61-65} \) the interaction between the fixed spins embedded into the 2D TI and the HESs were modeled phenomenologically. In contrast, here we pay special attention to the detailed forms of the HF interactions within a 2D TI.

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and valid for \( \mathbf{k} = (k_x, k_y) \) close to the \( \Gamma \) point, i.e., close to \( \mathbf{k} = (0, 0) \). The basis states of the model are the two Kramer pairs \( |E\pm\rangle \) and \( |H\pm\rangle \). Details on the derivation of the BHZ model are found in Refs. 1, 25, and 76. For a 2D QW, the BHZ Hamiltonian is

\[
\mathcal{H}_0 = \sum_{\mathbf{k}} \mathbf{c}^\dagger_{\mathbf{k}} \mathcal{H}_0(\mathbf{k}) \mathbf{c}_{\mathbf{k}},
\]

where \( \mathbf{c}_{\mathbf{k}} = (c_{\mathbf{k}_+}, c_{\mathbf{k}_-})^\dagger \) is a vector of creation operators and

\[
\mathcal{H}_0(\mathbf{k}) = \begin{pmatrix} h(\mathbf{k}) & 0 \\ 0 & h^*(\mathbf{-k}) \end{pmatrix},
\]

with \( h(\mathbf{k}) = \begin{pmatrix} \varepsilon_{\mathbf{k}} + M_\mathbf{k} & A(k_x + i k_y) \\ A(k_x - i k_y) & \varepsilon_{\mathbf{k}} - M_\mathbf{k} \end{pmatrix}. \]

Here, \( \varepsilon_{\mathbf{k}} = -Dk^2, M_\mathbf{k} = M_{\mathbf{0}} - Bk^2 \), and \( k \equiv \sqrt{k_x^2 + k_y^2} \) have been introduced.77 The parameters \( A, B, D, \) and \( M_{\mathbf{0}} \) depend on the QW geometry.125 Importantly, varying the QW width changes the sign of \( M_{\mathbf{0}} \), which in turn makes the system go from a nontopological to a topological state with HESs.25

The Hamiltonian (4a) \emph{a priori} has periodic boundary conditions and thereby does not contain any edges. By introducing boundaries into the model, it is possible to derive explicitly the HESs in the TI state of the QW.78,79 This will be discussed further in Sec. VIA.

Within the envelope function approximation73–75 the states of the BHZ model are

\[
|E+\rangle = f_{E+}(z)|\Gamma_6, +\rangle + f_{E+}(z)|\Gamma_8, +\rangle, \quad (5a)
\]

\[
|H+\rangle = f_{H}(z)|\Gamma_8, +\rangle + 3/2), \quad (5b)
\]

\[
|E-\rangle = f_{E-}(z)|\Gamma_6, -\rangle + f_{E-}(z)|\Gamma_8, -\rangle, \quad (5c)
\]

\[
|H-\rangle = f_{H}(z)|\Gamma_8, -\rangle - 3/2), \quad (5d)
\]

where \( f_{E}(z) \) are the transverse envelope functions in the \( z \) direction perpendicular to the 2D QW and \( |\Gamma_{\mathbf{m}}, m_\mathbf{m}\rangle \) are the lattice periodic functions at \( k = 0 \) for the \( \Gamma_\mathbf{m} \) band with projection \( m_\mathbf{m} \) of the total angular momentum, \( \mathbf{J} = \mathbf{L} + \mathbf{S} \), on the \( z \) axis. Here, \( \mathbf{S} \) is the electron spin and \( \mathbf{L} \) is the orbital angular momentum (see Appendix A). The time-reversal operator \( \Theta \) connects states within a Kramer pair \( (\Theta|E\pm\rangle = \mp|E\mp\rangle \) and \( \Theta|H\pm\rangle = \mp|H\mp\rangle \)), and the two blocks in \( \mathcal{H}_0(\mathbf{k}) \) (4b) are related by time reversal. Here, we choose phase conventions of the envelope functions such that time-reversed partners have equal envelope functions. Moreover, \( f_{E+} \) and \( f_{H} \) are chosen real, whereas \( f_{E-} \) is chosen purely imaginary. (Appendix A gives more details on the envelope functions and the lattice periodic functions.)

The states \( |E\pm\rangle \) are seen to be mixtures of the \( S \)-like \( \Gamma_6 \) band and the \( P \)-like \( \Gamma_8 \) band with \( m_\mathbf{m} = \pm 1/2 \), whereas \( |H\pm\rangle \) consist only of the \( P \)-like \( \Gamma_8 \) band with \( m_\mathbf{m} = \pm 3/2 \). Hence the states have a definite total angular momentum projection, \( J_z|E\pm\rangle = \pm \sqrt{2}h|E\pm\rangle \) and \( J_z|H\pm\rangle = \pm \sqrt{2}h|H\pm\rangle \), but \( |E\pm\rangle \) are not eigenstates of \( J^2 \).

The HF interactions can only induce transitions between states with a difference of angular momentum projection of one unit: \( m_J - m_{J'} = \pm 1 \). Therefore we can already at this point see that only particular combinations of the BHZ states can be connected by HF interactions as seen in Fig. 1. Furthermore, it is evident that HF interactions relevant for both \( S \)- and \( P \)-like states need to be included to have a full description of the HF interactions in a HgTe TI.

The real-space basis functions of \( \mathcal{H}_0 \) (4a) for the 2D QW with periodic boundary conditions are

\[
\varphi_{k, \pm}(\mathbf{r}) = \frac{\sqrt{V_0}}{\sqrt{L_x L_y}} e^{i(k_x x + k_y y)}
\]

\[
\times \left[ f_{E+}(z) u_{\Gamma_6, \pm}(\mathbf{r}) + f_{E+}(z) u_{\Gamma_8, \pm}(\mathbf{r}) \right],
\]

\[
\varphi_{k, \pm}(\mathbf{r}) = \frac{\sqrt{V_0}}{\sqrt{L_x L_y}} e^{i(k_x x + k_y y)} f_{H}(z) u_{\Gamma_8, \pm}(\mathbf{r}),
\]

where \( \mathbf{r} = (x, y, z) \), \( L_x \) (\( L_y \)) is the QW length in the \( x \) (\( y \)) direction, and \( u_{\Gamma_{\mathbf{m}}, m_\mathbf{m}}(\mathbf{r}) \equiv \langle \mathbf{r} |\Gamma_{\mathbf{m}}, m_\mathbf{m}\rangle \) are the real-space lattice periodic functions at \( \mathbf{k} = 0 \). Moreover, we have included the atomic volume, \( v_a \) explicitly here as it is often done for HF related calculations.47–50 It depends on the choice of the individual normalization of the envelope functions and the lattice periodic functions, respectively, if \( v_a \) should be included explicitly,30 as discussed in Appendix B.

**IV. HYPERFINE INTERACTIONS WITHIN THE BHZ MODEL**

Next, we find the HF interactions within the BHZ model by using the states (7) for a 2D QW with periodic boundary conditions. As we shall see, these results are useful, since they allow us to find the HF interactions for any nanostructure created in a HgTe QW (see Sec. V).

**A. Outline of the way to find the hyperfine interaction matrix elements**

The HF interactions (1) are local in space on the atomic scale, so the important part of the wave function with respect to the HF interactions is the behavior around the nucleus. Hence, in the envelope function approximation, it is the rapidly varying lattice periodic functions \( u_{\Gamma_{\mathbf{m}}, m_\mathbf{m}}(\mathbf{r}) \) that play the central role, whereas the slowly varying envelope functions only are multiplicative factors at the atomic nucleus, as we shall see below.

We set out to find the HF interactions

\[
\mathcal{H}_{\text{HF}, i} = \sum_{\mathbf{k}, \mathbf{k}', \nu, \nu'} \langle \nu \nu' |\mathcal{H}_{\text{HF}, i}| \nu \nu' \rangle c_{\mathbf{k}' \nu'}^\dagger c_{\mathbf{k} \nu},
\]

for \( i = 1, 2, 3 \) in the basis (7), i.e., for \( \varphi_{k, \nu \nu'}(\mathbf{r}) \) with \( \nu = E, H \). We begin by describing the general way that we find the HF interaction matrix elements \( \langle \nu \nu' |\mathcal{H}_{\text{HF}, i}| \nu \nu' \rangle \). To this end, the integration over the entire system volume \( V \) is rewritten as a sum of integrals over each unit cell \( m \) of volume \( v_{\text{uc}} \), i.e.,

\[
\int_V \mathbf{d} \mathbf{r} \cdots = \sum_m \int_{v_{\text{uc}}} \mathbf{d} \rho \cdots,
\]

This should be understood in the following way: every space point \( \mathbf{r} \) can be reached by first a Bravais lattice vector.
\( \mathcal{R}_m \equiv (X_m, Y_m, Z_m) \) and then a vector \( \mathbf{r} \) within the \( m \)th unit cell, i.e., \( r = \mathcal{R}_m + \mathbf{r} \). The superscript \((m)\) on the unit cell volume \( v^{(m)} \) indicates that the integral is over the \( m \)th unit cell. Thus the matrix element is

\[
\langle \psi_{k'\tau'} | H_{HF,i} | \psi_{k\tau} \rangle = \sum_n \sum_{\mathcal{R}_m} \int_{v^{(m)}} d\mathbf{r} \, \psi_{k'\tau'}(\mathcal{R}_m + \mathbf{r}) h^n_{\mathbf{r}} \psi_{k\tau}(\mathcal{R}_m + \mathbf{r}).
\]

(10)

Here, one sum is over all unit cells \( \mathcal{R}_m \), whereas the other sum is only over those atoms at position \( \mathcal{R}_m \) with a nonzero nuclear spin. To proceed, we take \( \nu = \nu' = H \) as an illustrative example and obtain

\[
\langle \psi_{kH} | H_{HF,i} | \psi_{k'H} \rangle \simeq \frac{v_{\nu}}{L_x L_y} \sum_n \sum_{\mathcal{R}_m} e^{i(k' - k)\mathbf{R}_n,i} | f_H(Z_m) |^2 \times \int_{v^{(m)}} d\mathbf{r} \, u_{\mathbf{r},3/2}(\mathbf{r}) h^n_{\mathbf{r}} u_{\mathbf{r},3/2}(\mathbf{r}),
\]

(11)

where we have used the slow variation of the envelope functions on the atomic scale, \( f_H(\mathbf{r} + Z_m) \simeq f_H(Z_m) \), and the lattice periodicity of the lattice periodic functions, e.g., \( u_{\mathbf{r},3/2}(\mathcal{R}_m + \mathbf{r}) = u_{\mathbf{r},3/2}(\mathbf{r}) \) for all \( \mathcal{R}_m \). Here, \( \mathcal{R}_{m,2} \equiv (X_m, Y_m) \), and the integral over \( \mathbf{r} \) is over the \( m \)th unit cell, whereas \( h^n_{\mathbf{r}} \) is for the \( n \)th nuclei. For a specific nuclear spin \( n \), we now include only the integral over that particular unit cell containing the \( n \)th nuclear spin, since the HF interactions are local in space. In other words, if the nuclei spin \( n \) is not inside the integration volume of the unit cell \( m \), then the contribution is neglected, i.e.,

\[
\langle \psi_{kH} | H_{HF,i} | \psi_{k'H} \rangle = \frac{v_{\nu}}{L_x L_y} \sum_n \sum_{\mathcal{R}_m} e^{i(k' - k)\mathbf{R}_n,i} | f_H(Z_m) |^2 \times \int_{v^{(m)}} d\mathbf{r} \, u_{\mathbf{r},3/2}(\mathbf{r}) h^n_{\mathbf{r}} u_{\mathbf{r},3/2}(\mathbf{r}),
\]

(12)

where the unit cell integral now is independent of the unit cell position \( \mathcal{R}_m \). The sum is only over the lattice nuclei at \( \mathcal{R}_m \) with a nonzero nuclear spin. Therefore the system does not have discrete translational symmetry, so the sum cannot simply be made into an integral. Hence, the matrix elements are not diagonal in \( \mathbf{k} \) due to the nuclear spins at random lattice points.

In order to proceed, we need to evaluate the integral of the lattice periodic function over the unit cell in Eq. (12). To this end, the symmetry of the lattice periodic functions is important; the contact interaction \( H_{HF,i} \) is zero for \( P \)-like states, since they vanish on the atomic center, while matrix elements of \( H_{HF,i} \) for \( i = 2,3 \) vanish for \( S \)-like states due to their spherical symmetry. Here, we approximate the lattice periodic functions by a linear combination of atomic orbitals (LCAO) as

\[
u_{\mathbf{r},3/2}(\mathbf{r}) = \sum_{n=1}^N \alpha_T e^{i(k' - k)\mathbf{R}_n,i} | f_T(Z_m) |^2 \times \int_{v^{(m)}} d\mathbf{r} \, u_{\mathbf{r},3/2}(\mathbf{r}) h^n_{\mathbf{r}} u_{\mathbf{r},3/2}(\mathbf{r}),
\]

(14)

where the important contribution of the atomic wave functions centered on the Hg atom is included. In other words, integrals involving atomic wave functions centered on different atoms are neglected. Fischer et al. estimated that these nonlocal contributions are two to three orders of magnitude smaller for GaAs—even for the long-ranged potentials in \( h^n_{\mathbf{r}} \) in Eqs. (1b) and (1c).

Thus we have now outlined how to find the matrix elements \( \langle \psi_{kH} | H_{HF,i} | \psi_{k'H} \rangle \) for all three kinds of HF interactions (1). The matrix elements of the types \( \langle \psi_{kH} | H_{HF,i} | \psi_{k'H} \rangle \) and \( \langle \psi_{kH} | H_{HF,1} | \psi_{k'H} \rangle \) follow the same lines as above. The essential ingredients are the locality of the HF interactions, the periodicity of \( N_{\mu,i} \) and the slowly varying envelope functions. Next, we find the three HF interactions (1) within the BHZ model.

**B. The contact HF interaction for \( S \)-like states**

Now we find the contact HF interaction \( H_{HF,1} \) Eq. (1a) within the BHZ basis (7). We begin by noting that \( \langle \psi_{kH} | H_{HF,1} | \psi_{k'H} \rangle = 0 \) and \( \langle \psi_{kH} | H_{HF,1} | \psi_{k'H} \rangle = 0 \), since the contact interaction is only nonzero at the atomic center \( h^n_{\mathbf{r}} \propto \delta(\mathbf{r} - \mathbf{R}_n) \), where the \( \Gamma_8 \) \( P \)-like atomic orbitals vanish. Hence, only the \( \Gamma_8 \) \( S \)-like part of the \( \psi_{kH} \) states leads to nonzero matrix elements of \( H_{HF,1} \). Using the approach in Sec. IV A to find the matrix elements, we get

\[
\langle \psi_{kH} | H_{HF,1} | \psi_{k'H} \rangle = \frac{v_{\nu}}{L_x L_y} \sum_n \sum_{\mathcal{R}_m} e^{i(k' - k)\mathbf{R}_n,i} | f_E(T_i,Z_m) |^2 \times \int_{v^{(m)}} d\mathbf{r} \, u_{\mathbf{r},1/2}(\mathbf{r}) h^n_{\mathbf{r}} u_{\mathbf{r},1/2}(\mathbf{r}),
\]

(15)

for \( \tau, \tau' = \pm \). The \( \Gamma_8 \) states \( u_{\mathbf{r},1/2}(\mathbf{r}) \) simply factorize into a spin and an orbital part as \( u_{\mathbf{r},1/2}(\mathbf{r}) = u_{\mathbf{r},1/2}(\mathbf{r}) \uparrow (\downarrow) \), see, e.g., Eq. (A2). Using this and the explicit form of the contact
interaction $h_0^\parallel$ in Eq. (1a), we readily obtain
\[
\langle \psi_{k\epsilon_1} | H_{HF,1} | \psi_{k\epsilon_1'} \rangle = \frac{1}{L_x L_y} \sum_n e^{i(k-k') \cdot \mathbf{R}_n} A_{S,j_n}(Z_n) \times \frac{1}{\hbar} \left[ \frac{1}{2} I_{\epsilon_n \epsilon_1'} \delta_{\epsilon_1',-\epsilon_n} + \frac{1}{2} I_{\epsilon_n \epsilon_1} \delta_{\epsilon_1',-\epsilon_n} \right],
\]
where $I_{\epsilon_1,\epsilon_2} \equiv I_{\epsilon_1,\epsilon_2} + i I_{\epsilon_1,\epsilon_2}$ are the raising and lowering nuclear spin operators. In analog to the case of a quantum dot,\cite{45,46} we here introduce the position dependent contact HF coupling as\cite{47}
\[
A_{S,j_n}(Z_n) \equiv v_g |f_{E\tau}|(Z_n)|^2 A_{S,j_n}^{\text{Atomic}},
\]
which includes the atomic contact HF coupling
\[
A_{S,j_n}^{\text{Atomic}} = \frac{2\mu_0}{3} g_S H \beta \mu_N |u_{\epsilon_n}^\dagger(\mathbf{R}_n)|^2
\]
for the nuclear spin at site $n$ of isotope $j$. Here, $A_{S,j_n}(Z_n)$ depends on the real-space position of the nuclear spin. In contrast, $A_{S,j_n}^{\text{Atomic}}$ does not depend on the nuclear position, since it can be given in terms of the atomic orbital $\Psi^\parallel_{\epsilon_n}$ by using Eq. (13) as $A_{S,j_n}^{\text{Atomic}} \propto |u_{\epsilon_n}(\mathbf{R}_n)|^2 \simeq |N_{\epsilon_n,1/2}|^2 |\alpha_{j_1}|^2 |\Psi^\parallel_{\epsilon_n}(0)|^2$, i.e., $A_{S,j_n}^{\text{Atomic}}$ only depends on the nuclear isotope type $j_1$ at site $n$. Moreover, at the present level of approximation, we can freely replace the Bravais lattice vector $\mathbf{R}_n$ by the actual position of a nuclear spin within the nth unit cell in the envelope functions in Eq. (16) due to their slow variation. Finally, we arrive at the HF contact interaction in the BHZ basis as
\[
H_{HF,1} = \sum_n \sum_{k,k'} e^{i(k-k') \cdot \mathbf{R}_n} c_k^\dagger \tilde{H}_{HF,1} c_{k'},
\]
where $c_k = (c_{k,E}, c_{k,H+,1}, c_{k,H+,2}, c_{k,H-,1}, c_{k,H-,2})$ and\cite{47,48}
\[
\tilde{H}_{HF,1} = \frac{1}{2\hbar} A_{S,j_n}(Z_n) \begin{pmatrix} I_{\epsilon_n,0} & 0 & 0 \\ 0 & I_{-\epsilon_n,0} & 0 \\ 0 & 0 & 0 \end{pmatrix}.
\]
The sum is only over nonzero nuclear spins. Therefore it is now clear that the contact HF interaction contains elements $\propto I_{\epsilon_1,\epsilon_2}$, which connect the time-reversed blocks in the BHZ Hamiltonian (4b). Moreover, as illustrated in Fig. 1, only the $|E\pm\rangle$ states are connected by $H_{HF,1}$, since only these states contain a $S$-like symmetry part. In Table I, estimates of the atomic contact HF couplings $A_{S,j_n}^{\text{Atomic}}$ are given for the stable isotopes of HgTe with nonzero nuclear spin (see Appendix D for details).

### C. The HF interactions for $P$-like states

Next, we find the HF interactions within the BHZ basis (7) for $H_{HF,2}$ and $H_{HF,3}$, Eqs. (1b) and (1c), which are relevant for the $P$-like states. To begin with, we argue that the $\Gamma_i$, $S$-like states—part of the $E\pm$ states—do not contribute to the matrix elements $\langle \psi_{k\epsilon_1} | H_{HF,1} | \psi_{k\epsilon_1'} \rangle$ and $\langle \psi_{k\epsilon_1} | H_{HF,1} | \psi_{k\epsilon_1''} \rangle$ for $i = 2, 3$. (In contrast, the $\Gamma_3 P$-like part of $E\pm$ does contribute to these elements as will be shown below.) To understand this, the HF matrix elements are written in terms of the unit cell integrals over the atomic-like wave functions as outlined in Sec. IV A. Firstly, for the dipole-dipole-like HF interaction (1b), we have
\[
\int d\rho |\Psi_{\Gamma_i,\epsilon_n}^\parallel(\rho + d/2)|^2 h_0^\parallel \Psi_{\Gamma_i,\epsilon_n}^\parallel(\rho + d/2) = 0
\]
due to the rotational symmetry of the $S$-like orbitals around the atomic core.\cite{72} Secondly, we have
\[
\int d\rho |\Psi_{\Gamma_i,\epsilon_n}^\parallel(\rho + d/2)|^2 h_0^\parallel \Psi_{\Gamma_i,\epsilon_n}^\parallel(\rho + d/2) = 0
\]
due to opposite parities of the $S$- and $P$-like orbitals.\cite{83} The same matrix elements containing $h_0^{\parallel}$ instead of $h_0^\parallel$ are also zero, because the $S$-like states have zero orbital momentum, i.e., $L_n^\parallel \Psi_{\Gamma_i,\epsilon_n}^\parallel(\rho) = 0$.

Therefore only $P$-like states contribute, so we are now left with (see Sec. IV A)
\[
\langle \psi_{k\epsilon_1} | H_{HF,1} | \psi_{k\epsilon_1'} \rangle = \frac{v_g}{L_x L_y} \sum_n e^{i(k-k') \cdot \mathbf{R}_n} |f_{E\tau}|(Z_n)|^2 \times \int d\rho |\Psi_{\Gamma_i,\epsilon_n}^\parallel(\rho)|^2 h_0^\parallel \Psi_{\Gamma_i,\epsilon_n}^\parallel(\rho),
\]
\[
\langle \psi_{k\epsilon_1} | H_{HF,1} | \psi_{k\epsilon_1''} \rangle = \frac{v_g}{L_x L_y} \sum_n e^{i(k-k') \cdot \mathbf{R}_n} |f_{E\tau}|(Z_n)|^2 \times \int d\rho |\Psi_{\Gamma_i,\epsilon_n}^\parallel(\rho)|^2 h_0^\parallel \Psi_{\Gamma_i,\epsilon_n}^\parallel(\rho),
\]
and $\langle \psi_{k\epsilon_1} | H_{HF,1} | \psi_{k\epsilon_1'} \rangle = \langle \psi_{k\epsilon_1} | H_{HF,1} | \psi_{k\epsilon_1''} \rangle^*$, where $i = 2, 3$ and $\tau, \tau' = \pm$. Using the LCAO approach (13), the unit cell integrals over the lattice periodic functions now become integrals over the atomic-like wave functions as in Eq. (14). We write the atomic wave functions as a product of a radial part $\Psi_{\Gamma_i,\epsilon_n}^\parallel(\rho)$ and an angular part $\Psi_{\Gamma_i,\epsilon_n}^\parallel(\theta, \phi)$, i.e., $\Psi_{\Gamma_i,\epsilon_n}(\rho) = \Psi_{\Gamma_i,\epsilon_n}^\parallel(\rho) \Psi_{\Gamma_i,\epsilon_n}^\parallel(\theta, \phi)$, using spherical coordinates $(r, \theta, \phi)$ with the nucleus in the center. Since the integrals are over the two-atomic unit cell volume, they do not $a$ priori factorize into a product of radial and angular integrals. However, due to
the $1/r^3$ dependence of $h^a_i$ ($i = 2, 3$), the important part of the unit cell integrals are numerically within one or two Bohr radii $a_0$ from the atomic core, which is certainly within the unit cell volume. Therefore it is a good approximation to write the unit cell integrals [e.g., Eq. (14)] as

$$\int_{vuc} d\rho [\Psi^H_{\Gamma,im}(\rho - d/2)]^* h_{ij}^a \Psi^H_{\Gamma,im'}(\rho - d/2)$$

$$\approx \int_{0}^{r_{\text{max}}} dr' \int_{0}^{2\pi} d\phi \int_{0}^{\pi} d\theta \sin(\theta) [\Psi^H_{\Gamma,im}(r')] h_{ij}^a \Psi^H_{\Gamma,im'}(r'),$$

(24)

where the specific choice of $r_{\text{max}} \gtrsim a_0$ is not important for the numerical value of the integral.\footnote{Using the radial integral (25), we introduce the atomic P-like HF coupling for isotope $j$ (at site $n$) as}

$$A_{P,j}^{\text{Atomic}} \equiv \frac{\mu_0}{4\pi} g_p \mu_B g_s \mu_N (N_{\Gamma})^2 [\alpha_{\Gamma}]^2 \left(\frac{1}{r^3}\right),$$

(26)

which are estimated to be about one order of magnitude smaller than the atomic contact HF couplings $A_{S,j}^{\text{Atomic}}$ (18), see Table I. Here, it makes sense to have a common atomic HF coupling for the dipole-dipole-like coupling $h_{ij}^a$ and the orbital to nuclear-spin coupling $h_{ij}^b$, since the normalization constants for the LCAO lattice functions (13) are numerically approximately equal, $N_{\Gamma,1/2} \simeq N_{\Gamma,1/2} \equiv N_{\Gamma}$, as discussed in Appendix D.\footnote{Similarly, for the contact HF interaction only a single position dependent HF coupling was introduced in Eq. (17). Here, the explicit dependence on the position $Z_n$ of the nuclear spin has been suppressed in the notation for simplicity, i.e., $A_{P,j}^{\text{HF}}(Z_n) = A_{P,j}^{\text{HF}}$. Similarly, the matrix elements for the HF interaction $H_{\text{HF},3}$ between the electronic orbital momentum and the nuclear spins become}

$$\langle \Phi_{k,T} | H_{\text{HF},3} | \Phi_{k',T'} \rangle = \sum_n \frac{\epsilon^{(k'-k)}_{\mathbf{R}z,n} - A_{P,j}^{\text{HF}} \delta_{\mathbf{R}z,n}}{L_x L_y} 5\sqrt{3} \hbar,$$

(27c)

where we introduce the position dependent $P$-like HF couplings as

$$A_{P,j}^{\text{HF}} \equiv v_J f_H(Z_n)^2 A_{P,j}^{\text{Atomic}},$$

(28a)

$$A_{P,j}^{\text{HF}} \equiv v_J f_{\mathbf{R}z,n} A_{P,j}^{\text{Atomic}},$$

(28b)

$$A_{P,j}^{\text{HF}} \equiv v_J f_{\mathbf{R}z,n} A_{P,j}^{\text{Atomic}},$$

(28c)

and $A_{P,j}^{\text{HF}} = [A_{P,j}^{\text{HF}}]^*$. In comparison, for the contact HF interaction only a single position dependent HF coupling was introduced in Eq. (17). Here, the explicit dependence on the position $Z_n$ of the nuclear spin has been suppressed in the notation for simplicity, i.e., $A_{P,j}^{\text{HF}}(Z_n) = A_{P,j}^{\text{HF}}$. Similarly, the matrix elements for the HF interaction $H_{\text{HF},3}$ between the electronic orbital momentum and the nuclear spins become

$$\langle \Phi_{k,T} | H_{\text{HF},3} | \Phi_{k',T'} \rangle = \sum_n \frac{1}{L_x L_y} \epsilon^{(k'-k)}_{\mathbf{R}z,n} A_{P,j}^{\text{HF}} \times \frac{1}{\hbar} \left[ \delta_{r',r} \frac{1}{3} I_{z,n} + \delta_{-r',-r} \frac{1}{3} I_{r,n} \right].$$

(29a)

$$\langle \Phi_{k,T} | H_{\text{HF},3} | \Phi_{k',T'} \rangle = \sum_n \frac{1}{L_x L_y} \frac{\epsilon^{(k'-k)}_{\mathbf{R}z,n} A_{P,j}^{\text{HF}} \delta_{\mathbf{R}z,n}}{5\hbar},$$

(29b)

$$\langle \Phi_{k,T} | H_{\text{HF},3} | \Phi_{k',T'} \rangle = \sum_n \frac{1}{L_x L_y} \frac{\epsilon^{(k'-k)}_{\mathbf{R}z,n} A_{P,j}^{\text{HF}} \delta_{\mathbf{R}z,n}}{5\hbar},$$

(29c)

It is noteworthy that the heavy-hole-like states $H \pm$ only couple diagonally ($\tau = \tau'$) or Ising-like in Eqs. (27b) and (29b) in agreement with Ref. 47. Physically, this is because the $H \pm$ states have a difference of total angular momentum projection larger than one, $|m_j - m_{j'}| > 1$. Moreover, the coupling between the states $E \pm$ in Eqs. (27a) and (29a) is essentially like the coupling between the light hole states $|\Gamma_8, \pm 1/2\rangle$, since the $S$-like states do not contribute to the matrix elements of $H_{\text{HF},2}$ and $H_{\text{HF},3}$. For these matrix elements between the $E \pm$ states, the off-diagonal elements ($\tau = -\tau'$) are a factor of 2 larger than the diagonal elements ($\tau = \tau'$) in accordance with Ref. 51.

Using the matrix elements in Eqs. (27) and (29), we now finally arrive at the HF interactions relevant for the $P$-like states in the basis (7) as

$$H_{\text{HF},i} = \sum_n \frac{\epsilon^{(k'-k)}_{\mathbf{R}z,n}}{L_x L_y} \mathbf{c}_k^\dagger H_{\text{HF},i} \mathbf{c}_{k'},$$

(30)

for $i = 2, 3$, where

$$\mathbf{H}_{\text{HF},2} = \frac{1}{5\hbar} \begin{pmatrix}
-\frac{1}{3} A_{P,j}^{\text{EE}} I_{z,n} & -\frac{1}{3} A_{P,j}^{\text{EH}} I_{-n} & -\frac{1}{3} A_{P,j}^{\text{EE}} I_{n} & 0 & -\frac{1}{3} A_{P,j}^{\text{EE}} I_{-n} \\
-\frac{1}{3} A_{P,j}^{\text{EH}} I_{-n} & -\frac{1}{3} A_{P,j}^{\text{EE}} I_{n} & 0 & -\frac{1}{3} A_{P,j}^{\text{EE}} I_{-n} & 0 \\
-\frac{1}{3} A_{P,j}^{\text{EE}} I_{n} & 0 & 0 & -\frac{1}{3} A_{P,j}^{\text{EE}} I_{-n} & 0 \\
0 & -\frac{1}{3} A_{P,j}^{\text{EE}} I_{-n} & 0 & -\frac{1}{3} A_{P,j}^{\text{EE}} I_{n} & 0 \\
0 & 0 & 0 & 0 & -\frac{1}{3} A_{P,j}^{\text{EE}} I_{n}
\end{pmatrix},$$

(31a)
and
\[ \tilde{H}_{\text{HF},3} = -5 \tilde{H}_{\text{HF},2} \] (31b)
such that the total HF interaction for the \( P \)-like states becomes
\[ \tilde{H}_{\text{HF},P} = \tilde{H}_{\text{HF},2} + \tilde{H}_{\text{HF},3} = -4 \tilde{H}_{\text{HF},2}. \] (32)

Just as the contact HF interaction (20), the \( P \)-like HF interaction connects the time-reversed blocks by connecting the \( E\pm \) states. Moreover, the \( P \)-like HF interaction connects the states within the time-reversed blocks (e.g., \( E+ \) and \( H+ \)) in contrast to the contact HF interaction, see Fig. 1.

Interestingly, the sign of the dipole-dipole-like HF interaction (31a) is opposite to the contact HF interaction (20) and to the orbital to nuclear-spin coupling (31b). However, since the elements of \( \tilde{H}_{\text{HF},3} \) are larger than those of \( \tilde{H}_{\text{HF},2} \) in absolute value, the total HF interaction for the \( P \)-like states (32) ends up having the same sign as the contact HF interaction.

V. HYPERFINE INTERACTIONS FOR A NANOSTRUCTURE IN A HgTe QUANTUM WELL

Now, we show how the HF interactions for any nanostructure in a HgTe QW can be derived from our results in Eqs. (20) and (31) for a HgTe QW with periodic boundary conditions. Examples of such structures are quantum dots, mesoscopic rings, point contacts, and antidots. The Peierls substitution is needed in order to find its HF interactions within the BHZ framework. Utilizing the Peierls substitution (31) for a HgTe QW with periodic boundary conditions. Examples of such structures are quantum dots, mesoscopic rings, point contacts, and antidots.}

VI. HYPERFINE INTERACTIONS FOR A PAIR OF HELICAL EDGE STATES

Next, we deal with the HF interactions for a pair of HESs in a HgTe 2D Ti QW.

A. The helical edge states along the \( y \) axis

To find the HF interactions, we first give the envelope wave functions for a pair of HESs. These can be found by introducing a boundary in the BHZ model and requiring that the envelope functions vanish at the boundary. For a semi-infinite half-plane restricted to \( x > 0 \) and periodic boundary condition in the \( y \) direction, \( k_y \) is still a good quantum number. The HESs envelope functions running along the \( y \) direction become
\[ \psi_{\xi}(x,y) = \frac{1}{\sqrt{L_y}} e^{ik_y} b_{\xi}^\dagger(x) \chi_{\xi} \] for \( \xi = u,d \) (36)
For illustrative purposes, the HESs are drawn side by side even though equal energy HESs in fact are on top of each other.

The HESs only exist in the topological regime of the BHZ model where $M_0/B > 0$. The explicit forms above were derived under the assumption $0 \leq M_0/B \leq A^2/(4B^2)$, where $\lambda_{1,2}$ are purely real.89 This is the relevant regime for the realistic parameters for 2D TI in a HgTe QW of width 61 or 70 Å.

Using the time-reversal properties of the basis states of the BHZ model (as discussed in Appendix A), it is seen explicitly that $\Psi_{y,k}^{\mu}(x,y)$ and $\Psi_{y,-k}^{\nu}(x,y)$ constitute a Kramers pair, since they are connected by the time-reversal operator $\Theta$ as $\Theta \Psi_{y,k}^{\mu}(x,y) = -\Psi_{y,-k}^{\nu}(x,y)$ and $\Theta \Psi_{y,-k}^{\nu}(x,y) = \Psi_{y,k}^{\mu}(x,y)$. Often the $\Psi_{y,k}^{\mu}$ ($\Psi_{y,k}^{\nu}$) is referred to as the spin-up (spin-down) edge state, since it only consists of states with positive (negative) total angular momentum projection, see Eq. (37).

B. Hyperfine interactions for the helical edge states along the y axis

The HFI interactions are now readily found by inserting the envelope HESs along the $y$ axis (36) into the general HFI formula (35) for any structure in a HgTe QW. Using Eq. (20), the contact HFI interaction becomes

$$\gamma_{HF,y}^{(y)} = \frac{1}{2\hbar} \frac{B - D}{2B} \sum_{k_y} \sum_{n} \frac{\epsilon_{n}(k_y)}{L_y} A_{S_{\alpha},\beta} (\vec{Z}_n)$$

$$\times \left[ A_{k_y,k_y}^{(X_n)} s^\dagger_{n,k_y} c^\dagger_{y,k_y} - A_{-k_y,-k_y}^{(X_n)} s_{-n,k_y} c_{y,k_y} - A_{k_y,-k_y}^{(X_n)} I_{-n,k_y} c^\dagger_{y,k_y} s_{n,k_y} \right].$$

where $c^\dagger_{n,k_y}$ ($c_{n,k_y}$) are the creation (annihilation) operators for the HESs $\Psi_{y,k_y}^{\mu}(x,y)$ (36). We have emphasized the notation that $\mathcal{H}_{HF,y}^{(y)}$ is for HESs along the $y$ axis. The product of the transverse parts of the HESs at the nuclear spin $n$ is introduced as

$$A_{k_y,k_y}^{(X_n)} = g_{k_y}^{(y)}(x,y)g_{k_y}^{(y)}(L_y),$$

and includes the only dependence of $\lambda_n$ in $\mathcal{H}_{HF,y}^{(y)}$. Here we see that the contact HFI interactions can produce transitions between the HESs $\Psi_{y,k_y}^{\mu}(x,y)$ and $\Psi_{y,-k_y}^{\nu}(x,y)$ at the expense of a change in a nuclear spin state. In particular, elastic transitions within the Kramers pair $\Psi_{y,k_y}^{\mu}(x,y)$ and $\Psi_{y,-k_y}^{\nu}(x,y)$ are possible. This is just as if the HESs were spin-1/2 as used, e.g., in Refs. 61, 62, and 64. Hence, from the point of view of the electrons in the HESs the time reversal symmetry is broken. Of course, the composed system of electrons and nuclear spins is time-reversal invariant, since any system can be made time-reversal invariant by expanding it sufficiently.36

The HFI interaction due to the $P$-like states, $\mathcal{H}_{HF,P}^{(y)} = \mathcal{H}_{HF,2}^{(y)} + \mathcal{H}_{HF,3}^{(y)}$, is similarly found by inserting

\[ W_{k_y} = \left[ \frac{A^2}{4} - \frac{M_0}{B} (B^2 - D^2) \right] k_y + \frac{D\sqrt{B^2 - D^2}}{B} k_y + (B^2 - D^2) k_y^2. \]
where the dependence on \( Z_n \) is inside the HF couplings \( A_{\perp,z}^{\perp} \) (28). Here, we used the rewritings

\[
i[I_{+,n}A_{\perp,z}^{\perp} - I_{-,n}A_{\perp,z}^{\perp}] = -2I_{+,n} \text{Im}(A_{\perp,z}^{\perp})
\]

and

\[
i[I_{+,n}A_{\perp,z}^{\perp} + I_{-,n}A_{\perp,z}^{\perp}] = +2I_{+,n} \text{Im}(A_{\perp,z}^{\perp}),
\]

which build on the fact that \( A_{\perp,z}^{\perp} = i \text{Im}(A_{\perp,z}^{\perp}) \) due to the phase conventions of \( f_{\perp,z} \) as purely imaginary and \( f_H \) as real. This HF interaction also permits transitions between the two HESs—especially within the Kramers pair—just as the contact HF interaction (39). The terms \( \propto c_{z,i}^c c_{x,i}^d \) in the HF interaction (41) affect transitions within a single HES. These are more unusual than their counterparts in the contact HF interaction (39), since they do not only contain terms involving \( I_{x,n} \), but also \( I_{\perp,n} \). Hence the HF interaction (41) due to the \( P \)-like states has terms like a \( I_x S_z \) coupling, which are not present in, e.g., a Heisenberg model. These terms \( \propto I_{\perp,n}c_{z,i}^c c_{x,i}^d \) stem from the fact that the HF interactions due to the \( P \)-like states (31) couple the states \( |H\pm\rangle \) and \( |E\pm\rangle \) within a single time-reversed block of \( H_0 \). In order to shine more light on the origin of the HF interactions (39) and (41), they are given in Appendix E in terms of nondiagonal edge state spin operators using the picture of spin-1/2 HESs.

C. Hyperfine interactions for helical edge states along the \( x \) axis: curious differences

The HF interactions presented above are for HESs running along the \( y \) axis. Now, we find various interesting differences in the HF interactions for HESs running along the \( x \) axis.

The HESs are found in the same way as in Sec. VIA. The only difference is that we consider the HESs localized near a boundary given by the \( x \) axis instead of the \( y \) axis, i.e., we study the semi-infinite half-plane defined by \( y > 0 \). The HESs along the \( x \) axis are given by

\[
\psi_{\pm,x,k_x}(x,y) = \frac{1}{\sqrt{L_x}} e^{ik_x x} g_{x,k_x}(y), \quad \chi_x = n \left( \begin{array}{c} \alpha \\ \beta \end{array} \right) \left( \begin{array}{c} \sqrt{\beta^2 - D^2} \\ B - D \end{array} \right), \quad \chi_x^d = n \left( \begin{array}{c} \alpha \\ \beta \end{array} \right) \left( \begin{array}{c} \sqrt{\beta^2 - D^2} \\ B - D \end{array} \right),
\]

i.e., the imaginary unit \( i \) does not appear in the \( E\pm \) components of the spinors as for the HESs along the \( y \) axis, see Eq. (37). This is the mathematical origin of the differences between the HF interactions for the HESs in the two directions. These HESs also appear in Kramers pairs \( (\psi_{+,x,k_x}, \psi_{-,x,-k_x}) \) and \( (\psi_{+,x,k_x}, \psi_{-,x,k_x}) \) is referred to as spin-up (spin-down). The spin-up HES \( \psi_{+,x,k_x} \) has negative velocity such that \( E^x_k = E_0 - h\omega_{k_x} \), while the spin-down HES has positive velocity, i.e., \( E^d_k = E_0 + h\omega_{k_x} \). Hence the velocities of the HESs along the \( x \) and \( y \) axes have opposite signs, such that spin-\( \zeta \) always travels the same way along the boundary, see Fig. 2. Therefore it is natural that \( k_x \) has to be exchanged by \( -k_x \) to connect the HESs in the two perpendicular directions.

By inserting the HESs along the \( x \)-axis Eq. (42) into Eq. (35), the contact HF interaction becomes

\[
\mathcal{H}_{HF,1}(x) = \frac{1}{B - D} \sum_{k_x} e^{i(k_x - k_x')x} \psi_{+,x,k_x}(x,y) L_x \left( \begin{array}{c} \chi_{x'} \\ \chi_{x'}^d \end{array} \right). \quad (44)
\]

where \( \Lambda_{\perp,x}^{(2)}(\chi_{x'}) = g_{x,k_x}(\chi_{x'}) g_{x,-k_x}(\chi_{x'}) \). Interestingly, the sign of the terms producing inter HES transitions is opposite to the one in \( \mathcal{H}_{HF,1}^{(3)} \) (39). This difference stems from the imaginary unit \( i \) in \( \chi_{x'}^d \) (37), which is absent in \( \chi_{x'} \) (43). Moreover, the sign of \( k_x \) and \( k_x' \) is opposite in the \( \Lambda \) functions for \( \mathcal{H}_{HF,1}^{(3)} \) (44) and \( \mathcal{H}_{HF,1}^{(3)} \) (39), respectively. This is natural in order to maintain the propagation direction of the HES—spin \( \zeta = u,d \), see Fig. 2.

The HF interaction due to the \( P \)-like states for the HESs at the \( x \) axis becomes

\[
\mathcal{H}_{HF,P}(x) = \frac{2}{15\hbar} \sum_{k_{x,x',}} e^{i(k_{x,x'} - k_{x})x} L_x \left( \begin{array}{c} 2 - \frac{B - D}{B} A_{\perp,x}^{\perp} \left( \begin{array}{c} \Lambda_{\perp,x}^{(2)} \end{array} \right) \left( \begin{array}{c} \chi_{x'} \\ \chi_{x'}^d \end{array} \right) \right) \left( \begin{array}{c} \Lambda_{\perp,x}^{(2)} \end{array} \right) (x) \left( \begin{array}{c} \chi_{x}
\right) \left( \begin{array}{c} \chi_{x'}^d \end{array} \right) \right),
\]

\[
+ \left[ 2\sqrt{3} \frac{A \sqrt{B^2 - D^2}}{|A|B} \text{Im}(A_{\perp,x}^{\perp}) (x) + \frac{(B - D)A_{\perp,x}^{\perp} + (B + D)A_{\perp,x}^{\perp} \text{Im}(A_{\perp,x}^{\perp}) (x)}{B} \left( \begin{array}{c} \Lambda_{\perp,x}^{(2)} \end{array} \right) (x) \left( \begin{array}{c} \chi_{x'} \\ \chi_{x'}^d \end{array} \right) \right),
\]

(45)
where the inter HES transition terms again have an opposite overall sign compared to $\mathcal{H}_{\text{HF,p}}^{(3)}$ (41). Another noteworthy difference is the exchange of the terms $\lambda_{n,n'} c^\dagger_{k,n} c_{k',n'}$ in $\mathcal{H}_{\text{HF,p}}^{(3)}$, by $I_{n,n'} c^\dagger_{k,n} c_{k',n'}$ in $\mathcal{H}_{\text{HF,p}}^{(3)}$, i.e., intra-HES transitions are coupled to the nuclear spin operators perpendicular to the propagation direction. These differences again stem from the elementary unit (or the lack thereof) in the spinors. Furthermore, the signs of $k_n$ and $k'_n$ are again interchanged in the $\Lambda$ functions by comparing $\mathcal{H}_{\text{HF,p}}^{(3)}$ and $\mathcal{H}_{\text{HF,p}}^{(3)}$.

### D. Position averaged hyperfine interactions

In HgTe, about 19% of the atoms have a nonzero nuclear spin and these can be assumed to be randomly distributed. In the HF interactions for the HESs, the unit-cell position of every nuclear spin is included. This information is sample dependent and often valuable insights can be found without it. Therefore we now consider the HF interactions averaged over the unit-cell position of the nuclear spins in analogy to impurity averaging. To be specific, we focus here on the HF interactions (39) and (41) for the HESs along the $y$ axis. Mathematically, the position averaged of some quantity $\mathcal{F}$ is introduced as

$$ \mathcal{F} = \frac{1}{A_{N}} \int_A d\mathcal{R}_{x_{\alpha}} \cdots \int_A d\mathcal{R}_{x_{\alpha}N} \mathcal{F}(\mathcal{R}_{x_{\alpha}}, \ldots, \mathcal{R}_{x_{\alpha}N}), $$

where $N$ is the number of nonzero nuclear spins covered by the HESs. We only average over the positions $\mathcal{R}_{x_{\alpha}N} \equiv (\Lambda_x, Z_{\alpha}n)$ in the cross-section area $A$ of the HESs along the $y$ axis. Therefore we keep the positions $\mathcal{R}_{y_{\alpha}}$, which break translational invariance along the edge and ultimately can lead to backscattering.

Now we study the position averaged HF Hamiltonians. However, one can equally well average position at a later stage of a calculation, if it is physically relevant for a particular phenomenon, e.g., position averaging of the transition rates. Using the normalization of $f_{\text{HF}}$ in Appendix B, the position averaged contact HF interaction (39) becomes

$$ \mathcal{H}_{\text{HF,1}}^{(3)} = \frac{1}{4\hbar^2} \frac{B-D}{2B} N \sum_{\mathcal{R}_{x_{\alpha}N}} \sum_n \sum_{k_n,k'_n} e^{i(k_n-k'_n)\mathcal{R}_{x_{\alpha}N}} \frac{A_{\text{Atomic}}^{\text{Atomic}}} {N} \left( \Lambda_{n,n'} c^\dagger_{k,n} c_{k',n'} \right) $$

$$ - \left( \Lambda_{n,n'} c^\dagger_{k,n} c_{k',n'} - \Lambda_{-n,-n'} c^\dagger_{k,n} c_{k',n'} \right), $$

(47)

where the cross section area $A$ is given in terms of the QW thickness $W_{x}$ and the HES width $W_{y}$ as $A = W_x W_y$, such that $\int_A d\mathcal{R}_{x_{\alpha}N} = 1$. Here, $W_{y}$ is on the order of a few decay lengths $\lambda_{y,1}^{-1}$ and the number of atoms covered by the HESs is $N = (L_{A}/1)a$. We observe that the position dependent HF coupling $A_{\text{Atomic}}^{\text{Atomic}} / N$ due to the position averaging as in the case of quantum dots.

The position averaged of the product of transverse functions, $\Lambda_{n,n'} = \int_0^{W_y} d\mathcal{R}_{x_{\alpha}} g^\dagger_{n}(\mathcal{X}_{n}) g_{n'}(\mathcal{X}_{n'})$, is now independent of the positions $\mathcal{X}_{n}$. It can be well approximated by replacing $W_{y}$ by $\infty$ in the upper limit, which gives

$$ \Lambda_{k,k'} = \sqrt{\frac{2\lambda_1 \lambda_2 (\lambda_1 + \lambda_2)} {2\lambda_1 \lambda_2 (\lambda_1 + \lambda_2)}} \left( \frac{1} {\lambda_1 + \lambda_1} - \frac{1} {\lambda_1 + \lambda_2} - \frac{1} {\lambda_1 + \lambda_2} + \frac{1} {\lambda_1 + \lambda_2} \right) \right), $$

(48)

where $\lambda_i$ and $\lambda'_i$ depend on $k_n$ and $k'_n$, respectively. It is evident that $\Lambda_{k,k'} = \Lambda_{k',k}$, since $g_{n}$ in Eq. (38a) is real. Moreover, $\Lambda_{k,k'} = 1$ due to the normalization of $g_{n}$. Furthermore, in the particle-hole symmetric limit $D = 0$, we have $g_{-k}(x) = g_{k}(x)$ such that $\Lambda_{k,k'}^{(D=0)} = \Lambda_{-k,-k'}^{(D=0)} = \Lambda_{k,-k'}^{(D=0)}$. Hence the position averaged contact HF interaction (47) becomes isotropic in the particle-hole symmetric limit. Since the BHZ model is valid only close to the $\Gamma$ point, we expand $\Lambda_{k,k'}$ to lowest order in $k_{y}$ and $k_{y}'$ for $D \neq 0$, i.e., $\Lambda_{k,k'} \approx \eta_{k,k'}$, where

$$ \eta_{k,k'} \equiv 1 - \frac{D^2}{8M_{0}^2 (B^2 - D^2)} (k_{y} - k_{y}')^2. $$

(49)

Hence the lowest-order expansion fulfills $\eta_{k,k'} = \eta_{k,-k'}$ and $\eta_{-k,-k'} = \eta_{k,-k'}$ such that the position averaged contact HF interaction (47) simplifies to

$$ \mathcal{H}_{\text{HF,1}}^{(3)} = \frac{1}{4\hbar^2} \frac{B-D}{2B} N \sum_{k_n,k'_n} \sum_n e^{i(k_n-k'_n)\mathcal{R}_{x_{\alpha}N}} \frac{A_{\text{Atomic}}^{\text{Atomic}}} {N} \left( \Lambda_{n,n'} c^\dagger_{k,n} c_{k',n'} \right) $$

$$ \times \left[ \eta_{k,k'} I_{\text{c}} c^\dagger_{k,n} c_{k',n'} - \eta_{k,-k'} I_{\text{c}} c^\dagger_{k,n} c_{-k',n'} \right], $$

(50)

to lowest order in $k_{y}$ and $k_{y}'$. In this limit, $\mathcal{H}_{\text{HF,1}}^{(3)}$ therefore has uniaxial anisotropy.

The position averaged HF interaction due to the $P$-like states in Eq. (41) becomes

$$ \mathcal{H}_{\text{HF,1}}^{(3)} = \frac{2}{15\hbar^2} \frac{B-D}{2B} N \sum_{n} \sum_{k_n,k'_n} e^{i(k_n-k'_n)\mathcal{R}_{x_{\alpha}N}} \frac{A_{\text{Atomic}}^{\text{Atomic}}} {N} \left( \Lambda_{n,n'} c^\dagger_{k,n} c_{k',n'} \right) $$

$$ \times \left[ \eta_{k,k'} \left( I_{\text{c}} c^\dagger_{k,n} c_{k',n'} \right) \right. $$

$$ \left. - \eta_{k,-k'} \left( I_{\text{c}} c^\dagger_{k,n} c_{-k',n'} \right) \right], $$

(51)

by using the expansion $\Lambda_{k,k'} \approx \eta_{k,k'}$ and the normalization conditions for $f_{\text{HF}}$ and $f_{\text{HF}}$ (see Appendix B). Interestingly, the terms in $\mathcal{H}_{\text{HF,1}}^{(3)}$ (41) coupling $I_{\text{c}} c^\dagger_{k,n} c_{k',n'}$ vanish in the position averaging, since $f_{\text{HF}}(z)$ is even and $f_{\text{HF}}(z) = 0$ such that $A_{\text{HF}}^{\text{HF}} \propto \int d\mathcal{R}_{x_{\alpha}} f_{\text{HF}}(\mathcal{R}_{x_{\alpha}})$ = 0. Furthermore, even in the particle-hole symmetric limit $D = 0$, $\mathcal{H}_{\text{HF,1}}^{(3)}$ is not isotropic in contrast to the contact HF interaction.

The total position averaged HF interaction

$$ \mathcal{H}_{\text{HF}}^{(3)} = \mathcal{H}_{\text{HF,1}}^{(3)} + \mathcal{H}_{\text{HF,2}}^{(3)} $$

in the small wave-vector limit is

115411-10
TABLE II. Estimates of the effective HF couplings (53) for a pair of HESs. In parentheses, we give the percentage of the HF coupling stemming from the HF Hamiltonians due to P-like states, e.g., 4[(B - D)/(15B)]A_{Atomic} / A_{\perp}. Here, we use the atomic HF couplings in Table I and the BHZ model parameters.1,94 B and D only for a 70-Å-thick QW.

<table>
<thead>
<tr>
<th></th>
<th>199Hg</th>
<th>201Hg</th>
<th>123Te</th>
<th>125Te</th>
</tr>
</thead>
<tbody>
<tr>
<td>A_{jn}^+ (\mu eV)</td>
<td>1.1</td>
<td>-0.38</td>
<td>-12</td>
<td>-14</td>
</tr>
<tr>
<td>(%)</td>
<td>(77%)</td>
<td>(75%)</td>
<td>(73%)</td>
<td>(73%)</td>
</tr>
<tr>
<td>A_{jn}^- (\mu eV)</td>
<td>0.30</td>
<td>-0.11</td>
<td>-3.5</td>
<td>-4.2</td>
</tr>
<tr>
<td>(%)</td>
<td>(14%)</td>
<td>(12%)</td>
<td>(12%)</td>
<td>(12%)</td>
</tr>
</tbody>
</table>

now found from Eqs. (50) and (51) to be

$$H_{HF}^{(3\perp)} \simeq \frac{1}{2N} \sum_{n,k_x,k_y} e^{i(k_x^0-k_x)} \left[ A_{jn}^+ N \eta_{k_x,k_y} I_{x,n} \left( c_{k_x^0,n}^c c_{k_x^0,n}^d - c_{k_x^0,n}^d c_{k_x^0,n}^c \right) - A_{jn}^- N \eta_{k_x,k_y} \left( I_{-n} c_{k_x^0,n}^c c_{k_x^0,n}^d + I_{+n} c_{k_x^0,n}^d c_{k_x^0,n}^c \right) \right]$$

(52)

where effective HF couplings were introduced as

$$A_{jn}^+ = \frac{B - D}{4B} A_{S,jn} + \frac{4}{15} \frac{7B + 5D}{2B} A_{P,jn}$$

$$A_{jn}^- = \frac{B - D}{B} \left( \frac{1}{4} A_{S,jn} + \frac{4}{15} A_{P,jn} \right)$$

(53a)

(53b)

Hence the total position averaged HF interaction $\langle H_{HF}^{(3\perp)} \rangle$ has uniaxial anisotropy. Estimates of $A_{jn}^+$ and $A_{jn}^-$ are given in Table II. Remarkably, the part of the effective HF couplings due to the P-like states dominates for the coupling $A_{jn}^+$, but not for $A_{jn}^-$. One reason is that the HESs have their main contribution on the H states compared to the E states, since $\langle \chi^0_y^T \rangle \simeq (-1.036, -0.93, 0, 0)$ for a 70-Å-thick QW.94 Moreover, not only the H states are P-like states, but also partly the E states, see Eq. (5).

We remark that the position averaged HF interactions for the HESs along the x axis Eqs. (44) and (45) follow along the same lines. The only difference in the total HF interaction in Eq. (52) is an opposite sign of the inter HES transition terms (apart from the replacements $\gamma_{jn} \rightarrow X_{jn}$ and $k_y \rightarrow k_j$). For typical parameters,96 the number of atoms covered by the HESs is about $N \sim 10^7$ per μm edge, where about 19% of these atoms have a nonzero nuclear spin.

VII. DISCUSSION, SUMMARY, AND OUTLOOK

In this paper, we have provided benchmark results within the BHZ model for the form and magnitude of (i) the contact HF interaction in Eq. (20), (ii) the dipole-dipole-like HF interaction in Eq. (31a), and (iii) the coupling of the electrons orbital momentum to the nuclear spin in Eq. (31b).

All the HF interactions couple the time-reversed blocks of the BHZ Hamiltonian (4b)—just as the Rashba spin-orbit coupling and the bulk inversion asymmetry terms.9 However, in contrast to the Rashba and bulk inversion asymmetry terms, the HF interactions break time-reversal symmetry from the electronic point of view. Therefore the HF interactions couple directly the Kramers pair of counterpropagating HESs of opposite wave numbers (k and -k), and thereby open for elastic backscattering. In contrast, the Rashba spin-orbit interaction combined with other scattering mechanisms can only couple the HESs inelastically.13,14,16,63 Hence our careful microscopic modeling of the HF interactions confirms that elastic backscattering spin-flip processes indeed are present as correctly anticipated on physical grounds in previous works on the interaction between HESs (modeled as spin-(1/2) and one or more fixed magnetic moments.61-65

Furthermore, we estimated the atomic HF constants relevant for a HgTe QW, see Table I. These estimates are generally smaller by an order of magnitude or so compared to similar estimates for GaAs by Fischer et al.47,100 This is natural, since heavier elements often have lower HF couplings due to their higher principal quantum number of the outermost electron [see, e.g., Eqs. (D4) and (D5)]. As a consequence, the typical time for polarizing the nuclear spins by a current through the HESs of a HgTe QW is increased to hours or days compared to seconds for a GaAs QW in the quantum hall regime.54

From the HF Hamiltonians within the BHZ model, we derived a general formula (35) for the HF interactions for any nanostructure in a HgTe QW. The input of this formula is the envelope function of the given structure, where the effects of bulk inversion asymmetry,8 Rashba spin-orbit coupling,76 and magnetic fields21 can be included. From this formula, we found the HF interactions for a pair of HESs. Interestingly, the HF Hamiltonians depend on the orientation of the boundary at which the HESs propagate: the sign of the terms creating inter-HES transitions is opposite for perpendicular boundaries. This has not been considered previously in works on HESs coupled to fixed spins.61-65 On the level of transition rates between the HESs,61,62,64 such a difference is less important, since the rates are proportional to the HF matrix elements squared. However, this sign might play a role for more delicate phenomena such as Kondo physics53,55 or for HESs circulating one or more fixed spins.

We also found that the HF interactions due to the P-like states couple the intra-HES transitions to both nuclear spin components perpendicular to the propagation direction of the HESs, see Eqs. (41) and (45). The unusual terms coupling $I_{x,n} (I_{x,n})$ to the intra-HES transitions for propagation along the y axis (x axis) were not included in previous studies.51-65 These terms might complicate the nature of nuclear spin polarization and its associated Overhauser effective magnetic field101 in a nontrivial way. For instance, this could affect the spin-orbit interaction induced backscattering processes between the HESs in the presence of a finite Overhauser field discussed in Ref. 64.

Finally, we averaged over the positions of the nuclear spins to remove the sample dependent information. This revealed that the total HF Hamiltonian is quite generally anisotropic and, moreover, that the contribution due to P-like states can dominate over the contact HF contribution, see Table II and Eq. (52). Therefore it can be important to include the HF interactions (1b) and (1c) relevant for P-like states for the HESs. Moreover, we found that the coupling of $I_{x,n} (I_{x,n})$ to the intra-HES transitions for propagation along the y axis (x axis) vanishes in the position averaging of the HF Hamiltonians. In this sense, these couplings are somewhat fragile compared to...
the usual coupling of \( I_{\gamma} \) to the intra-HES transitions. On the other hand, position averaging at a later stage of a calculation might allow interesting effects from these unusual terms to survive.

In passing, we remark that the nuclear spins can open a very small energy gap in the HES spectrum. This can be shown by averaging out all spacial directions of the nuclear spin positions in the total HF interaction. Treating the nuclear spins as a semiclassical field of zero mean value, the energy gap becomes proportional to the in-plane field. The ensemble averaged energy gap \( \delta \) is proportional to \( N^{-1/2} \) and estimated to be on the order of \( 10^{-4} \) \( \mu \text{eV} \) for a micrometer-sized edge, which seems out of the current experimental range.

ACKNOWLEDGMENTS

We are especially grateful to Jan Fischer and Dietrich Rothe for helpful correspondence on their work in Refs. 47–50 and 76, respectively. We also thank Laurens Molenkamp, Bjorn Trauzettel, Andrzej Kdziora, Jens Piaske, and Karsten Flensberg for useful discussions. Both AML and GP are supported by Grant No. MAT2011-24331 and by the ITN Flensberg for useful discussions. Both AML and GP are supported by Grant No. MAT2011-24331 and by the ITN Grant 234970 (EU). AML acknowledges the Juan de la Cierva program (MICINN), Grant No. FIS2009-07277, and the Carlsberg Foundation. Furthermore, we acknowledge FIS2010-22438-E (Spanish National Network for Physics of Out-of-Equilibrium Systems).

APPENDIX A: ON THE BHZ MODEL STATES

This Appendix describes various details of the BHZ states \(|E\pm\rangle\) and \(|H\pm\rangle\). In particular, the time-reversal properties and the phase conventions of the envelope functions are discussed. The states in the BHZ model as presented in Ref. 25 are given by

\[
|E+\rangle = f_1(z)|\Gamma_6, + 1/2\rangle + f_2(z)|\Gamma_8, + 1/2\rangle, \quad (A1a)
\]
\[
|H+\rangle = f_3(z)|\Gamma_6, + 3/2\rangle, \quad (A1b)
\]
\[
|E-\rangle = f_2(z)|\Gamma_6, - 1/2\rangle + f_3(z)|\Gamma_8, - 1/2\rangle, \quad (A1c)
\]
\[
|H-\rangle = f_4(z)|\Gamma_6, - 3/2\rangle, \quad (A1d)
\]

similar to Eq. (5), but without specifying any phase conventions for the envelope functions \(f_n(z)\). The lattice periodic functions can be given as

\[
|\Gamma_6, + 1/2\rangle = |S|\uparrow, \quad (A2a)
\]
\[
|\Gamma_6, - 1/2\rangle = |S|\downarrow, \quad (A2b)
\]

and

\[
|\Gamma_8,3/2\rangle = +\frac{1}{\sqrt{2}}[|P_1\rangle + i|P_5\rangle]|\uparrow\rangle, \quad (A3a)
\]
\[
|\Gamma_8,1/2\rangle = -\frac{\sqrt{2}}{3}[P_2\rangle]|\uparrow\rangle + \frac{1}{\sqrt{6}}[|P_1\rangle + i|P_5\rangle]|\downarrow\rangle, \quad (A3b)
\]
\[
|\Gamma_8,-1/2\rangle = -\frac{\sqrt{2}}{3}[P_2\rangle]|\downarrow\rangle - \frac{1}{\sqrt{6}}[|P_1\rangle - i|P_5\rangle]|\uparrow\rangle, \quad (A3c)
\]
\[
|\Gamma_8,-3/2\rangle = -\frac{1}{\sqrt{2}}[|P_1\rangle - i|P_5\rangle]|\downarrow\rangle, \quad (A3d)
\]

where the Bloch amplitudes \(|S\rangle, |P_1\rangle, |P_5\rangle, \) and \( |P_2\rangle \) transform the same way as the well-known orbitals with the same names.\(^{75,105}\) The orbitals are connected to the spherical harmonics.\(^{73,96}\) Thus \(|\Gamma_8,m_j\rangle\) correspond to \(|j = 3/2,m_j = l = 1, s = 1/2\rangle\) in the angular momentum representation using the total angular momentum \(J = L + S\) as a good quantum number, where \(S\) is the electron spin in the basis \(|\uparrow\downarrow\rangle\). Likewise, \(|\Gamma_6,m_j\rangle\) simply corresponds to the \(l = 0\) state. Note that the split-off band \(\Gamma_6\) with \(j = 1/2\) and \(l = 1\) is neglected in the BHZ model. Here, \(|S\rangle\) is chosen to be purely imaginary\(^{106}\) and \(|P_2\rangle, |P_4\rangle, |P_5\rangle\) to be real.\(^{73}\) Furthermore, we follow the convention by Bernevig et al.\(^{25}\) and Novik et al.\(^{105}\) by using an overall opposite sign\(^{106}\) for the \(\Gamma_6\) states in terms of the \(P\) states in Eq. (A3) compared to other authors.\(^{73,109}\) This sign change is not important for the purposes of this paper.

Next we discuss the phase conventions for the envelope functions made in the main text. The envelope functions \(f_n(z) (n = 1,\ldots,6)\) are found from the Luttinger-Kane model at \(k_x = k_y = 0\) and therefore has to fulfill the following differential equations:\(^{25,76}\)

\[
Tf_n(z) - \frac{\sqrt{2}}{3} P_0 \partial_z f_{n+3}(z) = E_{k=0} f_n(z), \quad (A4a)
\]
\[
-\frac{\sqrt{2}}{3} P_0 \partial_z f_n(z) + W_{-} f_{n+3}(z) = E_{k=0} f_{n+3}(z), \quad (A4b)
\]

for \(n = 1,2\) only [i.e., only for the two pairs \((f_1,f_2)\) and \((f_2,f_3)\)]. Similarly,\(^{25,76}\)

\[
W_{+} f_n(z) = E_{k=0} f_n(z), \quad \text{for } n = 3,6 \text{ only}. \quad (A5)
\]

Here, we have introduced the real operators

\[
T = E_c(z) + \frac{\hbar^2}{2m_e} k_z [2F(z) + 1] k_z, \quad (A6a)
\]
\[
W_{\pm} = E_c(z) + \frac{\hbar^2}{2m_e} k_z [2\gamma_2(z) \mp \gamma_1(z)] k_z, \quad (A6b)
\]

where \(k_z = -i\partial_z\), \(E_{c(z)}\) is the conduction (valence) band edge, \(m_e\) the bare electron mass, \(\gamma_1,2\) are the Luttinger parameters,\(^{110}\) and \(F(z)\) is a real function including the remote \(\Gamma_6\) bands perturbatively.\(^{76}\) The parameters \(\gamma_2, F,\) and \(E_{c(z)}\) are different in the HgTe and CdTe layers of the heterostructure, which leads to the \(z\) dependence. The solution of these equations will also give the energy for that particular solution (energy band) \(E_{k=0} = k = (0,0)\). From Eq. (A5), it follows that we can choose \(f_2(z) = f_3(z)\), which is simply denoted as \(f_H(z)\) in the main text. Furthermore, Eq. (A4) allows us to choose \(f_3(z) = f_2(z)\) and \(f_4(z) = f_3(z)\), which are called \(f_{\text{FER}}(z)\) and \(f_{\text{FER}}(z)\), respectively, in the main text. By comparison of Eq. (A4) and their complex conjugates, it follows that we can choose \(f_1(z)\) real and \(f_2(z)\) purely imaginary as in Ref. 76.

Now we turn our attention to the time-reversal properties of the states \(|E\pm\rangle\) and \(|H\pm\rangle\). The time-reversal operator \(\Theta\) is defined up to an arbitrary phase factor. Here, we use \(\Theta = -i\sigma_z K\), where \(K\) is the complex conjugation operator and \(\sigma_z\) a Pauli matrix in electron spin space. The time-reversal operator \(\Theta\) acts differently in different bases (due to the complex conjugation), so one should stick to the same basis throughout out a calculation.\(^{96}\) The \(|\Gamma_1,m_j\rangle\) states under the time-reversal operator follow from Eqs. (A2) and (A3) by using that the \(P\)-like states are real, the \(S\)-like states are pure
imaginary and that $\Theta | \uparrow \rangle = + | \downarrow \rangle$ and $\Theta | \downarrow \rangle = - | \uparrow \rangle$, i.e.,

$$
\begin{align*}
\Theta | \Gamma_6, \pm 1/2 \rangle &= \mp | \Gamma_6, \mp 1/2 \rangle, \\
\Theta | \Gamma_8, \pm 1/2 \rangle &= \pm | \Gamma_8, \mp 1/2 \rangle, \\
\Theta | \Gamma_8, \pm 3/2 \rangle &= \mp | \Gamma_8, \mp 3/2 \rangle.
\end{align*}
$$

Therefore we can now evaluate, e.g., $\Theta | E \rangle$ by using Eq. (A7) and that $f_{E \Gamma_4}$ is real and $f_{E \Gamma_5}$ is purely imaginary, which gives $\Theta | E \rangle = - | E \rangle$. Hence our conventions lead to

$$
\begin{align*}
\Theta | E \pm \rangle &= \mp | E \mp \rangle, \\
\Theta | H \pm \rangle &= \pm | H \mp \rangle,
\end{align*}
$$

which fulfill $\Theta^2 = -1$ as expected. We remark that that Rothe et al.\textsuperscript{111} find opposite signs under time-reversal (i.e., $\Theta | E \pm \rangle = \pm | E \mp \rangle$ and $\Theta | H \pm \rangle = \pm | H \mp \rangle$), simply because an opposite overall sign was chosen in the definition of the time-reversal operator.\textsuperscript{111} In Ref. 67, the same signs as in Eq. (A8) are found.

**APPENDIX B: NORMALIZATION OF THE BHZ STATES**

In this Appendix, the normalization of the envelope functions and lattice periodic functions within the envelope function approximation is discussed. To this end, we use $\varphi_{k,H^+}(r)$ in Eq. (7b) as an example. The entire wave function is normalized in the usual way, i.e.,

$$
\int_V dr |\varphi_{k,H^+}(r)|^2 = 1,
$$

where $V$ is the volume of the entire system. The normalization of the entire wave function (B1) leaves a freedom to normalize the envelope function and the lattice periodic function in the most convenient way for the problem at hand. Various choices are found in the literature, see, e.g., footnote 2 in the review of Coish and Baugh.\textsuperscript{30}

To see how this normalization choice works in practice, we begin by separating the left-hand side of the normalization condition (B1) into a product of the envelope function and the lattice periodic function normalization, respectively. To this end, the normalization condition (B1) is rewriting by dividing the integral over the entire space into a sum of integrals over the unit cells as in Eq. (9), i.e.,

$$
1 = \frac{v_u}{L_x L_y} \int_V d\mathbf{r} |f_H(z)|^2 |u_{\Gamma_1 \pm \frac{1}{2}}(\mathbf{r})|^2
$$

$$
= \frac{v_u}{L_x L_y} \sum_{\mathbf{R}_n} \int_{vuc} d\rho |f_H(\rho_z + \mathbf{Z}_n)|^2 |u_{\Gamma_1 \pm \frac{1}{2}}(\mathbf{R}_n + \rho)|^2
$$

$$
\approx \frac{v_u}{L_x L_y} \sum_{\mathbf{R}_n} \int_{vuc} d\rho |f_H(\mathbf{Z}_n)|^2 |u_{\Gamma_1 \pm \frac{1}{2}}(\rho)|^2
$$

$$
= \frac{v_u}{L_x L_y} \left[ \int_{vuc} d\rho |u_{\Gamma_1 \pm \frac{1}{2}}(\rho)|^2 \right]
$$

where we used in the third equality that the envelope function—by construction—is slowly varying on the scale of the unit cell, so $f_H(\rho_z + \mathbf{Z}_n) \simeq f_H(\mathbf{Z}_n)$, and that the lattice periodic functions are periodic with the lattice, i.e., $u_{\Gamma_1 \pm \frac{1}{2}}(\mathbf{R}_n + \rho) = u_{\Gamma_1 \pm \frac{1}{2}}(\rho)$. Therefore we arrive at

$$
1 = \frac{v_u}{L_x L_y} \int_V d\mathbf{r} |f_H(z)|^2 \left[ \int_{vuc} d\rho |u_{\Gamma_1 \pm \frac{1}{2}}(\rho)|^2 \right],
$$

where the normalization of the entire wave function in Eq. (B1) have been written as a product of the normalization of the envelope function and lattice periodic function part, respectively. Thus it is now clear that some freedom exists in the normalization choice.

In this paper, we normalize the lattice periodic function as Fischer et al.,\textsuperscript{47-50} i.e.,

$$
\int_{vuc} d\rho |u_{\Gamma_1 \pm \frac{1}{2}}(\rho)|^2 = \frac{v_u}{L_x L_y} = 2
$$

using the fact that a zinc-blende crystal, like HgTe or GaAs, contains two atoms per unit cell, $v_u = 2v_{uc}$. This normalization has the advantage that the atomic HF constants found in the main paper are independent of the number of atoms in the unit cell.\textsuperscript{30} Moreover, the envelope function is normalized as

$$
\frac{1}{L_x L_y} \int_V d\mathbf{r} |f_H(z)|^2 = 1,
$$

such that Eq. (B3) is fulfilled.

The normalization procedure follows the same lines as above for the other BHZ basis functions, e.g., all lattice periodic functions are normalized to the number of atoms in the unit cell. When the wave function is not a simple product of an envelope function and a lattice periodic function, then it should be used that different lattice periodic functions are orthogonal, i.e.,

$$
\int_{vuc} d\rho u_{\Gamma_1 \pm \frac{1}{2}}(\rho) u_{\Gamma_1 \pm \frac{1}{2}}(\rho) = 2\delta_{\Gamma_1 \pm \frac{1}{2}},
$$

Finally, it should be noted that for the $E \pm$ states, we end up with a combined normalization for the two envelope functions, i.e.,

$$
\int d\mathbf{z} \left[ \int_{vuc} d\rho |f_{E \Gamma_1}(\rho)|^2 + |f_{E \Gamma_2}(\rho)|^2 \right] = 1.
$$

APPENDIX C: DETAILS ON THE CALCULATION OF THE ATOMIC INTEGRALS OF THE HYPERFINE INTERACTIONS FOR P-LIKE STATES

This Appendix deals with the integrals over the atomic wave functions of the form

$$
\int_{vuc} d\rho \left[ \psi_{\Gamma_1, m, j}(\rho + d/2) \right]^* \psi_{\Gamma_1, m, j}(\rho + d/2),
$$

which appear in the matrix elements of $H_{HF,2}$ and $H_{HF,3}$ in Sec. IV C. The atomic wave functions are written as

$$
\psi_{\Gamma_1, m, j}(r) = R_{\Gamma_1, m, j}(r) Y_{\Gamma_1, m}(\theta, \phi),
$$

i.e., a product of a radial and an angular part as in the main text. The angular part
of the wave functions $\tilde{\Psi}_{\Gamma_{m,n}}(\theta, \phi)$ are combinations of the usual spherical harmonics $Y^m_\theta(\theta, \phi)$ and the electronic spin-1/2 (|↑⟩ and |↓⟩) and inherit the symmetry of the bands.\cite{47,48} i.e.,

$$
\Psi_{\Gamma_{m+2}}(\theta, \phi) = -Y_1^1(\theta, \phi)|↑⟩,
$$

\begin{equation}
\Psi_{\Gamma_{m+1}}(\theta, \phi) = -\frac{2}{3} Y_0^0(\theta, \phi)|↑⟩ - \frac{1}{3} Y_1^1(\theta, \phi)|↓⟩, \tag{C2}
\end{equation}

$$
\Psi_{\Gamma_{m-2}}(\theta, \phi) = -Y_1^1(\theta, \phi)|↓⟩,
$$

which are all eigenfunctions of $J_z = L_z + S_z$ (with eigenvalue $\hbar m_j$). $\mathbf{J}^2 = (\mathbf{L} + \mathbf{S})^2$ (with $j = 3/2$), $\mathbf{L}^2$ (with $l = 1$ due to $P$ states), and $S^2$ (with $s = 1/2$). To be consistent with the HZH model, we use the same overall sign as Refs. 25 and 107, which is opposite to the one used in, e.g., Refs. 73 and 109 [see also Appendix A, Eq. (A3), and endnote 108]. However, this overall sign cancels out in the matrix elements between $P$ states and therefore has no effect here.

To find the integrals (C1), the spherical approximation Eq. (24) is used. This is an excellent approximation, since most of the weight of the integrals are close to the atomic core. To facilitate the calculations, the HF dipole-dipole-like interaction for a single nuclear spin $\hbar n^2$ Eq. (1b) is rewritten as (choosing the origin at the nuclear spin, i.e., $\mathbf{r}_n = \mathbf{r} - \mathbf{R}_n \rightarrow \mathbf{r}$)

$$
\hbar^2 n^2 = \frac{\mu_0}{4\pi} \gamma_e \gamma_y \frac{1}{\mathbf{r}^2} \left[ 1 + \frac{\mathbf{r}^2}{2} \right] ^2 \times \left[ 2 S_x I_{x,n} - \frac{1}{2} (S_y I_{y,n} + S_z I_{z,n}) \right] + \frac{3}{2} \mathbf{r}^2 \left( S_x I_{x,n} + S_z I_{z,n} \right) + 6 \frac{\mathbf{r}^2}{2} \left( S_x I_{x,n} + S_z I_{z,n} \right) + 6 \frac{\mathbf{r}^2}{2} \left( S_y I_{y,n} + S_z I_{z,n} \right). \tag{C3}
$$

This is written in such a way that the integrals [like Eq. (24)] consist of a radial integral over $\alpha_r \gamma_e \gamma_y/\mathbf{r}^2$ times a sum of angular integrals. The terms in the curly bracket become the sum of angular integrals, where the space dependencies are seen to form spherical tensor operators or sums thereof. Therefore the Wigner-Eckart theorem is useful to identify the integrals that are zero, see, e.g., Ref. 96. As an example, for the element of a Hg nuclear spin between the $\Psi_{\Gamma_{r,3/2}}(\mathbf{r})$ states, appearing in the matrix element $\langle \phi_{\mathbf{k}', \mathbf{r}'}|H_{\text{HF}, 2}^\text{atom}|\phi_{\mathbf{k}, \mathbf{r}}\rangle$, is found to be (after some calculations)

$$
\int_0^{\alpha_r} \frac{d\alpha_{r'}}{\alpha_{r'}} \int_0^{2\pi} d\phi \int_0^{\pi} d\sin(\theta) \left| \Psi_{\Gamma_{r, 3/2}}(\mathbf{r}) \right|^2 \hbar^2 \frac{\Psi_{\Gamma_{r, 3/2}}(\mathbf{r}')}{\mathbf{r}} \hbar^2 \frac{\Psi_{\Gamma_{r, 3/2}}(\mathbf{r})}{\mathbf{r}} \delta_{\mathbf{r}, \mathbf{r}'} \left( -\frac{1}{5} \tau \hbar I_{z,n} \right) \tag{C4}
$$

using Eqs. (C2) and (C3) and the definition (25). The rest of the integrals for $\hbar^2 n^2$ are found similarly.

Finally, we note that the integrals (C1) involving $\hbar^2 n^2$ (1c) are much simpler to evaluate. The integrals in the spherical approximation (24) again separate into the radial integral (1/r^3)Hg/Te times a sum of angular integrals, which can be found by using the rewriting $\mathbf{L}_n \cdot \mathbf{I}_n = L_{+, n} I_{z,n} + \frac{1}{2}(L_{+, n} I_{-, n} + L_{-, n} I_{z,n})$ and Eq. (C2).

APPENDIX D: ESTIMATION OF THE ATOMIC HF CONSTANTS

In this Appendix, we estimate the atomic HF couplings Eqs. (18) and (26),

$$
A_{\text{atomic}}^\text{S,}\gamma_n = \frac{2\mu_0}{3} g_e \mu_B g_J \mu_N |u_{\Gamma_n}(\mathbf{R}_n)|^2, \tag{D1a}
$$

$$
A_{\text{atomic}}^\text{P,}\gamma_n = \frac{\mu_0}{4\pi} g_e \mu_B g_J \mu_N |N_{\Gamma_n}|^2 |u_{\Gamma_n}(\mathbf{R}_n)|^2 \left( \frac{1}{\mathbf{r}^2} \right)^{\frac{1}{2}}, \tag{D1b}
$$

along the same lines as Fischer et al.\cite{47} These estimates are given in Table I. Below, we go through the ingredients to make these estimates.

Within the LCAO approach (13), the lattice periodic functions within a unit cell are written as a linear combination of the two atomic orbitals. The relative weight between the two orbitals is related to the ionicity and found to be\cite{112,113}

$$
\alpha_{\text{Te}} \simeq \sqrt{0.8} \quad \text{and} \quad \alpha_{\text{Hg}} \simeq \sqrt{0.72}, \tag{D2}
$$

which is taken to be the same for the $\Gamma_n$ and $\Gamma_8$ bands.\cite{47}

Moreover, the $g$ factors for the various isotopes are\cite{31}

$$
g_{\text{Te}}^{\text{Hg}} = 1.01, \quad g_{\text{Te}}^{\text{Hg}} = -0.37, \tag{D3a}
$$

$$
g_{\text{Te}}^{\text{Te}} = -1.47, \quad g_{\text{Te}}^{\text{Te}} = -1.78. \tag{D3b}
$$

These are seen to vary in sign, which is the reason for the sign variation of the HF couplings.

Furthermore, to estimate the HF couplings, the atomic wave functions $\Psi_{\Gamma_n, m}^\text{Hg/Te}$ also have to be given explicitly. The angular part follows the band symmetry as in Eq. (C2). As for the radial part, we follow Fischer et al. and approximate it by a hydrogenic radial eigenfunction\cite{96} $R_n(r)$ with an effective charge $e Z_{\text{eff}}$ replacing the actual charge of the nucleus $eZ$ in order to include atomic effects, etc., i.e., $Z_{\text{eff}} < Z$. The outermost electrons in Hg (Te) have the principal quantum number $n = 6$ ($n = 5$) such that $R_n^\text{Hg/Te}(r) = R_{6(5),1}(r)$ and $R_n^\text{Hg/Te}(r) = R_{6(5),0}(r)$. Clementi et al.\cite{114,115} have calculated the effective charges $Z_{\text{eff}}$ for various atoms and orbitals and found that $Z_{\text{eff}}(\text{Te}, 5s) = 12.5$, $Z_{\text{eff}}(\text{Te}, 5p) = 10.8$ and $Z_{\text{eff}}(\text{Hg}, 6s,6p) = 11.2$, which obviously is much smaller than the bare nuclear charges $eZ = 52e$ for Te and $eZ = 80e$ for Hg.

Using $|u_{\Gamma_n}(\mathbf{R}_n)|^2 \simeq (N_{\Gamma_n, 1/2})^2 |\alpha_j|^2 |\Psi_{\Gamma_n}(\mathbf{0})|^2$ with the hydrogenic orbital $\Psi_{\Gamma_n}(\mathbf{r}) = R_{0}^\text{Hg/Te}(r) Y_0^0(\theta, \phi)$ for isotope $j$, we can now give the atomic contact HF coupling as

$$
A_{\text{atomic}}^\text{S,}\gamma_n \simeq \frac{2\mu_0}{3} g_e \mu_B g_J \mu_N |N_{\Gamma_n, 1/2}|^2 |\alpha_j|^2 \left( \frac{Z_{\text{eff}}(j, s)}{\alpha_0 n^3} \right)^2, \tag{D4}
$$

where $\alpha_0 = 4\pi\epsilon_0 e\hbar^2/(m_e e^2)$ is the Bohr radius and $\epsilon_0$ is permittivity of free space.
The hydrogenic interactions in atomic orbitals also makes it easy to calculate $1/r^3$ in Eq. (25) numerically, which shows that neither the nuclear length scale $r_n$ nor $r_{\text{max}}$ make a difference in practice. Hence we can use
\[
\left( \frac{1}{r^3} \right)_r \simeq \int_0^\infty dr r^2 |R_{n,l}(r)|^2 \frac{1}{r^3} \sim \left[ Z_{\text{eff}}(j, p) \right]^3 \frac{3 \alpha_j^3}{n^3}, \tag{D5}
\]
to find the HF coupling $A_{ij}^{\text{atomic}}$ for the $P$ states.

Therefore now we only need one more ingredient to be able to estimate the HF couplings, namely the normalization constants $N_{\Gamma,m_j}$ of the lattice periodic functions in the LCAO approach Eq. (13). The normalization condition (B4) leads to
\[
\int \alpha_{\Gamma,m_j}^2 \psi_{\Gamma,m_j}(r) \left[ \frac{1}{2} \frac{d}{dr} \right]_r \left[ \frac{1}{2} \frac{d}{dr} \right]_r \psi_{\Gamma,m_j}(r) = \frac{2}{N_{\Gamma,m_j}}, \tag{D6}
\]
where $+(-)$ corresponds to $\Gamma_8$ $(\Gamma_6)$. First of all, we note that
\[
N_{\Gamma,m_j} = N_{\Gamma,-m_j},
\]
due to the similar form of the atomic wave functions for $\pm m_j$, see, e.g., Eq. (C2). Using the hydrogenic eigenstates, we can therefore now numerically find the normalization constants $N_{\Gamma,m_j}$. Numerically, these do depend weakly on how the Wigner-Seitz unit cell of the zinc-blende crystal is approximated, in contrast to the unit cell integrals involving $\hbar^2$ for $\Gamma = 2, 3$ in Sec. IV C. We have tested various spherical and cubic approximations to the primitive Wigner-Seitz unit cell all with the same volume as the Wigner-Seitz unit cell, namely $v_{\text{uc}} = 16|d|^3/(3\sqrt{3})$, where $|d| = 0.279$ nm is the distance between the Hg and Te atoms in unit cell, see, e.g., p. 58 in Ref. 33. Such a weak dependence is also found in the estimate for GaAs by Fischer et al.\textsuperscript{47} From our various approximate unit cell calculation, we found that a good estimate for the normalization constants are $(N_{\Gamma_8,1/2})^2 \simeq (N_{\Gamma_8,3/2})^2 \simeq 3.6$ and $(N_{\Gamma_6,1/2})^2 \simeq 2.7$. Therefore we can use approximately equal normalization constants for $N_{\Gamma_8,\pm 1/2}$ and $N_{\Gamma_6,\pm 3/2}$, which allows for the introduction of a common atomic $P$-like HF constant in Eq. (26). Therefore we now have all the ingredients to make the estimates with the results seen in Table I.

APPENDIX E: HYPERFINE INTERACTIONS IN TERMS OF EDGE STATE SPIN OPERATORS

Here, we reformulate the HF interactions (39) and (41) for the HESSs along the $y$ axis in order to give some more insights into their form. Having in mind the spin-1/2 picture of a pair of HESSs discussed in Sec. VI A, we are lead to introduce the
\[\text{nondiagonal edge states spin operators as}\]
\[\begin{align}
g_{k',k',x} &= \frac{\hbar}{2} \left( c_{k',a}^\dagger c_{k',d} + c_{k',d}^\dagger c_{k',a} \right), \tag{E1a} \\
g_{k',k',y} &= \frac{\hbar}{2} \left( c_{k',a}^\dagger c_{k',a} + c_{k',d}^\dagger c_{k',d} \right), \tag{E1b} \\
g_{k',k',z} &= \frac{\hbar}{2} \left( c_{k',a}^\dagger c_{k',a} - c_{k',d}^\dagger c_{k',d} \right), \tag{E1c}
\end{align}\]
together with the operator $\mathcal{J}_{k,k'} = \frac{\hbar}{2} \left( c_{k'a}^\dagger c_{k'a} + c_{k'd}^\dagger c_{k'd} \right)$ and the raising and lowering operators $s_{k',k'} = \pm i s_{k',k'}$ for the edge state spin. Here, for instance, $s_{k',k'}$ moves a particle in the state $\Psi_{k',k'}^d$ into the state $\Psi_{k',k'}^u$ and in this sense raises the edge state spin (while also changing the wave vector). In the case of $k = k'$, the edge state spin operators (E1) coincide with the usual spin-1/2 operators\textsuperscript{97} and $\mathcal{J}_{k,k'}$ is the particle number operator (times $\hbar/2$). The contact HF interaction (39) in terms of the edge state spin operators (E1) becomes
\[\mathcal{H}_{\text{HF}}^{(y)} = \frac{1}{2\hbar^2} \sum_{k,k',\Gamma} \frac{L_{y}}{N_{\Gamma}} A_{S,j,k'}(Z_n)\]
\[\times \left\{ (\mathcal{A}_{k',k}^{(X)} + \mathcal{L}_{k',k}^{(X)} I_{\Gamma} a_{k,k'} z) \right\} + (\mathcal{A}_{k',k}^{(Y)} - \mathcal{L}_{k',k}^{(Y)} I_{\Gamma} a_{k,k'} z) \right\} + (\mathcal{A}_{k',k}^{(Z)} - \mathcal{L}_{k',k}^{(Z)} I_{\Gamma} a_{k,k'} z) \right\} + \mathcal{J}_{k,k'} \right\}.
\]
Using the edge state spin operators (E1), the HF interaction (41) due to the $P$-like states becomes
\[\mathcal{H}_{\text{HF}}^{(p)} = \frac{2}{15\hbar^2} \sum_{k,k',\Gamma} \frac{L_{y}}{N_{\Gamma}} \left[ \frac{2 - B - D}{B} \right] A_{P,j,k'}^{E} \left\{ (\mathcal{A}_{k',k}^{(X)} - \mathcal{L}_{k',k}^{(X)} I_{\Gamma} a_{k,k'} z) \right\} + \mathcal{J}_{k,k'} \right\}.
\]
where
\[\mathcal{J}_{k,k'} = \mathcal{L}_{\Gamma} a_{k,k'} z \right\}.
\]
in both HF interactions, the edge state spin-flipping terms $I_{\pm} a_{k,k'} z$ appear. Moreover, in the HF interaction for $P$-like states, the unusual coupling $I_{\Gamma} a_{k,k'} z$ is found as discussed in the main text. Note that the terms including the operator $\mathcal{J}_{k,k'}$ vanish to second order in $k$ and $k'$ in the position averaging and also in the particle-hole symmetric limit, see Sec. V ID.
HYPERFINE INTERACTIONS IN TWO-DIMENSIONAL...
This overall sign-change compared to the conventional one does not come from the spherical harmonics as given by Sakurai, see, e.g., Winkler. Generally, it is convenient to have the parameter $P_0 = -\frac{\hbar}{m_0} \langle S | p_\alpha | P_\alpha \rangle$ with the opposite sign compared to the convention in Winkler, where $P_0 = +\frac{\hbar}{m_0} \langle S | p_\alpha | P_\alpha \rangle$. Note that this sign has no effect on the time-reversal properties of the states.

Using a Gaussian distributed semiclassical field from the nuclear spins, we can derive the ensemble averaged energy gap to be approximately $E_\text{g} \simeq \sqrt{\frac{\hbar^2}{m_0}} A_{\text{HF}}$. Here, the effective in-plane HF coupling constant is given by $A_{\text{HF}} \equiv \sum_j \frac{n_j}{2} (A_j^+)^2 (I_j + 1)$, where the sum is over the nuclear isotope types $j = \{199\text{Hg}, 201\text{Hg}, 113\text{Te}, 115\text{Te}, 123\text{Te}, 199\text{Hg}, 201\text{Hg}, 113\text{Te}, 115\text{Te}\}$. Sometimes an imaginary unit is actually included explicitly and not absorbed into the notation of, e.g., Table C1 in Appendix C of Ref. 73. Sometimes an imaginary unit $i$ is often conventionally chosen to be purely imaginary, see, e.g., Table C1 in Appendix C of Ref. 73. Sometimes an imaginary unit $i$ is often conventionally included explicitly and not absorbed into the notation of $|S\rangle$ as it is done here, see, e.g., Chuang. Generally, it is convenient to have $|S\rangle$ purely imaginary such that the parameter $P_0 = \frac{\hbar}{m_0} \langle S | p_\alpha | P_\alpha \rangle$ connecting $S$- and $P$-like bands in $k \cdot p$ theory becomes real, since the $P$-like states are real. However, the choice of having $|S\rangle$ purely imaginary affects the time-reversal properties of the $|E \pm \rangle$ states.

This overall sign-change compared to the conventional one does not come from the spherical harmonics as given by Sakurai, see, e.g., Winkler. For many purposes, this sign does not play a role, since it is simply an overall phase factor. However, the matrix elements between $\Gamma_6$ and $\Gamma_3$ states change sign. This is taken care of in Refs. 25 and 107 by changing the sign of the definition of the $P_0$ parameter in the $k \cdot p$ theory, so the $k \cdot p$ Hamiltonian looks formally the same. Therefore Refs. 25 and 76 use $P_0 = -\frac{\hbar}{m_0} \langle S | p_\alpha | P_\alpha \rangle$ with the opposite sign compared to the convention in Winkler. Where $P_0 = +\frac{\hbar}{m_0} \langle S | p_\alpha | P_\alpha \rangle$. Note that this sign has no effect on the time-reversal properties of the states.

Even though the spherical harmonic $Y_{\ell=0}^{m=0} = 1/\sqrt{4\pi}$ corresponding to the $|S\rangle$ state is real, the state $|S\rangle$ is often conventionally chosen to be purely imaginary, see, e.g., Table C1 in Appendix C of Ref. 73. Sometimes an imaginary unit $i$ is actually included explicitly and not absorbed into the notation of $|S\rangle$ as it is done here, see, e.g., Chuang. Generally, it is convenient to have $|S\rangle$ purely imaginary such that the parameter $P_0 = \frac{\hbar}{m_0} \langle S | p_\alpha | P_\alpha \rangle$ connecting $S$- and $P$-like bands in $k \cdot p$ theory becomes real, since the $P$-like states are real. However, the choice of having $|S\rangle$ purely imaginary affects the time-reversal properties of the $|E \pm \rangle$ states.

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