Dirac-point models: Hilbert space geometry and topology

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- Quick review of Hilbert space geometry: Berry curvature and Quantum metric (Fubini-Study metric). (abstract)

- Special features when applied to Bloch states in the Brillouin zone (semiclassical dynamics, non-commutative geometry)

- Application to graphene-like models:
  - (a) the gapless case
  - (b) broken time-reversal symmetry and the Chern Insulator (anomalous/zero field QHE).

- One-way light and the photonic analog
Hilbert space geometry induced on a manifold of quantum states:

\[ |\Psi(g)\rangle = \sum_{i=1}^{N} a_i(g) |i\rangle \]

\[ \langle i|j \rangle = \delta_{ij} \]

orthonormal fixed basis in Hilbert space

\[ g = \{ g^\mu, \mu = 1, 2, \ldots, d \} \]
coordinates on a continuous d-dimensional manifold

U(1) “Berry gauge” ambiguity of quantum mechanics: nothing physical is affected by

\[ |\Psi(g)\rangle \rightarrow e^{i\phi(g)} |\Psi(g)\rangle \]
Only (Berry) gauge-invariant quantities can have physical meaning, e.g. \( \langle \Psi(g) | \Psi(g) \rangle = 1 \)

- non-gauge-invariant derivative:
  \[
  |\partial_\mu \Psi(g)\rangle = \sum_i \frac{\partial a_i(g)}{\partial g^\mu} |i\rangle
  \]

- gauge-invariant (covariant) derivative:
  \[
  |D_\mu \Psi(g)\rangle = |\partial_\mu \Psi(g)\rangle - |\Psi(g)\rangle \langle \Psi(g) | \partial_\mu \Psi(g)\rangle
  \]
  \[
  = |\partial_\mu \Psi(g)\rangle - iA_\mu(g) |\Psi(g)\rangle \quad \langle \Psi(g) | D_\mu \Psi(g) \rangle = 0
  \]

\[A_\mu(g) = -i \langle \Psi(g) | \Psi(g) \rangle \]

Berry connection ("vector potential")
From this we get two related fundamental Berry-gauge-invariant geometrical quantities:

\[ \langle D_\mu \Psi(g) | D_\nu \Psi(g) \rangle = G_{\mu\nu}(g) + i F_{\mu\nu}(g) \]

Positive Hermitian

Positive real symmetric (Fubini-Study) "metric"

imaginary antisymmetric Berry curvature

\[ F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu \]

- dimensionless, gauge-invariant quantum distance between two normalized states in Hilbert space

\[ d(g, g')^2 = 1 - |\langle \Psi(g) | \Psi(g') \rangle|^\lambda, \lambda \geq 1. \]
• The **Berry curvature** is by now very familiar.

• The **quantum metric** that accompanies it is less familiar. It is a distinct but related property.

• Because the two combine to give a positive Hermitian matrix the absolute (unsigned) value of the Berry curvature provides a
Application to Bloch states, $g = k$, manifold = Brillouin zone:

- Geometry comes not just from Bloch states, but also on how they are embedded in real space.

- The Berry curvature and metric control the semiclassical physics of the the response to quasi-uniform electromagnetic fields that only vary on lengthscales much larger than the unit cell.

$$x_{R\alpha} = R + a_{\alpha}$$

**Spatial embedding**

$$H = \sum_{R, R', \alpha, \beta} t_{\alpha\beta}(R - R') c_{R\alpha}^\dagger c_{R'\beta}$$

**Labels**
- unit cells
- different orbitals in unit cell
Bloch states:

\[ H |\Psi_n(k)\rangle = E_n(k) |\Psi_n(k)\rangle \]

- States with different \( k \) are orthogonal, don’t form a manifold. Need to extract “periodic part”

\[ U(k; \{a_\alpha\}) = \sum_{R_\alpha} e^{ik \cdot (R+a_\alpha)} c_{R_\alpha}^\dagger c_{R_\alpha} \]

- Definition of the manifold of states depends the spatial positions \( \{a_\alpha\} \) of the orbitals within the unit cell:

\[ |\Phi_n(k; \{a_\alpha\})\rangle = U^{-1}(k; \{a_\alpha\}) |\Psi_n(k)\rangle \]
The gauge-dependent Berry connection defines the “mean position” of the electron in the unit cell:

\[ A_n^a(k) = -i \langle \Phi_n(k) | \nabla_k^a \Phi_n(k) \rangle \]

\[ = x_n^a(k) - i \langle \Psi_n(k) | \nabla_k^a \Psi_n(k) \rangle \]

\[ x_n(k) = \sum_\alpha a_\alpha \langle \Psi_n(k) | n_{R\alpha} | \Psi_n(k) \rangle \]

depends on choice of unit cell
The “mean position” in the unit cell is ambiguous, but its derivatives (wrt to time, k) are not!
\[ [k_a, k_b] = i(e/\hbar)F_{ab}(\mathbf{x}), \quad F_{ab} = \nabla_a A_b - \nabla_b A_a \]

\[ [x_n^a, x_n^b] = i\mathcal{F}_{n}^{ab}(\mathbf{k}), \quad \mathcal{F}_{n}^{ab}(\mathbf{k}) = \nabla_k^a A_n^b - \nabla_k^b A_n^a \]

- non commutative geometry!

Semiclassical equations of motion in phase space

\[
H = \varepsilon_n(\mathbf{k}) + V(\mathbf{x})
\]

\[
\hbar \frac{dk_a}{dt} = -\nabla_a V(\mathbf{x}) + eF_{ab}(\mathbf{x}) \frac{dx^b}{dt}
\]

\[
\hbar \frac{dx^a}{dt} = \nabla_k^a \varepsilon(\mathbf{k}) + \hbar \mathcal{F}_{n}^{ab}(\mathbf{k}) \frac{dk_b}{dt}
\]

Lorentz force

Group velocity

Karplus-Luttinger

"anomalous velocity"

describes redistribution of charge inside unit cell as \( k \) changes
• The Topological invariant **Chern number** for a 2D Brillouin zone does **not** depend on the embedding in space:

\[
c_n = \frac{1}{2\pi} \int_{BZ} d^2 k \ F_n(k; \ \{a_\alpha\})
\]

**Controls QHE (TKNN 1982)**

• Moving the positions of the orbitals changes the Berry curvature distribution in the BZ (and hence changes the semiclassical equations of motion), but does **not** change the Chern invariant
Graphene:

- Dirac points are protected against mass generation because:
- They are at different k-points
- Spin-orbit coupling is absent (negligible), and both time reversal and inversion symmetry are present:

\[ \mathcal{F}_n(k) = \mathcal{F}_n(-k) \]  
\text{inversion}  

\[ \mathcal{F}_n(k) = -\mathcal{F}_n(-k) \]  
\text{Time-reversal}  

\[ \mathcal{F}_n(k) = 0 \]
gapless graphene:

- when Berry curvature vanishes, Berry phase is Z2 topological invariant of 1D path in k-space:

\[ e^{i \oint \mathbf{A} \cdot d\mathbf{k}} = -1 \]

Euclidean metric \( d_{kk'}^2 = |k - k'|^2 \)

(or \( \min_{G} |k - k' + G|^2 \))
The conduction and valence bands combine into a single smooth genus-3 manifold in the Hilbert space picture,

Brillouin zone is torus (genus 1)

Genus 3 manifold (two bands joined by two Dirac points)
“Pseudospin conservation” and the “quantum distance” (Fubini-Study metric)

- Since the Berry curvature field vanishes, the only remaining ingredient of the “quantum geometry” is the metric $\mathcal{G}$ which measures quantum distance.

- Significance: semiclassical (long-wavelength) scattering processes are **suppressed when there is a large “quantum distance” between initial and final states.** THIS IS THE “PSEUDOSPIN CONSERVATION” near the Dirac points.
when more bands are included, geodesics are no longer null, metric becomes positive definite

spatial positions of the orbitals must be correctly assigned to give the correct geodesics
mass generation

- I will forget spin and superconductivity (leave full classification of 56 mass terms to C. Chamon!)

- Breaking inversion or translation (Kekule) leads to “boring” semiconduction.

- Breaking T (FDMH 1988) leads to “zero-field QHE” or “Chern insulator”.

- QHE comes from **Berry curvature** of the $k$-space Bloch-state band-structure, not Bohm-Aharonov in real space.

- This model has proved very useful for studying anomalous Hall efect, and **more recently provided the initial building block for topological insulator models**:

- Has extensions to photonics (“one-way light”) (FDMH and Raghu.), now experimentally realized at MIT (Joanopoulos group).
2D zero-field Quantized Hall Effect


- 2D quantized Hall effect: $\sigma^{xy} = \nu e^2/h$. In the absence of interactions between the particles, $\nu$ must be an integer. There are no current-carrying states at the Fermi level in the interior of a QHE system (all such states are localized on its edge).

- The 2D integer QHE does NOT require Landau levels, and can occur if time-reversal symmetry is broken even if there is no net magnetic flux through the unit cell of a periodic system. (This was first demonstrated in an explicit “graphene” model shown at the right.)

- Electronic states are “simple” Bloch states! (real first-neighbor hopping $t_1$, complex second-neighbor hopping $t_2 e^{i\phi}$, alternating onsite potential $M$.)

FIG. 1. The honeycomb-net model (“2D graphite”) showing nearest-neighbor bonds (solid lines) and second-neighbor bonds (dashed lines). Open and solid points, respectively, mark the $A$ and $B$ sublattice sites. The Wigner-Seitz unit cell is conveniently centered on the point of sixfold rotation symmetry (marked “*”) and is then bounded by the hexagon of nearest-neighbor bonds. Arrows on second-neighbor bonds mark the directions of positive phase hopping in the state with broken time-reversal invariance.

FIG. 2. Phase diagram of the spinless electron model with $|t_2/t_1| < \frac{1}{3}$. Zero-field quantum Hall effect phases ($\nu = \pm 1$, where $\sigma^{xy} = \nu e^2/h$) occur if $|M/t_2| < 3\sqrt{3}|\sin \phi|$. This figure assumes that $t_2$ is positive; if it is negative, $\nu$ changes sign. At the phase boundaries separating the anomalous and normal ($\nu = 0$) semiconductor phases, the low-energy excitations of the model simulate undoubled massless chiral relativistic fermions.
Landau levels of a single Dirac equation (as a function of B)

- massless case

- massive case
add the two Dirac points
(spinless case, double it to include spin)

Broken Inversion symmetry

Broken time-reversal symmetry (QHE)
• bulk bands are separated, upper and lower bands have opposite chern number

• spectral flow between bands through edge states.
chiral edge states (QHE)
2D Topological insulator edge states (unbroken T-reversal symmetry)

Topological Insulators (Kane + Mele)

Spin ↑

Spin ↓

+ Rashba SOC
Still stable!
(kramers degeneracy)

T-invariant

two conjugate copies of model, (Kane and Mele)

The 2D “Chern insulator” is the first of the “topological insulator” models, though a physical realization has not yet been found.
Graphene model with complex second neighbor hopping is very useful!

- Quantum Hall effect with simple Bloch states
- Used for anomalous Hall effect studies (Nagaosa), add disorder etc.
- used for testing/developing fundamental band-structure formulas for orbital magnetization (Vanderbilt)
- Quantum Spin Hall effect (Kane and Mele)
- Analog system for photonic edge states (Haldane and Raghu)
quantum Hall effect vs Photonics
(with S. Raghu)

- Quantum Hall effect:
  - involves charged interacting fermions (electrons) in strong magnetic fields (Landau levels) in an incompressible collective quantum state.

- Photonics (photon band gap materials, etc)
  - involves neutral non-interacting non-conserved bosons (photons) propagating as waves: not really “quantum”, and definitely not incompressible!

Superficially, it seems unlikely that there could be any similarities between the two systems!
• The **integer** quantum Hall effect (as opposed to the **fractional** one discovered by Tsui and Stormer 1982) can be understood in terms of non-interacting electrons (plus the Pauli principle)

• The quantum Hall effect requires broken time reversal symmetry, but not necessarily a uniform magnetic flux: (it can occur without Landau levels, with “simple” Bloch states (**zero-field quantum Hall effect**)

• One aspect of the integer QHE (”Chiral” edge states) does not need the Pauli principle, and is a “band-structure” property!

**THE EDGE STATES WILL SURVIVE IN PHOTONICS!**
Wall between two quantum Hall regions of opposite sign

Two chiral edge modes, one associated with each Dirac point
Photonic bands (2D array of dielectric rods)
side view of dirac points
with faraday, no wall
edge modes!
• need to get a thin slab, with a gap around Dirac point for all modes

• one-way transmission, no elastic reflection at bends

• unlike electrons, photons can be absorbed

• Faraday effect is weak. Magneto-optical coupling better....

• but interesting possibilities for “Berry phase engineering”
Analogs of quantum Hall edge states in photonic crystals

- Predicted theoretically that using magnetooptic (time-reversal-breaking) materials, photonic analogs of electronic quantum Hall systems could be created where topologically-protected edge modes allow light to only travel along edges in one direction, with no possibility of backscattering at obstacles!

- Effect was experimentally confirmed recently at MIT (Wang et al., Nature 461, 775 (8 October 2009)).

- Obvious potential for technological applications! (one-way loss-free waveguides)

Figure 2 | Photonic CESs and effects of a large scatterer. a, CES field distribution ($E_z$) at 4.5 GHz in the absence of the scatterer, calculated from finite-element steady-state analysis (COMSOL Multiphysics). The feed (from Wang et. al)