Topological Properties of Quantum States of Condensed Matter: some recent surprises.

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I. Berry phases, zero-field Hall effect, and "one-way light"

II. Anomalous and Spin Hall effect, Topological insulators

III. Non-abelian FQHE states

Berry curvature and dynamics of Bloch electrons

- anomalous velocity (Karplus and Luttinger 1957)

Lorentz force

$$\hbar \frac{d\boldsymbol{k}}{dt} = e\left(\boldsymbol{E}(\boldsymbol{r}) + \frac{d\boldsymbol{r}}{dt} \times \boldsymbol{B}(\boldsymbol{r})\right)$$

$$\frac{d\boldsymbol{r}}{dt} = \frac{1}{\hbar}\boldsymbol{\nabla}_k \varepsilon_n(\boldsymbol{k}) + \frac{d\boldsymbol{k}}{dt} \times \boldsymbol{\Omega}_n(\boldsymbol{k})$$

a band-structure property distinct from the energy bands (Berry curvature)

group velocity

The “anomalous velocity” is absent if time-reversal **and** inversion symmetry are **both** present.

alternate notation (used here)

$$\mathcal{F}_n^{ab}(\boldsymbol{k}) = \epsilon^{abc}(\Omega_n(\boldsymbol{k}))_c$$

- The Karplus-Luttinger term was derived from a Kubo fomula, and gives rise to the “intrinsic” part of the anomalous Hall effect in ferromagnetic metals.
- It was very controversial, and dismissed as deriving from an “obvious error” by a number of authors at the time, who felt it violated “fundamental principles”
- A modern interpretation (Sundaram and Niu 1999) identifies it as the effect of the “Berry curvature”.

symplectic form (collect time derivatives on left hand side of equation)

$$\begin{pmatrix} \frac{e}{\hbar}F_{ab} & -\delta_a^b \\ \delta_b^a & \mathcal{F}_n^{ab} \end{pmatrix} \frac{d}{dt} \begin{pmatrix} r^b \\ k_b \end{pmatrix} = \frac{1}{\hbar} \begin{pmatrix} \nabla_a \mathcal{H} \\ \nabla_k^a \mathcal{H} \end{pmatrix}$$

antisymmetric matrix

$$\det = 1 + \frac{e}{\hbar} F_{ab} \mathcal{F}_n^{ab}$$

$$= 1 + \frac{e}{\hbar} \epsilon_{abc} \mathcal{F}_n^{ab}(\boldsymbol{k}) B^c$$

$$\mathcal{H}(\boldsymbol{r}, \boldsymbol{k}) = \varepsilon_n(\boldsymbol{k}) + eV(\boldsymbol{r})$$

$$F_{ab}(\boldsymbol{r}) = \nabla_a A_b(\boldsymbol{r}) - \nabla_b A_a(\boldsymbol{r})$$

magnetic field

$$\mathcal{F}_n^{ab}(\boldsymbol{k}) = \nabla_k^a \mathcal{A}_n^b(\boldsymbol{r}) - \nabla_k^b \mathcal{A}_n^a(\boldsymbol{k})$$

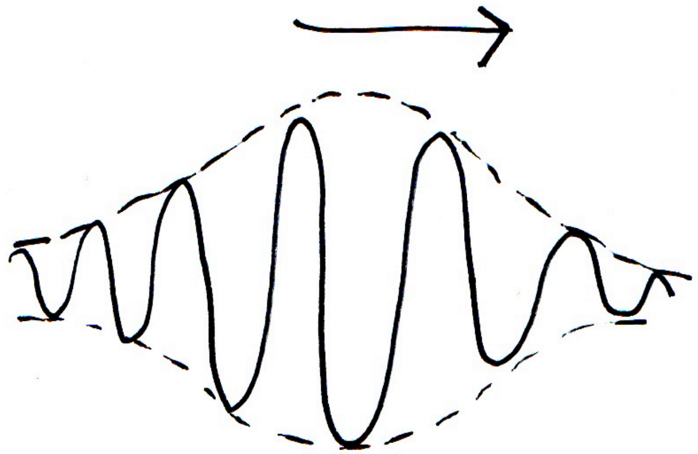
Berry curvature

modified Phase-space volume element!

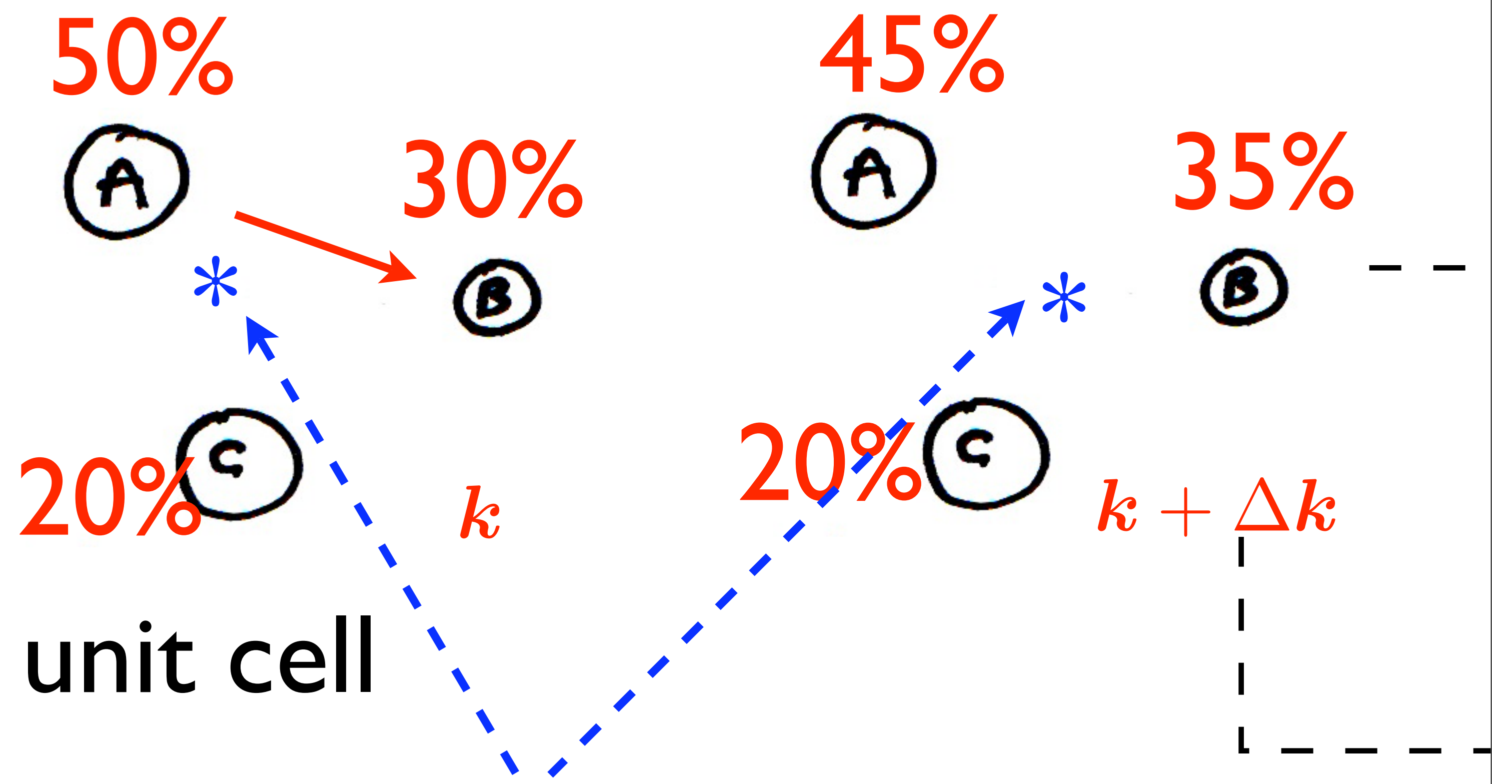
- The symplectic form identifies the conserved phase-space volume element (Louiville theorem) (to lowest order in B) as

$$\frac{1}{(2\pi)^3}\int_{\mathrm{BZ}} d^3\boldsymbol{k}\int d^3\boldsymbol{r}\left(1+\frac{e}{\hbar}\epsilon_{abc}\mathcal{F}(\boldsymbol{k})_n^{ab}B^c(\boldsymbol{r})\right)$$

(Xiao,Shi, and Niu,2006)



group velocity is motion of
<u>envelope</u> of wavepacket

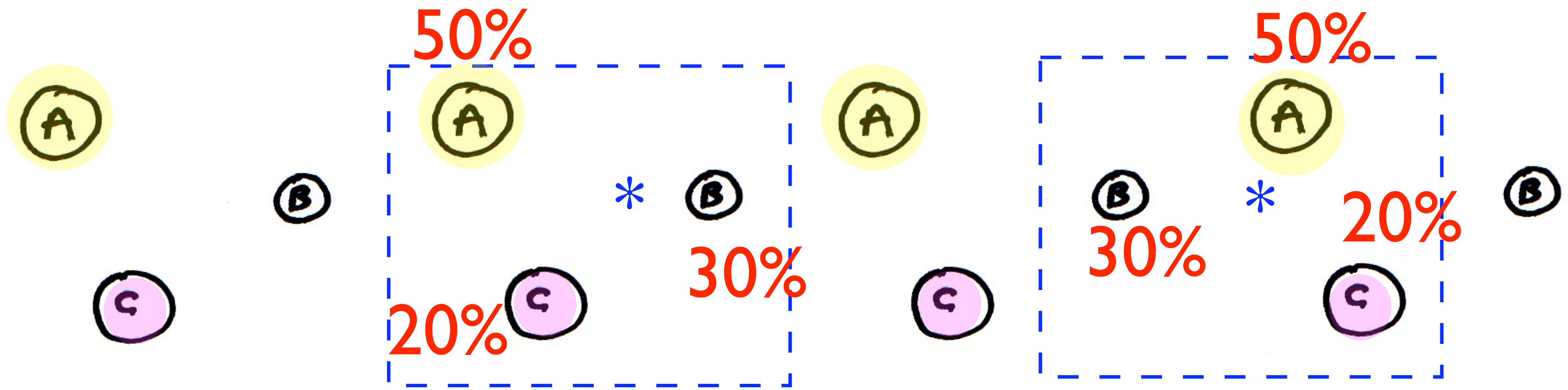


- anomalous velocity is motion of "average position of electron in unit cell" (with more than one orbital in the cell)

- as k changes (wavepacket is accelerated), "average position" $*$ in unit cell moves, relative amplitude on different orbitals (diferent atoms) changes.

- This internal motion is the "anomalous velocity".

Ambiguity of the "mean position in the unit cell"



- The "average position" depends on the (arbitrary) choice of unit cell.
- <u>Displacements</u> and <u>velocity</u> of the "average position" are unambiguous.

The Berry connection and curvature.

$$|\Psi_n(\boldsymbol{k})\rangle = \sum_{\boldsymbol{R},i} a_{n,i}(\boldsymbol{k}) e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{r}_i)} |\boldsymbol{R}, i\rangle$$

Bloch state

positions of orbitals inside unit cell

unit cell

orbitals inside unit cell

$$|\Psi_n(\boldsymbol{k})\rangle \rightarrow e^{i\chi_n(\boldsymbol{k})}|\Psi_n(\boldsymbol{k})\rangle$$

"Berry gauge" transformation

$$\mathcal{A}_n^a(\boldsymbol{k}) = -i\langle\Psi_n(\boldsymbol{k})|\nabla_k^a \Psi_n(\boldsymbol{k})\rangle$$

<u>Berry connection</u>
(analog of vector potential in k-space)

$$\mathcal{A}_n^a(\boldsymbol{k}) \rightarrow \mathcal{A}_n^a(\boldsymbol{k}) + \nabla_k^a \chi_n(\boldsymbol{k})$$

effect of "Berry gauge" transformation

non-commutative geometry of the "average position" in the unit cell:

- formal operator involves the Berry connection:

$$r_n^a = -i\nabla_k^a - \mathcal{A}_n^a(\boldsymbol{k})$$

Berry curvature

- commutation relation:

$$[r_n^a, r_n^b] = i\mathcal{F}_n^{ab}(\boldsymbol{k}) \quad \equiv i(\nabla_k^a \mathcal{A}_n^b(\boldsymbol{k}) - \nabla_k^b \mathcal{A}_n^a(\boldsymbol{k}))$$

- compare to

$$k_a = -i\nabla_a - ieA_a(\boldsymbol{r})/\hbar \qquad [k_a, k_b] = ieF_{ab}(\boldsymbol{r})/\hbar$$

electromagnetic vector potential

significance of the Berry curvature

$$\mathcal{F}_n^{ab}(\boldsymbol{k}) = \epsilon^{abc}(\Omega_n(\boldsymbol{k}))_c$$

- It is gauge invariant.
- It depends not just on the Hamiltonian, but on how it is embedded in (Euclidean) space.
- This means that it contains information about how the electron system responds to uniform electromagnetic fields:

$$H_0 = \sum_{\boldsymbol{r},\boldsymbol{r}'} h(\boldsymbol{r},\boldsymbol{r}')|\boldsymbol{r}\rangle\langle\boldsymbol{r}'| \qquad H(t) = \sum_{\boldsymbol{r},\boldsymbol{r}'} h(\boldsymbol{r},\boldsymbol{r}')e^{i\phi(\boldsymbol{r},\boldsymbol{r}',t)}|\boldsymbol{r}\rangle\langle\boldsymbol{r}'|$$

$$\phi(\boldsymbol{r},\boldsymbol{r}',t) = (e/\hbar)\left(\boldsymbol{E}\cdot(\boldsymbol{r}-\boldsymbol{r}')t + \tfrac{1}{2}\boldsymbol{B}\cdot\boldsymbol{r}\times\boldsymbol{r}'\right)$$

time-reversal (T) and inversion symmetry (I)

- if either (antiunitary) T or (unitary) I is unbroken,

$$\varepsilon_n(\boldsymbol{k}) = \varepsilon_n(-\boldsymbol{k})$$

- if (antiunitary) T is unbroken,

$$\mathcal{F}_n^{ab}(\boldsymbol{k}) = -\mathcal{F}_n^{ab}(-\boldsymbol{k})$$

- if (unitary) I is unbroken,

$$\mathcal{F}_n^{ab}(\boldsymbol{k}) = +\mathcal{F}_n^{ab}(-\boldsymbol{k})$$

- if both (antiunitary) T and (unitary) I is unbroken,

$$\mathcal{F}_n^{ab}(\boldsymbol{k}) = 0$$

k-space analogs of electromagnetic quantities:

- Berry phase as analog of Bohm-Aharanov phase:

$$e^{i\phi_{BA}(\Gamma)} = \exp i(e/\hbar) \oint_{\Gamma} A_a(\boldsymbol{r}) dr^a$$

measures magnetic flux through a closed path in real space

$$e^{i\phi_{B}(\Gamma')} = \exp i \oint_{\Gamma'} \mathcal{A}^a(\boldsymbol{k}) dk_a$$

measures "Berry flux" through a closed path in k-space

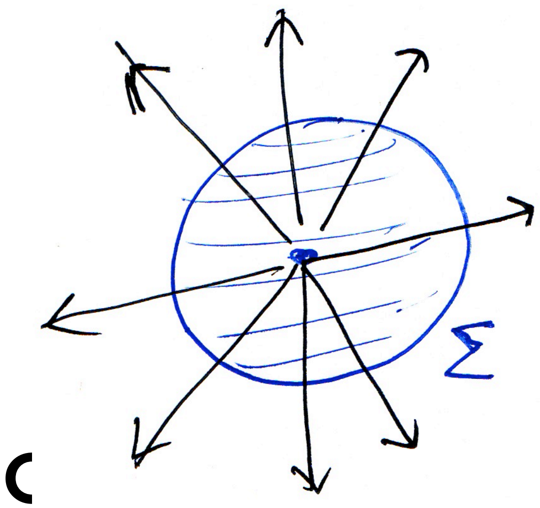
e.g.: The Berry phase around closed constant energy paths in k-space can give a correction to Landau-level quantization in a uniform magnetic field.

Chern number and Dirac monopole quantization:

$$(e/\hbar)\int_{\Sigma} d^2 r_a B^a(\boldsymbol{r}) \equiv (e/\hbar)\int_{\Sigma} d^2 F = 2\pi \times \text{integer}$$

$$d^2 r_a \equiv \tfrac{1}{2}\epsilon_{abc}\, dr^b \wedge dr^c \qquad d^2 F \equiv \tfrac{1}{2} F_{ab}\, dr^a \wedge dr^b$$

$$\int_{\Sigma'} d^2\mathcal{F} = 2\pi \times \text{integer} \qquad d^2\mathcal{F} \equiv \tfrac{1}{2}\mathcal{F}^{ab}_n(\boldsymbol{k})\, dk_a \wedge dk_b$$



- This is the integrated flux through any closed 2-manifold in k-space
- The 2D Brillouin zone (BZ) is a 2-torus, so the integral of Berry curvature over the 2D BZ is 2π times the (integer) Chern number.

- this works because by Stokes theorem, the Berry phase is given by

$$e^{i\phi_B(\Gamma)} = \exp i \oint_\Gamma \mathcal{A}^a(\boldsymbol{k}) dk_a = \exp i \int_\mathcal{M} d^2 F \qquad \Gamma = \partial\mathcal{M}$$

$\mathcal{M}$ Γ

$$\exp i \int_{\mathcal{M}-\mathcal{M}'} d^2\mathcal{F} = \exp i \int_\Sigma d^2\mathcal{F} = 1$$

where Σ is a closed 2-manifold.

where is any 2-surface bounded by the closed path

Chern invariants of non-degenerate bands:

(these vanish if time-reversal symmetry is present)

- 2D case, k-space = (k_x,k_y) :

$$\frac{1}{2\pi}\int_{2DBZ} dk_x dk_y \mathcal{F}_n^{xy} = C_n$$

2D integer QHE

chern number

- 3D case: the intersection of 3D bands with 2D plane normal to a lattice translation is a 2D bandstructure. If the band is non-degenerate, Gauss law is obeyed (no monopoles), so.

$$\frac{1}{2\pi}\int_{3DBZ} d^3k\, \mathcal{F}_n^{ab} = C_n \epsilon^{abc} (G_n^0)_c$$

a primitive reciprocal vector, (which indexes a family of lattice planes)

chern number

3D integer QHE = 2D integer QHE on each plane

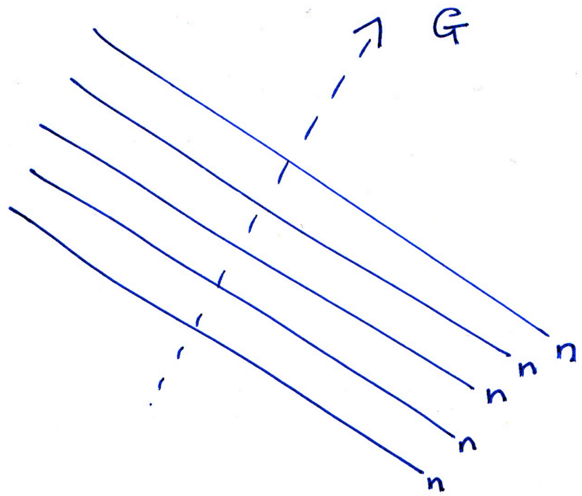
Quantum Hall effect:

- number of states in a filled band varies with B!

$$\frac{d(N/V)}{dB^a} = \frac{e}{\hbar}\epsilon_{abc}\frac{1}{(2\pi)^3}\int_{\mathrm{BZ}} d^3\boldsymbol{k}\mathcal{F}_n^{bc}(\boldsymbol{k})$$

- By the Streda formula, if there is a gap at the Fermi level,

$$\sigma_H^{ab} = \frac{e^2}{h}\frac{\epsilon^{abc}}{2\pi}\sum_{n(\mathrm{occ})} C_n(G_n^0)_c$$



(this is an integer 2D QHE in each plane of a family of parallel lattice planes)

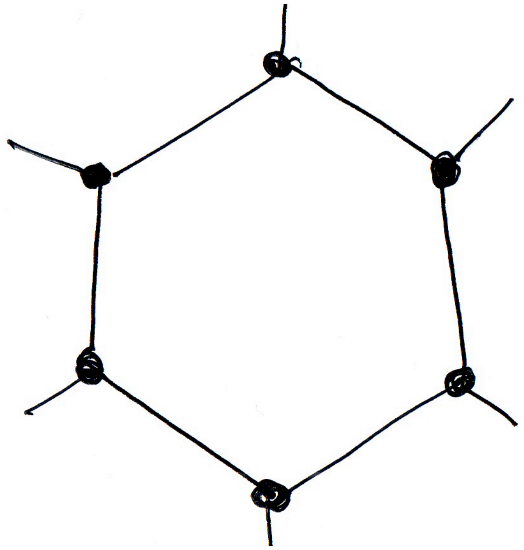
Accidental degeneracies

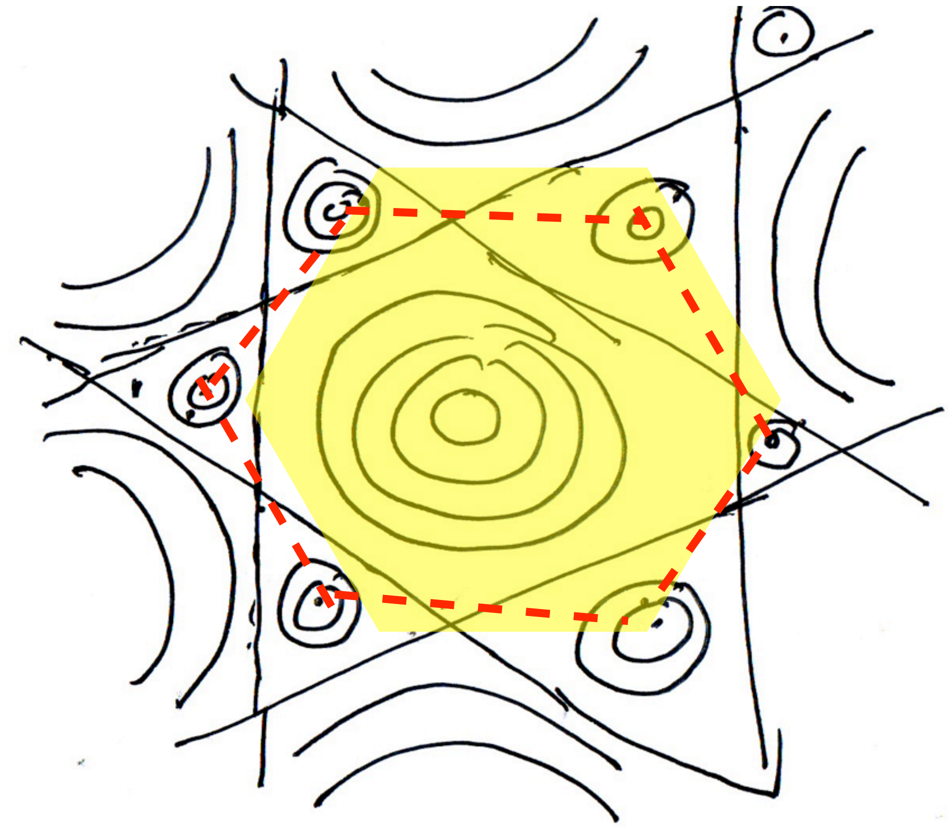
- Three generic classes:
- “orthogonal”: hamiltonian “is real symmetric” : NO Berry curvature; vary TWO parameters to find an “accidental degeneracy” between levels
- “unitary”: hamiltonian is complex, has Berry curvature, vary THREE parameters to find an “accidental” degeneracy between levels
- “symplectic” (Kramers degeneracy), vary FIVE parameters to find an “accidental” degeneracy between two Kramers doublets
- First case: time-reversal symmetry without spin-orbit coupling, third case, time-reversal symmetry with spin-orbit coupling.

topologically-stable “Dirac points” occur at “accidental” degeneracies between bands.

A simple model 2D bandstructure.

- “Graphene”:





has spatial inversion and time-reversal symmetry

Two distinct “Dirac points” at BZ corners.

why does graphene have two Dirac points?

- (a) because the corners of the BZ have threefold symmetry, and degenerate bands make doublet representation of C3v point group?
- NO, because Dirac points dont disappear when three-fold rotation symmetry is broken! - they just move to generic points (related by inversion symmetry).
- correct answer: because time-reversal symmetry and inversion symmetry are unbroken, and no spin-orbit coupling: ("orthogonal" case, vary TWO parameters, kx, ky, to find an "accidental" degeneracy.)
- Immediately destroyed (gap opens) if EITHER of these two symmetries is broken! THEN GET UNITARY CASE.

2D zero-field Quantized Hall Effect

FDMH, Phys. Rev. Lett. 61, 2015 (1988).

- 2D quantized Hall effect: $\sigma^{xy} = \nu e^2/h$. In the absence of interactions between the particles, ν 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 $t_2 e^{i\varphi}$, alternating onsite potential M.)

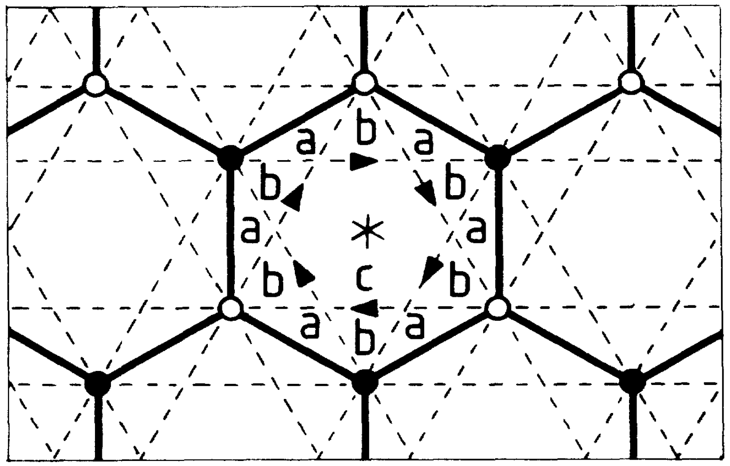


FIG. 1. The honeycomb-net model ("2D graphite") showing nearest-neighbor bonds (solid lines) and second-neighbor bonds (dashed lines). Open and solid points, respectively, mark the A and B sublattice sites. The Wigner-Seitz unit cell is conveniently centered on the point of sixfold rotation symmetry (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.

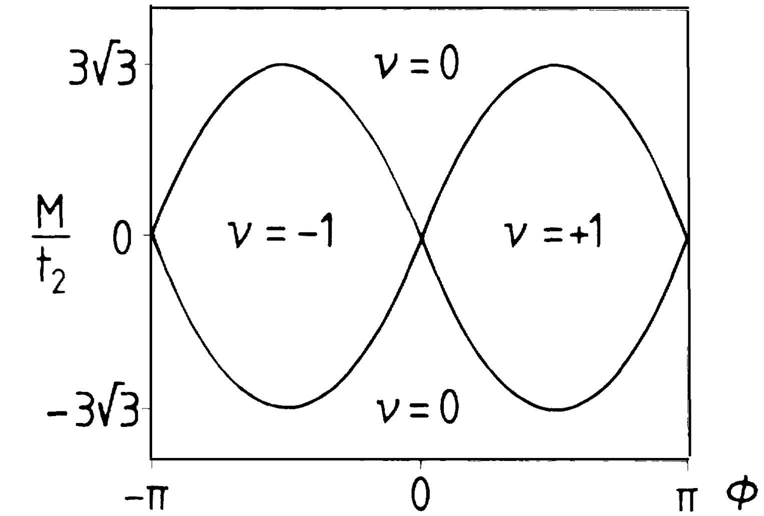
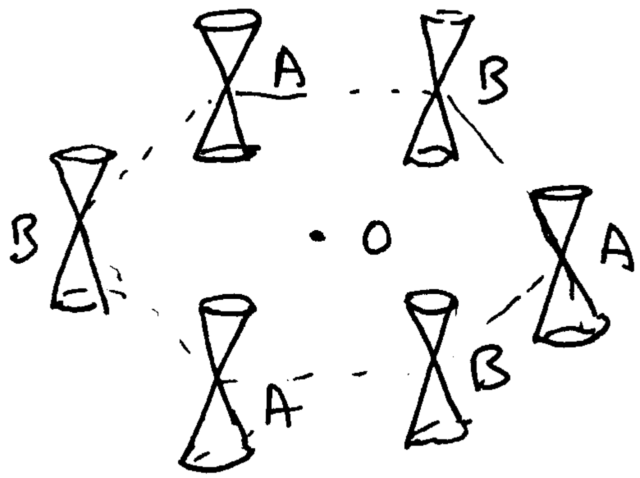
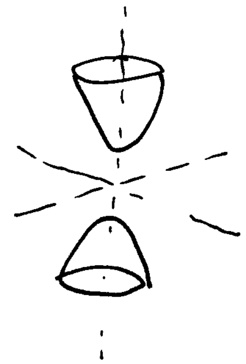


FIG. 2. Phase diagram of the spinless electron model with $|t_2/t_1| < \frac{1}{3}$. Zero-field quantum Hall effect phases ($\nu = \pm 1$, where $\sigma^{xy} = \nu e^2/h$) occur if $|M/t_2| < 3\sqrt{3}|\sin\phi|$. This figure assumes that t_2 is positive; if it is negative, ν changes sign. At the phase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

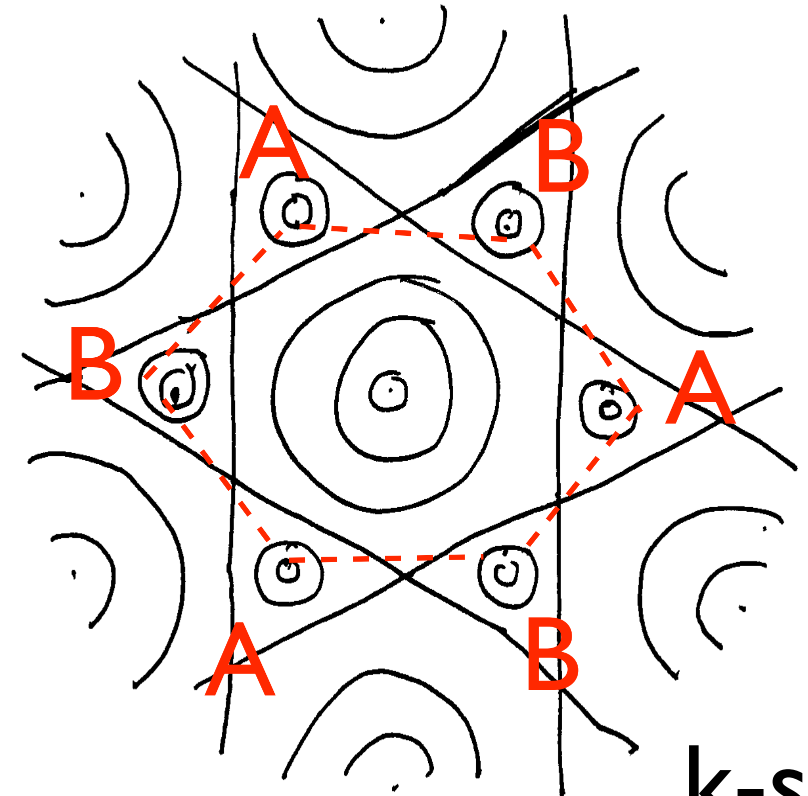
2D “graphene” bandstructure



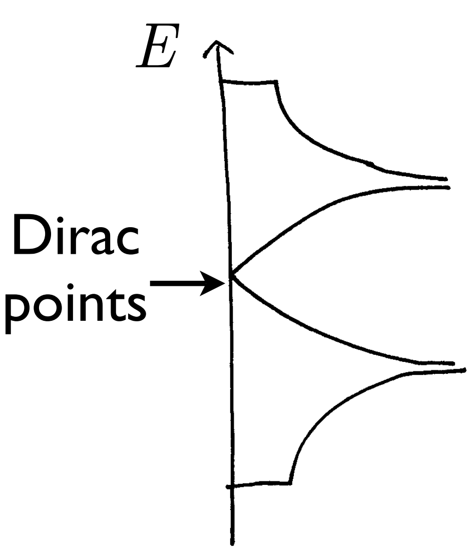
two distinct “Dirac points” (at corners of hexagonal Brillouin zone)



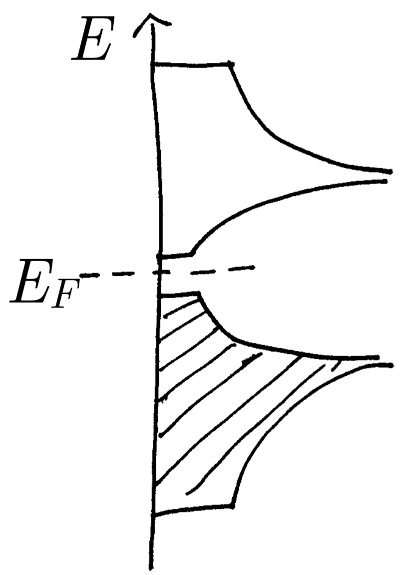
Breaking either inversion (I) or time-reversal (T) symmetry opens a “mass gap” at Dirac points.)



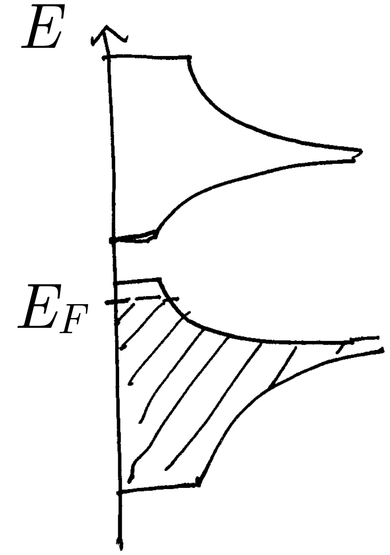
k-space



density of states (massless)



massive case (bulk insulator)



massive case (bulk metal)

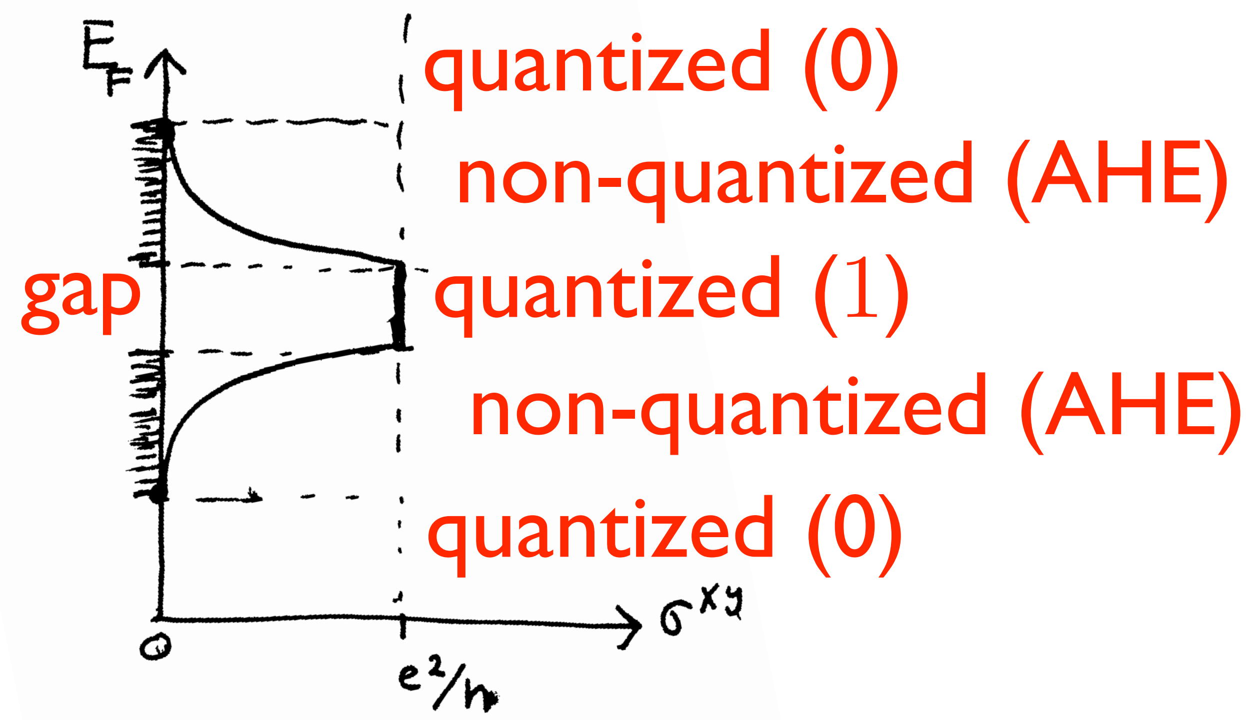
Break only T: $m_A = m_B$

same sign Berry curvature near A and B points

Break only I: $m_A = -m_B$

opposite sign Berry curvature near A and B points

- Intrinsic (Karplus Luttinger) Hall conductivity interpolates between quantized Hall conductance from edge states



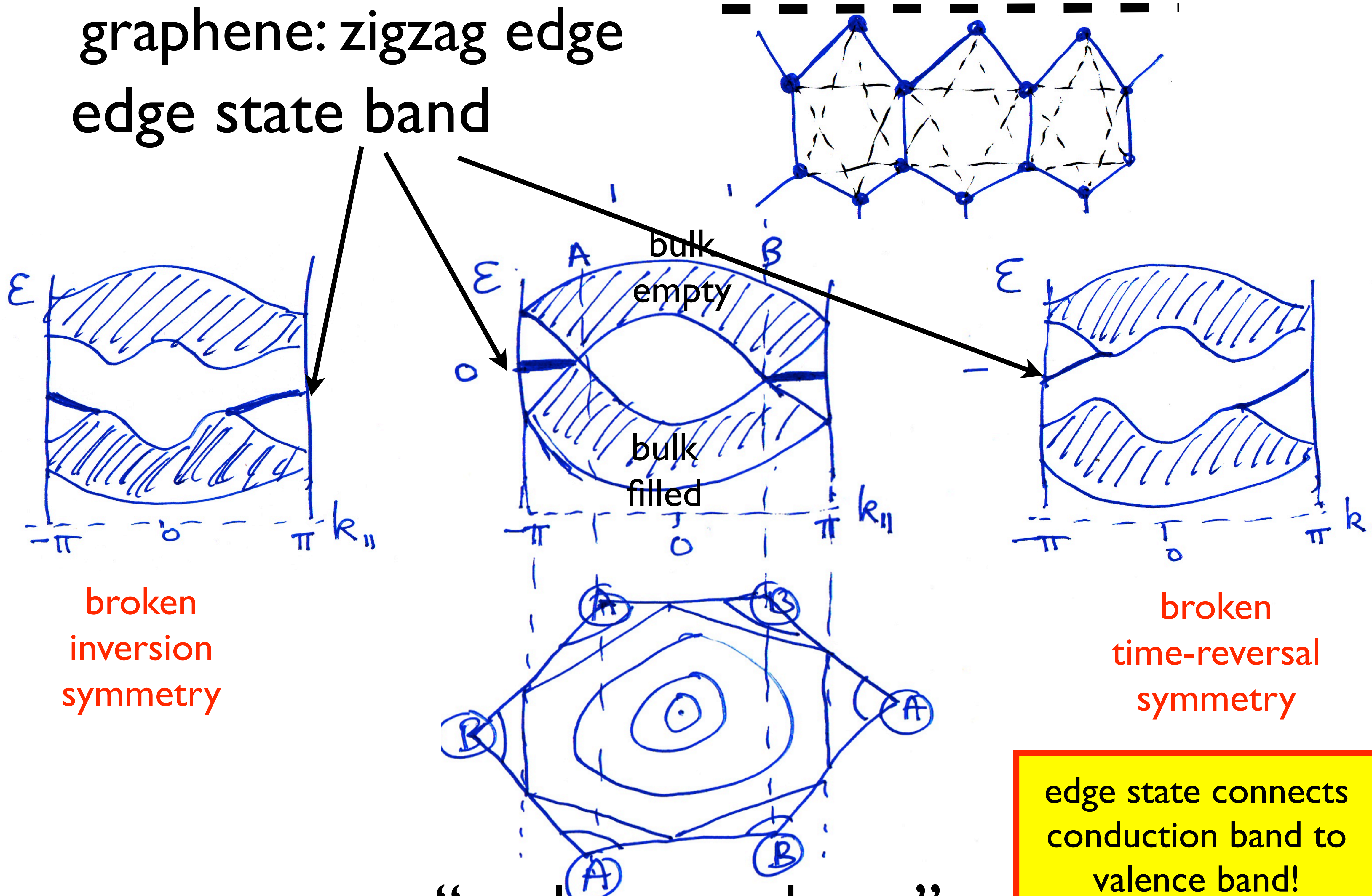
Graphene model with second neighbor hopping is very useful!

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

- Unitary case: 2π Berry flux “monopole” in three parameter space.
- If parameters are kx, ky, and the “mass” (gap) parameter, total “flux” π passes through the k-plane “near” the weakly-gapped Dirac point. These points dominate the Chern number integral.

graphene: zigzag edge

edge state band



broken
inversion
symmetry

broken
time-reversal
symmetry

"gapless graphene"

edge state connects
conduction band to
valence band!

quantum Hall effect vs Photonics

- Quantum Hall effect:

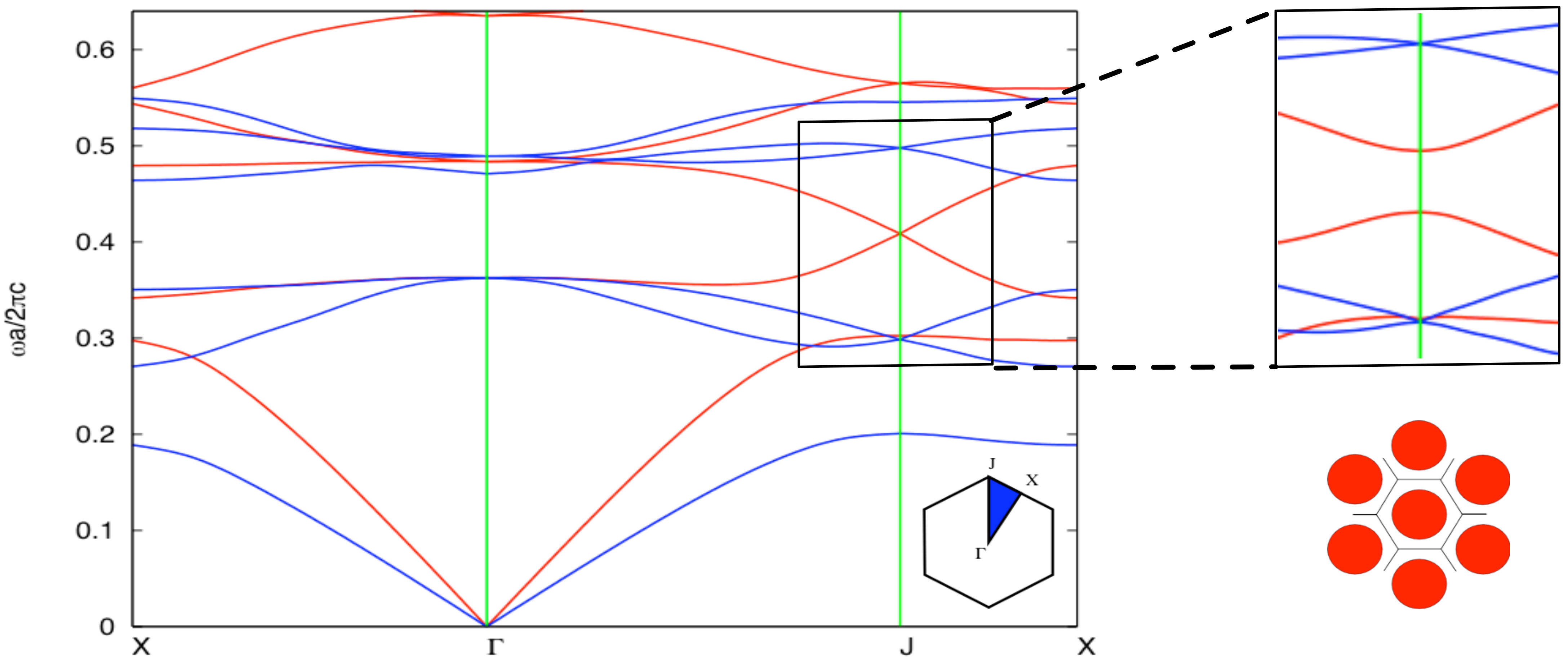
  - involves charged interacting fermions (electrons) in strong magnetic fields (Landau levels) in an incompressible collective quantum state.

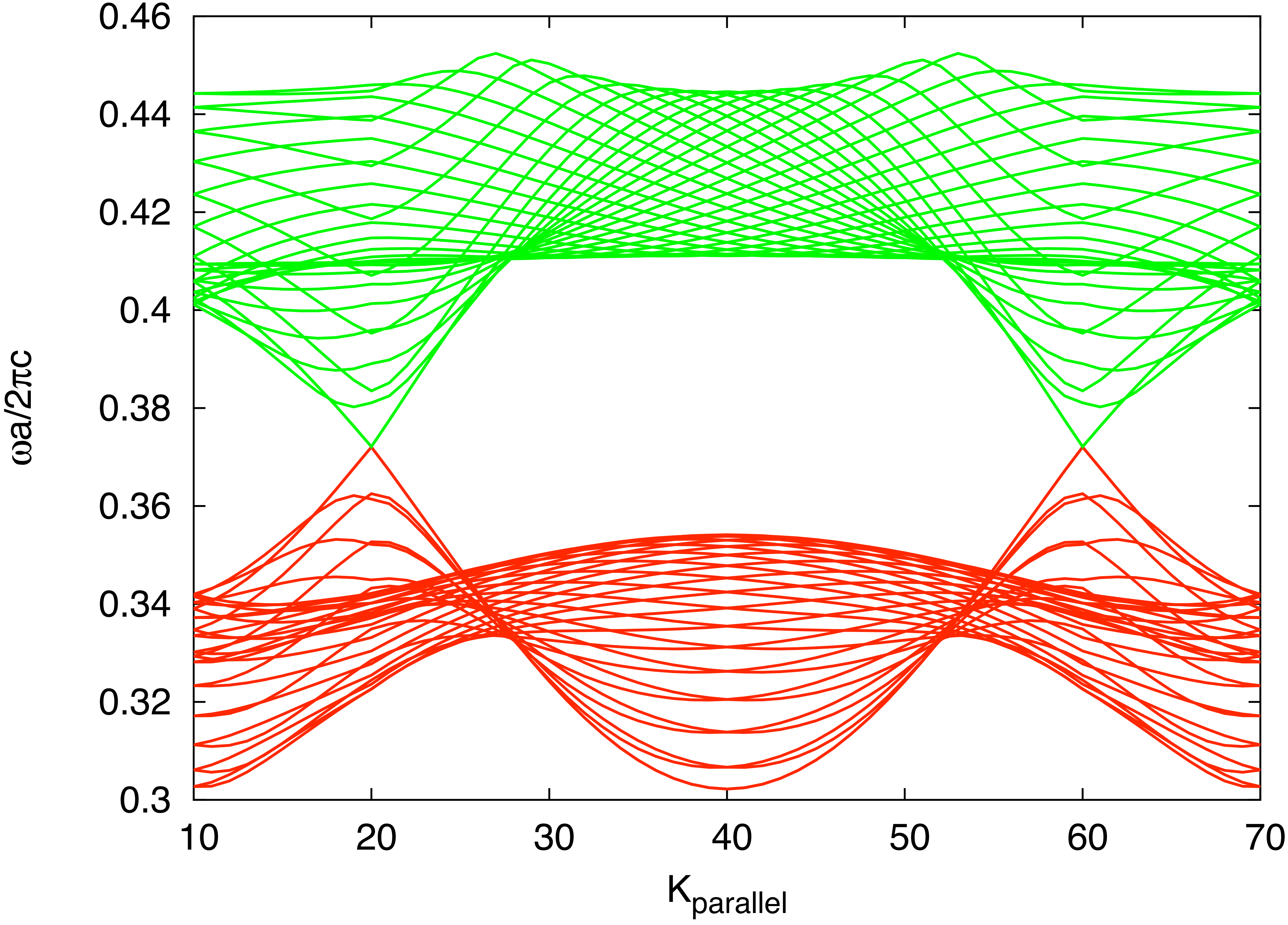
- Photonics (photon band gap materials, etc)

  - involves neutral non-interacting non-conserved bosons (photons) propagating as waves: not really "quantum", and definitely not incompressible!

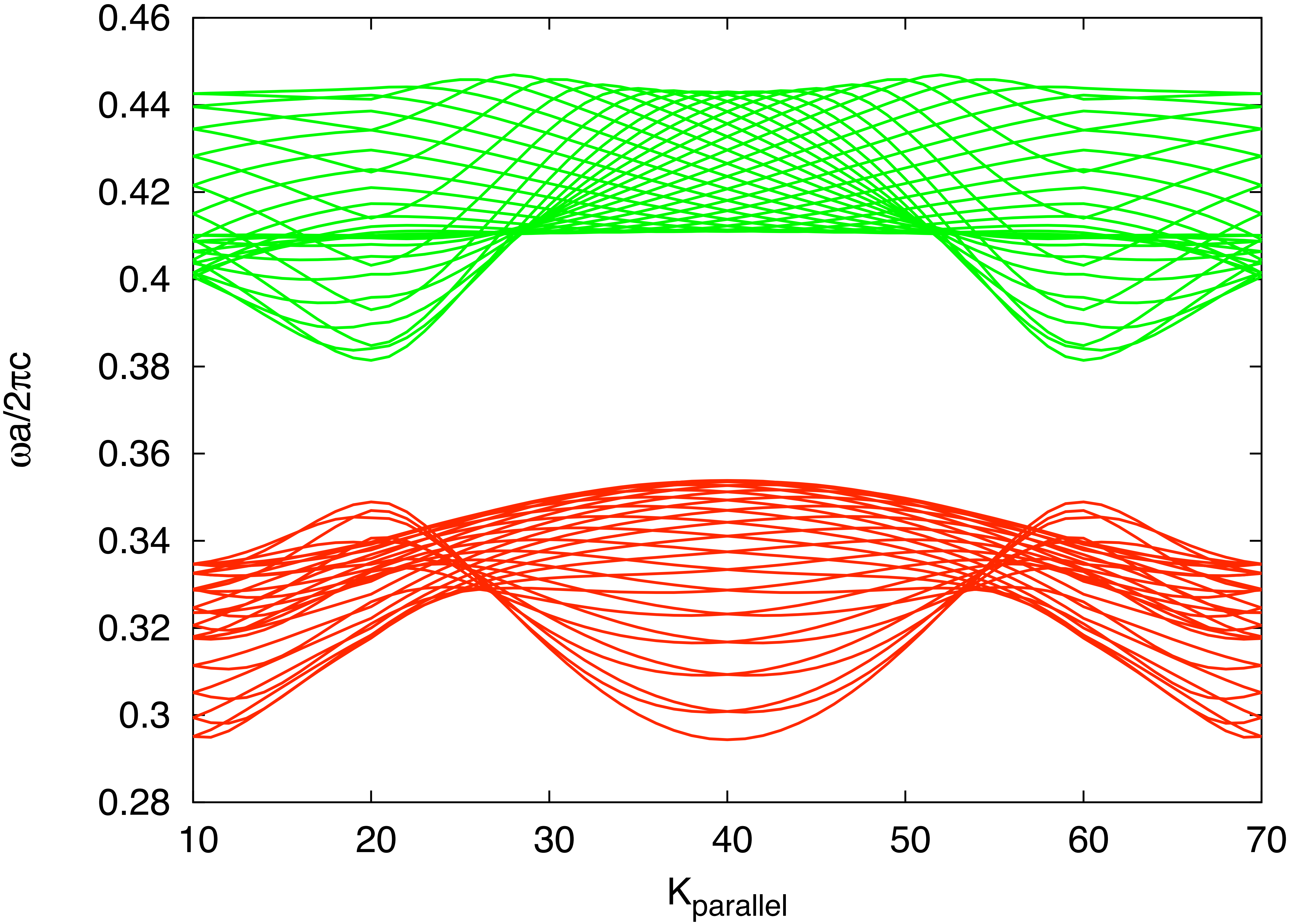
Superficially, it seems unlikely that there could be any similarities between the two systems!

Photonic bands (2D array of dielectric rods)

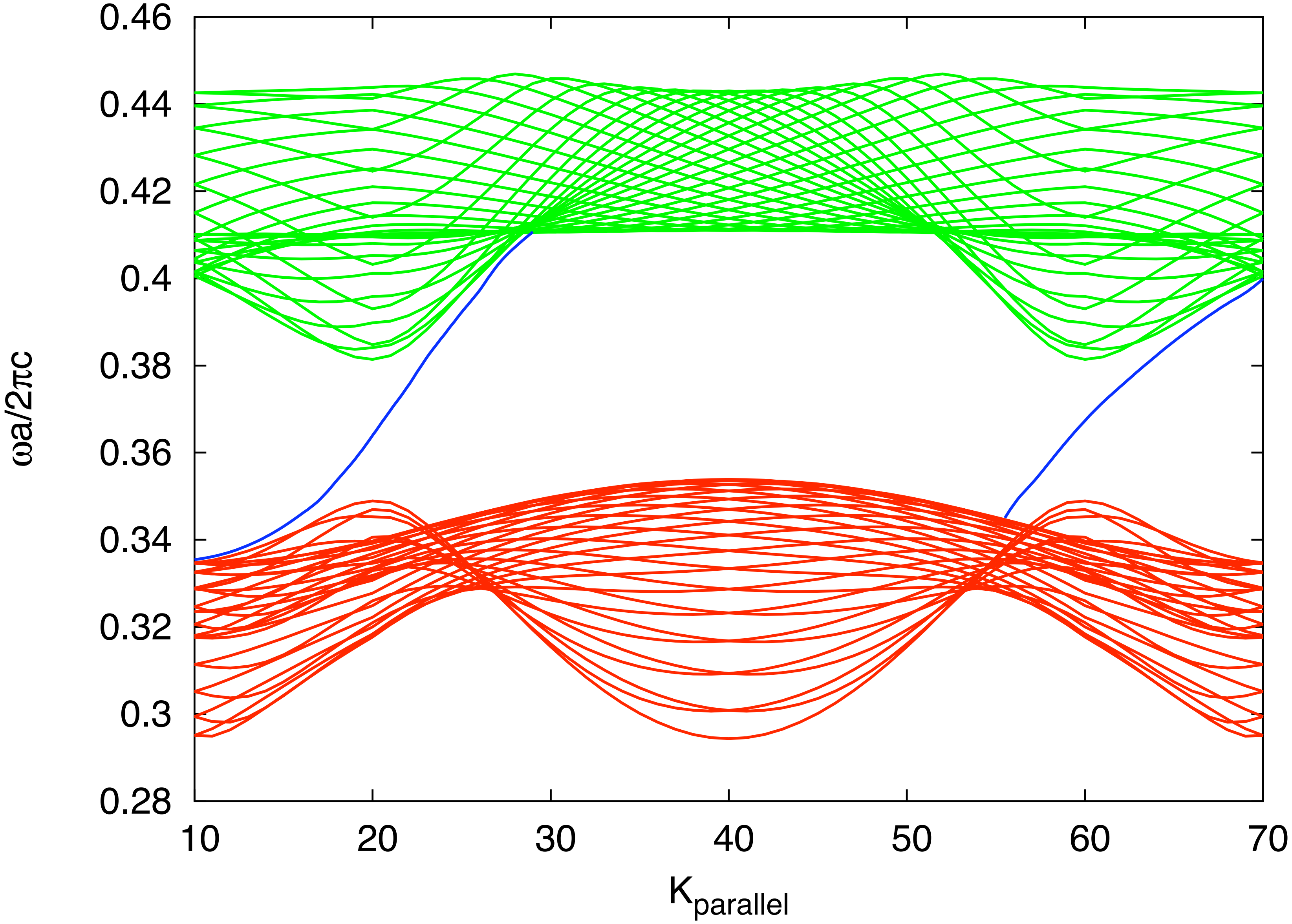




side view of dirac points

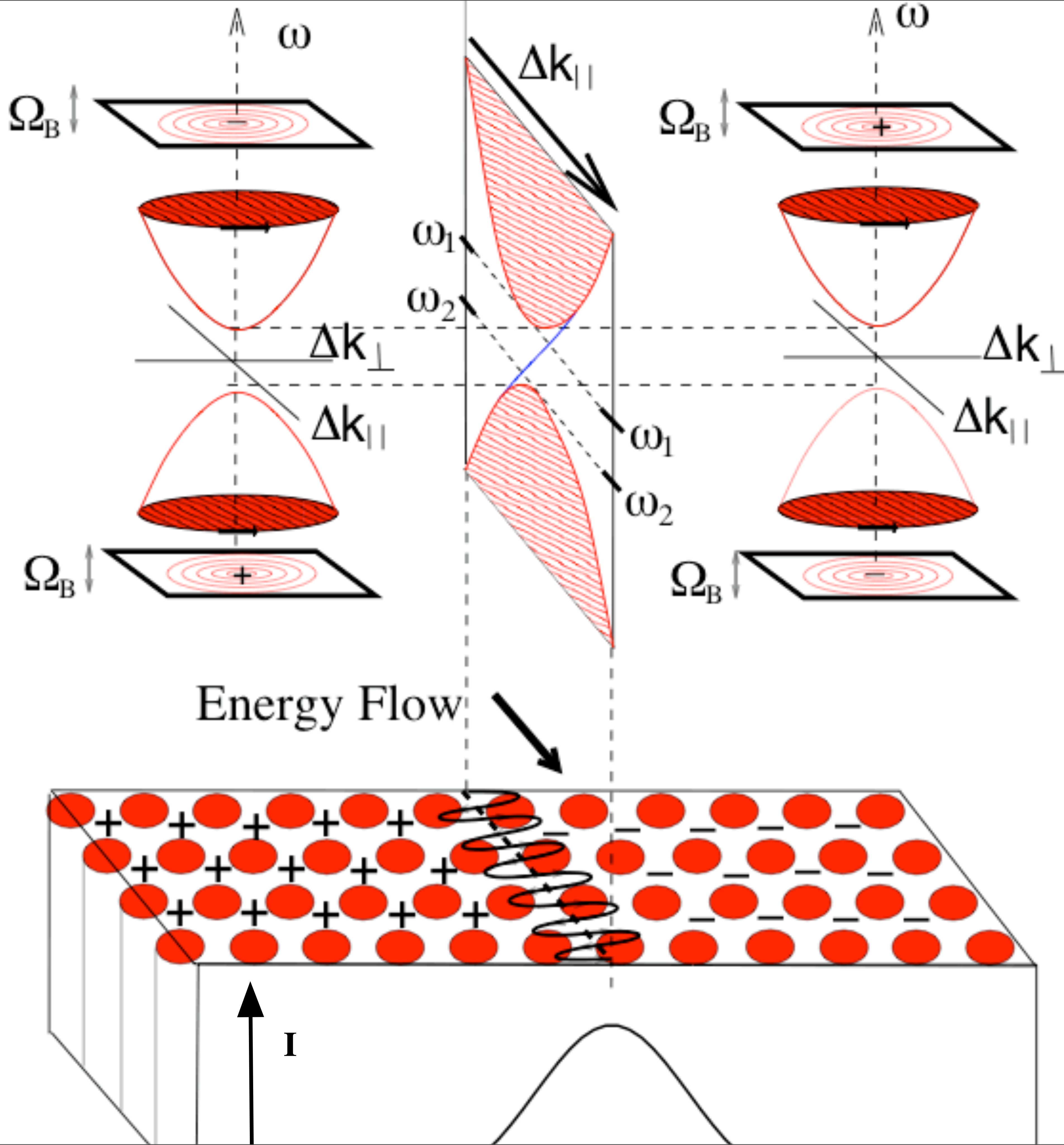


with faraday, no wall



0.46
0.44
0.42
0.4
0.38
0.36
0.34
0.32
0.3
0.28
ωa/2πc
10
20
30
40
50
60
70
Kparallel

edge modes!


ω
Ω_B
Δk_||
Δk_⊥
ω_1
ω_2
Energy Flow
I

- 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...
- but interesting possibilities for “Berry phase engineering”
- Berry phases also from broken inversion, but no edge modes