Existence of bulk chiral fermions and crystal symmetry

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We consider the existence of bulk chiral fermions around points of symmetry in the Brillouin zone of nonmagnetic 3D crystals with negligible spin-orbit interactions. We use group theory to show that this is possible, but only for a reduced number of space groups and points of symmetry that we tabulate. Moreover, we show that for a handful of space groups the existence of bulk chiral fermions is not only possible but unavoidable, irrespective of the concrete crystal structure. Thus our tables can be used to look for bulk chiral fermions in a specific class of systems, namely that of nonmagnetic 3D crystals with sufficiently weak spin-orbit coupling. We also discuss the effects of spin-orbit interactions and possible extensions of our approach to Weyl semimetals, crystals with magnetic order, and systems with Dirac points with pseudospin 1 and 3/2. A simple tight-binding model is used to illustrate some of the issues.

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I. INTRODUCTION

Electrons in the vicinity of the $K$ points in graphene, have linear dispersion relations and behave like massless chiral fermions. More concretely, the dynamics of electrons around these points is governed by the relativistic, two-dimensional massless Dirac hamiltonian $H_0 \sim \sigma_x k_x + \sigma_y k_y$, and many of the exotic electronic properties of graphene stem from this fact. This also turns graphene into a potential laboratory for two-dimensional relativistic dynamics, incorporating massless fermions, gauge fields and curved gravitational backgrounds. Moreover, optical lattices that could be used to simulate relativistic systems with trapped cold atoms can be fashioned after graphene with control over the properties of the system. Obviously three-dimensional analogs of graphene are potentially very interesting.

Strictly speaking, the massless Dirac hamiltonian $H_0$ describes only the low energy, orbital dynamics of electrons in graphene. As reviewed in Section III, spin-orbit coupling in graphene gives fermions a very small mass. This mass is so small that for most practical purposes spin and orbital degrees of freedom decouple and $H_0$ provides an effective description of an enormous variety of phenomena.

In this paper we will consider 3D analogs of graphene, i.e., crystals with orbital electron dynamics governed by the 3D two-component massless Dirac hamiltonian $H_0 \sim v \sigma \cdot \vec{k}$, also known as the Weyl hamiltonian. This hamiltonian describes massless chiral fermions, right-handed for $v > 0$, left-handed otherwise. Henceforth we will use the term ‘orbital Weyl point’ to refer to points around which the low energy dynamics in the absence of spin-orbit couplings is described by the 3D Weyl hamiltonian, with an additional twofold degeneracy due to electron spin. We will also speak of ‘bulk chiral fermions’, keeping in mind that, as in graphene, they are exactly chiral in the limit of vanishing spin-orbit interactions. Also note that it is pseudospin, not electron spin, which is parallel (or antiparallel) to $\vec{k}$ in the chiral limit and that, in these systems, pseudospin is purely orbital in origin.

These should be distinguished from other systems where the total hamiltonian, including electron spin and spin-orbit interactions, adopts the form of the Weyl hamiltonian. These include surface states in topological insulators, as well as novel three-dimensional ‘Weyl semimetals’. The spectrum of these systems, unlike graphene and its 3D analogs considered in this paper, remains gapless for arbitrary values of the spin-orbit couplings. Actually, some Weyl semimetals have strong spin-orbit interactions. Possible extensions of our methods to Weyl semimetals will be considered in the last Section.

It is well known that Weyl points have topological properties and no fine-tuning or symmetries are usually necessary for their existence. But symmetry, while not necessary, can sometimes be sufficient for the existence of Weyl points. That is what we show in this paper, where we investigate the role played by the space groups of crystals with time reversal symmetry (TRS) in the existence of orbital Weyl points.

The main results of this paper are summarized in Tables. Only crystals with one of the 19 space groups in these tables can have orbital Weyl points at points of symmetry. Moreover, crystals with space groups in Table must have orbital Weyl points at the listed points, irrespective of the actual crystal structure. For crystals with space groups in Table the situation is only slightly different: At the listed points both orbital Weyl points and non-degenerate bands with quadratic dispersion relations are possible. These results are relevant to nonmagnetic 3D crystals with sufficiently weak spin-orbit interactions and to cold atoms in optical lattices.

The rest of the paper is organized as follows. Our main results, contained in Eq. (2) and Tables, are explained in Section II. Section III considers the effects of spin-orbit interactions on the orbital Weyl points, and a simple tight-binding model is constructed and analyzed in
Section IV. Possible extensions of our approach to Weyl semimetals, crystals with magnetic order and other types of Dirac points are considered in Section V. An outline of the methods used to obtain Tables I–II is given in the Appendix.

II. ORBITAL WEYL POINTS AND CRYSTAL SYMMETRY

Our strategy is based on the fact that the form of the hamiltonian in the vicinity of a point of symmetry $\vec{K}_1$ is strongly constrained by the symmetries of the point in question [19,22]. These include $\mathcal{G}_{\vec{K}_1}$—the little group [23,24] of the vector $\vec{K}_1$—and combinations of TRS with space group elements. Since we are interested in systems with very weak spin-orbit interactions, we will consider first the structure of the orbital or spin-independent part of the hamiltonian. The transformation properties of orbital wavefunctions are described by single-valued representations of the space group.

As explained in the Appendix, we have carried out a survey of all the single-valued irreducible representations of the 230 space groups at points of symmetry in the Brillouin zone (BZ). We find that, for most space groups, the constraints on the form of the hamiltonian around points of symmetry are incompatible with the structure of the Weyl hamiltonian. The comparatively few exceptions are listed in Tables I–II. In all cases, two electronic bands transform according to a single-valued irreducible representation (IR) of $\mathcal{G}_{\vec{K}_1}$. Near the point of symmetry, i.e., for $\vec{K} = \vec{K}_1 + \vec{k}$, the degeneracy is broken by $k$-dependent terms and the hamiltonian takes the form

$$H(\vec{k}) = v_x \sigma_x k_x + v_y \sigma_y k_y + v_z \sigma_z k_z + O(k^2) \quad (1)$$

where $v_x = v_y$ for uniaxial crystals and $v_x = v_y = v_z$ for cubic crystals. After appropriate rescalings of the components of $\vec{k}$ for non-isotropic crystals, this is just the Weyl hamiltonian $H \sim v \vec{\sigma} \cdot \vec{k}$, with the sign of $v$ equal to the product of the signs of $v_i$. The points of symmetry and IRs where this happens are listed in the last column of Tables I–II in standard notation [22].

TRS reverses the sign of $\vec{K}$. In those cases where $-\vec{K}_1$ is not equivalent to $\vec{K}_1$, we get a copy of the Weyl hamiltonian at the mirror point $-\vec{K}_1$, and fermions have, in addition to the pseudospin index associated to the Pauli matrices $\sigma_i$, a ‘valley’ index. As shown in the Appendix, the total hamiltonian is then given by the 4 × 4 matrix

$$H(\vec{k}) = v \begin{pmatrix} \vec{\sigma} \cdot \vec{k} & 0 \\ 0 & \vec{\sigma} \cdot \vec{k} \end{pmatrix} + O(k^2) \quad (2)$$

This describes two degenerate massless fermions of the same chirality, right-handed for $v > 0$, left-handed otherwise. Somewhat surprisingly, we find that this doubling continues to take place even when $-\vec{K}_1 \equiv \vec{K}_1$, i.e., for TRS invariant momenta. In that case, Eq. (2) describes two distinct fermions of the same chirality at the same point in the BZ. There is still a ‘valley’ index but, unlike in graphene, it can not be associated with two different points in the BZ. This happens for the six space groups with simple (P) Bravais lattices in Table III.

The groups in Table I have one important feature in common: The IRs in the last column of the table include all the IRs at the point of symmetry. This means that, at that point, all the bands must form degenerate pairs with Weyl hamiltonians. In other words, any crystal with space group in Table I will have bulk chiral fermions described by Eq. (2), irrespective of the concrete chiral structure. On the other hand, the space groups in Table II have, besides the listed small IRs $K_3$ and $H_3$, which are two-dimensional and give rise to orbital Weyl points, other one-dimensional small IRs ($K_1$, $K_2$, $H_1$, $H_2$) not related to Weyl points. In this case, both orbital Weyl points and non-degenerate bands with quadratic dispersion relations are possible at the listed points of symmetry.

| Space Group | IRs |
|-------------|-----|
| 182         | $P6_322$ | $D_6^2$ | $K_3$ |
| 181         | $P6_322$ | $D_6^2$ | $K_3$, $H_3$ |
| 180         | $P6_322$ | $D_6^2$ | $K_3$, $H_3$ |
| 179         | $P6_322$ | $D_6^2$ | $K_3$ |
| 178         | $P6_322$ | $D_6^2$ | $K_3$ |
| 177         | $P6_22$  | $D_4^2$ | $K_3$, $H_3$ |
| 154         | $P321$   | $D_3^2$ | $K_3$, $H_3$ |
| 152         | $P321$   | $D_3^2$ | $K_3$, $H_3$ |
| 150         | $P321$   | $D_3^2$ | $K_3$, $H_3$ |

TABLE II: Hexagonal and trigonal space groups with orbital Weyl points. The small IRs listed are all 2d and refer to the symmetry points $K(\frac{1}{4}, \frac{1}{4}, 0)$ and $H(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$, with components in the conventional basis of Ref. 22. The stars have two vectors ($\vec{K}_1$, $-\vec{K}_1$) in all cases.
It is well known that spin-orbit interactions in graphene open a gap and give fermionic excitations a small mass. In the case of graphene, the intrinsic spin-orbit hamiltonian is proportional to \( \sigma_z \otimes s_z \otimes \tau_z \), where \( s_z \) and \( \tau_z \) are Pauli matrices for electron spin and valley indices respectively. Around each valley, the hamiltonian can be written in terms of 4 \( \times 4 \) matrices

\[
H_0 + H_{so} = v(\alpha_x k_x + \alpha_y k_y) + \beta \Delta \quad \text{(4)}
\]

where \( \alpha_i = \sigma_i \otimes \mathbf{1}_x \), \( \beta = \pm \sigma_z \otimes s_z \) and \( \Delta \) is the strength of the spin-orbit coupling. The matrices satisfy the Clifford algebra

\[
\{\alpha_i, \alpha_j\} = 2\delta_{ij}, \quad \{\alpha_i, \beta\} = 0, \quad \beta^2 = 2 \quad \text{(5)}
\]

This identifies Eq. (4) as the Dirac hamiltonian for 4-component fermions with mass \( m = \Delta \) and spectrum \( E_{\pm} = \pm \sqrt{\Delta^2 + v^2 k^2} \).

For the space groups in Tables I-II, the most general \( k \)-independent spin-orbit hamiltonian compatible with spatial symmetries and TRS takes the form

\[
H_{so} = \frac{1}{4} (\Delta_x \sigma_x \otimes s_x + \Delta_y \sigma_y \otimes s_y + \Delta_z \sigma_z \otimes s_z) \otimes \mathbf{1}_\tau \quad \text{(6)}
\]

where \( \Delta_x = \Delta_y \) for uniaxial crystals and \( \Delta_x = \Delta_y = \Delta_z \) for cubic crystals. Actually, this valley independent form of the spin-orbit interaction is valid on the basis \((e_1, e_2, ie_z, -ie_z)\) of orbital wavefunctions introduced in the Appendix. If one uses the more conventional basis \((e_1, e_2, e_1^*, e_2^*)\), then one has to append the valley matrix \( \tau_z \) to the \( x \) and \( z \) components in Eq. (6). Note that, in the conventional basis, instead of Eq. (2), we would have Eq. (A6).

The spectrum of the total hamiltonian \( v\sigma \cdot \vec{k} + H_{so} \) can be computed numerically and one finds that, in general, gaps are generated and all fermionic excitations acquire masses. Cubic crystals, where \( H_{so} \) is isotropic and depends on a single parameter \( \Delta \), are an exception and can be treated analytically. In this case the spectrum is given by

\[
E_{\pm}^- = -\frac{\Delta}{4} \pm \sqrt{\frac{\Delta^2}{2} + v^2 k^2}
\]

\[
E_{\pm}^+ = \frac{\Delta}{4} \pm vk
\]

and contains massless excitations. This spectrum is radically different from that of the Dirac hamiltonian appropriate for 2D graphene. Note, in particular, that the linear bands \( E_{\pm}^+ \), together with \( E_{\pm}^- \), form a triplet (see Fig. 1), following the usual rules for addition of angular momenta with \( L = S = 1/2 \) and \( \vec{J} = \vec{L} + \vec{S} \). This is only natural: assembling pseudospin and spin into a 4-component object is equivalent to taking the Kronecker product of two \( j = 1/2 \) irreducible representations of the \( SO(3) \) rotation group and this product decomposes according the rules of angular momentum composition.

Thus, unlike in 2D where strong spin-orbit interactions simply destroy the orbital Weyl points and turn massless
fermions into massive excitations, here we also get Dirac points with $J = 1$. In the next Section we will present a model that in the absence of spin-orbit has, besides orbital Weyl points, Dirac points with pseudospin-one. The points with pseudospin-one would be split by strong spin-orbit interactions into Weyl points with $J = 1/2$ and novel Dirac points with $J = 3/2$. Subduction of IRs can be used in principle to extend the analysis to non-cubic groups.

Henceforth we will assume that spin-orbit interactions are weak and can be ignored. In this limit the dynamics is well described by the 3D Weyl hamiltonian –albeit with an additional two-fold degeneracy due to spin– and, as a consequence, the systems considered in this paper may share some of the properties of Weyl semimetals.

### IV. A TIGHT-BINDING EXAMPLE

As a practical application, we present a tight-binding model with space group $214 I4_1 32(O^3)$, the first entry in Table I. According to our previous analysis, any lattice with this space group must have orbital Weyl points at $P$. Here we consider a lattice with four atoms per primitive unit cell, with cartesian coordinates $\vec{r}_1 = a/8(1,1,1)$, $\vec{r}_2 = a/8(1,1,3)$, $\vec{r}_3 = a/8(3,1,5)$ and $\vec{r}_4 = a/8(3,1,7)$. To each atom we associate a Bloch function

$$\Phi_i(\vec{k}) = \sum_{\vec{t} \in T} e^{i\vec{k} \cdot (\vec{r}_i - \vec{t})} \varphi(\vec{r} - \vec{r}_i - \vec{t})$$

where the sum runs over all the points in the Bravais lattice and $\varphi(\vec{r})$ is an $s$-wave atomic orbital. Each atom has three nearest neighbors (NN), with bonds parallel to the three cartesian planes. In terms of the reduced cartesian components of the wave vector $\vec{k} = 2\pi/a(k_x, k_y, k_z)$ the NN tight-binding hamiltonian is given by

$$H(\vec{k}) = t \begin{pmatrix} 0 & e^{i\frac{\pi}{2} (k_z - k_y)} & e^{i\frac{\pi}{2} (k_y - k_z)} & e^{i\frac{\pi}{2} (k_z - k_x)} \\ e^{-i\frac{\pi}{2} (k_z - k_y)} & 0 & e^{i\frac{\pi}{2} (k_y + k_z)} & e^{i\frac{\pi}{2} (k_x + k_y)} \\ e^{-i\frac{\pi}{2} (k_z + k_x)} & e^{-i\frac{\pi}{2} (k_x + k_y)} & 0 & e^{i\frac{\pi}{2} (k_y + k_z)} \\ e^{i\frac{\pi}{2} (k_z + k_x)} & e^{i\frac{\pi}{2} (k_x + k_y)} & e^{-i\frac{\pi}{2} (k_y + k_z)} & 0 \end{pmatrix}$$

(9)

to confirm that they actually are Weyl points, as predicted. The four Bloch functions $\Phi_i$ form the basis of a reducible representation $\mathcal{H}$ that can be decomposed into small IRs as $\mathcal{H}(\Phi_1, \ldots, \Phi_4) = P_2(e_1, e_2) + P_3(u_1, u_2)$. Up to normalizations, the symmetry-adapted vectors are given by $e_1 \sim (1, \beta_2, -1, i\beta_2)$, $e_2 \sim (-\beta_2, -1, -\beta_2, i)$,
with \( \beta_2 = (1 + \sqrt{3})(1 - i)/2 \), and identical expressions for \( u_1, u_2 \) with \( \beta_2 \) replaced by \( \beta_3 = (1 - \sqrt{3})(1 - i)/2 \). Using a unitary transformation \( U_P \) to change to the symmetry adapted basis and expanding around the point \( P \) yields

\[
U_P^\dagger H(\vec{k}) U_P = \frac{\pi t}{\sqrt{3}} \left( \frac{1}{\sqrt{3}} + \sigma \cdot \vec{k} \right) - \frac{\pi}{\sqrt{3}} \frac{H_{23}(\vec{k})}{-\sigma \cdot \vec{k}} + O(k^2)
\]

where \( H_{23}(\vec{k}) \) is given by

\[
H_{23}(\vec{k}) = \frac{1}{\sqrt{2}} \left( \begin{array}{ccc}
\omega k_z & \omega^* k_x - i \omega k_y & -k_z \\
\omega^* k_x + i \omega k_y & \omega k_z & 0 \\
-k_z & 0 & \omega k_z \\
\end{array} \right)
\]

with \( \omega = e^{2\pi i/3} \). There are thus two orbital Weyl points at \( P \) with different energies \( \pm t\sqrt{3} \) and opposite chiralities. The existence of orbital Weyl points of opposite chirality is of course to be expected from fermion doubling which requires the net chirality of the BZ to vanish, although the fact that they appear at coincident points is peculiar to this model. Note also the linear couplings between the two points. Due to the split in energies, these couplings contribute corrections \( O(k^2) \) to the \( 2 \times 2 \) effective hamiltonians around the orbital Weyl points and do not spoil their structure. A similar expansion around \(-K_1\) confirms that, due to TRS, each orbital Weyl point is degenerate in energy with another point of the same chirality. Restoring the lattice constant yields a Fermi velocity \( v_F = \frac{2|t|}{\sqrt{3}} \). Note however that, as no symmetry connects the orbital Weyl points with different chiralities and energies, going beyond the NN approximation is expected to give different Fermi velocities for them.

Fig. 2 exhibits linear bands around the \( \Gamma \) and \( H \) points as well. Their nature is, however, very different from that of the orbital Weyl points at \( P \). Let’s consider, for the sake of concreteness, the \( \Gamma \) point. In this case, the representation associated with the Bloch functions decompose into IRs of dimension one and three, \( \mathcal{H} = A_1 + T_2 \). Transforming to the appropriate symmetry-adapted basis and linearizing yields

\[
U_T^\dagger H(\vec{k}) U_T = t \left( \begin{array}{ccc}
3 & 0 & 0 \\
0 & -1 & -i \pi k_z \\
0 & i \pi k_z & -1 \\
\end{array} \right) + O(k^2)
\]

Up to a constant energy, the \( 3 \times 3 \) block can be written

\[
H_{T_2}(\vec{k}) = \pi t \vec{J} \cdot \vec{k}
\]

where \( (J_{ij})_{jk} = -i \epsilon_{ijk} \) are spin-1 matrices. Thus, around this Dirac point, electrons behave more like massless spin-one particles, with spectrum \( E(\vec{k}) = 0, \pm v_F|\vec{k}|^2 \) and \( v_F = \frac{2|t|}{\sqrt{3}} \). Indeed, one can check that, while the \( E = 0 \) component is longitudinally polarized, the other two are transverse, just like the propagating components of a photon. Pseudospin-one Dirac points have been reported in some two-dimensional and three-dimensional systems.

A look at Fig. 2 shows that, even if the Fermi level coincides with one of the orbital Weyl points at \( P \), band overlap will cause the dynamics to be dominated by large electron (or hole) pockets. The existence of band overlap can be traced in this case to the 3-fold degeneracies in Fig. 2 which force one of the bands arising from the orbital Weyl points to bend over. As 3d IRs exist only for cubic groups, we may modify the model by making the hopping parameters \( t_\perp \) associated with bonds parallel to the \( OXY \)-plane different from the rest. This reduces the symmetry to the tetragonal subgroup \( 14_2 \) and eliminates the 3-fold degeneracies at \( \Gamma \) and \( H \). Fig. 4 shows the bands for \( \epsilon = 0.4 \). In the absence of spin-orbit interactions the system would behave like a gapless semiconductor with massless carriers for 1/4 and 3/4 fillings, with positive or negative chirality depending on the filling.

V. DISCUSSION

In this paper we have studied the interplay between crystal symmetry and the existence of bulk chiral fermions in nonmagnetic 3D crystals with weak spin-orbit coupling. We have shown that the space group plays a determinant role, as summarized in Tables II and III. As Weyl semimetals depend on the existence of magnetic order or strong spin-orbit interactions, we have explored an entirely different corner in the space of candidate 3D crystals with bulk chiral fermions. We have also considered the effects of spin-orbit interactions and shown that, unlike in 2D, these may give rise to new critical points supporting massless fermions for different values of the pseudospin. For sufficiently weak spin-orbit interactions the dynamics is well described by the 3D Weyl hamiltonian and the systems considered in this paper may share some of the properties of Weyl semimetals.

There are two obvious uses for the information in Tables II and III. First, one can look for orbital Weyl points in nonmagnetic crystals with weak spin-orbit interactions and space groups in the tables, either in theoretically
computed electronic bands or experimentally. The other use is the design of 3D lattices with Weyl points. This may allow for a physical realization of massless chiral fermions with cold atoms in optical lattices. Note that the physical relevance as well as the feasibility of detecting chiral fermions in actual crystals will be affected by structure dependent features such as the position of the Fermi level and the amount of band overlap. But knowing that the bulk chiral fermions have to be there is obviously a good starting point. As shown in the example of Section IV, we can then try to engineer the required properties by modifying the initial system.

There are several possible extensions to this work. One is to consider the existence of orbital Weyl points away from points of symmetry. All the points in a line of symmetry, except for the endpoints, have the same group $G_K$. Therefore, symmetry alone can not imply the existence of bulk chiral fermions at a particular point in the line, although it will indicate whether this is possible at all. But it can, in some cases, imply the existence along the line of ‘semi-Dirac’ points, where the dispersion relations are linear only for some directions. For generic points in the BZ, symmetry alone has little to say and a different kind of analysis may be useful.

Sometimes not two, but three bands become degenerate at a Dirac point. This is the case with the $\Gamma$ and $H$ points in the example of Section IV. This is possible for some cubic space groups, and group theory can be used to determine the IRs and points of symmetry where this may happen. As shown in Section III, turning on spin-orbit interactions will give rise to novel Dirac points with pseudospin 3/2. Other, more complicated linear Hamiltonians are also possible and may be physically relevant. Group theory can be used to classify or even predict the existence of the different types of Dirac points.

In this paper we have analyzed all the single-valued irreducible representations at points of symmetry in the BZ. These are appropriate for orbital degrees of freedom. By considering instead double-valued IRs we could study the existence of Weyl points where the total Hamiltonian, including electron spin and spin-orbit interactions, takes the form of the 3D Weyl Hamiltonian. Thus, we could extend our analysis to TRS invariant Weyl semimetals. Double-valued IRs have been recently applied to the study of ‘Dirac semimetals’.

So far we have restricted ourselves to TRS invariant crystals. The reasons are mostly practical. The symmetries of crystals with magnetic order are classified by the 1651 magnetic space groups, instead of the 230 ordinary (Fedorov) space groups that classify crystals with TRS. The amount of work required to examine the points of symmetry and irreducible corepresentations for all the magnetic groups is, obviously, much greater. Moreover, unlike ordinary space groups, there are few databases with the magnetic space groups of crystals with magnetic order.

Nevertheless, some of the results in this paper can also be applied to spinless electrons in crystals with magnetic order. The reason is that, by construction, the 19 entries in Tables I-II describe situations where the 3D Weyl Hamiltonian is invariant under the ‘grey’ or ‘type II’ Shubnikov space group associated to an ordinary (Fedorov) space group by the addition of the TRS operation. Now, all the magnetic space groups derived from the Fedorov space group with the BNS settings are subgroups of the grey group. As a consequence, the corresponding Weyl Hamiltonian is automatically invariant under all the magnetic groups derived from the ordinary space groups listed in our tables. For instance, the Weyl Hamiltonians at the $P$ point of group 214 are automatically invariant under the derived magnetic groups 214.68 and 214.69 (in the BNS settings).

One still has to check that the degeneracy of the two bands at the point of symmetry, necessary for the existence of the Weyl point, is maintained under the lower symmetry of the magnetic space group. If this is not the case but the effects of the magnetic order are small, the Weyl point will survive, but move away from the point of symmetry. The main difference when dealing with crystals with magnetic order is that we can not exclude the possibility of finding bulk chiral fermions around points of symmetry for space groups not listed in Tables I-II. That happens whenever the Weyl Hamiltonian is invariant under the magnetic subgroup of the grey space group, but not under the grey space group itself.

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Appendix A

In this Appendix we outline the methods used to obtain Tables I-II and Eq. (3). Symmetry operations belonging to the space group $G$ will be written $g = \{\alpha|\bar{v}\}$, where $\alpha$ and $\bar{v}$ denote the rotation and translation parts respectively. Let $\{e_i(\vec{K})\}$ be a basis of orbital wave functions that transform linearly under the action of $G$, $e_i(\vec{K}) \rightarrow e_j(\alpha \vec{K}) R_{ij}(g)$, where we sum over repeated indices. Invariance of the Hamiltonian under $G$ means that, for any wavefunction $\psi$, $(H)\psi = (H)\psi_\alpha$, where $\psi_\alpha$ is the transformed of $\psi$ by the group element $g$. Expanding this condition on the basis $\{e_i(\vec{K})\}$ yields, in matrix notation

$$R^\dagger(g)H(\alpha \vec{K})R(g) = H(\vec{K})$$

(A1)
where $H_{ij}(\vec{k}) = \langle e_i(\vec{k}) | H | e_j(\vec{k}) \rangle$. Time reversal $\theta$ is an antiunitary operation that acts on orbital wavefunctions by complex conjugation, $e_i(\vec{k}) \rightarrow e_i(\vec{k})^* = e_j(-\vec{k})\Theta_{ij}$, where $\Theta_{ij}$ is a unitary matrix and reverses the momentum $\vec{k}$. Invariance under $\theta$ implies

$$\Theta^\dagger H(-\vec{k})\Theta = H^*(\vec{k}) \quad (A2)$$

We will also have to consider combined antiunitary operations of the form $\theta g$. In this case invariance of the Hamiltonian implies

$$T^\dagger(g)H(-\alpha\vec{k})T(g) = H^*(\vec{k}) \quad (A3)$$

where $T(g) = \Theta R^*(g)$. Eqs. (A1) hold if restricted to $\mathcal{G}_{K_1}$, i.e., $\alpha K_1 \equiv K_1$. By definition, the matrix $\alpha$ belongs to the vector representation $V^{23,24}$ if the basis functions $\{e_i(\vec{k})\}$ belong to the small IR $R$ of $\mathcal{G}_{K_1}$, terms of order $n$ in $\vec{k}$ in an expansion of the l.h.s. of Eq. (A4) will transform according to the product $R^* \times R \times [V]^n$, where $R^*$ is the complex conjugate of $R$ and $[V]^n$ denotes the $n$-th symmetric power of the representation $V^{23,24}$.

Consider for instance Eq. (A1) with $g$ restricted to the little group of $K_1$, $\mathcal{G}_{K_1}$, i.e., $\alpha K_1 \equiv K_1$. The IRs that pass this last test are listed in the last column of Tables 1 and 11. These IRs have an important property: There is always a basis where $H(-\vec{k}_1 + \vec{k}) \simeq v \vec{\sigma} \cdot \vec{k}$. The off-diagonal blocks between $K_1$ and $\bar{K}_1$ vanish by translation invariance, and we have

$$H(\vec{k}) = v \left( \begin{array}{cc} \vec{\sigma} \cdot \vec{k} & 0 \\ 0 & -\vec{\sigma}^* \cdot \vec{k} \end{array} \right) + O(k^2) \quad (A6)$$

We can make the symmetry between $K_1$ and $\bar{K}_1$ obvious by using the $SU(2)$ transformation $\sigma_g \vec{\sigma}^* \sigma_y = -\vec{\sigma}$ to change the basis at $-\bar{K}_1$ so that the 4th basis is $(e_1, e_2, ie_2^*, -ie_1^*)$. On this basis the Hamiltonian takes the form given in Eq. (2).

The case $-\vec{K}_1 \equiv \bar{K}_1$ is more subtle, and we have two possibilities. If $R$ is a real 2d IR, then TRS applies $(e_1, e_2)$ onto itself, with $e_1^* = e_1$. In this case, $\Theta = 1$ and Eq. (A2) requires $H(-\vec{k}) = H(\vec{k})^*$, which is not satisfied by the Weyl Hamiltonian. Thus 2d real IRs are excluded from Table 1. For complex and pseudoreal 2d IRs we have taken $e_1, e_2, e_1^*, e_2^*$ or $(e_1, e_2, ie_2^*, -ie_1^*)$, and everything proceeds as in the previous case. The main difference is that now the off-diagonal blocks need not vanish by translation symmetry. However, a detailed case by case analysis using space group and TRS invariance shows that the off-diagonal terms are at least of $O(k^2)$. This completes the proof of Eq. (2).

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41 We have also examined the ‘physically irreducible’ 2d representations, i.e., pairs of conjugate 1d representations degenerate by TRS. These are never compatible with the Weyl hamiltonian.