Geometric Semimetals

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Weyl and Dirac Semimetals as a Laboratory for High-Energy Physics,
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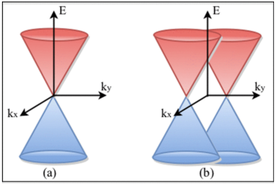
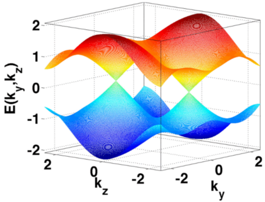
Outline

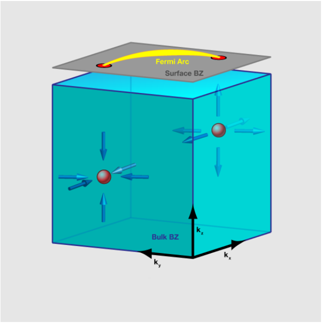
- Introduction to Weyl and multifold semimetals
- Real-space geometry in semimetals
- Momentum-space geometry and geometric semimetals
  (Y.-P. Lin and G. Palumbo, Phys. Rev. B 109, L201107 (2024))
- Conclusions and Outlook

3D Weyl Semimetals

In Weyl semimetals, the valence and conductance bands in the energy spectrum touch each other at special nodal points, which behave as magnetic monopoles in momentum space.







Weyl cones appear in materials that break either inversion ($\mathbf{k} \to -\mathbf{k}$) or time-reversal symmetry.

Abelian Berry Connection

Bloch wave-vector: $|u(\mathbf{k})\rangle = (u^1(\mathbf{k}), u^2(\mathbf{k}), ..., u^{\aleph}(\mathbf{k}))^\top$.
The gauge redundancy in a non-degenerate Bloch state is encoded in the arbitrary phase in $|u\rangle$

$$|u\rangle \to e^{i\alpha(\mathbf{k})}|u\rangle,$$

where $\alpha(\mathbf{k})$ is a momentum-dependent function.
We can build an Abelian gauge connection in momentum space as follows

$$\mathcal{A}_j = i\langle u|\partial_j|u\rangle, \quad \mathcal{A}_j \to \mathcal{A}_j - \partial_j\alpha,$$

with $\partial_j \equiv \partial_{k_j}$, while the gauge-invariant Berry curvature is given by

$$\mathcal{F}_{jk} = \partial_j\mathcal{A}_k - \partial_k\mathcal{A}_j.$$

Weyl fermions and momentum-space monopoles

Low-energy Weyl Hamiltonian (H. Weyl, 1929)

$$H_{3D} = k_x\sigma^x + k_y\sigma^y + k_z\sigma^z,$$

where $\boldsymbol{k} = (k_x, k_y, k_z)$ are the momenta and $\sigma^{x,y,z}$ are the Pauli matrices.

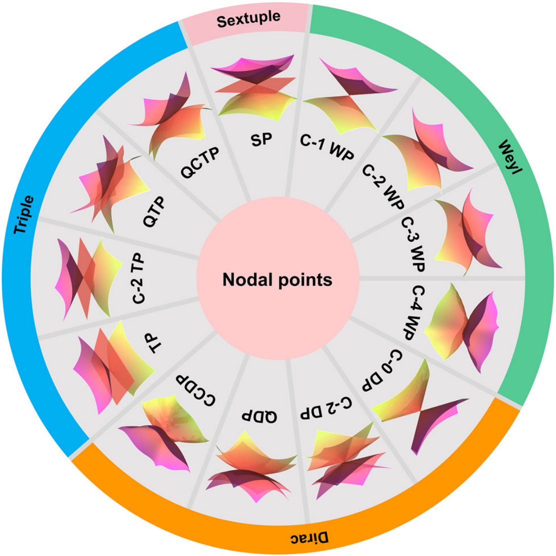
The Berry curvature around the Weyl point is given by

$$\mathcal{F}_{jk} = \epsilon_{jkl} \frac{k_l}{2(k_x^2 + k_y^2 + k_z^2)^{3/2}},$$

$$C = \frac{1}{2\pi}\int_{S^2} dk^j \wedge dk^k \mathcal{F}_{jk} = \pm 1,$$

which is the topological charge (first Chern number) of a momentum-space Dirac monopole.

3D multifold topological semimetals



picture taken from T. Yang at al., Matter 7, 320 (2024)

Higher Chern number

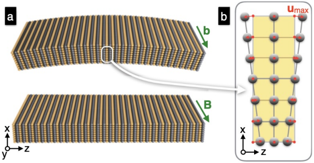
picture taken from : I. Robredo et al, EPL 147, 46001 (2024)

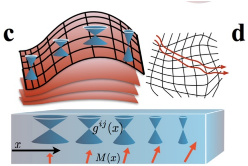
It has been shown that these systems support quantum anomalies although their effective field-theory description break Lorentz symmetry.

Notice that these systems violate the Nielsen-Ninomiya theorem!

Real-space geometry

An effective curved background in Weyl semimetals can be induced by introducing strain or linear dislocations and disclinations.



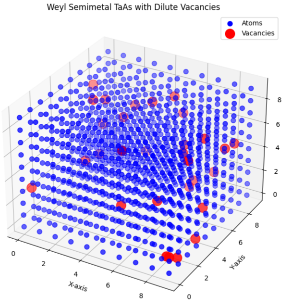


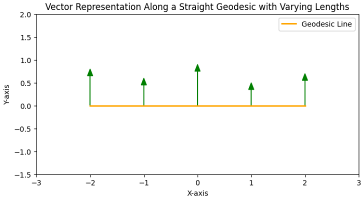
geometrical objects	space	physical systems
$R = T = \Omega = 0$	flat space	ideal crystal
$R = \Omega = 0,\ T \neq 0$	state of absolute parallelism	systems with dislocations (deformed crystals)
$T = \Omega = 0,\ R \neq 0$	Riemann space	systems with disclinations (liquid crystals, spin glasses)
$R \neq 0,\ T \neq 0,\ \Omega = 0$	Riemann Cartan space	theory of dislocations and disclinations
$R \neq 0,\ T \neq 0,\ \Omega \neq 0$	affine-metric space	gauge theory of linear and point defects

(Table from A. V. Grachev et al., The Gauge Theory of Point Defects, 1989).

From vacancies to non-metricity

Vacancies (point defects) in crystals give rise to an effective non-metricity tensor Q_{ijk} in the continuum low-energy regime.





$$Q_{ijk} = \nabla_i \tilde{g}_{jk} = W_i \tilde{g}_{jk}.$$

In the absence of torsion (no linear dislocations), the non-metricity is uniquely characterized by a vector field, known as Weyl connection W_i (G. P., arXiv:2412.04743).

Momentum-space geometry: quantum metric

The Berry curvature is the imaginary part of the quantum geometric tensor (Provost and Vallee, Comm. Math. Phys. 1980)

$$\chi_{jk} = g_{jk} + (i/2)\Omega_{jk},$$

where g_{jk} is the quantum metric given by

$$\begin{aligned} g_{jk} = & \frac{1}{2}(\langle \partial_j u | \partial_k u \rangle + \langle \partial_k u | \partial_j u \rangle \\ & - \langle \partial_j u | u \rangle \langle u | \partial_k u \rangle - \langle \partial_k u | u \rangle \langle u | \partial_j u \rangle). \end{aligned}$$

This is a Riemannian metric and quantifies, for instance, the infinitesimal distance between two quantum states (it is also known as Fubini-Study and Bures metric).

Importantly, this gauge invariant quantity can me measured in experiments.

Topological charge from the quantum metric

$$\Omega_{jk} = \epsilon_{jk}\,(2\sqrt{\bar{g}}),$$

where $\bar{g} = \det g_{\bar{j}\bar{k}}$ is the determinant of the 2×2 quantum metric tensor defined in the proper 2D subspace.

In spherical coordinates:

$$g_{\theta\theta} = 1/4, \quad g_{\phi\phi} = \sin^2\theta/4, \quad g_{\theta\phi} = 0.$$

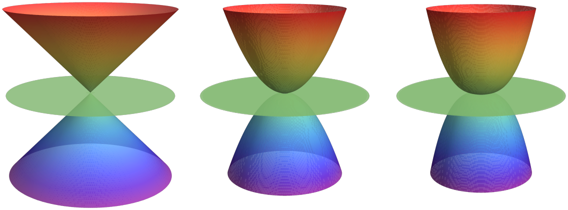
This corresponds to the metric of a sphere S^2, of fixed radius $r = 1/2$.

$$Q = \frac{1}{2\pi}\int_{S^2}\Omega = \frac{1}{2\pi}\iint(2\sqrt{g})\,d\theta d\phi = 1.$$

(G. Palumbo and N. Goldman, PRL 2018)

3D Geometric semimetals

We consider a class of inversion and time-reversal-symmetric ($T^2 = 1$) multifold semimetals characterized by real Bloch bands (zero Berry curvature), with the nodal points protected by sublattice and rotation symmetries.



These systems are characterized by the quantum metric trace

$$\mathrm{Tr}\, g_{\mathbf{k}} = \frac{s_\alpha(s_\alpha + 1)}{|\mathbf{k}|^2},$$

where s_α is the pseudo-spin.

Simplest example of geometric semimetal

For a suitable tight-binding model, we can linearize around the Weyl-like nodal points, which are described by the following momentum-space Hamiltonian

$$\mathcal{H}_{\mathbf{k}}^{(0,1)} = \frac{1}{\sqrt{2}} \begin{pmatrix} -k_z\sqrt{2} & k_x & k_y & 0 \\ k_x & 0 & 0 & k_x \\ k_y & 0 & 0 & k_y \\ 0 & k_x & k_y & k_z\sqrt{2} \end{pmatrix} = k_i \beta^i .$$

$E_{\pm}^{(1)} = \pm\sqrt{k_x^2 + k_y^2 + k_z^2}$, $E_0^{(2)} = 0$.

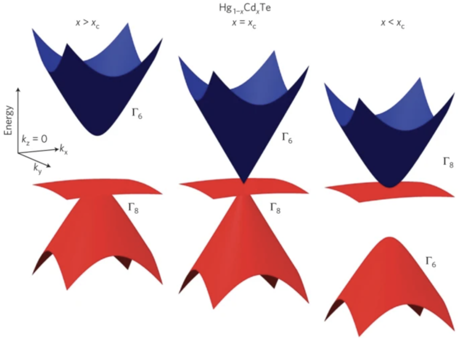
The geometric invariant is given by

$$G = \frac{1}{2\pi} \oint d\mathbf{S}_{\mathbf{k}} \cdot \hat{\mathbf{k}} \, \mathrm{Tr}\, g_{\mathbf{k}} = s_\alpha(s_\alpha + 1) = 2.$$

It can be simulated in synthetic matter systems such as ultracold atoms, superconducting quantum circuits and metamaterials.

Kane fermions in quantum materials

Massless Kane fermions are been experimentally observed in zinc-blende crystal (M. Orlita et al., Nat. Phys. 10, 233 (2014)).



All the three bands are doubly degenerated (doubly degenerate spin-1 quasiparticle).
Massless Kane fermions respect time-reversal symmetry but are topologically trivial. Moreover, the corresponding quantum metric trace is not quantized.

Conclusions and Outlook

- I have briefly discussed the role of the quantum metric in nodal-point semimetals.
- I have shown the existence of nodal-point semimetals that although topologically trivial, are nevertheless characterized by a quantized number related to the quantum metric trace.
- It would be important to show the absence of quantum anomalies in these systems by employing non-relativistic quantum field theory.
- It would be interesting to study the real-space geometry in these systems and build a more general phase-space geometric formalism (bi-metric phase-space theory).

Muito obrigado!