Existence of Dirac cones in the Brillouin zone of diperiodic atomic crystals according to group theory

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Received 8 October 2015, revised 17 December 2015

Abstract

We have considered non-magnetic materials with weak spin–orbit coupling, that are periodic in two non-collinear directions, and finite in the third, orthogonal direction. In some cases, the combined time-reversal and crystal symmetry of such systems, allows the existence of Dirac cones at certain points in the reciprocal space. We have investigated in a systematic way, all points of the Brillouin zone of all 80 diperiodic groups and have found sufficient conditions for the existence of $s = 1/2$ Dirac fermions, with symmetry-provided band touching at the vertex of the Dirac cones. Conversely, complete linear dispersion is forbidden for orbital wave functions belonging to two-dimensional (2D) irreducible representations (irreps) of little groups that do not satisfy certain group theoretical conditions given in this paper. Our results are illustrated by a tight-binding example.

Keywords: Dirac cones, diperiodic systems, symmetry

(Some figures may appear in colour only in the online journal)
Brillouin zone of all 80 diperiodic groups and have found sufficient conditions for the existence of $s = 1/2$ Dirac fermions. Symmetry also provides the band touching at the vertex of the cones. In spite of the extensive research related to the interplay between the symmetry and the properties of Dirac (Weyl) materials, to the best of our knowledge no systematic analysis of the connection between the symmetry of diperiodic systems and the appearance of Dirac cones in their energy spectrum has been performed until now. Our paper therefore aims to fill in this gap. Apart from the general idea, the results of [12] cannot be just simply applied to our case, where the reduced dimensionality of the system leads to different mathematical conditions. For example, a combined time-reversal and crystal symmetry provides the Dirac cones at the Brillouin zone corners of eight diperiodic groups belonging to the hexagonal system. At the end of the paper, we provided an example to illustrate our results.

2. Method

We will consider the two-dimensional (2D) Hamiltonian in the $k$-space in the vicinity of a point of symmetry. It turns out that the Taylor expansion of the Hamiltonian around that point combined with its symmetry properties gives certain constrains on the first order derivatives. We will use this fact to connect it with the appearance of Dirac cones in the band structure. The necessary group theoretical tools are nicely described in the book by Cornwell [14], for example.

Let $k_0$ be a real vector from the (2D) Brillouin zone of a diperiodic group and $q$ a 2D, real vector of a small modulus, $G(k_0)$ is a little group of the wave vector (a set of all elements of the diperiodic group which rotational parts transform $k_0$ to its equivalent) and $G_0(k_0)$ is a point group of the wave vector (a set that consists of rotational parts of elements of $G(k_0)$ only). Further, let $e_j(r, k_0)$, be orbital wave functions belonging to an irreducible representation (irrep) of $G(k_0)$. For any diperiodic group such irreps are either one-dimensional (1D) or 2D [15]. Since $e_j(r, k_0)$ are Bloch functions, $R$ must be allowed [16] (relevant [14], small [17]) irrep of $G(k_0)$. Let $\hat{H}(k_0)_j = \{ e_j(r, k_0) \hat{H}_0(r)|e_j(r, k_0) \}$. The original Hamiltonian $\hat{H}_0(r)$ is real. Let us assume that $R$ is 2D. It follows, that for every element $(\hat{g} | r)$ (in Seitz notation) of $G(k_0)$:

$$e_j((\hat{g} | r)^{-1} r, k_0) = \sum_{l=1}^{2} \hat{R}((\hat{g} | r))_{ij} e_j(r, k_0).$$  \hspace{1cm} (1)

The Taylor expansion of the Hamiltonian $\hat{H}(k)$ in the vicinity of the point $k_0$ reads [18, 19]:

$$\hat{H}(k_0 + q) \approx \hat{H}(k_0) + \sum_{j=0}^{3} (v_j, q) \hat{d}_j,$$  \hspace{1cm} (2)

where $\hat{d}_{1,2,3} (\hat{d}_0)$ are usual Pauli matrices (is a 2D unit matrix) and

$$(\forall j = 0, 1, 2, 3) v_j = \frac{1}{2} \left\{ \frac{\partial}{\partial q} Tr[\hat{d}_j \hat{H}(k_0 + q)] \right\}_{q=0}.$$  \hspace{1cm} (3)

Notes: The first column gives the number of the corresponding group, while the second column contains its Hermann–Mauguin notation. The third column gives the group factorisation into the semi-direct product of the translational subgroup $T$, and a point group. Superscripts for groups $Dg71$ and $Dg72$ indicate that those differ by the orientation of the symmetry elements of $D_{4h}$ with respect to the primitive translations. The responsible irrep denotes an irrep that generates a pair of Dirac cones. The point group of the wave vector is given in parentheses.

## Table 1. Diperiodic groups having symmetry-allowed Dirac cones at the Brillouin zone corners ($K$-points). Notations of diperiodic groups are according to [13].

| Diperiodic group | Responsible irrep ($G_d(K)$) |
|-----------------|-----------------------------|
| 68              | $p 3 2 1 \ T D_3$           |
| 70              | $p 3 1 m \ T C_{3v}$        |
| 71              | $p 3 1 2 m \ T D_{3d}$      |
| 72              | $p 3 2 m 1 \ T D_{3d}$      |
| 76              | $p 6 2 2 \ T D_6$           |
| 77              | $p 6 m m \ T C_{d}$         |
| 79              | $p 5 2 m \ T D_{3h}$        |
| 80              | $p 6 m m m \ T D_{3h}$      |

are 2D, real vectors. If we assume a double degeneracy of the electron energy level $E_0$ at $k_0$, we get for the energy in the vicinity of this point:

$$E_{i, 2} = E_0 + q \cdot v_0 \pm \sqrt{\sum_{j=1}^{3} (q \cdot v_j)^2} = E_0 + q \cdot v_0 \pm \sqrt{u_1 q_1^2 + u_2 q_2^2},$$  \hspace{1cm} (4)

where

$$u_{1, 2} = \frac{1}{2} \sum_{j=1}^{2} v_j \pm \frac{1}{2} \left( \sum_{j=1}^{3} v_j^2 \right) - 4 \sum_{j=1}^{3} \sum_{j=1}^{3} (v_j \times v_j),$$  \hspace{1cm} (5)

are eigenvalues of the quadratic, 2D matrix $\hat{S} = \sum_{j=1}^{3} |v_j\rangle \langle v_j|$. $q_1, 2$ are projections of $q$ along orthonormalised eigenvectors of $\hat{S}$, $\langle v_j| = v_j = v_j$ and $T$ denotes transposition. The matrix $\hat{S}$ is symmetric and positively semi-definite, so $u_1 \geq u_2 \geq 0$. For $u_1, 2$ both different than zero, (4) represents a pair of Dirac cones that is tilted for non-zero $v_0$. Combined TRS and crystal symmetry can make one or both $u_2$ vanish. We will investigate means to avoid such cases below.

3. Results

By the Taylor expansion of corresponding commutation relations between the Hamiltonian $\hat{H}(k)$ and matrices of irreps of $G(k)$ around $k_0$ up to the first order [12], we get

$$\hat{W} = \hat{R}((\hat{g} | r)) \hat{W}(\hat{R}^T((\hat{g} | r)) \otimes \hat{g}^T),$$  \hspace{1cm} (6)

where $(\hat{g} | r)$ is an element of $G(k_0)$, $\hat{g}^T$ is the reduction of $\hat{g}$ to the diperiodic plane, $\hat{R}((\hat{g} | r))$ is the matrix of the irrep $R$ of $G(k_0)$ that corresponds to the element $(\hat{g} | r)$, $*$ is the complex conjugation, $\otimes$ denotes the Kronecker product and...
\[
\hat{W}^* = \sum_{j=0}^{3} \hat{\sigma}_j \otimes \langle \psi \rangle.
\]

We will now state the group theoretical conditions that ensure the existence of Dirac cones touching at the vertex.

1. If \( R \) is a 2D irrep of \( G(\mathbf{k}_0) \), two bands will touch at \( \mathbf{k}_0 \).

2. In order to make bands split along every direction away from the \( \mathbf{k}_0 \), this point must be of locally maximal symmetry.

3. In order for \( \psi_1, \psi_2, \psi_3 \) not to vanish simultaneously, \((R^* \otimes R - \Gamma_1) \otimes \Gamma_{2D PV}^*\) must contain at least one \( \Gamma_1 \), where \( \Gamma_{2D PV}^* \) is the 2D polar-vector representation of \( G(\mathbf{k}_0) \) and \( \Gamma_1 \) is the totally symmetric (unit) representation of \( G(\mathbf{k}_0) \).

4. In order for \( u_2 \) not to vanish from symmetry reasons, in addition to \( O_3 \), \((R^* \otimes R - \Gamma_1) \otimes \text{det}(\Gamma_{2D PV}^*)\) must contain at least one \( \Gamma_1 \), where the number corresponding to an element \( \hat{g} \) of \( G(\mathbf{k}_0) \) by an irrep \( \text{det}(\Gamma_{2D PV}) \) is \( \text{det}(\hat{g}^*) \).

Note that since \( R^* \otimes R \) always contains \( \Gamma_1 \), the conditions \( O_3 \) and \( O_4 \) are mathematically well defined. These two conditions are derived from (6). The next conditions are due to TRS (reality of the original Hamiltonian \( \hat{H}_0(\mathbf{r}) \)).

5. For \( -\mathbf{k}_0 \) equivalent to \( \mathbf{k}_0 \), if \( R \) is a real irrep then \( u_2 = 0 \), but if \( R \) is pseudo-real or complex, then the energy level \( E_0 \) is four times degenerate and the presence of Dirac cones must be investigated on a case-by-case basis.

6. If \( -\mathbf{k}_0 \) is not equivalent to \( \mathbf{k}_0 \) but there exists an element \( (\hat{R}^*|\mathbf{t}) \) of the diperiodic group such that \( \hat{R}\mathbf{k}_0 \) is equivalent to \( -\mathbf{k}_0 \), then the combination of this element and complex conjugation leads in principle to an additional constrain [12]. However, it turned out that when conditions \( O_1-O_4 \) were fulfilled, the condition \( O_6 \) led to no further restrictions.

Finally, we state the condition that shows when the Dirac cones predicted to exist by \( O_1-O_6 \) are tilted. In order to make our results more general, we did not use this condition.

7. For Dirac cones to be untitled \( (v_0 = 0 \), \( \Gamma_{2D PV}^* \) must not contain \( \Gamma_1 \).

We have used conditions \( O_1-O_6 \) to investigate Brillouin zones [15, 20] of all 80 diperiodic groups. It turned out that only eight diperiodic groups fulfilled the conditions. All of them are symmorphic and belong to the hexagonal system, so their Brillouin zone is hexagon-shaped. Symmetry allowed, isotropic Dirac cones are located at the hexagon’s corners (K-points) and groups are listed in the table 1.

4. Discussion

We can see that the table 1 contains Dg80—the symmetry group of monolayer graphene. The same group is the symmetry group of the kagome lattice, which has Dirac cones at the K-points, within the tight-binding model [21]. Planar, graphene-like silicon (silicene) and germanium (germanene) also have Dirac cones at the K-point, within the tight-binding [22] and \( \text{ab initio} \) [23] method. In addition, \( \text{ab initio} \) calculations on non-planar, low-buckled silicene and germanene, show Dirac cones in the energy dispersion [24]. This configuration belongs to the diperiodic group Dg72 that is listed in the table 1. Recently, first principles calculations have shown a pair of Dirac cones at the K-point of the low-buckled SiGe compound [25]. Strictly speaking, this compound belongs to the group Dg69, which is not listed in the table 1. Still, as the authors of [25] also stated, Si and Ge atoms are chemically similar because their electronegativities are nearly identical, and so we can take the crystal structure of the SiGe compound effectively as being composed of only one type of atom. Such a crystal would be isostructural with the low-buckled silicene and germanene discussed above. The crystal structures of the mentioned compounds are shown in figure 1. On the other hand, the monolayer MoS\(_2\) belongs to Dg78, which does not satisfy our conditions. Dirac cones in the energy spectrum of this material are absent [26]. Examples of crystal structures belonging to other groups from table 1 are given in figure 2. All shown structures generate Dirac cones regardless of the type of orbitals used for building the LCAO MO wave functions. For example, the structure presented in figure 2 belonging to Dg68, would have two pairs of Dirac cones within the tight-binding model from the s-type orbitals, if one takes enough neighbours into account. For completeness, one has to note that figure 2 does not exhaust all possibilities.
It is also important to note that it is not guaranteed that the Fermi level will cross the energy near the contact points of the cones. Note that in order for the Dirac cones to appear, orbital wave functions must transform according to a responsible irrep from table 1. Orbital double degeneracy can appear also when two mutually conjugated, 1D irreps related by TRS, form a 2D physically irreducible representation. Since then $u_2 = 0$, these cases were excluded from consideration. The condition $O_1$ is sufficient (but not necessary) for the band touching at $k_0$. For this reason the Dirac cones touching each other accidentally can appear in other parts of Brillouin zone and in diperiodic groups other than those listed in table 1. Such is the case, for example, in $S$-graphene, which belongs to the rectangular system and whose anisotropic Dirac cones appear at points belonging to the $\Gamma Y$ and $M X$ directions of its Brillouin zone [27]. Alternatively, in systems where orbital and spin degrees of freedom cannot be separated, the above analysis does not apply. Some topological insulators, where the spin–orbit coupling is large, have a pair of Dirac cones at the Brillouin zone center (the $\Gamma$-point) [28].

5. An illustrative example

As an example we will consider a tight-binding model on a structure that arises from the site 1a of the diperiodic group Dg80. The crystal structure of the example is shown in figure 3. In order to ensure the presence of at least one pair of orbital wave functions that belong to a responsible irrep from table 1, we can choose for this particular example any type of orbitals except the $s$-type. For simplicity let us use $p$-orbitals for building the tight-binding wave functions. The primitive cell of this structure contains one atom which is located at the origin. Let $a_1$ and $a_2$ be the primitive lattice vectors as indicated in figure 3; the orbital $\phi = +f_p p_{\frac{3}{2}}$ is directed along $a_1$ and $\phi = f_y$ is directed along $a_1 - a_2$. $f_z$ where the $z$-axis is perpendicular to the diperiodic plane. Electronic levels of such a system are classified as $'+A E_2$ for the $K$-point (point group $D_{3d}$). In contrast to graphene, in which $p_z$ orbitals located at two atoms in the primitive cell belong to the irrep $E'$, the in-plane orbitals of our example belong to the irrep $E'$. Both irreps generate a pair of Dirac cones. The six nearest neighbours of the central atom are located at vertices of a regular hexagon, with the central atom located at its center. By taking into account the system’s symmetry, we get for its Hamiltonian:

$$
\begin{align*}
[H(k)]_{11} &= t_2 + t_9 w + (t_4 - t_1) r_1, \\
[H(k)]_{22} &= t_2 + t_9 w + (t_4 - t_1) r_3, \\
[H(k)]_{12} &= [H(k)]_{21} = \frac{1}{2} t_2 + \frac{1}{2} t_9 w + (t_3 - t_4) r_2, \\
[H(k)]_{13} &= [H(k)]_{31} = [H(k)]_{23} = 0, \\
[H(k)]_{33} &= t_0 + t_9 w,
\end{align*}
$$

(8)
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... presents a pair of Dirac cones, exactly as ... 

\( \varepsilon_1,2 = t_2 + \frac{2}{3}(t_3 + \frac{1}{2} t_4)w \) 

\[ \pm \frac{2}{3} |t_4 - t_1| \sqrt{\sum_{j=1}^{3} r_j^2 - \sum_{j>p>j'} r_j r_{j'}}, \]

\[ \varepsilon_3 = t_0 + \eta w. \] (12)

We take \( k = (b_1 + b_2)/3 + q \), for the expansion around the K-point. \( b_1, b_2 \) are primitive vectors of the reciprocal lattice such that \( b_j \cdot a_i = 2\pi \delta_{ij} \). For small \( q = |q| \) we get \( (a = |a_1| = |a_2|) \):

\[ \varepsilon_{1,2} \approx t_2 - (t_3 + \frac{1}{2} t_4) \pm \frac{\sqrt{3}}{2} a |t_4 - t_3| q. \] (13)

which, since \( t_4 \neq t_3 \), presents a pair of Dirac cones, exactly as predicted by our theory!

For the \( \Gamma \)-point (the center of the Brillouin zone), the in-plane orbitals belong to an irrep \( E_{1a} \) of the point group \( D_{6h} \). This irrep does not satisfy the condition \( O_2 \) so the dispersion in the vicinity of this point should be quadratic. The expansion around \( k_0 = 0 \), for small \( q \) reads:

\[ \varepsilon_{1,2} \approx t_2 + 2t_3 + t_4 - \frac{1}{2} a_q \left( t_3 + \frac{1}{2} t_4 \pm \frac{1}{2} |t_3 - t_4| q \right)^2. \] (14)

The quadratic dispersion in the last formula is another confirmation of our prediction.

6. Conclusions

In summary, we have determined the points in the Brillouin zone of non-magnetic, diperiodic atomic crystals, with weak spin–orbit interaction, where symmetry allows linear, cone-like dispersion in the vicinity of these points. We have formulated a set of group theoretical conditions which guarantee Dirac-like energy dispersion. Out of all 80 diperiodic groups investigated, only eight of them fulfill these conditions. All of them are symmorphic and belong to the hexagonal system. For all of them, Dirac cones are located at the corners of hexagons (K-points) that present the borders of the Brillouin zone. Our prediction is confirmed by tight-binding and density functional theory calculations on numerous examples published in the literature. On the other hand, Dirac-type dispersion is symmetry-forbidden for orbital wave functions belonging to any allowed, 2D irrep that is not listed in table 1. In the course of our work, we have also investigated all other parts of the Brillouin zone, i.e. without the condition \( O_2 \). We have found that for some non-symmorphic diperiodic groups, there are lines of symmetry in the Brillouin zone which fulfill the conditions \( O_1 \) and \( O_3 \)–\( O_6 \). In such cases, there is only Dirac-like dispersion in the direction that is perpendicular to those lines. This is another example where the absence of complete Dirac cones is caused by the presence of too many band contacts [29].

One of the conditions used, is sufficient but not necessary, so our analysis does not exhaust all cases. Two bands can touch each other accidentally but even in that case, there are...
group theoretical conditions which must be satisfied in order to avoid quadratic dispersion. An analysis of these cases is beyond the scope of this paper, as are questions regarding the stability of Dirac cones, or how to achieve that the Fermi level crosses the energy at the contact point of the cones.

Acknowledgments

This work was supported by the Serbian Ministry of Education, Science and Technological Development under project numbers OI 171005 and III 45016.

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