Beyond-Dirac fermions in a three-band Graphene-like toy model

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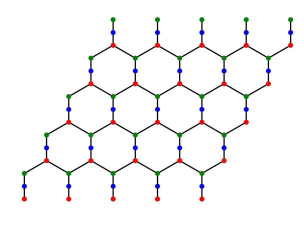
Outline of the Talk

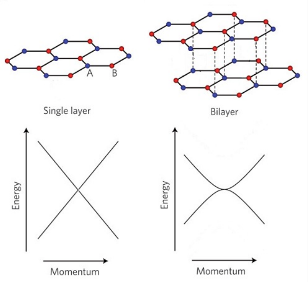
- Motivation (toy model building)
- Review of $SU(2)$ nature of Dirac fermions
- Main three-band continuum Hamiltonian of interest
- A winding number understanding
- Symmetry perspective
- Graphene-like lattice model



- Relevance to 3D
- Geometric phase understanding

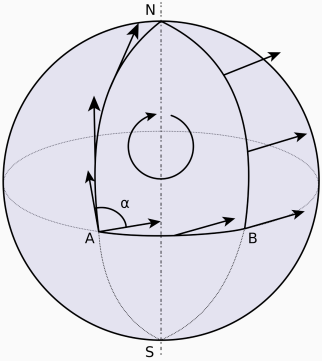
Motivation

- Geometry of some parameter-dependent wavefunctions
- Imp examples: QHE, Topological Insulators/Semi-metals
- Often reciprocal momenta of bands are our parameters
- Familiar Dirac cones on Honeycomb lattice



- Suppression of backscattering, Klein tunneling, Hall Effects
- Naive Q: Why Berry phase winding of π ?

Geometric Phase



- Arrows are of quantum mechanical origin for us
- Owing to phase differences of wavefunctions essentially
- But not fully...
- Notable examples: Focault's pendulum, Pancharatnam's phase in Light polarization

Berry Phase Formulas

- Berry connection

$$\gamma_n = \int_{\mathcal{C}} d\mathbf{R} \cdot \mathcal{A}_n(\mathbf{R})$$

where

$$\mathcal{A}_n(\mathbf{R}) = i\langle n(\mathbf{R})|\nabla_{\mathbf{R}}|n(\mathbf{R})\rangle$$

- Berry curvature

$$\mathbf{\Omega}_n(\mathbf{R}) = \nabla_{\mathbf{R}} \times \mathcal{A}_n(\mathbf{R}).$$

$$\gamma_n = \int_{\mathcal{S}} d\mathbf{S} \cdot \mathbf{\Omega}_n(\mathbf{R})$$

- parameter **R** may be reciprocal momenta
- Berry phase winding around a degeneracy
- Chern number of a filled gapped band

Why π?

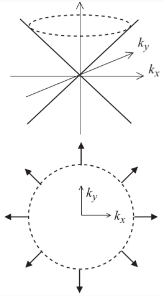
- Formal argument goes back to Berry's 1984 paper..
- A general two-band Hamiltonian with a degeneracy: $H = a\sigma_x + b\sigma_y + c\sigma_z$
- $H = \mathbf{B} \cdot \mathbf{S}$ in other words for $S = \frac{1}{2}$
- Berry phase is 0.5 solid angle subtended by path in Bloch sphere
- 0.5 comes due to $S = \frac{1}{2}$ $SU(2)$ structure
- For two parameters, use symmetries to get rid of one
- Thus solid angle is 2π
- $\implies$ Berry phase is π

Why π?

- A pictorial/operational demo:

$$-i \lim_{N\to\infty} \sum_{j=0}^{N-1} \log\langle j|j+1\rangle$$

- Recall Dirac cone wavefunctions



$$H_K^{\mathrm{Dirac}}(\mathbf{p}) = \begin{pmatrix} 0 & p_x - ip_y \\ p_x + ip_y & 0 \end{pmatrix}$$

$$v_1(\mathbf{p}) = \frac{1}{\sqrt{2}}(e^{-i\theta_{\mathbf{p}}}, 1)^T,$$

$$v_2(\mathbf{p}) = \frac{1}{\sqrt{2}}(-e^{-i\theta_{\mathbf{p}}}, 1)^T,$$

$$-i \lim_{N\to\infty} \sum_{j=0}^{N-1} \log\left(\frac{1+\exp[i(\theta_{j+1}-\theta_j)]}{2}\right)$$

$$-i \int_0^{2\pi} d\theta \quad \frac{i}{2} = \pi,$$

Go beyond π?

- More than two bands...
- Actually, can do it if we relax the degeneracy condition
- Gapped Dirac cones can enclose any fraction of π
- With degeneracy condition, look for three band generalizations...
- A simple case:

$$H_K^{3B}(\mathbf{p}) = \begin{pmatrix} 0 & p_x + ip_y & 0 \\ p_x - ip_y & 0 & p_x + ip_y \\ 0 & p_x - ip_y & 0 \end{pmatrix}$$

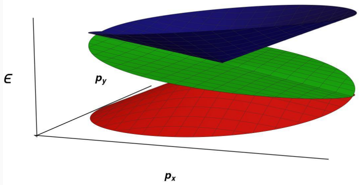
- Essentially, $H = \mathbf{B} \cdot \mathbf{S}$ for $S = 1$ now
- Therefore, Berry phase is 0 mod 2π
- Notable case: $\alpha - T_3$ model (Orsay group)

Three-band continuum Hamiltonian

- Instead consider

$$H_K^{3A}(\mathbf{p}) = \begin{pmatrix} 0 & p_x - ip_y & p_x - ip_y \\ p_x + ip_y & 0 & p_x + ip_y \\ p_x + ip_y & p_x - ip_y & 0 \end{pmatrix}$$

- Let's look at the spectrum



- Line degeneracies emanate from a central three-fold degeneracy
- Already gives a sense of non-Dirac geometry
- Goal to understand the geometry of this ...

Some context

- Lot of attention Three-fold degeneracies/triple point fermions
- both in 2D and 3D

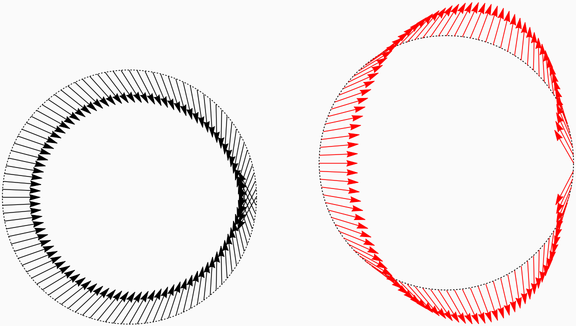
[14] D. Green, L. Santos, and C. Chamon, Phys. Rev. B **82**, 075104 (2010).
[15] B. Dóra, J. Kailasvuori, and R. Moessner, Phys. Rev. B **84**, 195422 (2011).
[16] Z. Lan, N. Goldman, A. Bermudez, W. Lu, and P. Öhberg, Phys. Rev. B **84**, 165115 (2011).
[17] D. F. Urban, D. Bercioux, M. Wimmer, and W. Häusler, Phys. Rev. B **84**, 115136 (2011).
[18] J. Wang, H. Huang, W. Duan, and Z. Liu, J. Chem. Phys. **139**, 184701 (2013).
[19] A. Raoux, M. Morigi, J.-N. Fuchs, F. Piéchon, and G. Montambaux, Phys. Rev. Lett. **112**, 026402 (2014).
[20] G. Giovannetti, M. Capone, J. van den Brink, and C. Ortix, Phys. Rev. B **91**, 121417(R) (2015).
[21] G. Palumbo and K. Meichanetzidis, Phys. Rev. B **92**, 235106 (2015).
[22] Y. Xu and L.-M. Duan, Phys. Rev. B **96**, 155301 (2017).
[23] L. Wang and D.-X. Yao, Phys. Rev. B **98**, 161403(R) (2018).

[25] G. W. Winkler, Q. S. Wu, M. Troyer, P. Krogstrup, and A. A. Soluyanov, Phys. Rev. Lett. **117**, 076403 (2016).
[26] H. Weng, C. Fang, Z. Fang, and X. Dai, Phys. Rev. B **93**, 241202(R) (2016).
[27] Z. Zhu, G. W. Winkler, Q. S. Wu, J. Li, and A. A. Soluyanov, Phys. Rev. X **6**, 031003 (2016).
[28] H. Weng, C. Fang, Z. Fang, and X. Dai, Phys. Rev. B **94**, 165201 (2016).
[29] G. Chang, S.-Y. Xu, S.-M. Huang, D. S. Sanchez, C.-H. Hsu, G. Bian, Z.-M. Yu, I. Belopolski, N. Alidoust, H. Zheng *et al.*, Sci. Rep. **7**, 1688 (2017).
[30] I. C. Fulga and A. Stern, Phys. Rev. B **95**, 241116(R) (2017).
[31] G. Chang, S.-Y. Xu, B. J. Wieder, D. S. Sanchez, S.-M. Huang, I. Belopolski, T.-R. Chang, S. Zhang, A. Bansil, H. Lin *et al.*, Phys. Rev. Lett. **119**, 206401 (2017).
[32] C. Zhong, Y. Chen, Z.-M. Yu, Y. Xie, H. Wang, S. A. Yang, and S. Zhang, Nat. Commun. **8**, 15641 (2017).
[33] J. Yu, B. Yan, and C.-X. Liu, Phys. Rev. B **95**, 235158 (2017).
[34] X. Zhang, Z.-M. Yu, X.-L. Sheng, H. Y. Yang, and S. A. Yang, Phys. Rev. B **95**, 235116 (2017).
[35] H. Yang, J. Yu, S. S. P. Parkin, C. Felser, C.-X. Liu, and B. Yan, Phys. Rev. Lett. **119**, 136401 (2017).

- almost all spin-1 cases
- One notable exception in 3D (“Nexus” fermions, Ref. 29)
- Precursor: Heikkila, Volovik, New J. Phys. 17, 093019, (2015)

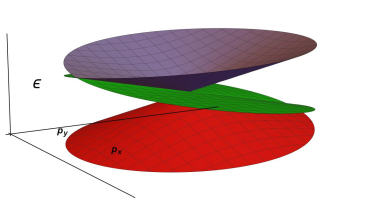
Geometry of H^{3A}

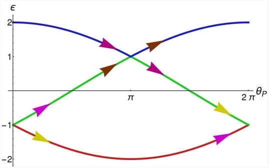
- Ref. 29's argued beyond-Weyl band structure
- Similarly, we are going beyond-Dirac in 2D here..
- Can explicitly see how in this toy model
- Line degeneracies are important
- This precludes Berry phase calculation
- Monitor arrow plots...



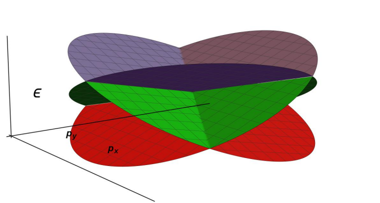
Geometry of H^{3A}

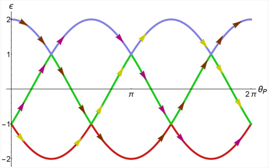
- The three bands are intertwined ..





- Contrast with $\begin{pmatrix} 0 & p_x - ip_y & p_x + ip_y \\ p_x + ip_y & 0 & p_x - ip_y \\ p_x - ip_y & p_x + ip_y & 0 \end{pmatrix}$





- Main message: Analytic movement across line degeneracies

Geometry of H^{3A}

- Explicit Eigensystem:

$$\epsilon_1^{3A}(\mathbf{p}) = -2p\cos\left(\frac{\theta_\mathbf{p}+\pi}{3}\right) \;;= \frac{1}{\sqrt{3}}\begin{pmatrix}\omega^2 e^{-i\frac{2\theta_\mathbf{p}}{3}} & \omega\; e^{i\frac{2\theta_\mathbf{p}}{3}} & 1\end{pmatrix}^T$$

$$\epsilon_2^{3A}(\mathbf{p}) = 2p\cos\left(\frac{\theta_\mathbf{p}}{3}\right) \;;= \frac{1}{\sqrt{3}}\begin{pmatrix}e^{-i\frac{2\theta_\mathbf{p}}{3}} & e^{i\frac{2\theta_\mathbf{p}}{3}} & 1\end{pmatrix}^T$$

$$\epsilon_3^{3A}(\mathbf{p}) = -2p\cos\left(\frac{\theta_\mathbf{p}-\pi}{3}\right) \;;= \frac{1}{\sqrt{3}}\begin{pmatrix}\omega\; e^{-i\frac{2\theta_\mathbf{p}}{3}} & \omega^2 e^{i\frac{2\theta_\mathbf{p}}{3}} & 1\end{pmatrix}^T$$

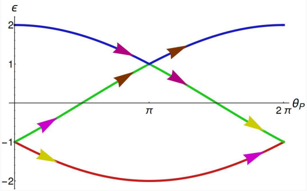
- $e^{i2\theta_\mathbf{p}/3}$ or $z^{1/3}$ are non-analytic in complex plane
- For analytic embedding, need three Riemann surfaces
- e.g. at spectrum level,

$$\Big\{\epsilon_1^{3A}(\mathbf{p}) = 2p\,\mathrm{Re}\left[\omega^2\sqrt[3]{e^{i\theta_\mathbf{p}}}\right], \epsilon_2^{3A}(\mathbf{p}) = 2p\,\mathrm{Re}\left[\sqrt[3]{e^{i\theta_\mathbf{p}}}\right],$$

$$\epsilon_3^{3A}(\mathbf{p}) = 2p\,\mathrm{Re}\left[\omega\sqrt[3]{e^{i\theta_\mathbf{p}}}\right]\Big\}$$

Geometry of H^{3A}: A winding number understanding

- $e^{i2\theta_{\mathbf{p}}/3}$ factors makes the analytic movement explicit

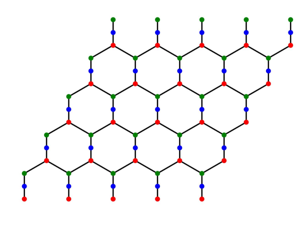


- This motivates to write winding numbers using these factors
- However, we can't circuit the three-fold degeneracy once
- Rather, need **three** circuits
- Beyond-Dirac comes because wavefunctions wind **twice**

Bands	Model	$\theta_{\mathbf{p}}$	H	v_i
2	Dirac	1	1	1(t), 1(b)
	QBT	1	2	2(t), 2(b)
3	H_K^{3B}	1	1	1(t), 2 (m), 1(b)
	H_K^{3A}	3	3	2(t), 2 (m), 2(b)

Symmetry Analysis

- Where could H^{3A} come from?
- Essentially, three copies of honeycomb hoppings...



- For regular two band (spinless) honeycomb,
  $\mathcal{C}_2$ (inversion or π rotation around centre of hexagon)
  $\mathcal{T}$ (time reversal)
  $\mathcal{P}_x$,$\mathcal{P}_y$ (x,y reflections)
  protect Dirac cone degeneracies
- Aside: $\mathcal{C}_3$ fixes them at $\mathbf{K}/\mathbf{K}'$ in honeycomb Brillouin zone

Symmetry Analysis: $SU(3)$ structure

- For two bands such a spinless symmetry analysis gives

$$\mathcal{H}^{\text{Dirac}} = \sum_{\mathbf{p}} \hat{c}^{\dagger}_{\mu\alpha}(\mathbf{p})\, H^{\text{Dirac}}_{\mu\alpha,\mu'\alpha'}\, \hat{c}_{\mu\alpha}(\mathbf{p}) \tag{1}$$

$$H^{\text{Dirac}}_{\mu\alpha,\mu'\alpha'} = p_x\left(\tau^{3}_{\mu\mu'} \otimes \sigma^{1}_{\alpha\alpha'}\right) + p_y\left(\tau^{0}_{\mu\mu'} \otimes \sigma^{2}_{\alpha\alpha'}\right) \tag{2}$$

which is nothing but Dirac cones at two valleys

- τ Pauli matrices index valleys, σ index sublattice
- In this way of writing, H^{3A} looks like (at one valley)

$$H^{3\text{A}}_{K}(\mathbf{p}) = p_x(\Lambda_1 + \Lambda_4 + \Lambda_6) + p_y(\Lambda_2 + \Lambda_5 - \Lambda_7) \tag{3}$$

where Λ_i are Gell-Mann matrices (generators of $SU(3)$)

- Whereas

$$H^{3\text{B}}_{K}(\mathbf{p}) = p_x(\Lambda_1 + \Lambda_6) + p_y(\Lambda_2 + \Lambda_7) \tag{4}$$

only use a subset (spin-1 generators of $SU(2)$) not surprisingly

Symmetry Analysis: $SU(3)$ structure

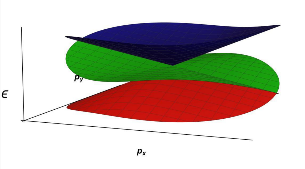
- H^{3A} involves all off-diagonal Gell-Mann matrices
- Inspired by the lattice, only impose $\mathcal{C}_2$, $\mathcal{T}$ and $\mathcal{P}_x$,$\mathcal{P}_y$ but no $\mathcal{C}_3$
- Also, anticipating valley structure along with sublattice ($\tau_i \otimes \Lambda_j$) with functional coefficients $f_{ij}(\mathbf{p})$
- Locality gets rid of half, those involving τ_x, τ_y
- Further reduce using above symmetries, to lowest order...

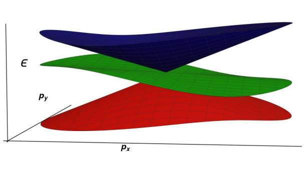
$$
\begin{aligned}
H = p_x\, \tau^3 \otimes (f^- \Lambda^1 + l_1^- (\Lambda^4 + \Lambda^6) + n^- \Lambda^8) \, + \\
p_y\, \tau^0 \otimes (g^- \Lambda^2 + m_2^- (\Lambda^5 - \Lambda^7)) \, + \\
\tau_0 \otimes (f^+ \Lambda^1 + n^+ \Lambda^8 + l_1^+ (\Lambda^4 + \Lambda^6))
\end{aligned}
$$

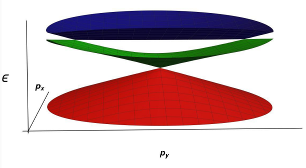
- large (8) parameter space for these Hamiltonians
- Aside: Imposing $\mathcal{C}_3$ can't accomodate the H^{3A} geometry

Symmetry Analysis: What we learnt?

- Categorize the various resulting band structures
- H^{3A} like band structure requires fine-tuning...
- Generic situation at the bottom:







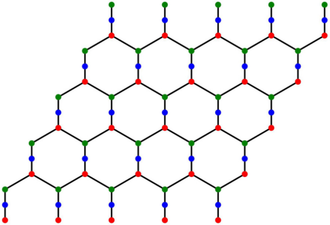
- However, this multiple Dirac Cone organization is deriving from the $SU(3)$ structure
- Also, “mass” term $(\tau_0 \otimes \Lambda_8)$ is allowed by symmetry

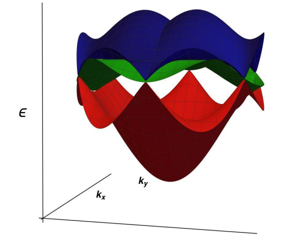
The Lattice Band structure

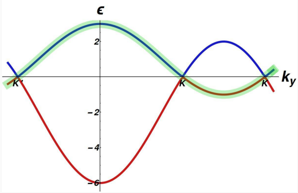
- Graphene-like Lattice hoppings with 3 sites per unit cell

$$\mathcal{H} = \sum_{n_1,n_2} \mathcal{H}_{ab} + \mathcal{H}_{ac} + \mathcal{H}_{bc}, \tag{22}$$

$$\begin{aligned}
\mathcal{H}_{ab} &= -t\, \hat{c}^{\dagger}_{(n_1,n_2),a}(\hat{c}_{(n_1,n_2),b} + \hat{c}_{(n_1,n_2-1),b} + \hat{c}_{(n_1+1,n_2-1),b}) \\
&\quad + \text{H.c.}, \\
\mathcal{H}_{ac} &= -(t+\delta t_0)\hat{c}^{\dagger}_{(n_1,n_2),a}\hat{c}_{(n_1,n_2),c} \\
&\quad - (t+\delta t_1)\hat{c}^{\dagger}_{(n_1,n_2),a}(\hat{c}_{(n_1,n_2-1),c} + \hat{c}_{(n_1+1,n_2-1),c}) + \text{H.c.}, \\
\mathcal{H}_{bc} &= -(t+\delta t_0)\hat{c}^{\dagger}_{(n_1,n_2),b}\hat{c}_{(n_1,n_2),c} \\
&\quad - (t+\delta t_1)\hat{c}^{\dagger}_{(n_1,n_2),b}(\hat{c}_{(n_1,n_2+1),c} + \hat{c}_{(n_1-1,n_2+1),c}) + \text{H.c.}
\end{aligned} \tag{23}$$



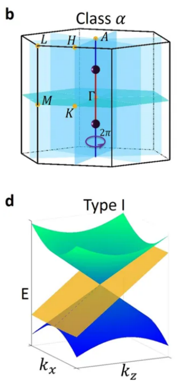


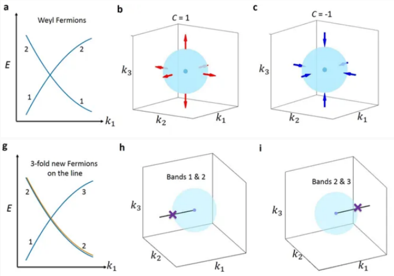


- With symmetry allowed deformations, get the generic case
- with lattice induced curvature in bands

Relevance to 3D

- turns out in 3D, such three-fold degeneracy can be guaranteed by symmetry
- Details in Ref. 29, G. Chang et al, Sci Rep (2017)
- Include proposed materials (Tungsten Carbide)





Relevance to 3D

- Beyond-Weyl implied because any sphere enclosing three-fold degenerate point encounters a gapless point due to emanating line degeneracies
- H^{3A} had the same feature/bug in 2D for any loop enclosing the three-fold degneracy
- Inspite of this, we can understand the geometry in the 2D quite well
- These gapless points are not a fundamental roadblock
- Analytic movement across them governs the geometry
- In fact, can give a 2D non-Abelian topological invariant
- Suspect our 2D understanding can help complete the 3D story
- Aside: Borophene material has our lattice

Non-Abelian Geometry of H^{3A}

- Since, the bands are intertwined, adiabatic evolution can not remain in a single "band"
- it will happen across the three "bands"
- $|\psi_a(t)\rangle = e^{-i\int^t dt'\epsilon_b(\lambda(t'))} \; U_{ab}(\lambda(t))|n_b(\lambda(t))\rangle$
- Under Schrodinger evolution, $\dot{U}_{ab}|n_b\rangle + U_{ab}|\dot{n}_b\rangle = 0$
- this leads to Non-Abelian Berry geometry (Wilczek & Zee)
- in 2D, can evaluate the holonomy $U = \mathcal{P}\left[e^{-i\oint \mathcal{A}_i d\lambda_i}\right]$
- $(\mathcal{A}_i)_{ba} = -i\langle n_a|\partial_{\lambda_i}|n_b\rangle$ and U are 3×3 matrices
- $U_K = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \qquad U_{K'} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}$
- can also compute Non-Abelian Berry curvature ($\mathcal{F}_{xy}$), trace of its powers
- doesn't give a signed invariant

Conclusions and Outlook

- Details in Phys. Rev. B 100, 125152 (2019).
- A toy model of beyond-Dirac fermions
- Wavefunction Geometry is explicit
- pertinent to understanding 3D Nexus fermions
- Physical properties, Effect of Interactions: further topics

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