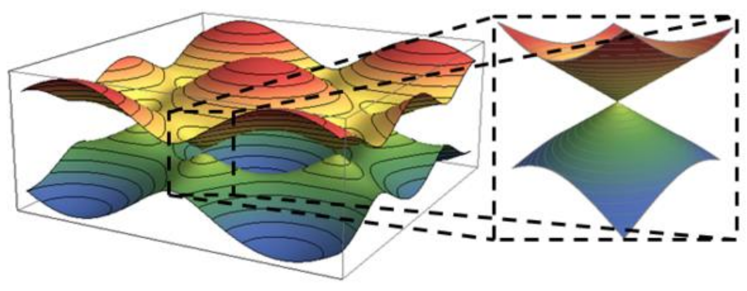
# Centrosymmetric, non-symmorphic, non-magnetic, spin-orbit coupled layers without Dirac cones: a tight-binding example

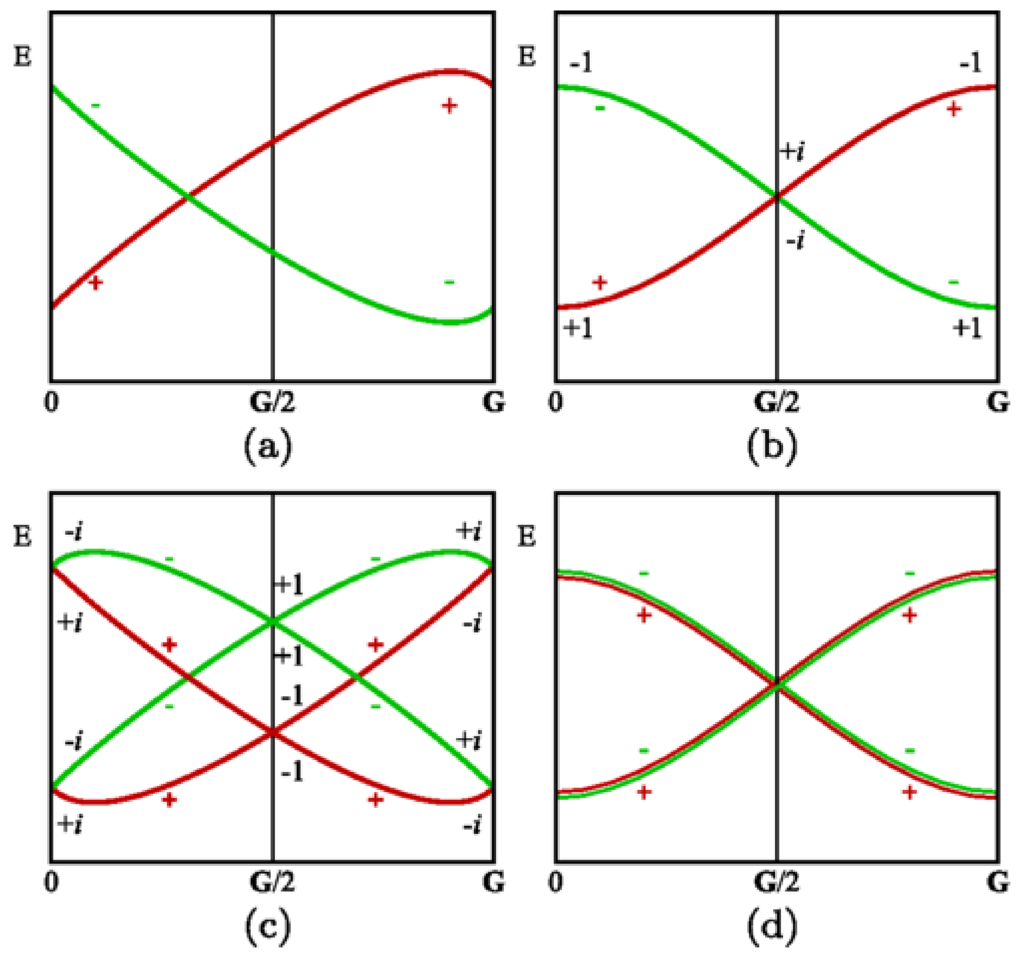
V. Damljanović

*Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11000 Belgrade, Serbia;* e-mail: damlja@ipb.ac.rs

**Abstract:**
It is believed that the existence of Dirac cones in the Brillouin zone (BZ) of time-reversal symmetric, two-dimensional (2D) materials with strong spin-orbit coupling (SOC) is closely connected with the presence of spatial inversion and non-symmorphic symmetry [1]. This belief is indeed confirmed in many cases published in the literature; however, a detailed group-theoretical analysis shows that this does not always hold [2]. Here we illustrate the mentioned fact by a tight-binding model from s-orbitals, on a structure that belongs to a non-symmorphic, gray, layer double group with spatial inversion. The band structure of the model consists of two double-degenerate bands, touching only along a line at the BZ edge. Further, we show that neglecting SOC leads to unaltered Hamiltonian, up to numerical values of the parameters. Finally, we state some 2D materials described in the literature, with the symmetry of our model.

Dirac cones in graphene (Wiki):



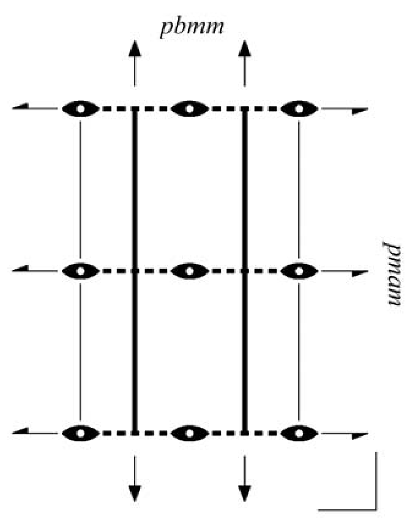



S. M. Young and C. L. Kane: **Dirac semimetals in two dimensions**, *Physical Review Letters* **115**, 126803 (2015)

474 citations (Web of Science, 08.08.2023.)!
*Phys. Rev. Lett.* - M21a – highest category (10 points)!

Figure 1
A nonsymmorphic symmetry {g|t} leads to band crossings on a g invariant line or plane in momentum space. (a) Without other symmetries, pairs of bands intersect an odd number of times as they cross the BZ. (b) With time-reversal symmetry, with Θ2=+1, the crossing occurs at the zone boundary G/2, where eiG·t=−1. For Θ2=−1, Kramers pairs at k=0 and G/2 connect as in (c), leading to a line node in an invariant plane or a Weyl node on an invariant line. The labels indicate the eigenvalues ±λeik·t of {g|t}. (d) With inversion and time-reversal symmetry, all states are degenerate (they are offset for clarity), and the crossing occurs at G/2.

Their main message: spin-orbit coupling + non-symmorphic symmetry + time reversal symmetry + space inversion = Dirac cones in the band structure.
Our main message: not so fast ☺ !

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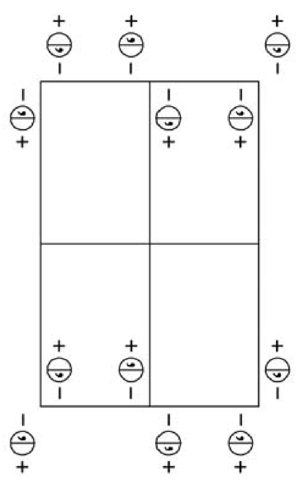
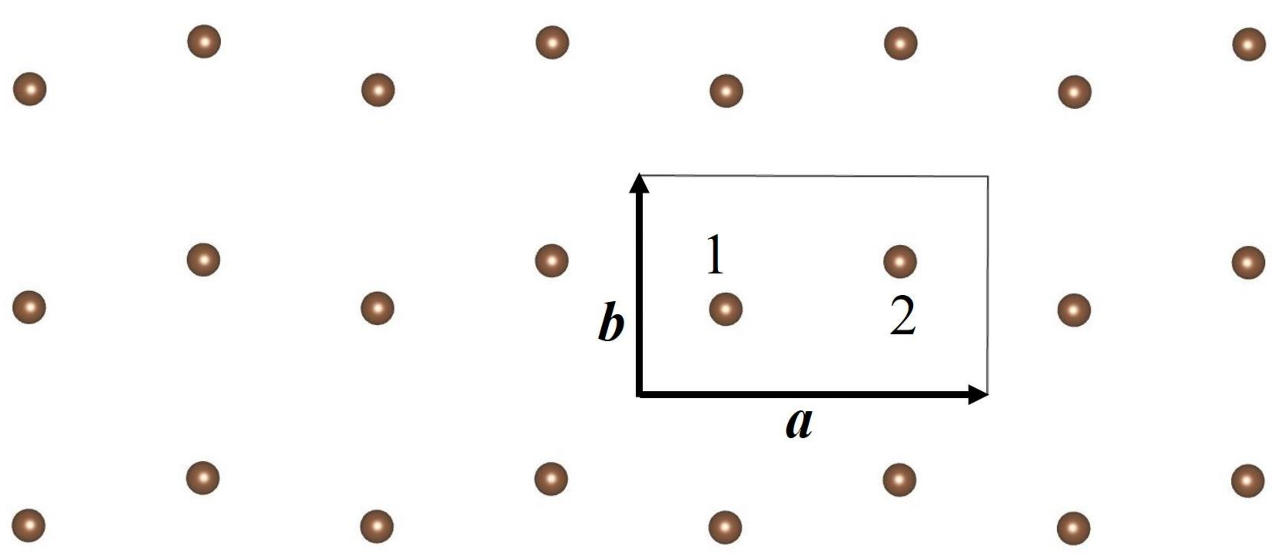
$P\,2_1/m\;2/a\;2/m$






Tight binding model from s - orbitals.
Third neighbours included.
Basis: $\{s_1\uparrow, s_2\uparrow, s_1\downarrow, s_2\downarrow\}$.

- spin-orbit coupling included
- non-symmorphic symmetry present
- space inversion symmetry present
- time-reversal symmetry present

$$\hat{H}_{TBM}(\boldsymbol{k}) = \begin{pmatrix} \hat{H}_\uparrow(\boldsymbol{k}) & \hat{0} \\ \hat{0} & \hat{H}_\downarrow(\boldsymbol{k}) \end{pmatrix}$$

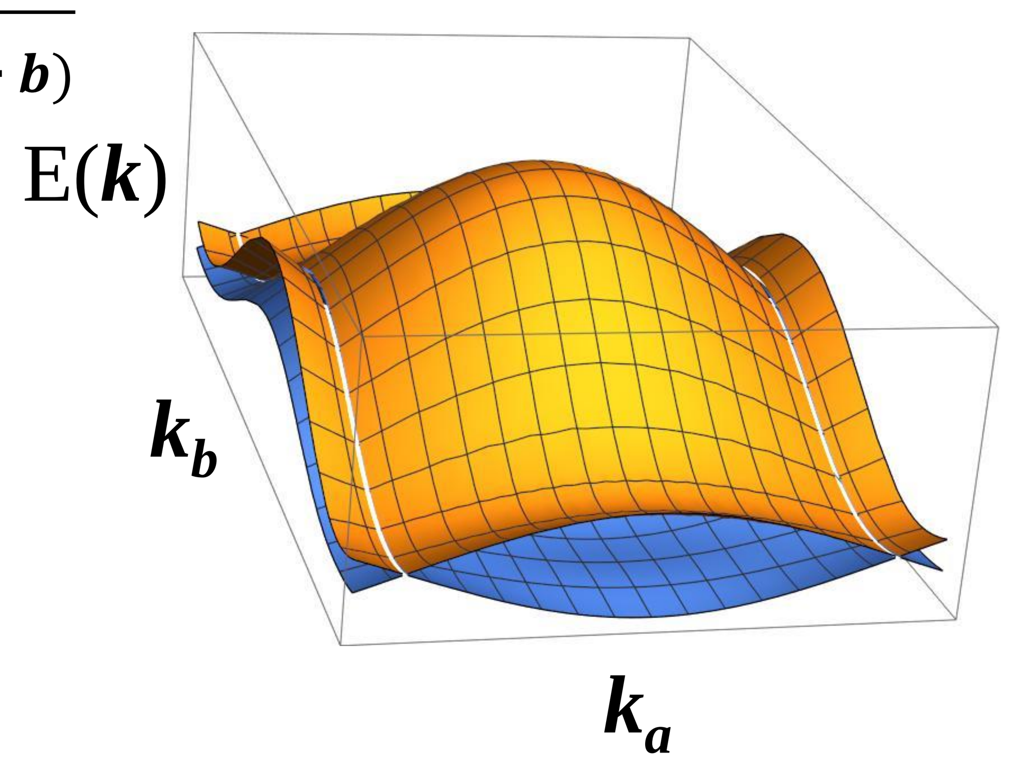
$$\hat{H}_\uparrow(\boldsymbol{k}) = \hat{H}_\downarrow(\boldsymbol{k}) =$$
$$= \begin{pmatrix} a_0 + 2a_1\cos(\boldsymbol{k}\cdot\boldsymbol{b}) & 2e^{-i\boldsymbol{k}\cdot\boldsymbol{a}/2}\cos\left(\frac{\boldsymbol{k}\cdot\boldsymbol{a}}{2}\right)\left(b_1 + b_3e^{-i\boldsymbol{k}\cdot\boldsymbol{b}}\right) \\ 2e^{i\boldsymbol{k}\cdot\boldsymbol{a}/2}\cos\left(\frac{\boldsymbol{k}\cdot\boldsymbol{a}}{2}\right)\left(b_1 + b_3e^{i\boldsymbol{k}\cdot\boldsymbol{b}}\right) & a_0 + 2a_1\cos(\boldsymbol{k}\cdot\boldsymbol{b}) \end{pmatrix}$$

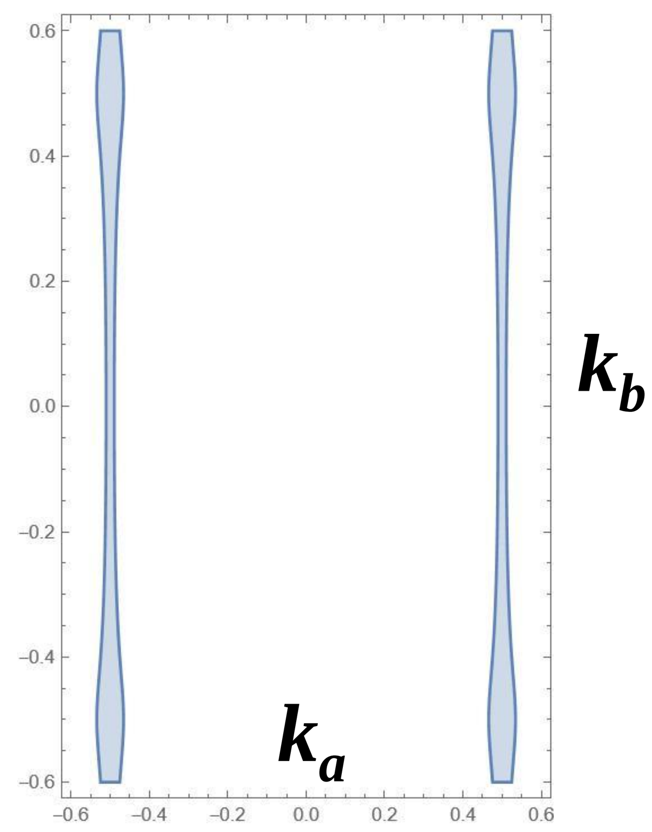
$$E_{1,2}^{\uparrow}(\boldsymbol{k}) = E_{1,2}^{\downarrow}(\boldsymbol{k}) = a_0 + 2a_1\cos(\boldsymbol{k}\cdot\boldsymbol{b}) \pm 2\left|\cos\left(\frac{\boldsymbol{k}\cdot\boldsymbol{a}}{2}\right)\right|\sqrt{b_1^2 + b_3^2 + 2b_1b_3\cos(\boldsymbol{k}\cdot\boldsymbol{b})}$$

Touching of two doubly-degenerate bands ($|a_0| > |b_1| > |a_1| > |b_3|$):

$$\cos\left(\frac{\boldsymbol{k}\cdot\boldsymbol{a}}{2}\right) = 0 \qquad \boldsymbol{k} = \pm\frac{1}{2}\boldsymbol{k}_a + y\boldsymbol{k}_b \qquad -\frac{1}{2} \le y \le \frac{1}{2}$$

Lines of 4-fold degeneracy, no Dirac cones!




**Conclusions:**
It is possible that prerequisites imposed by Young and Kane lead to lines of degeneracies, instead of point-like degeneracies. Instead of Dirac cones, Dirac lines appear. Young and Kane assumed that there is splitting away from ***G***/2 point in all directions, however, they never provided justification for this assumptions.

**Literature:**
[1] S. M. Young and C. L. Kane: Dirac semimetals in two dimensions, *Phys. Rev. Lett.* **115**, 126803 (2015).
[2] N. Lazić, V. Damljanović and M. Damnjanović: Fully linear band crossings at high symmetry points in layers, *J. Phys. A: Math. Theor*. **55**, 325202 (2022).