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Linear dispersions in two-dimensional materials: a crystal with symmetry *pbma1'* as an example

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Symmetry determines forms of band structures in the vicinity of special points in the reciprocal space of one-, two- and three-dimensional materials. Tight binding model on a crystal with four sites per primitive cell that belongs to gray layer single group *pbma* (45.2.315 or *pbma1'* in the magnetic layer groups notation) is calculated. Fortune teller states (FT) are obtained at the Brillouin zone (BZ) corners, as predicted by group theory for non-magnetic materials with negligible spin-orbit coupling. We show further that besides these FT states, another interesting band degeneracy arises as a consequence of symmetry.

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1. Introduction

Symmetry is widely applied concept in solid-state physics. Predictions of crystal field splitting of electron energy levels in three-dimensional (3D) crystals [1], determination of phonon-displacement patterns in graphene [2, 3] and spin ordering in nano-tubes [4], are just a few among many examples. Group theoretical results are derived from irreducible (co)representations of little groups of the wave vector and the whole space groups. Those are tabulated and available for (3D) space groups [5, 6]. For layer groups, which are symmetries of two-dimensional (2D) materials, [7] tabulates little groups characters, while [8] gives characters of the (whole) graphene layer group. Recently, the representations of all layer groups, both single- and double-, with and without time-reversal symmetry (TRS), were also published [9].

Not only band degeneracies, but also dispersions near band contacts, are determined by symmetry. Ref. [10] gives analysis of band dispersions dictated by all symmorphic little groups in 3D. A few decades later, sufficient conditions for existence of Weyl fermions near high-symmetry points (HSPs) in Brillouin zone (BZ) of (3D) space groups were derived [11]. Recently, a full classification of linear dispersions near HSPs in layers has been reported [12]. Fully linear Hamiltonians are mutually distinguished not only by the dimensionality, but also by the functional dependence of energy on the wave vector near band contacts. Fortune teller dispersion (FT), theoretically predicted earlier [13], is seen in surface layers of silicone by angular resolved photo-emission spectroscopy (ARPES) [14].

While group theory gives band contacts and dispersions in their vicinity, it does not predict the position of the Fermi level. Also, symmetry alone does not guarantee that no other bands cross the Fermi level, once it is conveniently placed (*i.e.* it does not guarantee clean Fermi surface). Here we report the realization of FT states from a tight-binding model and show that it is impossible for FT states to be the only dispersions near given energy, at least when spin-orbit coupling (SOC) is neglected and for FT states arising from essential band contacts at HSP. Our proof relies on topologically protected accidental band contacts tabulated in the literature [15–20].

2. Results and discussion

When SOC is neglected and the material is non-magnetic, the combined crystal symmetry and TRS give FT states near BZ corners of layer groups 33, 43 and 45 [13]. From these layer groups, space groups 29, 54 and 57 are obtained by adding pure vertical translation (notation for layer and space groups is according to [21] and [22], respectively). We calculated the electronic band structure within tight-binding approximation on a structure that belongs to layer groups 45 (site $4c$ with $z = 0.6$Å, $x = 0.2$), which is shown in Figure 1.

Tight-binding Hamiltonian arising from s-orbitals is:

$$\hat{H}(\mathbf{k}) = [f_0 + f_1 cos(\mathbf{k}\cdot\mathbf{a}_1)]\hat{I}_4 + \begin{pmatrix} 0 & b_0\left(1+e^{i\mathbf{k}\cdot\mathbf{a}_1}\right) & c_0 e^{i\mathbf{k}\cdot\mathbf{a}_1}\left(1+e^{i\mathbf{k}\cdot\mathbf{a}_2}\right) & g_0\left(1+e^{i\mathbf{k}\cdot\mathbf{a}_2}\right) \\ b_0\left(1+e^{-i\mathbf{k}\cdot\mathbf{a}_1}\right) & 0 & g_0\left(1+e^{i\mathbf{k}\cdot\mathbf{a}_2}\right) & c_0\left(1+e^{i\mathbf{k}\cdot\mathbf{a}_2}\right) \\ c_0 e^{-i\mathbf{k}\cdot\mathbf{a}_1}\left(1+e^{-i\mathbf{k}\cdot\mathbf{a}_2}\right) & g_0\left(1+e^{-i\mathbf{k}\cdot\mathbf{a}_2}\right) & 0 & b_0\left(1+e^{-i\mathbf{k}\cdot\mathbf{a}_1}\right) \\ g_0\left(1+e^{-i\mathbf{k}\cdot\mathbf{a}_2}\right) & c_0\left(1+e^{-i\mathbf{k}\cdot\mathbf{a}_2}\right) & b_0\left(1+e^{i\mathbf{k}\cdot\mathbf{a}_1}\right) & 0 \end{pmatrix}, \quad (1)$$

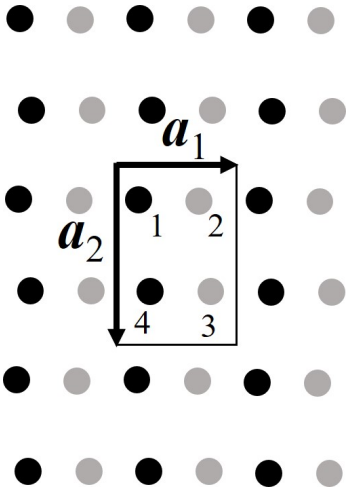

Figure 1: Crystal structure of the tight-binding model with $|\mathbf{a}_1|$ =2Å, $|\mathbf{a}_2|$ =3Å. All nuclei are of the same type. Black (gray) nuclei are located 0.6Å, above (below) the drawing plane. Fractional coordinates (in $\{\mathbf{a}_1, \mathbf{a}_2\}$-basis) for nucleus 1, 2, 3 and 4 are (0.2, 0.2), (0.7, 0.2), (0.8, 0.7) and (0.3, 0.7), respectively. We used program VESTA [23] for visualization.

where $\hat{I}_4$ is the four-dimensional unit matrix, $\mathbf{k}$ is a vector from the reciprocal space, while f_0, g_0, b_0, f_1 and c_0 (real numbers) are hopping parameters for the zeroth, first, second, third and fourth neighbor, respectively. The eigenvalues of $\hat{H}$ are bands denoted such that $E_1(\mathbf{k}) \leq E_2(\mathbf{k}) \leq E_3(\mathbf{k}) \leq E_4(\mathbf{k})$ for every wave vector $\mathbf{k}$. The full band structure for particular specified values of parameters is shown in Figure 2a) and near BZ corner in Figure 2b). Doubly degenerate lines are at BZ border as predicted by symmetry. The all four bands meet at the BZ corners. For closer look at dispersions near BZ corners, we expand the Hamiltonian in the vicinity of $(1/2, 1/2)$ in Taylor series up to linear (first) order:

$$\hat{H}(\mathbf{q}) \approx (f_0 - f_1)\hat{I}_4 + i \begin{pmatrix} 0 & -b_0\mathbf{q}\cdot\mathbf{a}_1 & c_0\mathbf{q}\cdot\mathbf{a}_2 & -g_0\mathbf{q}\cdot\mathbf{a}_2 \\ b_0\mathbf{q}\cdot\mathbf{a}_1 & 0 & -g_0\mathbf{q}\cdot\mathbf{a}_2 & -c_0\mathbf{q}\cdot\mathbf{a}_2 \\ -c_0\mathbf{q}\cdot\mathbf{a}_2 & g_0\mathbf{q}\cdot\mathbf{a}_2 & 0 & b_0\mathbf{q}\cdot\mathbf{a}_1 \\ g_0\mathbf{q}\cdot\mathbf{a}_2 & c_0\mathbf{q}\cdot\mathbf{a}_2 & -b_0\mathbf{q}\cdot\mathbf{a}_1 & 0 \end{pmatrix}. \tag{2}$$

The dispersion is:

$$E_{1,2,3,4} \approx f_0 - f_1 \pm \left| |b_0\mathbf{q}\cdot\mathbf{a}_1| \pm \sqrt{c_0^2 + g_0^2}\,|\mathbf{q}\cdot\mathbf{a}_2| \right|, \tag{3}$$

which is exactly FT type predicted in [13].

From (3) it follows that $E_1 = E_2$ and $E_3 = E_4$ if $\mathbf{q}\cdot\mathbf{a}_1 = 0$ or $\mathbf{q}\cdot\mathbf{a}_2 = 0$. These degeneracies are located at BZ borders and they are essential (caused by symmetry). However, there is another line of degeneracy $E_2 = E_3$, valid if $|b_0\mathbf{q}\cdot\mathbf{a}_1| = \sqrt{c_0^2 + g_0^2}\,|\mathbf{q}\cdot\mathbf{a}_2|$, which always has two solutions for sufficiently small $|\mathbf{q}|$. This degeneracy is accidental and it prevents the FT states to be the only states at the Fermi level, provided it continues across the whole BZ. Exact eigenvalues of full Hamiltonian (1) give lines of accidental degeneracies $E_2(\mathbf{k}) = E_3(\mathbf{k})$ for $|\mathbf{k}|$ not necessarily being small. These lines are indicated in red in Figure 2c). Such lines are not property of a model, but will always appear in group 45 as can be shown by the following argument. In the case with SOC included,

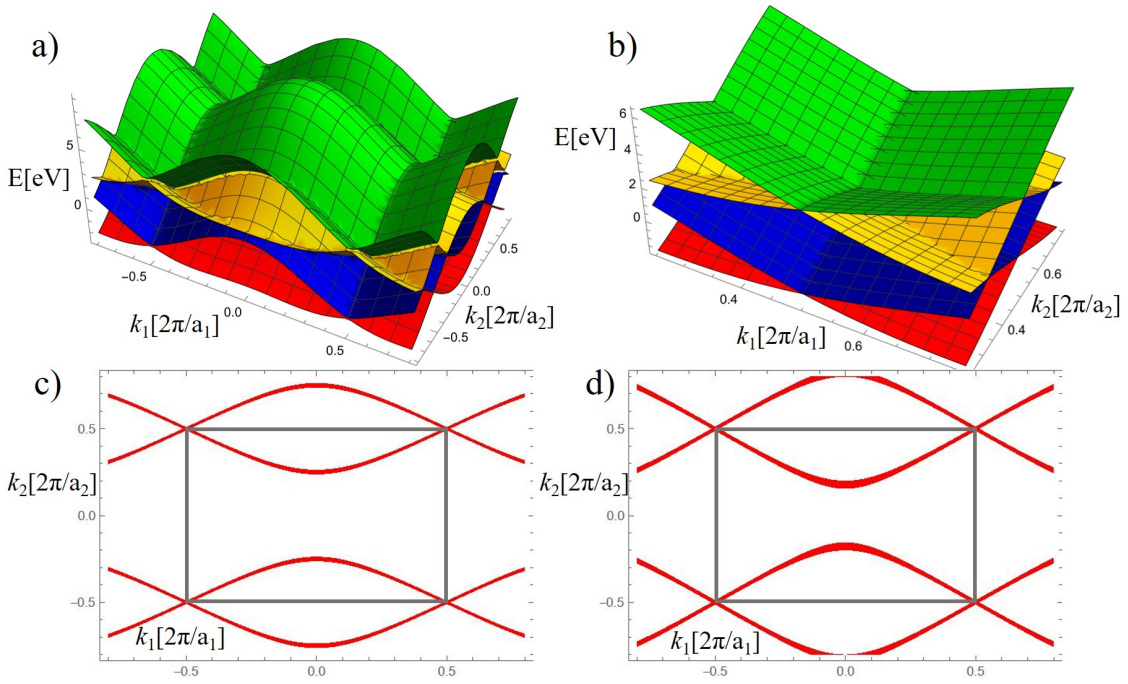

Figure 2: Band structure of the model: a) full band structure for f_0, g_0, b_0, f_1 and c_0 equal to $2eV$, $1.7eV$, $1.2eV$, $0.7eV$ and $0.3eV$, respectively, b) band structure near $(1/2, 1/2)$ showing FT dispersion, c) lines $E_2 = E_3$ (denoted in red) in **k**-space, d) lines $E_2 = E_3$ for f_0, g_0, b_0, f_1 and c_0 equal to $2.2eV$, $1.3eV$, $1.1eV$, $0.4eV$ and $0.1eV$, respectively. Grey rectangle in c) and d) denotes BZ border.

eight spinful non-degenerate bands are tangled together for groups 33, 43 and 45, giving electron filling of $8n$ as necessary condition for an insulator [17]. Since inclusion of SOC cannot close the gap, these eight bands (four if spin is not included) must be connected away from BZ corners, also in the absence of SOC. This means that the line $E_2 = E_3$ will always be present although its actual position depends on the parameters of the model. This is illustrated in Figure 2d) for slightly different values of parameters.

3. Conclusions

In summary we have confirmed that symmetry gives FT states unavoidably in the BZ corners of layer group 45, if the SOC is negligible and the magnetic order is absent. In addition, we showed that these FT states cannot be alone at the Fermi level and that there are always other bands that cross it. The same conclusion applies for remaining gray layer single groups with FT states (33 and 43). Our findings might help predicting new materials with anisotropic properties, or even suggest how to modify existing layered materials to obtain ones with these three symmetry groups.

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References

[1] H. Bethe, *Termaufspaltung in Kristallen*, *Annalen der Physik* **395**(2) (1929) 133–208.

[2] V Damljanović and R Gajić, *Phonon eigenvectors of graphene at high-symmetry points of the Brillouin zone*, *Physica Scripta* **T149** (2012) 014067.

[3] M. S. Dresselhaus, G. Dresselhaus, and A. Jorio, *Group Theory: Applications to the Physics of Condensed Matter*, Springer, 2008.

[4] Nataša Lazić and Milan Damnjanović, *Spin ordering in RKKY nanowires: Controllable phases in* ^{13}C *nanotubes*, *Phys. Rev. B* **90** (2014) 195447.

[5] Mois I. Aroyo, Asen Kirov, Cesar Capillas, J. M. Perez-Mato, and Hans Wondratschek, *Bilbao Crystallographic Server. II. Representations of crystallographic point groups and space groups*, *Acta Crystallographica Section A* **62** (2006) 115–128.

[6] Luis Elcoro, Barry Bradlyn, Zhijun Wang, Maia G. Vergniory, Jennifer Cano, Claudia Felser, B. Andrei Bernevig, Danel Orobengoa, Gemma de la Flor, and Mois I. Aroyo, *Double crystallographic groups and their representations on the Bilbao Crystallographic Server*, *Journal of Applied Crystallography* **50** (2017) 1457–1477.

[7] D. B. Litvin and T. R. Wike, *Character Tables and Compatibility Relations of the Eighty Layer Groups and Seventeen Plane Groups*, Plenum Press, 1991.

[8] V Damljanović, R Kostić, and R Gajić, *Characters of graphene's symmetry group Dg80*, *Physica Scripta* **T162** (2014) 014022.

[9] Božidar Nikolić, Ivanka Milošević, Tatjana Vuković, Nataša Lazić, Saša Dmitrović, Zoran Popović, and Milan Damnjanović, *Irreducible and site-symmetry-induced representations of single/double ordinary/grey layer groups*, *Acta Crystallographica Section A* **78** (2022) 107–114.

[10] A. A. Abrikosov and S. D. Beneslavskii, *Possible existence of substances intermediate between metals and dielectrics*, *Soviet Physics JETP* **32** (1971) 699–708.

[11] J. L. Mañes, *Existence of bulk chiral fermions and crystal symmetry*, *Phys. Rev. B* **85** (2012) 155118.

[12] N Lazić, V Damljanović, and M Damnjanović, *Fully linear band crossings at high symmetry points in layers: classification and role of spin–orbit coupling and time reversal*, *Journal of Physics A: Mathematical and Theoretical* **55** (2022) 325202.

[13] Vladimir Damljanović, Igor Popov, and Radoš Gajić, *Fortune teller fermions in two-dimensional materials*, *Nanoscale* **9** (2017) 19337–19345.

[14] Marek Kopciuszyński, Mariusz Krawiec, Lucyna Żurawek, and Ryszard Zdyb, *Experimental evidence of a new class of massless fermions*, *Nanoscale Horizons* **5** (2020) 679–682.

[15] Haruki Watanabe, Hoi Chun Po, Michael P. Zaletel, and Ashvin Vishwanath, *Filling-enforced gaplessness in band structures of the 230 space groups*, *Phys. Rev. Lett.* **117** (2016) 096404.

[16] Haruki Watanabe, Hoi Chun Po, Ashvin Vishwanath, and Michael Zaletel, *Filling constraints for spin-orbit coupled insulators in symmorphic and nonsymmorphic crystals*, *Proceedings of the National Academy of Sciences* **112** (2015) 14551–14556.

[17] Benjamin J. Wieder and C. L. Kane, *Spin-orbit semimetals in the layer groups*, *Phys. Rev. B* **94** (2016) 155108.

[18] J. Zhang, Y.-H. Chan, C.-K. Chiu, M. G. Vergniory, L. M. Schoop, and A. P. Schnyder, *Topological band crossings in hexagonal materials*, *Phys. Rev. Materials* **2** (2018) 074201.

[19] Moritz M. Hirschmann, Andreas Leonhardt, Berkay Kilic, Douglas H. Fabini, and Andreas P. Schnyder, *Symmetry-enforced band crossings in tetragonal materials: Dirac and Weyl degeneracies on points, lines, and planes*, *Phys. Rev. Materials* **5** (2021) 054202.

[20] Andreas Leonhardt, Moritz M. Hirschmann, Niclas Heinsdorf, Xianxin Wu, Douglas H. Fabini, and Andreas P. Schnyder, *Symmetry-enforced topological band crossings in orthorhombic crystals: Classification and materials discovery*, *Phys. Rev. Materials* **5** (2021) 124202.

[21] V Kopsky and D. B. Litvin, *International Tables of Crystallography Volume E: Subperiodic Groups*, Kluwer Academic Publishers, 2002.

[22] T Hahn, *International Tables of Crystallography Volume A: Space-Group Symmetry*, Springer, 2005.

[23] Koichi Momma and Fujio Izumi, *VESTA3 for three-dimensional visualization of crystal, volumetric and morphology data*, *Journal of Applied Crystallography* **44** (2011) 1272–1276.