Lattice theory of condensed matter

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Why study condmat systems?

They are very similar to relativistic strongly coupled QFT

- Dirac/Weyl points
- Quantum anomalies
- Strong coupling
- Spontaneous symmetry breaking

- Much simpler than QCD (the most interesting SC QFT)
- Relatively easy to realize in practice (table-top vs LHC)
- We (LQCD) can contribute to these fields of CondMat
- We can learn something new
  - ✓ new lattice actions
  - ✓ new algorithms
  - ✓ new observables/analysis tools

Why study condmat systems?

BUT BEWARE:	ENTROPY	VS	COMPLEXITY
QCD	Small (Log 1)		Large (Millenium problem)
CondMat	Large (all materials)		Small (mean-field often enough)

Why study condmat systems?

Some cond-mat systems/models are also very hard:

- Finite-density Hubbard model (high-Tc superconductivity)
- Frustrated systems
- Strange metals …
- Topological materials (non-interacting, but still beautiful)

Those systems are closest in spirit to lattice QCD

Some famous cond-mat physicists occasionally do something in HEP and LAT…

Particle Physics and Condensed Matter: The Saga Continues*

Frank Wilczek
Center for Theoretical Physics, MIT, Cambridge MA 02139 USA

April 20, 2016

pr 2016

Gapped Boundary Phases of Topological Insulators via Weak Coupling

May 2016

Nathan Seiberg and Edward Witten

Volume 130B, number 6 PHYSICS LETTERS 3 November 1983

THE ADLER–BELL–JACKIW ANOMALY AND WEYL FERMIONS IN A CRYSTAL

H.B. NIELSEN
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and

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How to build a lattice model of cond-mat system (in principle)?

Starting point: Schrödinger equation, periodic potential V(x) (we neglect phonons)

$$\left(\frac{\hat{p}_i^2}{2m_e} + \sum_i V(\hat{x}_i) + \sum_{i \neq j} U(\hat{x}_i, \hat{x}_j) \right) \psi = E\psi$$

Single-particle problem: Bloch states

$$\psi(x; k, n) = e^{ikx} u_n(k, x)$$

Lattice momenta
in the range
[-π/a .. π/a]
(modulo 2 π/a)

Periodic under
lattice shifts
x -> x + a
k -> k + 2 π/a

Bloch and Wannier functions

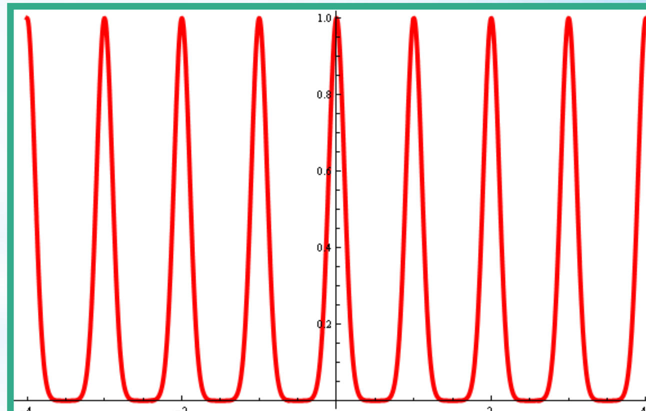
$$\left(\frac{(\hat{p}-k)^2}{2m_e}+V(\hat{x})\right)u(x;n,k)=E(n,k)\,u(x;n,k)$$

- Eigenvalue problem on a finite interval [0 .. a]
- Discrete spectrum - energy bands

Wannier functions:

$$w_{\vec{m}}(\vec{x})\equiv w(\vec{x}-a\vec{m})=\int_{-\pi/a}^{\pi/a}\frac{d^3\vec{k}}{(2\pi)^3}e^{i\vec{k}\cdot a\vec{m}}u\left(\vec{x};\vec{k}\right)$$

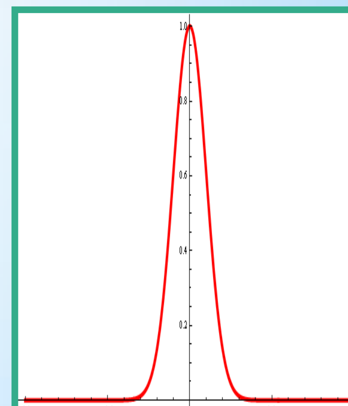
$$\psi\left(\vec{x};\vec{k},n\right)=\sum_{\vec{m}}w(\vec{x}-a\vec{m})\,e^{i\vec{k}\cdot a\vec{m}}$$



- Highly localized
- Approach atomic orbitals
- Not uniquely defined

$$\int d^3\vec{x}\,\bar{w}(\vec{x}-\vec{x}_i)\,\bar{w}(\vec{x}-\vec{x}_j)=\delta_{ij}$$

$=\Sigma_n$



Tight-binding model description

We replace the continuum motion of electrons by discrete hoppings between lattice centers:

$$\hat{H} = \sum_{ij} t_{ij} \hat{a}_i^\dagger \hat{a}_j$$

Fermionic creation/annihilation operators

Lattice sites

<u>Aim:</u> reproduce the Bloch spectrum

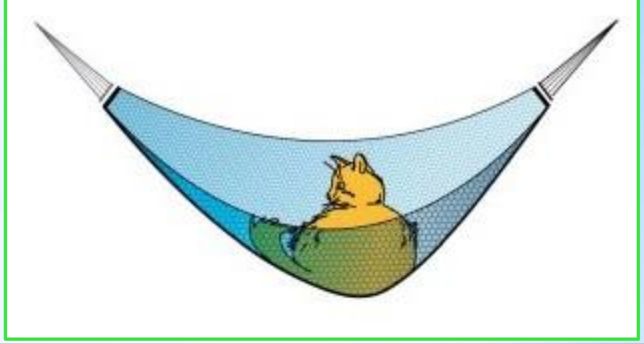
Typically not so easy: sometimes just fitting

<u>More systematic way:</u>

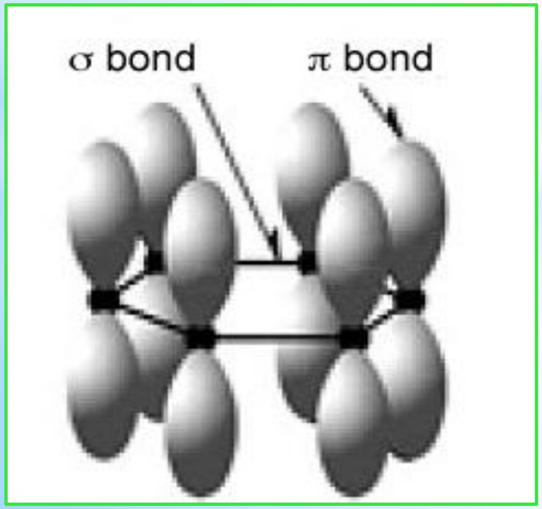
$$t_{ij} = \int d^3\vec{x}\, \bar{w}\left(\vec{x}-\vec{x}_i\right) \left(\frac{\hat{p}^2}{2m_e} + V\left(\vec{x}\right)\right) \bar{w}\left(\vec{x}-\vec{x}_j\right)$$

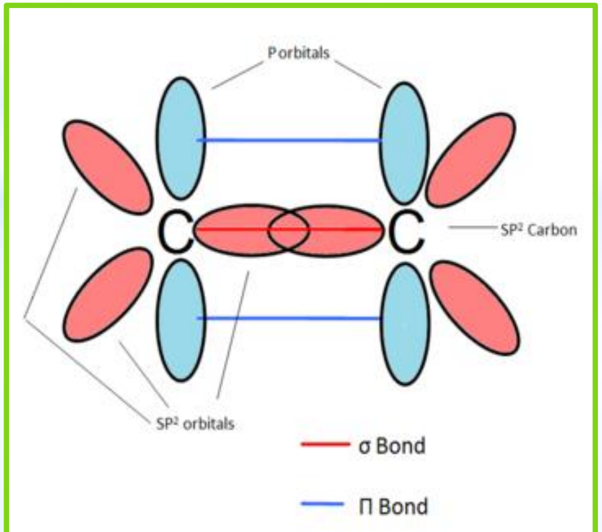
Just a few nearest-neighbors hoppings, due to localization of Wannier functions

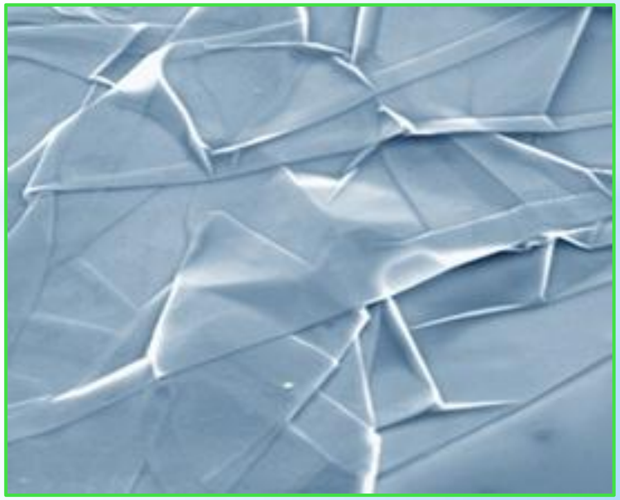
Graphene



- 2D carbon crystal with hexagonal lattice
- a = 0.142 nm – Lattice spacing
- π orbitals are valence orbitals (1 electron per atom)
- σ orbitals create chemical bonds







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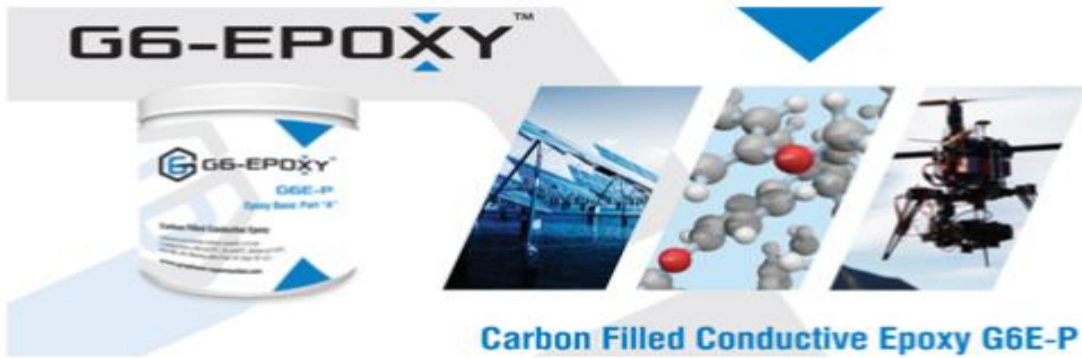

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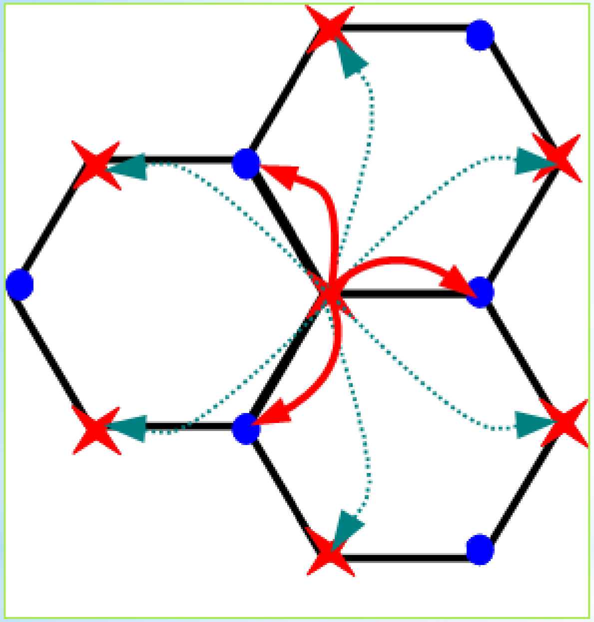
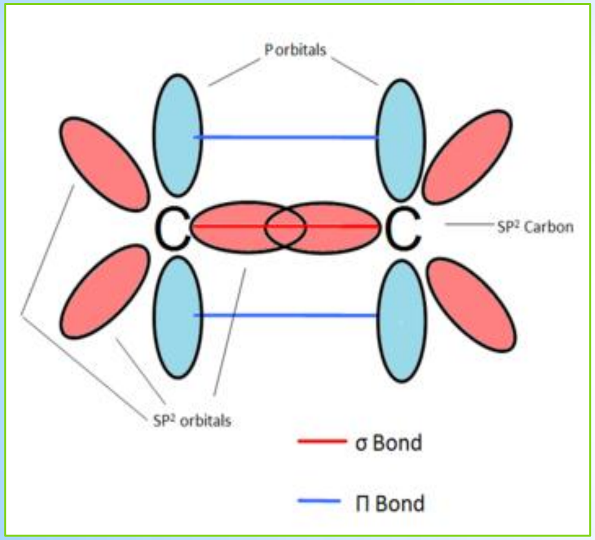
Tight-binding model of Graphene

Or The Standard Model of Graphene





Nearest-neighbor hopping

$t_n \sim 2.7\ eV$

Next-to-nearest neighbor

$t_{nn} \sim 0.1\ eV$

Spins unaffected

[Wallace 1947]

One of the best known and most precise tight-binding models !!!

-> High-precision numerics

Tight-binding model of Graphene

Or The Standard Model of Graphene

$$h_{ij} \equiv t_{ij}$$

- Single-particle Hamiltonian

$$\hat{H} = \sum_{ij} \hat{a}_i^\dagger h_{ij} \hat{a}_j$$

- Many-body Hamiltonian

$$\hat{H}_{tb} = -\kappa \sum_{\sigma=\uparrow,\downarrow} \sum_{<XY>} \left(\hat{a}^\dagger_{\sigma,X} \hat{a}_{\sigma,Y} + \hat{a}^\dagger_{\sigma,Y} \hat{a}_{\sigma,X} \right) \pm$$

$$\left\{ \hat{a}^\dagger_{\sigma_1 X}, \hat{a}_{\sigma_2 Y} \right\} = \delta_{XY} \delta_{\sigma_1 \sigma_2}$$

Energy spectrum of h ~ Bloch states

Spectrum of quasiparticles in graphene

Eigenstates are just the plain waves:

$$\psi\left(\vec{x}, A; \vec{k}\right) = \mathcal{N}_A\left(\vec{k}\right) e^{i\vec{k}\vec{x}}, \qquad \psi\left(\vec{x}, B; \vec{k}\right) = \mathcal{N}_B\left(\vec{k}\right) e^{i\vec{k}\vec{x}},$$

Cartesian coordinates

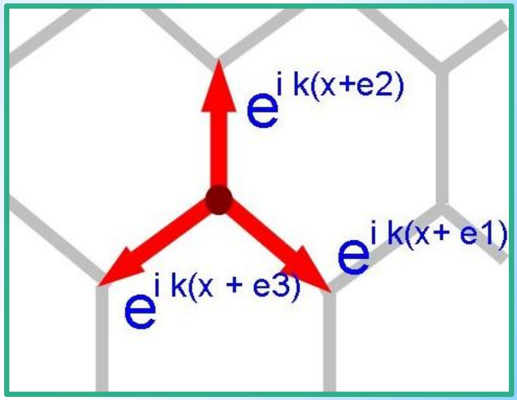
Sublattice indices

Wave vector

Schrödinger equation:

$$t\sum_a \mathcal{N}_B\left(\vec{k}\right) e^{i\vec{k}(\vec{x}+\vec{e}_a)} = \epsilon\mathcal{N}_A\left(\vec{k}\right) e^{i\vec{k}\vec{x}},$$

$$t\sum_a \mathcal{N}_A\left(\vec{k}\right) e^{i\vec{k}(\vec{x}-\vec{e}_a)} = \epsilon\mathcal{N}_B\left(\vec{k}\right) e^{i\vec{k}\vec{x}}$$

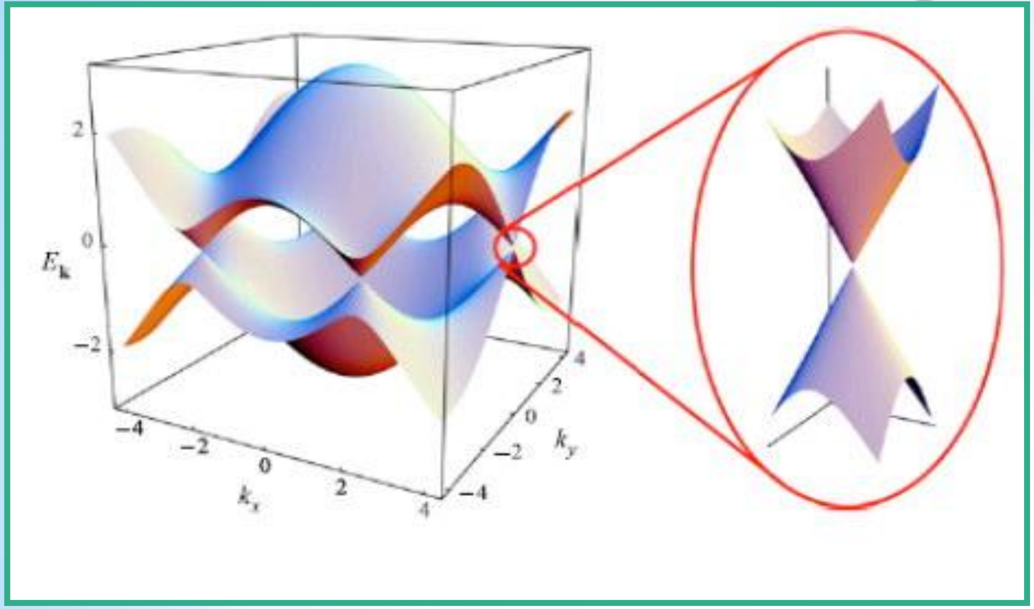


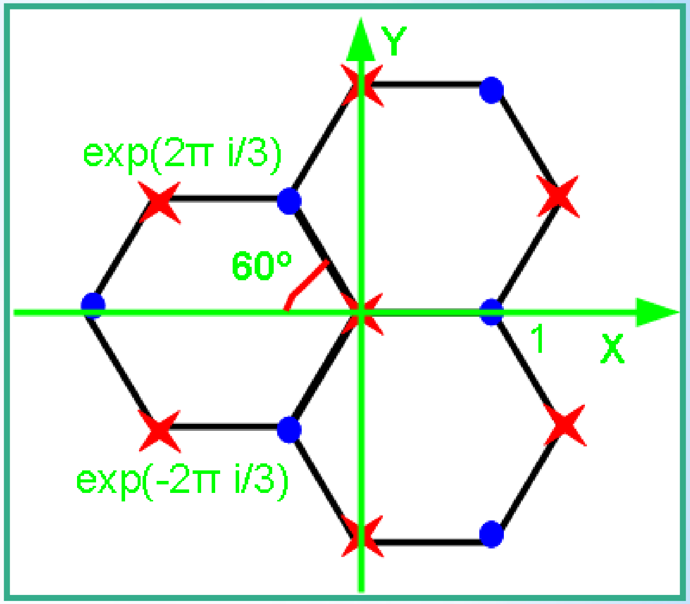
$$t\mathcal{N}_B\Phi = \epsilon\mathcal{N}_A, \qquad t\mathcal{N}_A\bar{\Phi} = \epsilon\mathcal{N}_B$$

$$\Rightarrow \quad \epsilon = \pm t\left|\Phi\right|$$

$$\Phi(k) = \sum_{a=1}^{3} e^{i\vec{k}\cdot\vec{e}_a}$$

Dirac points





$$\Phi\left(k_x, k_y\right) = \exp\left(ik_x a\right) + \\ + \exp\left(-ik_x \frac{a}{2} + ik_y \frac{\sqrt{3}a}{2}\right) + \exp\left(-ik_x \frac{a}{2} - ik_y \frac{\sqrt{3}a}{2}\right)$$

Dirac points: $$k_x^{(\pm)} = 0,\ k_y^{(\pm)} = \pm\frac{4\pi}{3\sqrt{3}a}$$

Phases for neighbors = elements of Z_3!!!

Dirac fermions

$$k_x = k_x^{(\pm)} + q_x, \; k_y = k_y^{(\pm)} + q_y$$

$$\Phi\left(k_x, k_y\right) = \frac{3a}{2}\left(q_y \pm i q_x\right) + O\left(q^2\right)$$

Linear dispersion relation

→ Dirac cones!!!

$$\epsilon = \pm v_F |q| + O\left(q^2\right)$$

“Non-relativistic” Dirac electrons

Fermi velocity

$$v_F = \frac{3\,a\,t}{2} \approx 1/300\,c$$

Dirac fermions

Let's expand the Schrödinger equation

$$t\Phi\,\psi_B = \epsilon\psi_A,\qquad t\bar{\Phi}\,\psi_A = \epsilon\psi_B \;\Rightarrow\; v_F\left(q_x + iq_y\right)\psi_B = \epsilon\psi_A,\qquad v_F\left(q_x - iq_y\right)\psi_A = \epsilon\psi_B$$

$$v_F\begin{pmatrix} 0 & q_x - iq_y \\ q_x + iq_y & 0 \end{pmatrix}\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} = \epsilon\begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix}$$

$$v_F\left(\sigma_x q_x + \sigma_y q_y\right)\psi = \epsilon\psi$$

- **Dirac/Weyl equation!!!**
- **Analogy continues with gauge fields**
- **Covariant derivatives emerge**

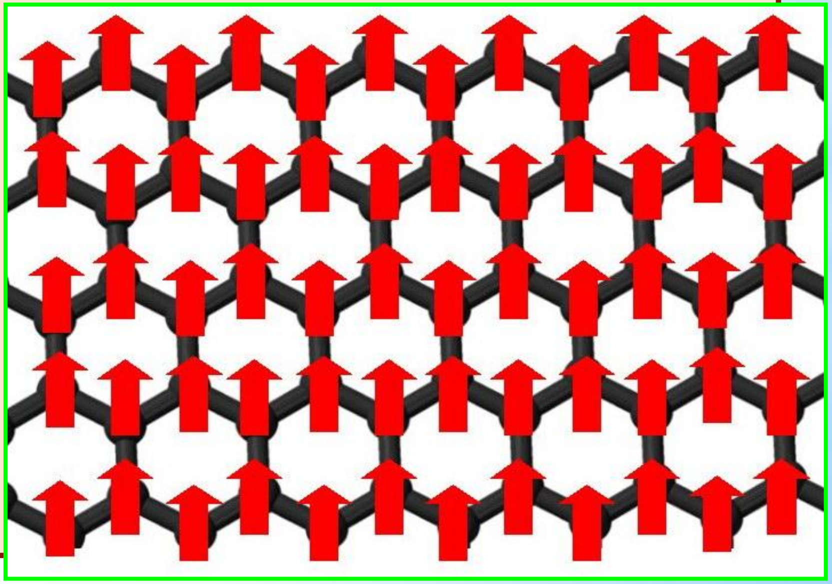
Particles and holes

- Each lattice site can be occupied by two electrons (with opposite spin)

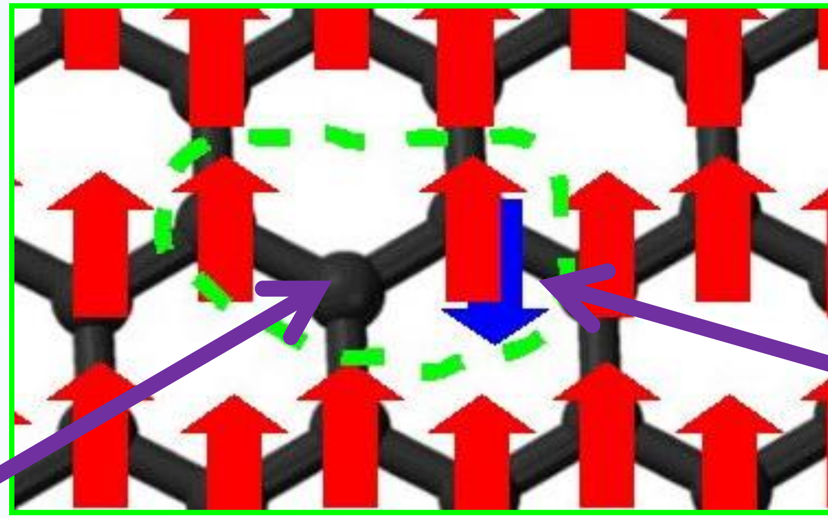
- The ground states is electrically neutral

- One electron (for instance $\uparrow$) at each lattice site

- «Dirac Sea»: hole = absence of electron in the state $\uparrow$



Particles and holes



Particle

Hole

Standard QFT vacuum: particles and holes

$$\hat{\psi}_{\uparrow,X} = \hat{a}_{\uparrow,X}, \quad \hat{\psi}_{\downarrow,X} = \pm\hat{a}^{\dagger}_{\downarrow,X},$$

Redefined creation/ annihilation operators

$$\hat{q}_X = \hat{\psi}^{\dagger}_{\uparrow,X}\,\hat{\psi}_{\uparrow,X} - \hat{\psi}^{\dagger}_{\downarrow,X}\,\hat{\psi}_{\downarrow,X}.$$

Charge operator

$$\hat{\psi}_{\uparrow,X}\,|0\rangle = 0,\ \hat{\psi}_{\downarrow,X}\,|0\rangle = 0$$

QFT vacuum conditions

$$\hat{H}_{tb} = -\kappa \sum_{\sigma=\uparrow,\downarrow}\sum_{<XY>}\left(\hat{\psi}^{\dagger}_{\sigma,X}\,\hat{\psi}_{\sigma,Y} + \hat{\psi}^{\dagger}_{\sigma,Y}\,\hat{\psi}_{\sigma,X}\right) + \\ + \sum_{\sigma=\uparrow,\downarrow}\sum_{X_1} m\,\hat{\psi}^{\dagger}_{\sigma,X_1}\hat{\psi}_{\sigma,X_1} - \sum_{\sigma=\uparrow,\downarrow}\sum_{X_2} m\,\hat{\psi}^{\dagger}_{\sigma,X_2}\hat{\psi}_{\sigma,X_2}$$

Hamiltonian does not change!!! Bipartite lattice!

Symmetries of the free Hamiltonian

2 Fermi-points
X 2 sublattices
= 4 components of the
Dirac spinor

$$(L, R, \bar{L}, \bar{R})$$

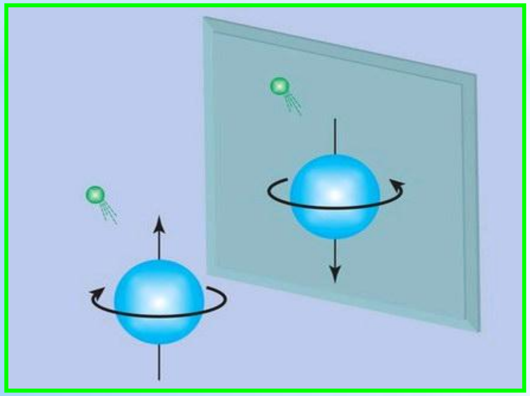
$$(+_A, -_B, +_A, -_B)$$

Physical spins = 2 Dirac flavours

Chiral U(4) symmetry
(massless fermions):
right ⟷ left

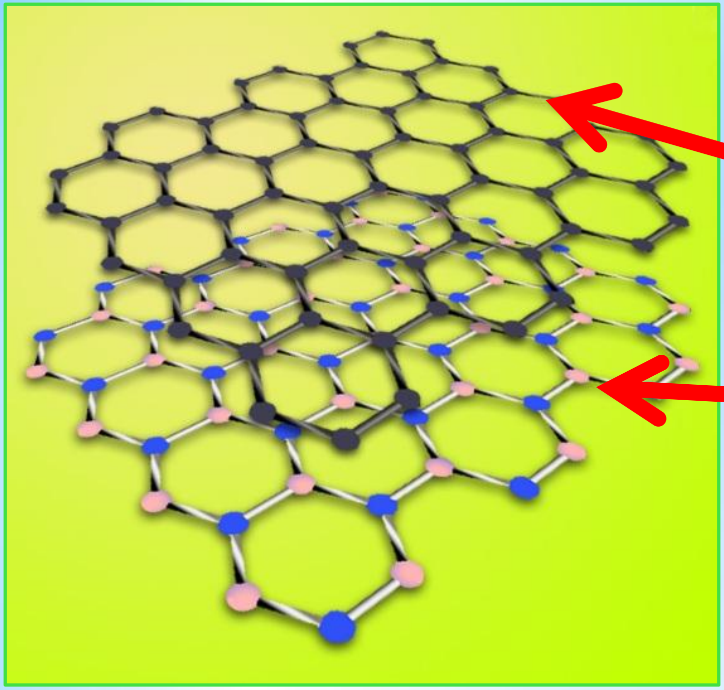
Discrete Z_2 symmetry
between sublattices

A ⟷ B



U(1) x U(1) symmetry: conservation
of currents with different spins

Giving mass to Dirac fermions



$$E = \sqrt{v_F^2 k^2 + m^2}$$

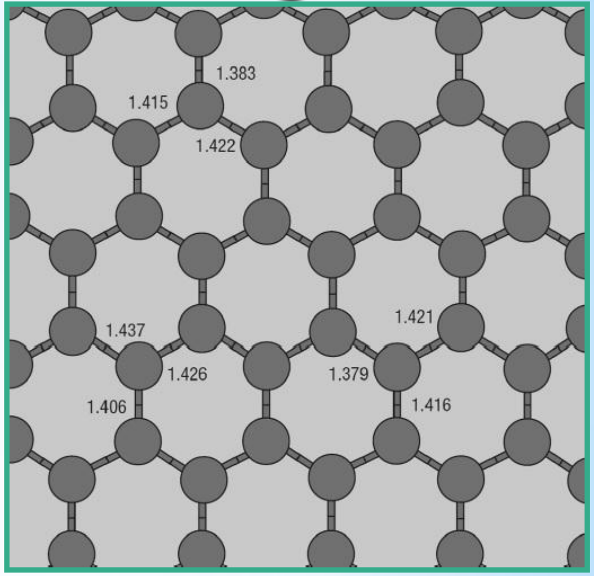
$$\hat{H}_{tb} = -\kappa \sum_{\sigma=\uparrow,\downarrow} \sum_{<XY>} \left(\hat{a}^\dagger_{\sigma,X} \, \hat{a}_{\sigma,Y} + \hat{a}^\dagger_{\sigma,Y} \, \hat{a}_{\sigma,X} \right) \pm$$

$$\pm \left(\sum_{\sigma=\uparrow,\downarrow} \sum_{X_1} m \, \hat{a}^\dagger_{\sigma,X_1} \hat{a}_{\sigma,X_1} - \sum_{\sigma=\uparrow,\downarrow} \sum_{X_2} m \, \hat{a}^\dagger_{\sigma,X_2} \hat{a}_{\sigma,X_2} \right)$$

«Valley» magnetic field`

Mechanical strain: hopping amplitudes change

$$H^{(1,2)} = \begin{pmatrix} 0 & S(P_0^{(1,2)}+p) \\ S^*(P_0^{(1,2)}+p) & \end{pmatrix} \approx$$
$$\approx \frac{3at}{2}\begin{pmatrix} 0 & \alpha(p_x \pm i p_y) \\ \alpha^*(p_x \mp i p_y) & 0 \end{pmatrix}$$



$$S(p) = t_1 + t_2 e^{-i(p^1-p^2)a} + t_3 e^{-ip^1 a}$$

$$p_x \to p_x \pm \frac{2t_2 - t_1 - t_2}{3} - \frac{\theta_3-\theta_1}{\sqrt{3}}$$
$$p_y \to p_y \pm \frac{t_3 - t_1}{\sqrt{3}} + \frac{2\theta_2 - \theta_1 - \theta_3}{3}$$

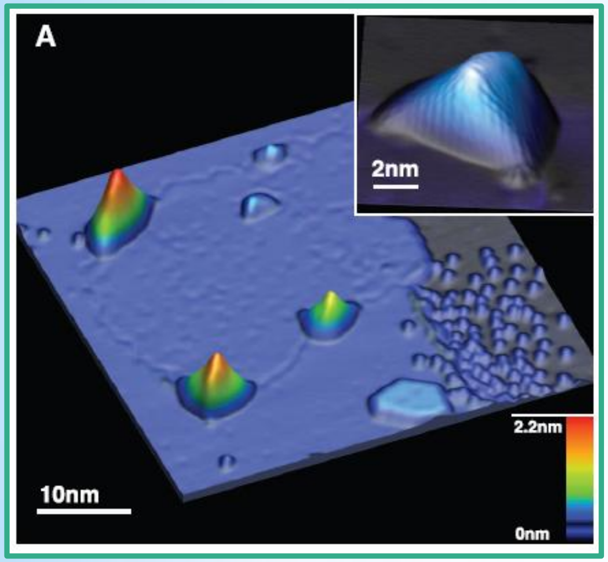
$$\theta_3 - \theta_1 = \vec{A}\cdot\vec{\tau}_3 = -A_x\sqrt{3}a\ ,$$
$$\theta_2 - \theta_1 = \vec{A}\cdot\vec{\tau}_2 = (-\frac{1}{2}A_x + \frac{\sqrt{3}}{2}A_y)\sqrt{3}a$$

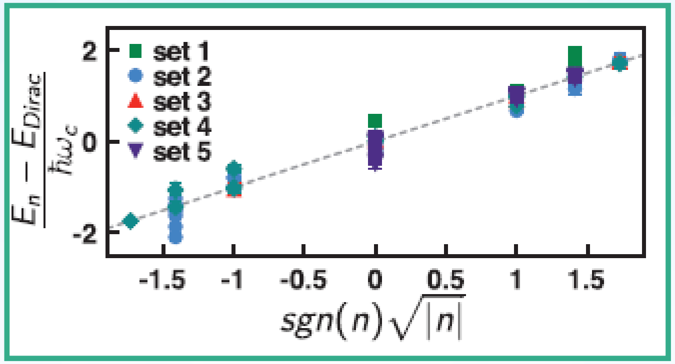
$$p_x \to p_x \pm \tilde{A}_x + A_x$$
$$p_y \to p_y \pm \tilde{A}_y + A_y$$

$$\tilde{A}_x = \frac{1}{2}(2t_2 - t_1 - t_3)\ , \qquad \tilde{A}_y = \frac{\sqrt{3}}{2}(t_3 - t_1)$$

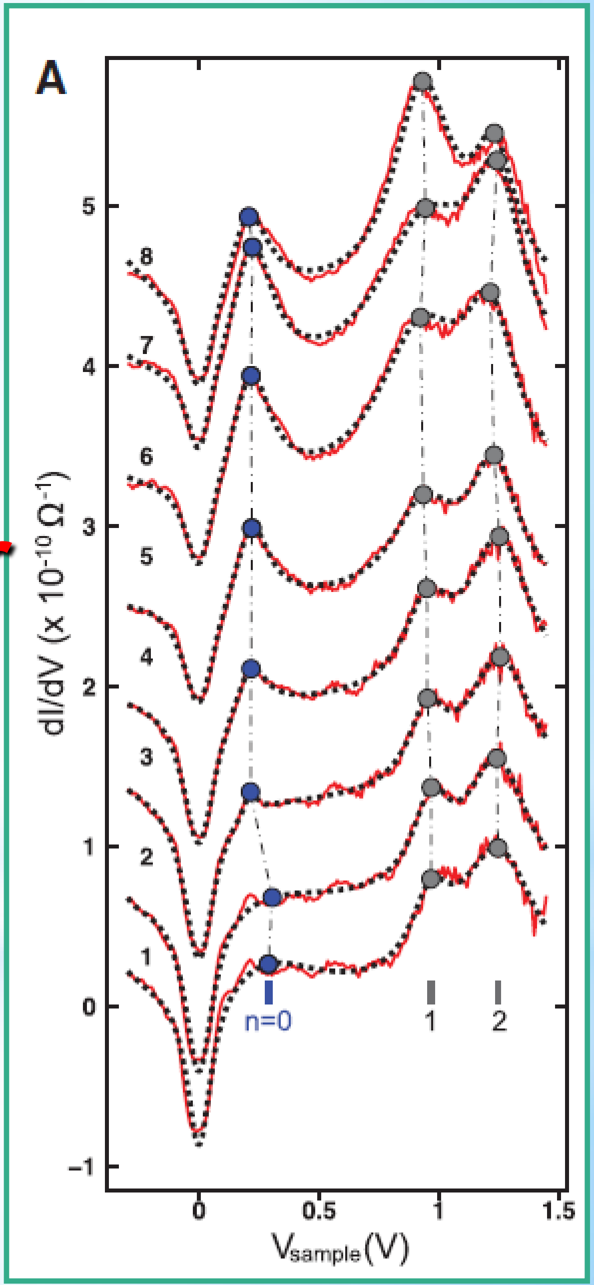
«Valley» magnetic field

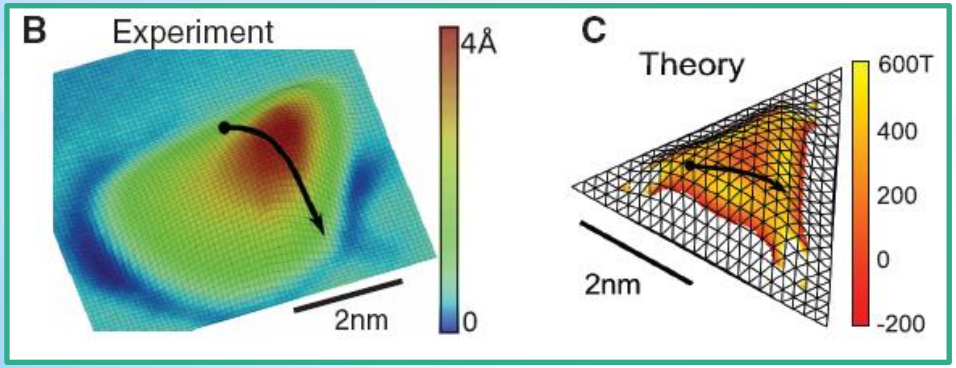
[N. Levy et. al., Science 329 (2010), 544]





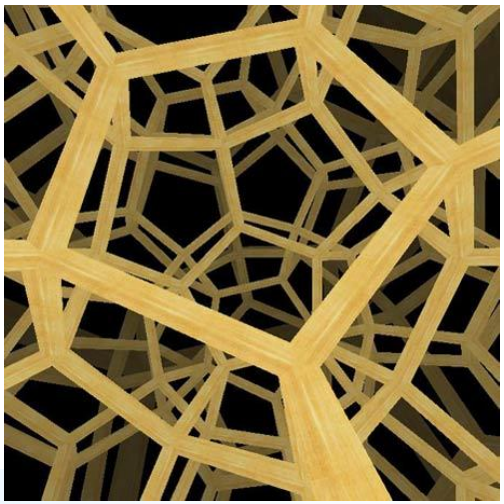
Fields of order of ~100 Tesla





(4D) Graphene as lattice discretization

Four-dimensional graphene and chiral fermions



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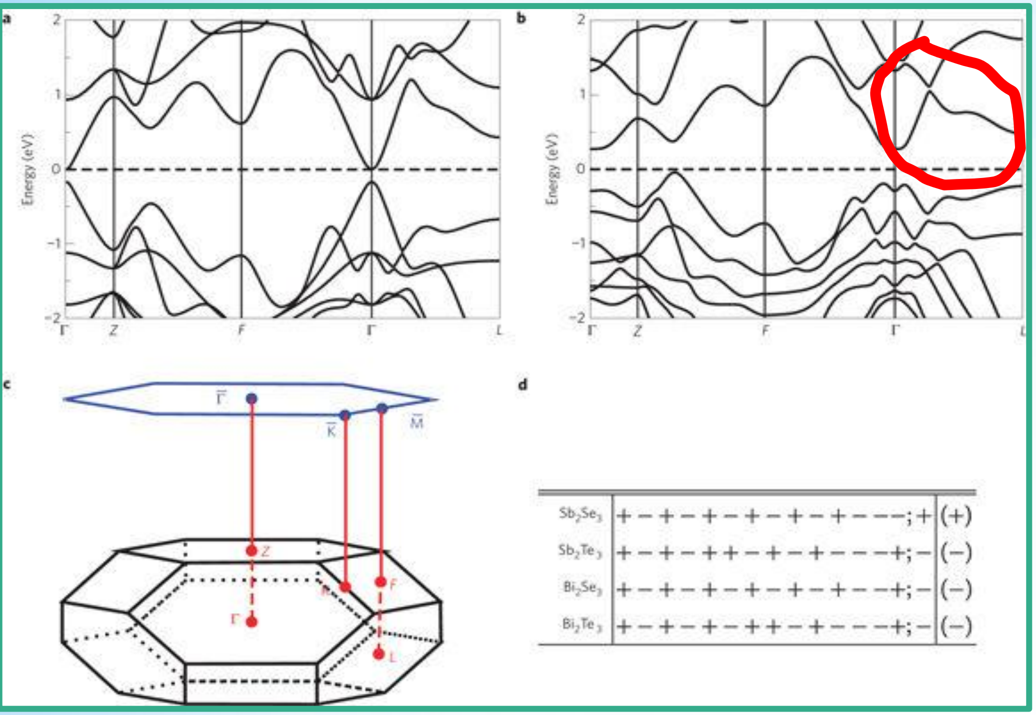
Abstract

- **Minimally doubled fermions**
- **(recall Nielsen-Ninomiya)**
- **Seem ideal for u- and d-quarks**
- **But … Some symmetry still broken**
- **Renormalization difficult**

Dirac semimetals, Topological insulators…



Bi_2Se_3, Bi_2Te_3, Sb_2Te_3

Top insulators/ Dirac semi-metals

[Zhang et al., Nature Physics 5, 438 - 442 (2009)]

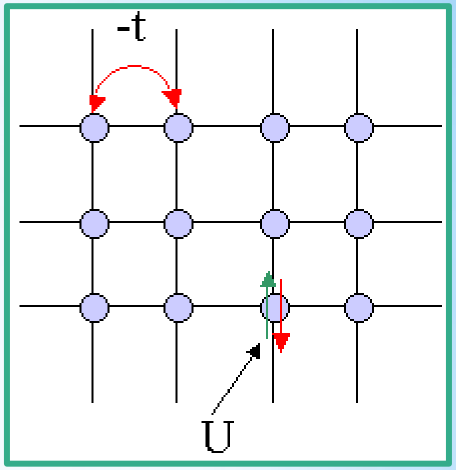
Wilson-Dirac fermions upon basis change

$$H(\mathbf{k}) = \epsilon_0(\mathbf{k})\mathbb{I}_{4\times4} + \begin{pmatrix} \mathcal{M}(\mathbf{k}) & A_1 k_z & 0 & A_2 k_- \\ A_1 k_z & -\mathcal{M}(\mathbf{k}) & A_2 k_- & 0 \\ 0 & A_2 k_+ & \mathcal{M}(\mathbf{k}) & -A_1 k_z \\ A_2 k_+ & 0 & -A_1 k_z & -\mathcal{M}(\mathbf{k}) \end{pmatrix}$$

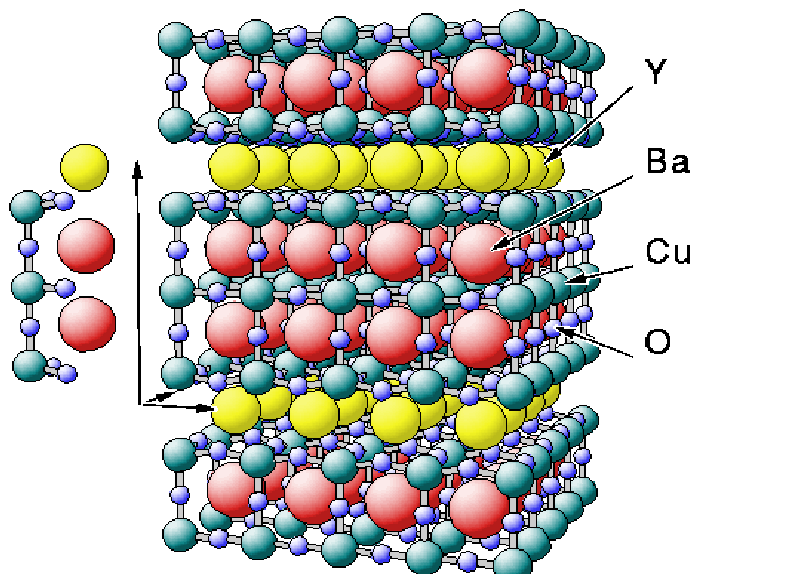
$$+ o(\mathbf{k}^2)$$

Hubbard model

$$\hat{H} = -t \sum_{\langle i,j \rangle,\sigma} (\hat{c}^\dagger_{i,\sigma}\hat{c}_{j,\sigma} + \hat{c}^\dagger_{j,\sigma}\hat{c}_{i,\sigma})$$



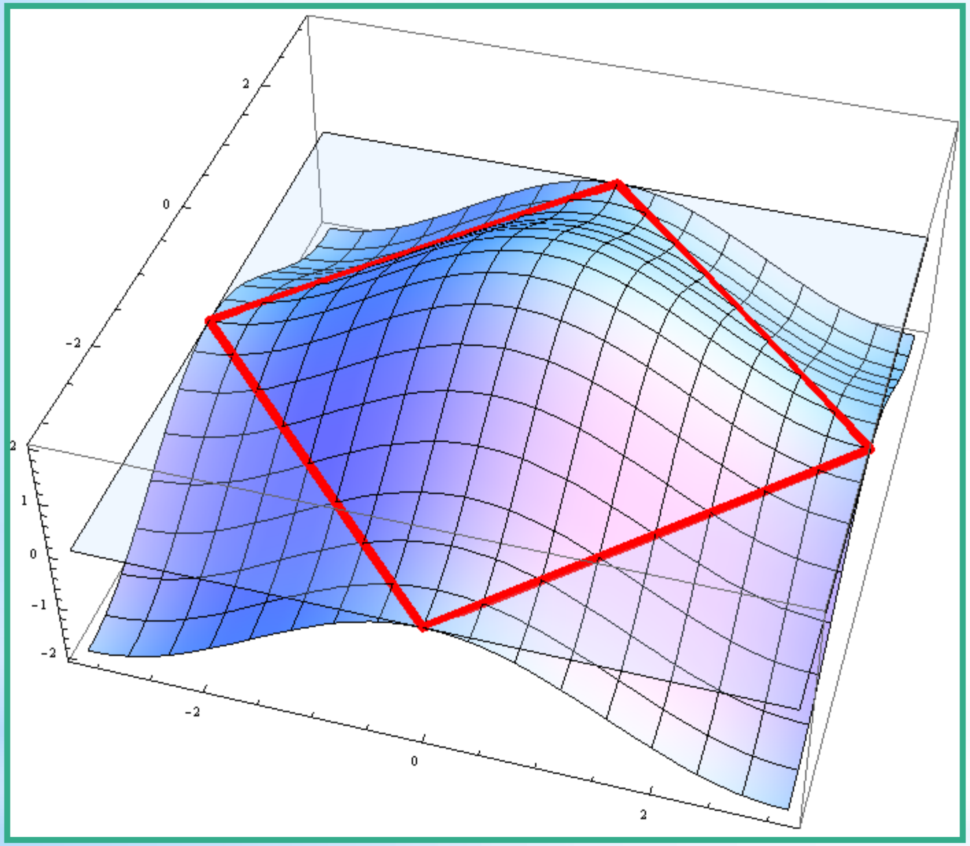
Electrons hopping on 2D square lattice
Simple imitation of layered structure of (many) high-Tc superconductors



$YBa_2Cu_3O_7$ (.3) lattice

Hubbard model

$$\Phi\left(k_x, k_y\right) = 2\cos\left(ak_x\right) + 2\cos\left(ak_y\right)$$



We need sign modulations of hoppings to get isolated zeros

→ Staggered fermions

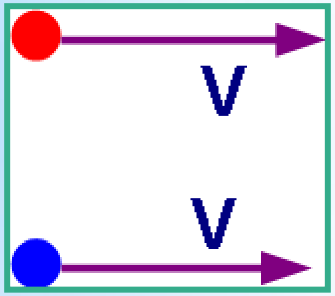
This time no Dirac points

Square “Fermi sphere“ at half-filling

Inter-electron interactions

Electrons in cond-mat move slowly

- **Fermi velocity v_F ~ c/300 (Graphene)**
- **Magnetic interactions suppressed by v_F^2**
- **Only Coulomb interactions are important**



- **Coulomb force ~ $(1-v^2/c^2)$**
- **Lorentz force ~ v^2/c^2**

$$H_{ee} = \frac{1}{2} \sum_{n,m,\sigma} \langle n_1 m_1 , n_2 m_2 | \frac{e^2}{|r_1 - r_2|} | n_3 m_3 , n_4 m_4 \rangle c^\dagger_{n_1 m_1 \sigma_1} c^\dagger_{n_2 m_2 \sigma_2} c_{n_4 m_4 \sigma_2} c_{n_3 m_3 \sigma_1}$$

Coulomb interactions in the tight-binding model

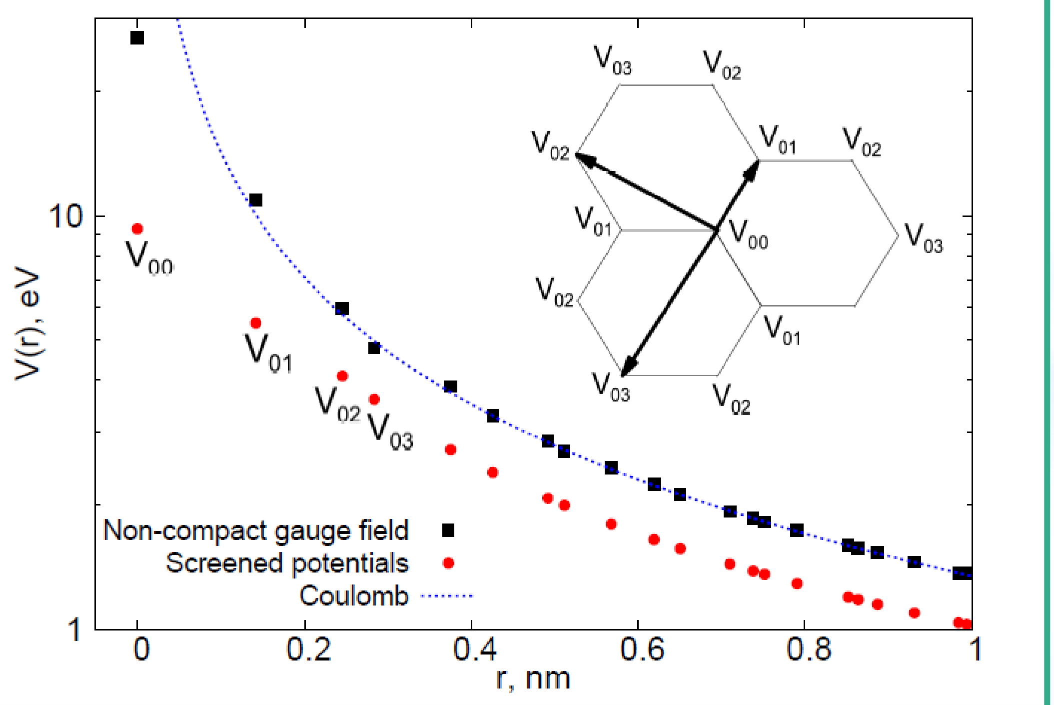
$$\hat{H}_I = \sum_{x,y} V_{xy} \hat{q}_x \hat{q}_y$$

Charge operator

$$\hat{q}_x = \hat{a}^\dagger_\uparrow \hat{a}_\uparrow + \hat{a}^\dagger_\downarrow \hat{a}_\downarrow - 1$$

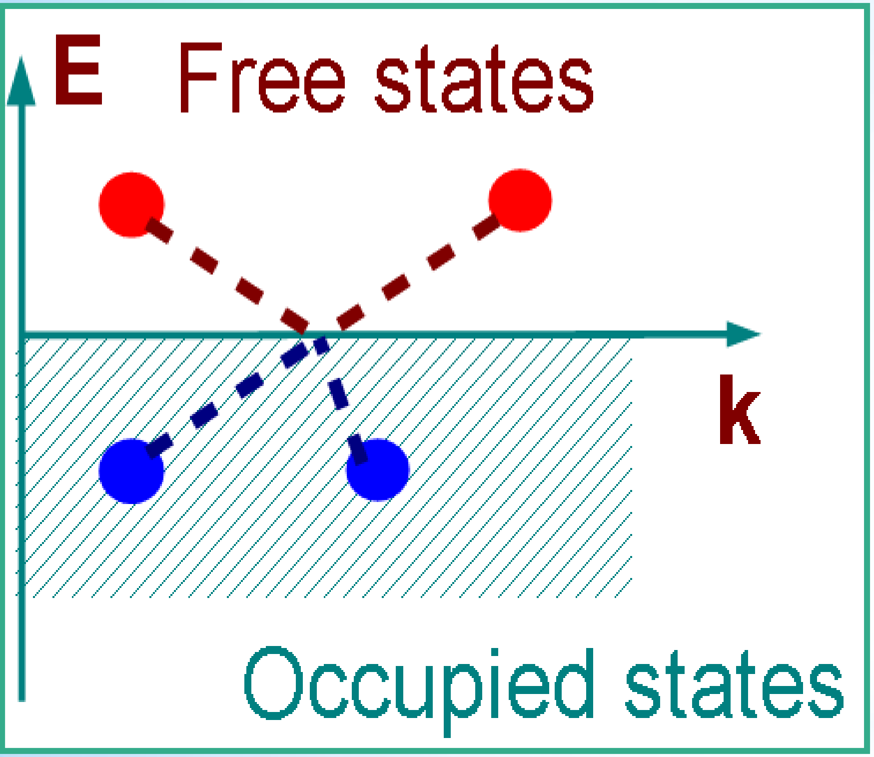
Ion charge

[Wehling et al. 1101.4007]



Screening is most important in 3D materials

Density of states and relevance of interactions



- Interactions mostly localized near Fermi surface
- How many free states for scattering?

Density of states near Fermi surface is important

Density of states and relevance of interactions

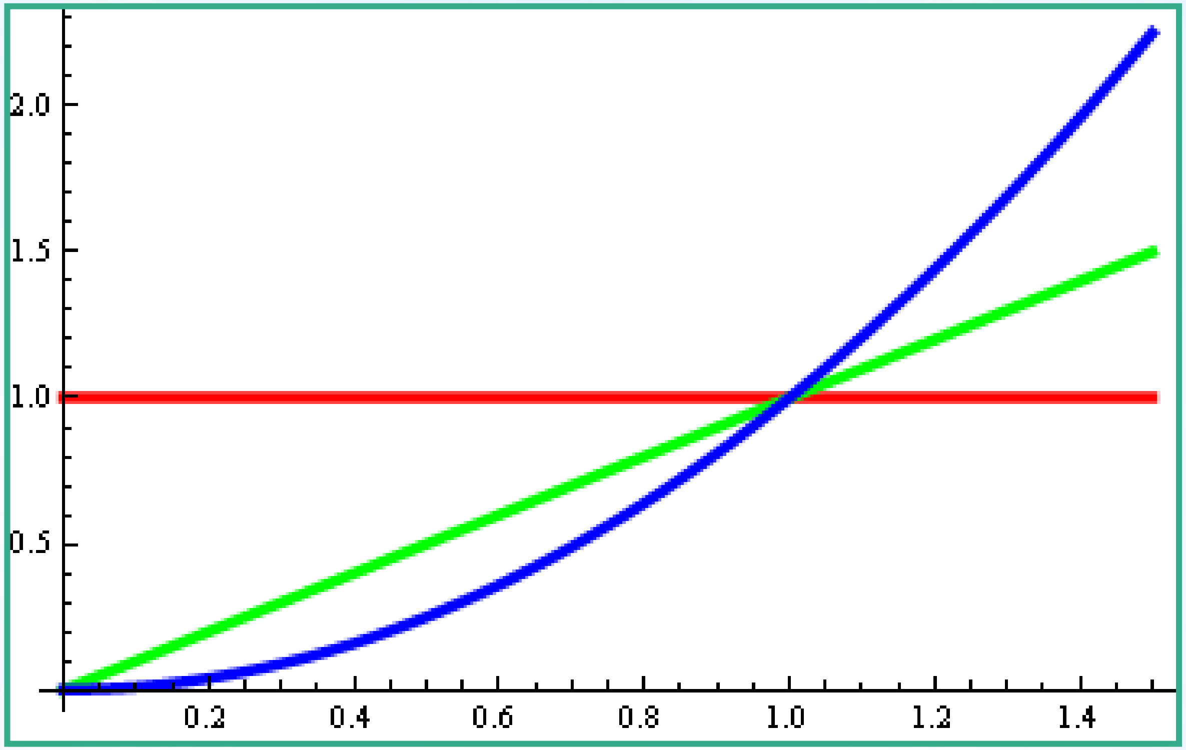
- ***d*** **spatial dimensions**
- **Dispersion law** $\varepsilon \sim |k|^{\alpha}$

$$k \sim \epsilon^{1/\alpha} \Rightarrow dn \sim d(k^d) \sim d\left(\epsilon^{d/\alpha}\right)$$

$$\rho\left(\epsilon\right) = dn/d\epsilon \sim \epsilon^{d/\alpha - 1}$$

- **DOS smaller in higher dimensions**
- **Interactions are weaker (screening)**
- **1D/2D systems strongly interacting**

DOS and interactions



- Hubbard model $\rho(\varepsilon) \sim const$
- Quadratic bands $d=2$, $a=2$, $\rho(\varepsilon) \sim const$
- Graphene $d=2$, $a=1$, $\rho(\varepsilon) \sim \varepsilon$
- Dirac semimetals $d=3$, $a=1$, $\rho(\varepsilon) \sim \varepsilon^2$

How to treat interactions?

$$\hat{H} = \sum_{x,y} \hat{\psi}_x^\dagger h_{xy}^{\psi} \hat{\psi}_y + \sum_{x,y} \hat{\chi}_x^\dagger h_{xy}^{\chi} \hat{\chi}_y + \frac{1}{2} \sum_{x,y} V_{xy} \hat{q}_x \hat{q}_y$$

Particles

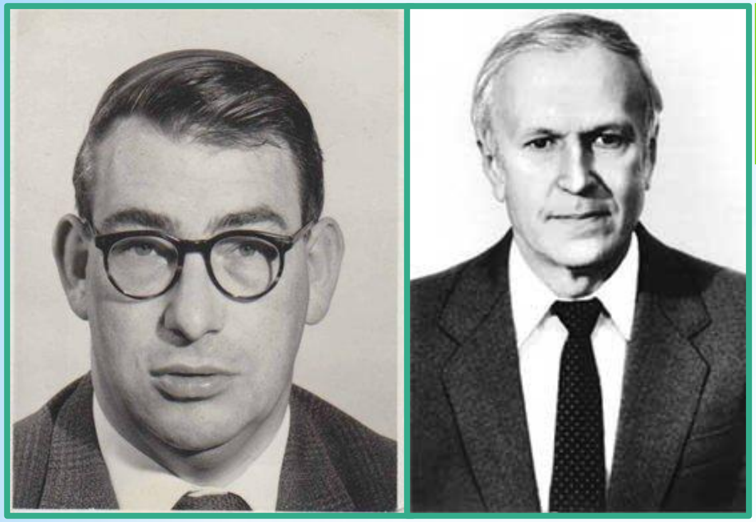
Holes

Interactions

1) Suzuki-Trotter decomposition

$$\mathrm{Tr}\, \exp\left(-\beta\left(\hat{H}_0 + \hat{H}_I\right)\right) =$$
$$= \mathrm{Tr}\left(e^{-\hat{H}_0 \Delta\tau} e^{-\hat{H}_I \Delta\tau} \ldots e^{-\hat{H}_0 \Delta\tau} e^{-\hat{H}_I \Delta\tau}\right) + O\left(\Delta\tau^2\right)$$

Hubbard-Stratonovich transformation



$$\exp\left(-\frac{ax^2}{2}\right) = \int\limits_{-\infty}^{+\infty} d\phi \exp\left(-\frac{\phi^2}{2a} + ix\phi\right)$$

$$\exp\left(-\tfrac{1}{2}A_{ij}x_jx_j\right) = \\ = \int\limits_{-\infty}^{+\infty} d\phi \exp\left(-\tfrac{1}{2}\phi_i\left(A^{-1}\right)_{ij}\phi_j + ix_i\phi_i\right)$$

Important: *[q_x,q_y] = 0*

$$\exp\left(-\hat{H}_I\Delta\tau\right) = \exp\left(-\frac{\Delta\tau}{2}\sum_{x,y}V_{xy}\hat{q}_x\hat{q}_y\right) =$$

$$= \int d\phi \exp\left(-\frac{\Delta\tau}{2}\sum_{x,y}\left(V^{-1}\right)_{xy}\phi_x\phi_y + i\Delta\tau\sum_x \phi_x\hat{q}_x\right)$$

Now only two fermionic fields

Integrating out fermions

$$\mathrm{Tr}\,\exp\left(-\hat{H}/T\right) = \int d\phi_1 \exp\left(-\frac{\Delta\tau}{2}\phi^1_x \left(V^{-1}\right)_{xy}\phi^1_y\right)$$

$$\ldots \int d\phi_n \exp\left(-\frac{\Delta\tau}{2}\phi^n_x \left(V^{-1}\right)_{xy}\phi^n_y\right) \times$$

$$\times\, \mathrm{Tr}\left(\exp\left(-\hat{H}_0\Delta\tau + i\sum_x \phi^1_x \hat{q}_x\right)\ldots\exp\left(-\hat{H}_0\Delta\tau + i\sum_x \phi^n_x \hat{q}_x\right)\right)$$

Useful identity for fermionic bilinears

$$\hat{B}_1 = \left(B_1\right)_{ij}\hat{\psi}^\dagger_i \hat{\psi}_j$$

$$\mathrm{Tr}\left(e^{\hat{B}_1}\ldots e^{\hat{B}_n}\right) = \det\left(1 + e^{B_1}\ldots e^{B_n}\right)$$

(To prove: use fermionic coherent states, see e.g. Montvay/Münster book)

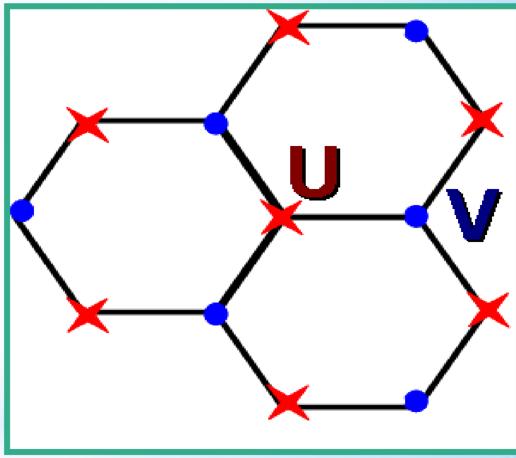
Action of Hubbard-Stratonovich fields

$$S_{HS}\left[\phi\right] = \int d\tau\, \phi_x V_{xy} \phi_y / 2$$

V_{xy} should be positive-definite matrix

Limits applicability of HS transform

For hex lattice $V < U/3$



Unscreened $V_{xy} \sim 1/|x-y|$

$[V^{-1}]_{xy} \sim \Delta_{xy}$

We recover electrodynamics

φ_x is the electrostatic potential

Back to continuous time

$$\mathrm{Tr}\,\exp\left(-\hat{H}/T\right) = \int d\phi_1 \exp\left(-\frac{\Delta\tau}{2}\phi^1_x\left(V^{-1}\right)_{xy}\phi^1_y\right)$$
$$\ldots\int d\phi_n \exp\left(-\frac{\Delta\tau}{2}\phi^n_x\left(V^{-1}\right)_{xy}\phi^n_y\right)\times$$
$$\times\det\left(1+\exp\left(-\left(h_\psi - i\phi^1_x\right)\Delta\tau\right)\ldots\exp\left(-\left(h_\psi - i\phi^n_x\right)\Delta\tau\right)\right)\times$$
$$\times\det\left(1+\exp\left(-\left(h_\chi + i\phi^1_x\right)\Delta\tau\right)\ldots\exp\left(-\left(h_\chi + i\phi^n_x\right)\Delta\tau\right)\right)$$

Path integral in continuous time

$$\mathrm{Tr}\,\exp\left(-\hat{H}/T\right) = \int \mathcal{D}\phi(\tau)\exp\left(-\int_0^{T^{-1}} d\tau\,\phi_x(\tau)\left(V^{-1}\right)_{xy}\phi_y(\tau)\right)\times$$
$$\times\det\left(1+\mathcal{T}\exp\left(-\int_0^{T^{-1}} d\tau\left(h_\psi - i\phi_x(\tau)\right)\right)\right)\times$$
$$\times\det\left(1+\mathcal{T}\exp\left(-\int_0^{T^{-1}} d\tau\left(h_\chi + i\phi_x(\tau)\right)\right)\right)$$

Single-particle Hilbert space

Time ordering

No kinetic term for the HS field!!!

Local form of the action

Single-particle Hilbert space X

anti-periodic functions on circle *L= 1/T*

$$\det\left(1+\mathcal{T}\exp\left(-\int d\tau h(\tau)\right)\right)=$$
$$=\det\left(\partial_\tau+h(\tau)\right)=$$
$$=\int\mathcal{D}\eta(\tau)\,\mathcal{D}\bar{\eta}(\tau)\exp\left(-\int d\tau\,\bar{\eta}(\tau)\left(\partial_\tau+h(\tau)\right)\eta(\tau)\right)$$

Path integral over fermionic fields

In practice, we still discretize the time

$$\det\left(\partial_\tau+h(\tau)\right)\approx$$
$$\approx\det\begin{pmatrix} 1 & -1+h(\tau_1)\Delta\tau & 0 & 0 & \ldots \\ 0 & 1 & -1+h(\tau_1)\Delta\tau & 0 & \ldots \\ \ldots & \ldots & \ldots & \ldots & \ldots \\ 1-h(\tau_1)\Delta\tau & 0 & \ldots & 0 & 1 \end{pmatrix}$$
$$\equiv\det(M)$$

Monte-Carlo simulations

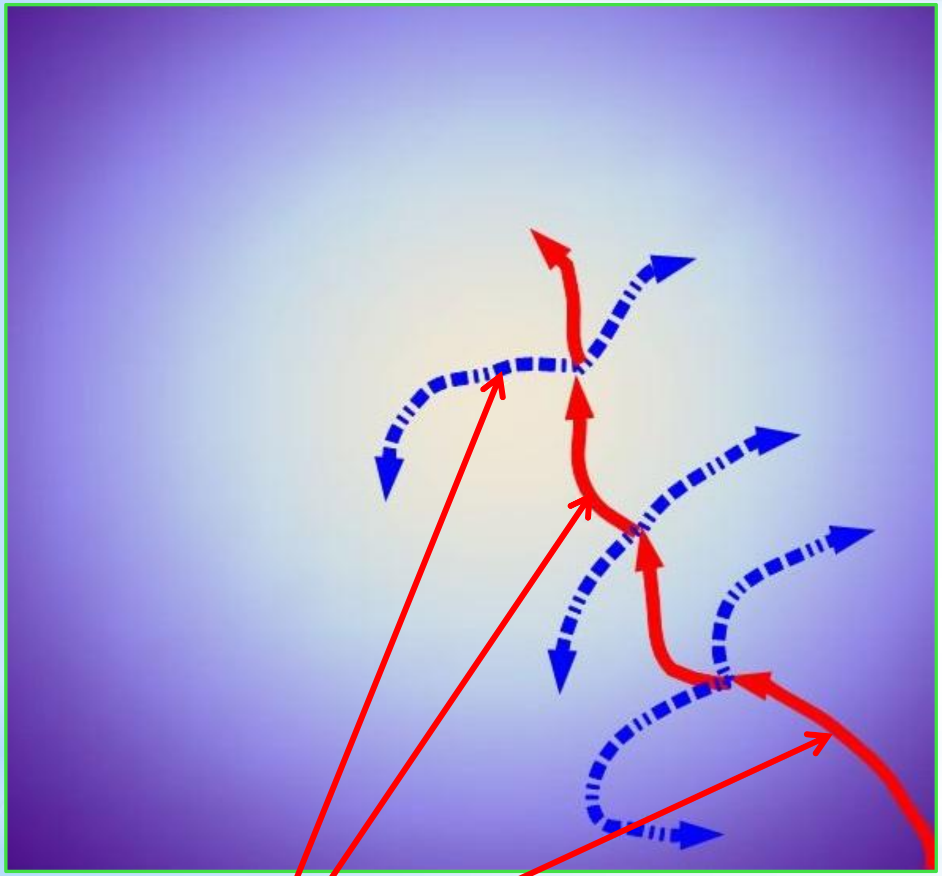
$$\mathrm{Tr}\,\exp\left(-\hat{H}/T\right) = \int d\phi \exp\left(-S_{HS}\left[\phi\right]\right) \times$$
$$\times \det\left(\partial_\tau - h_\psi + i\phi\right) \det\left(\partial_\tau - h_\chi - i\phi\right)$$

If $h_\psi = h_x$, the two dets are complex conjugate, Monte-Carlo possible !!!

$$\det\left(M_\psi\right) \det\left(M_\chi\right) = \det\left(M M^\dagger\right) =$$
$$= \mathcal{N} \int d\Phi \exp\left(-\Phi \left(M M^\dagger\right)^{-1} \Phi\right)$$

Pseudofermion fields

Hybrid Monte-Carlo
= Molecular Dynamics + Metropolis

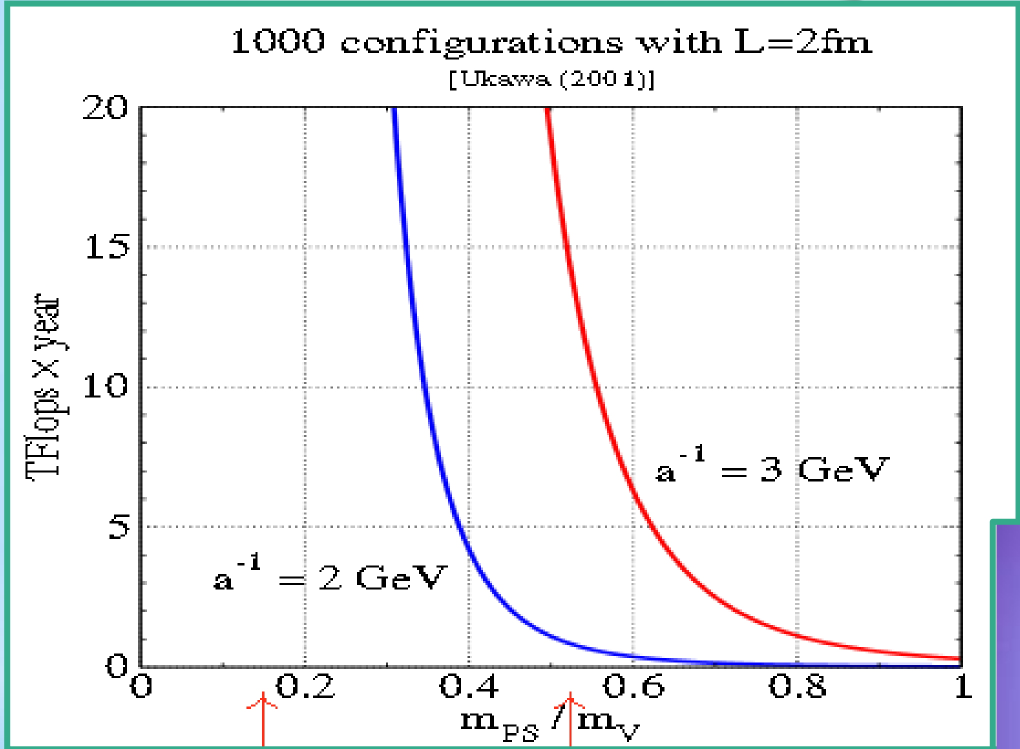


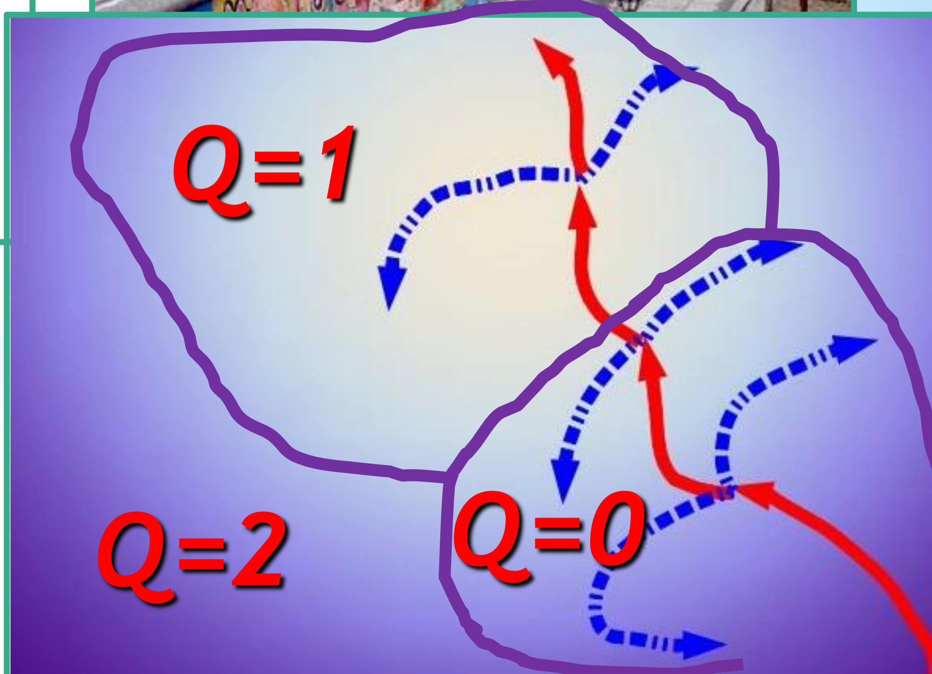
Molecular Dynamics Trajectories

- Use numerically integrated Molecular Dynamics trajectories as Metropolis proposals
- Numerical error is corrected by accept/reject
- Exact algorithm
- Ψ-algorithm [Technical]: Represent determinant as Gaussian integral

Chiral limit and Berlin wall

At *m->0* lattice QCD HMC slows down …





Potential barriers associated with topology

Chiral limit for graphene HMC

Test case: two-site model, single time

$$h_\psi = h_\chi = \begin{pmatrix} 0 & t \\ t & 0 \end{pmatrix}$$

$$e^{-h/T} = \begin{pmatrix} \cosh(\kappa) & \sinh(\kappa) \\ \sinh(\kappa) & \cosh(\kappa) \end{pmatrix}$$

$$\det\left(1 + e^{-h/T} e^{+i\phi}\right) \det\left(1 + e^{-h/T} e^{-i\phi}\right) =$$
$$= 1 + 2e^{-2\kappa} + 2e^{-2\kappa}\cos(\phi_1 - \phi_2) +$$
$$+ 2e^{-\kappa}\cos(\phi_1) + 2e^{-\kappa}\cos(\phi_2)$$

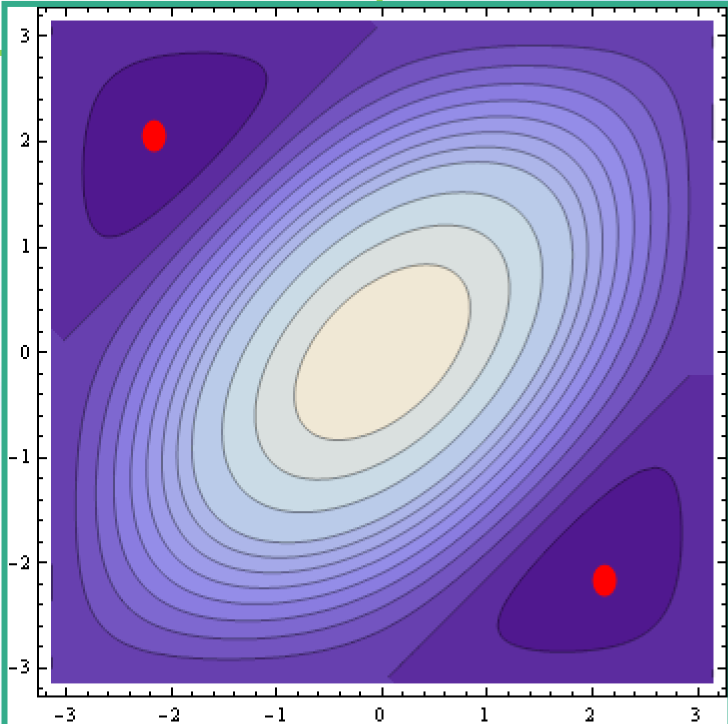
$$\kappa = t/T$$

Det zeros:

Discrete points

(N-2-dim in general)

HMC not stuck



No topology, no wall!

Mean-field approximation

- Dirac fermions
- On-site interactions only

$$\hat{H} = \sum_{x,y} \hat{\psi}^\dagger_x h_{xy} \hat{\psi}_y + U \sum_x \left(\hat{\psi}^\dagger_x \hat{\psi}_x - 2 \right)^2$$

4-component spinors

- We now transform

$$\exp\left(-\hat{H}_I \Delta\tau\right) = \prod_x \exp\left(-U \Delta\tau\, \hat{q}^2_x\right)$$

$$\hat{q}^2 = \left(\hat{\psi}^\dagger_\alpha \hat{\psi}_\alpha - 2\right)\left(\hat{\psi}^\dagger_\beta \hat{\psi}_\beta - 2\right) = \hat{\psi}^\dagger_\alpha \hat{\psi}_\alpha \hat{\psi}^\dagger_\beta \hat{\psi}_\beta - 4\hat{\psi}^\dagger_\alpha \hat{\psi}_\alpha + \text{const} =$$

$$= \hat{\psi}^\dagger_\alpha \hat{\psi}_\alpha \left(4 - \hat{\psi}_\beta \hat{\psi}^\dagger_\beta\right) - 4\hat{\psi}^\dagger_\alpha \hat{\psi}_\alpha = -\hat{\psi}^\dagger_\alpha \hat{\psi}_\alpha \hat{\psi}_\beta \hat{\psi}^\dagger_\beta = +\hat{\psi}^\dagger_\alpha \hat{\psi}_\beta \hat{\psi}_\alpha \hat{\psi}^\dagger_\beta =$$

$$= \hat{\psi}^\dagger_\alpha \hat{\psi}_\beta \left(\delta_{\alpha\beta} - \hat{\psi}^\dagger_\beta \hat{\psi}_\alpha\right) = R_{\alpha\beta} R_{\beta\alpha} + \hat{q} + \text{const}$$

$$R_{\alpha\beta} = \hat{\psi}^\dagger_\alpha \hat{\psi}_\beta, \qquad R^\dagger_{\alpha\beta} = R_{\beta\alpha}$$

Mean-field + Hubbard-Stratonovich

$$e^{-\hat{H}_I \Delta\tau} = \exp\left(U\Delta\tau \hat{R}_{\alpha\beta}\hat{R}_{\beta\alpha} - U\Delta\tau\hat{q}\right) =$$
$$= \exp\left(U\Delta\tau\, \hat{R}_{\alpha\beta}\hat{R}_{\beta\alpha}\right)\, \exp\left(-U\Delta\tau\,\hat{q}\right)$$

$$\exp\left(U\Delta\tau \hat{R}_{\alpha\beta}\hat{R}_{\beta\alpha}\right) =$$
$$= \int d\Phi_{\alpha\beta}\, e^{-\frac{\Delta\tau}{4U}\,\mathrm{Tr}\,\Phi^2 - \Delta\tau\Phi_{\alpha\beta}\,\hat{\psi}^\dagger_\alpha\hat{\psi}_\beta}$$

$$\left[\hat{R}_{\alpha\beta}, \hat{R}_{\beta\alpha}\right] = \left[\hat{R}_{\alpha\beta}, \hat{R}^\dagger_{\alpha\beta}\right] = 0$$

- $R_{\alpha\beta}$ cannot be treated as C-number
- By doing so we introduce an error of order $\Delta\tau^2$
- (Splitting single exp into the product over α, β)

Now we join back all exps, again error ~ $\Delta\tau^2$

Mean-field path integral

$$\mathcal{Z} = \int \mathcal{D}\Phi_{x,\alpha\beta}(\tau) \exp\left(-\frac{1}{4U} \sum_{x} \int_{0}^{T^{-1}} d\tau \, \mathrm{Tr}\, \Phi_x^2 \right) \times$$

$$\times \, \mathrm{Tr}\, \mathcal{T} \exp\left(- \int_{0}^{T^{-1}} d\tau \, \hat{\psi}^\dagger(\tau) \, h^\Phi(\tau) \hat{\psi}(\tau) \right)$$

Time-dependent single-particle Hamiltonian

$$h^\Phi_{x,\alpha;y,\beta}(\tau) = h_{x,\alpha;y,\beta} + \Phi_{x;\alpha\beta}(\tau)\delta_{xy} + \delta_{\alpha\beta}\delta_{xy}$$

- The mean-field Hamiltonian is Hermitian
- Exact identity with full integration
- Saddle points of the path integral ?
- Assume translational symmetry
- $\mathrm{Tr}(\Phi)$ decouples, compensates $\delta_{\alpha\beta}\, \delta_{xy}$

Mean-field path integral

We now minimize the effective action over all constant $\Phi_{x\alpha\beta}(\tau) = \Phi_{\alpha\beta}$

$$\frac{\mathrm{Tr}\,\Phi^2}{4UT} - \log \mathcal{Z}\left[\Phi\right] = T^{-1}\left(\frac{\mathrm{Tr}\,\Phi^2}{4U} + \mathcal{F}\left[\Phi\right]\right)$$

Partition function/Free energy of the free fermion gas with the Hamiltonian *$h[\Phi]$*

$$\mathcal{F}\left[\Phi\right] = -T\sum_i \ln\left(1 + e^{-\epsilon_i/T}\right)$$

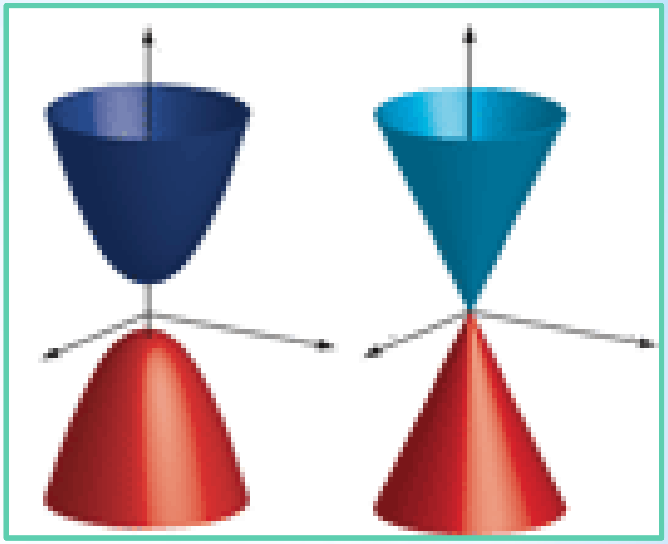
In the limit of zero temperature

$$\mathcal{F}\left[\Phi\right] = \sum_i \epsilon_i \Theta\left(-\epsilon_i\right)$$

Sum over all energy levels within the <u>Fermi sea</u> (below zero) !!!

Spontaneous chiral symmetry breaking

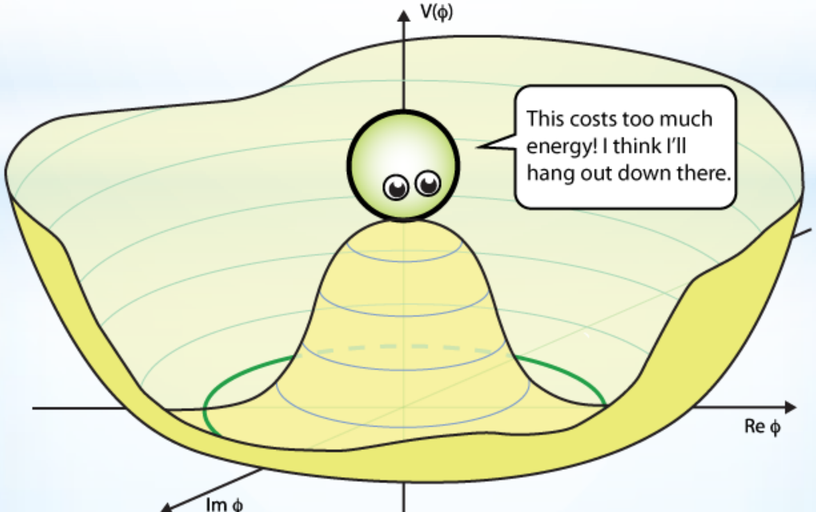
$$\Phi_x = \begin{pmatrix} 0 & me^{i\theta} \\ me^{-i\theta} & 0 \end{pmatrix}$$



To-be-Goldstone!

Mass term lowers all energies in the Fermi sea

$$\epsilon\left(\vec{k}\right) = \pm|\vec{k}| \Rightarrow \epsilon\left(\vec{k}\right) = \pm\sqrt{\vec{k}^2 + m^2}$$



Spontaneous chiral symmetry breaking

E.g. for 2D continuous Dirac fermions

$$\mathcal{F}[m] \sim -\int_0^\Lambda d^2k\sqrt{k^2+m^2} \sim$$

$$\sim m^3 - \left(m^2+\Lambda^2\right)^{3/2} \sim \text{const} - \alpha m^2 + \beta m^3 + \ldots$$

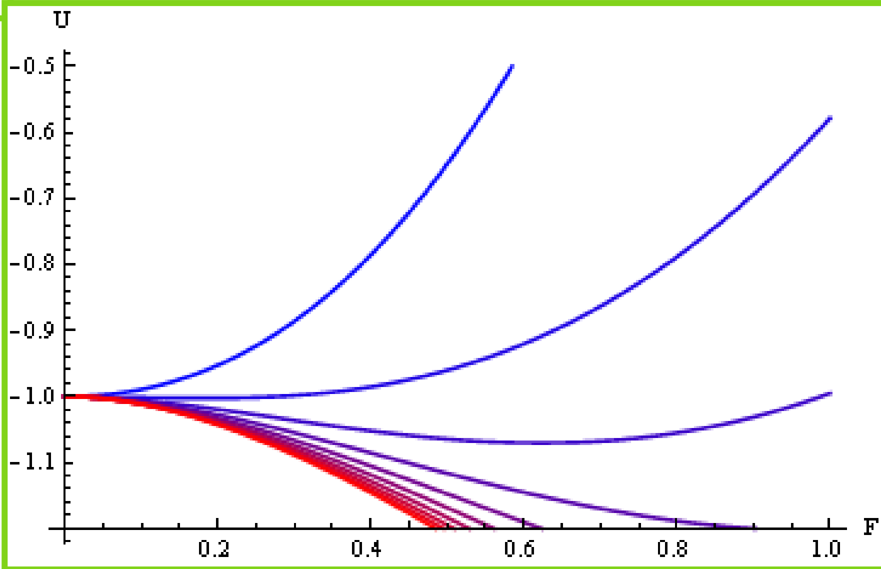
The whole effective action is

$$-\alpha m^2 + \frac{m^2}{4U} + \beta m^3 + \ldots$$

m=0 **unstable if**

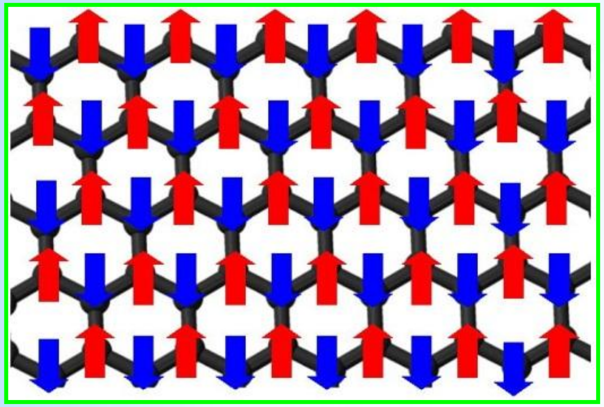
$$-\alpha + \frac{1}{4U} < 0$$

$$U > \alpha/4$$

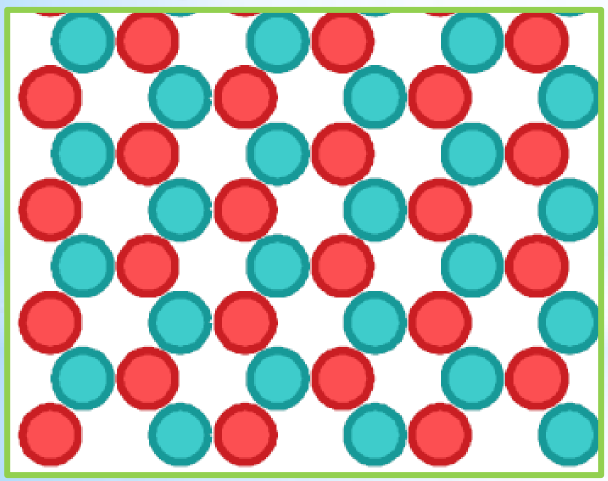


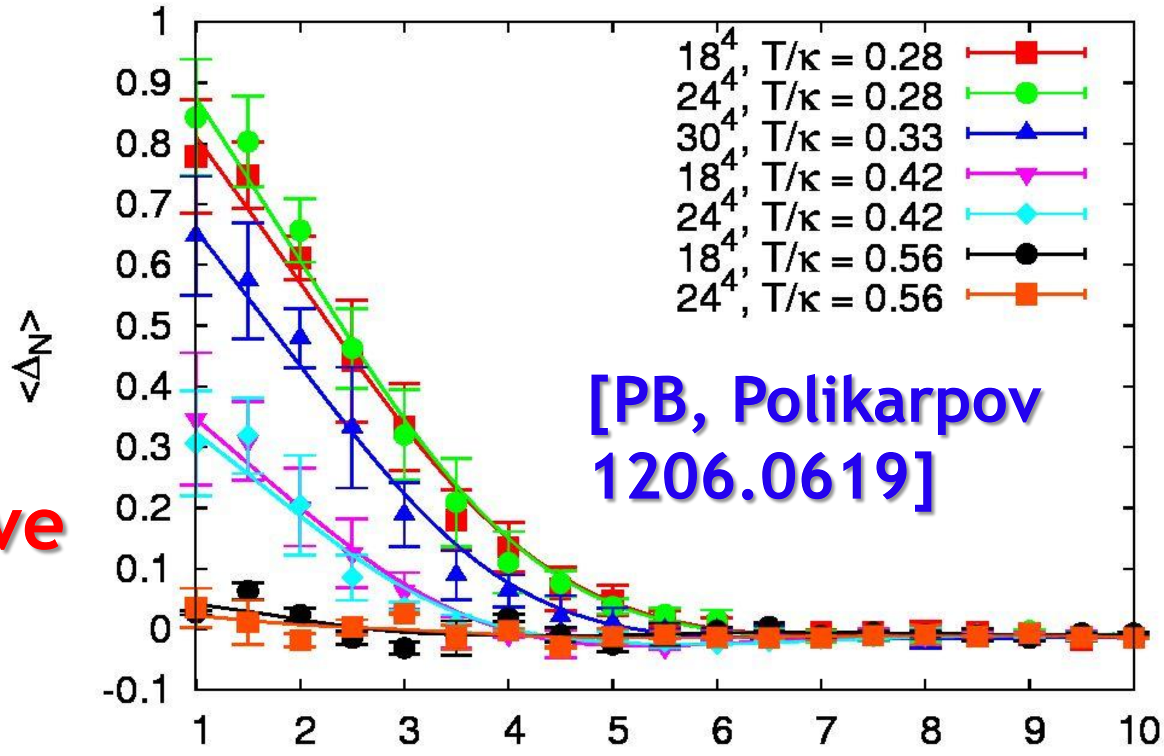
What happens in real graphene?

Spin density wave



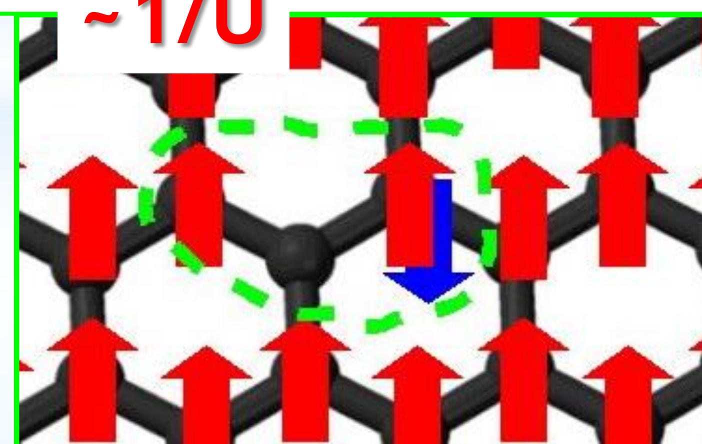
Charge density wave





~1/U

Mesons:
Particle-Hole
Bound states



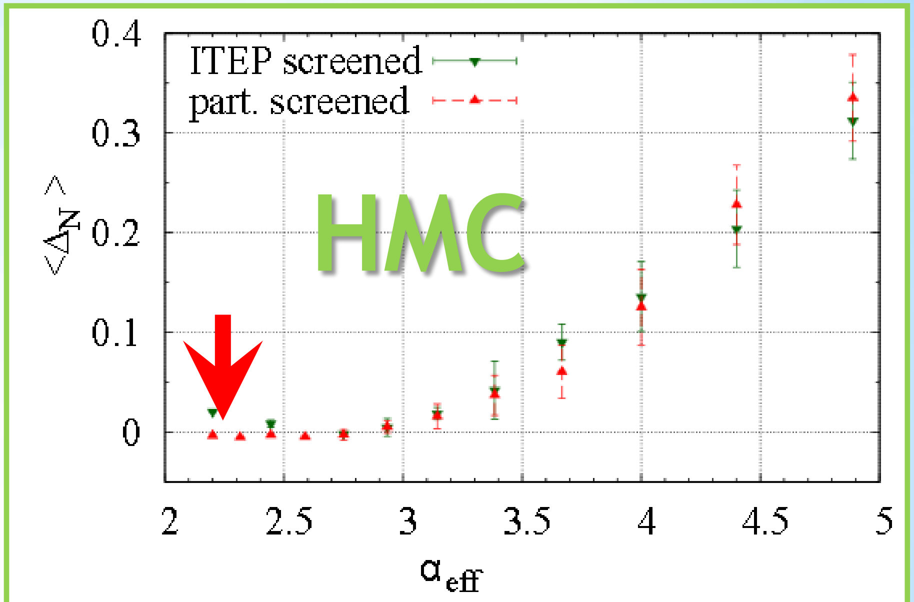
Real suspended graphene is a semimetal

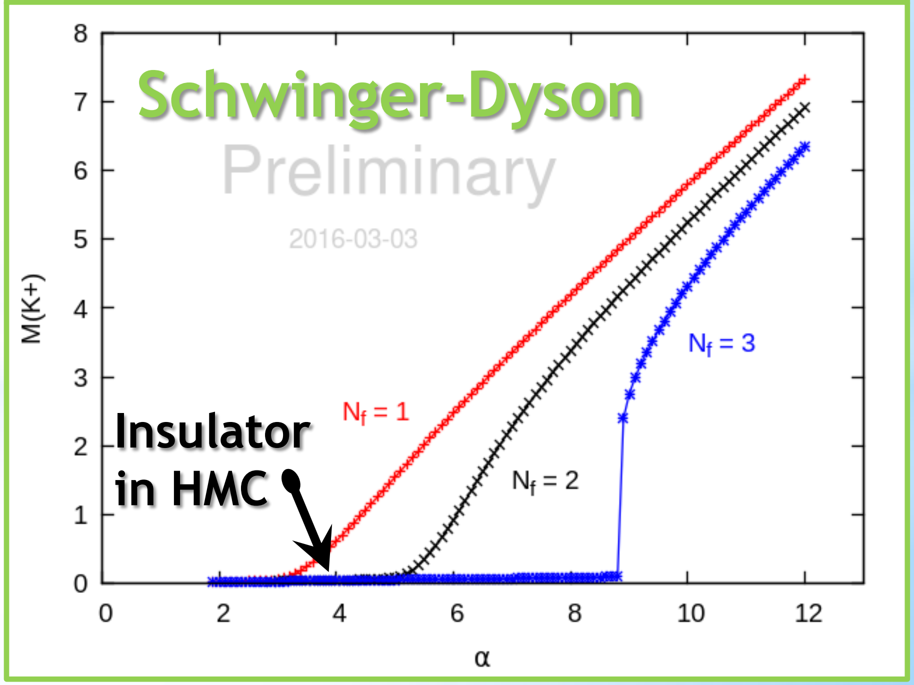
Experiments by Manchester group [Elias et al. 2011,2012]:
Gap < 1 meV

HMC simulations (ITEP, Regensburg and Giessen) [1304.3660,1403.3620]
Unphysical $\alpha_c \sim 3 > \alpha_{eff} = 2.2$

Schwinger-Dyson equations [Smekal,Bischoff, 1308.6199]
Unphysical $\alpha_c \sim 5 > \alpha_{eff} = 2.2$

In the meanwhile:
Graphene Gets a Good Gap on SiC [M. Nevius et al. 1505.00435] - interactions are not so important...





Hirsch transformation: "Discrete HS"

On-site interactions of spinful electrons

$$\exp\left(-\hat{H}_I \Delta\tau\right) = \exp\left(-U\Delta\tau\,(\hat{n}_\uparrow + \hat{n}_\downarrow - 1)^2\right) =$$
$$= \exp\left(-2U\Delta\tau\,\hat{n}_\uparrow\hat{n}_\downarrow - U\Delta\tau\,\hat{q}\right), \quad \hat{n}_\sigma^2 = \hat{n}_\sigma$$

$$\exp\left(-2\Delta\tau U\,\hat{n}_\uparrow\hat{n}_\downarrow + U\Delta\tau\hat{q}\right) \sim$$
$$\sim \frac{1}{2}\sum_{\sigma=\pm 1} \exp\left(2a\sigma\left(\hat{n}_\uparrow - \hat{n}_\downarrow\right)\right)$$

$$\tanh^2(a) = \tanh\left(\frac{U\Delta\tau}{2}\right)$$

Should be proven only for eigenvalues +/- 1 of electron number operators !!!

Partition function = sum over discrete spin-like variables !!!

Hirsch transformation: "Discrete HS"

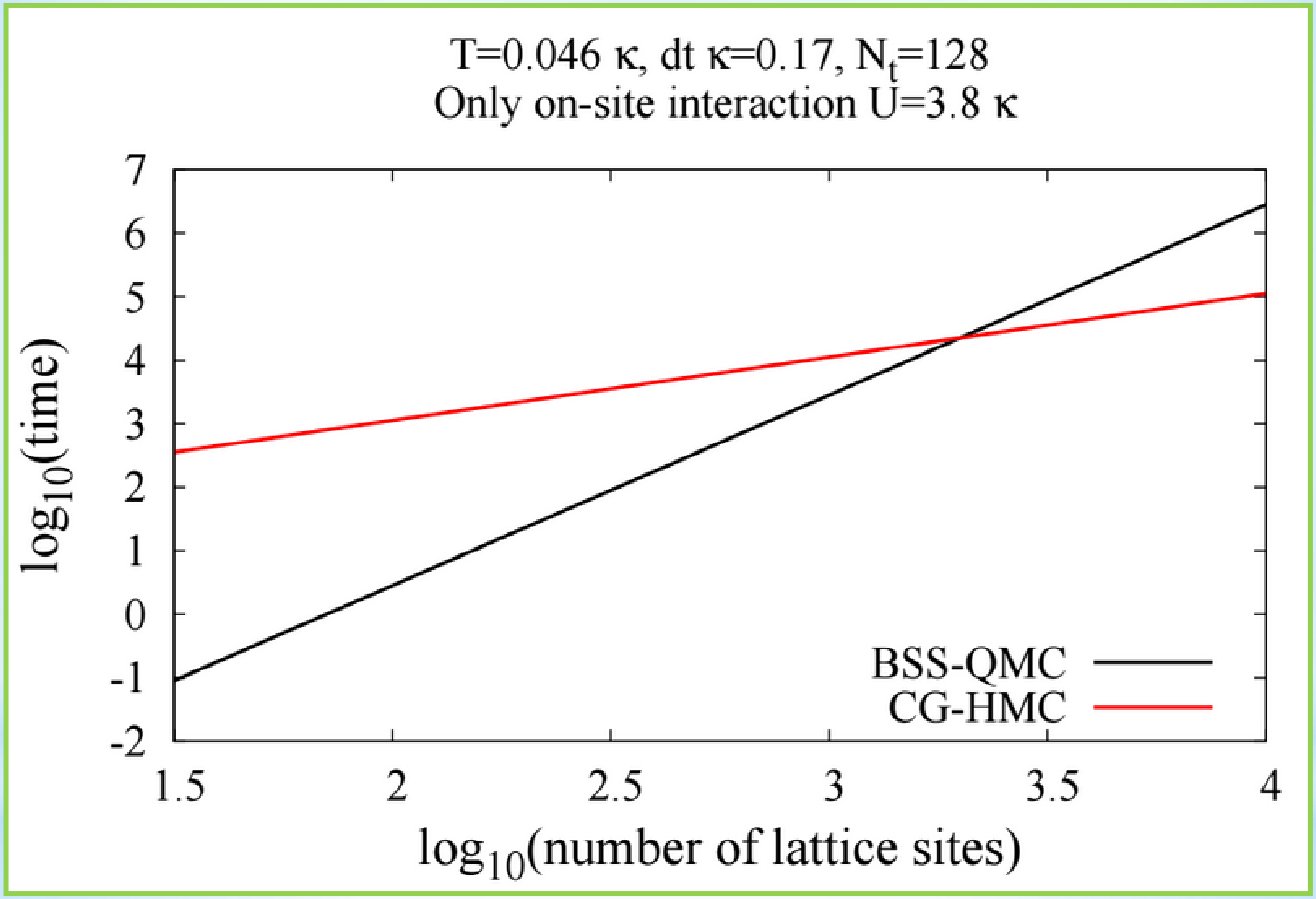
With more complicated interactions, other "Discrete HS" possible with larger number of terms, can be truncated allowing errors $\sim\Delta\tau^2$

Auxiliary field Quantum Monte-Carlo

[BSS-Blankenbecler,Scalapino,Sugar'81]

- Discrete updates of HS variables
- Metropolis accept-reject with determinants
- Fast re-calculation of determinant ratios
- Fermionic operator real
- Statistical noise significantly reduces
- Numerical cost ~ $(T^{-1}\,V)^3$

Aux.field QMC vs HMC

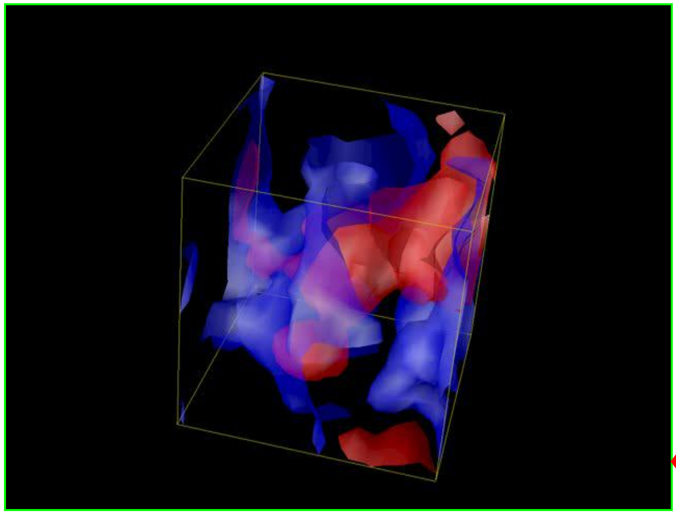


[Data of M. Ulybyshev, F. Assaad]

Quite different scaling with volume!!!

Diagrammatic Monte-Carlo

Sum over fields



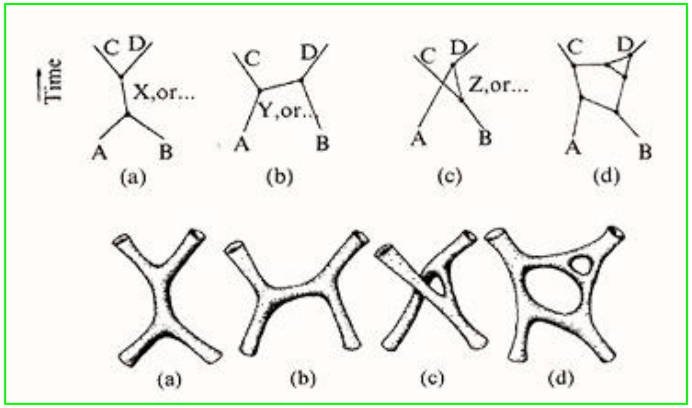
$$\mathcal{Z} = \mathrm{Tr}\, e^{-\hat{\mathcal{H}}/kT} =$$
$$= \int \mathcal{D}\phi\left(x^{\mu}\right)\, \exp\left(-S_E\left[\phi\left(x^{\mu}\right)\right]\right)$$

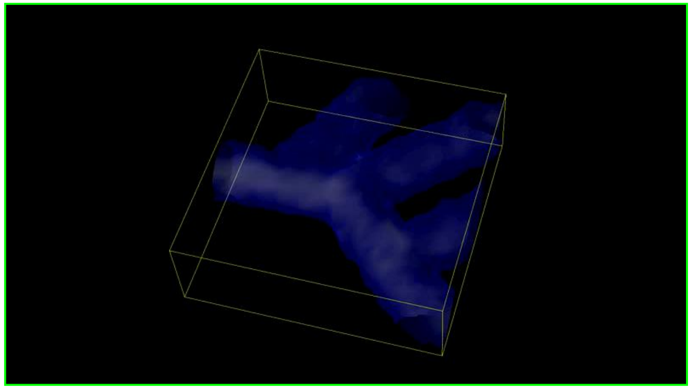
Euclidean action:

$$S_E = \int d^D x \left(\frac{1}{2}\, \partial_{\mu}\phi \partial_{\mu}\phi + \frac{m^2}{2}\, \phi^2 + V\left(\phi\right) \right)$$

Perturbative expansions

Sum over interacting paths



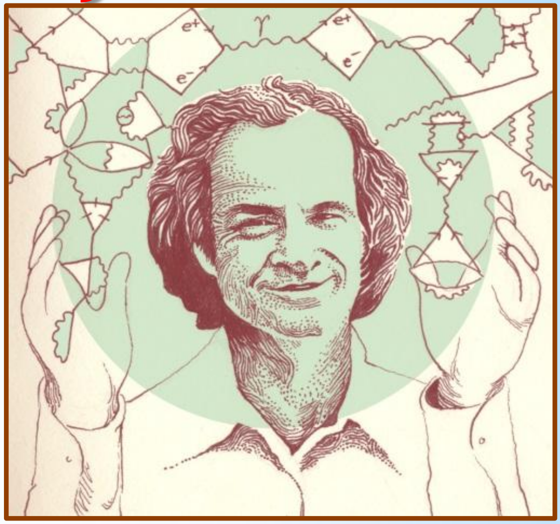


$$\mathcal{Z} = \sum_k \frac{\lambda^k}{k!} \exp\left(-L\left(\text{Paths connecting } k \text{ vertices}\right)\right)$$

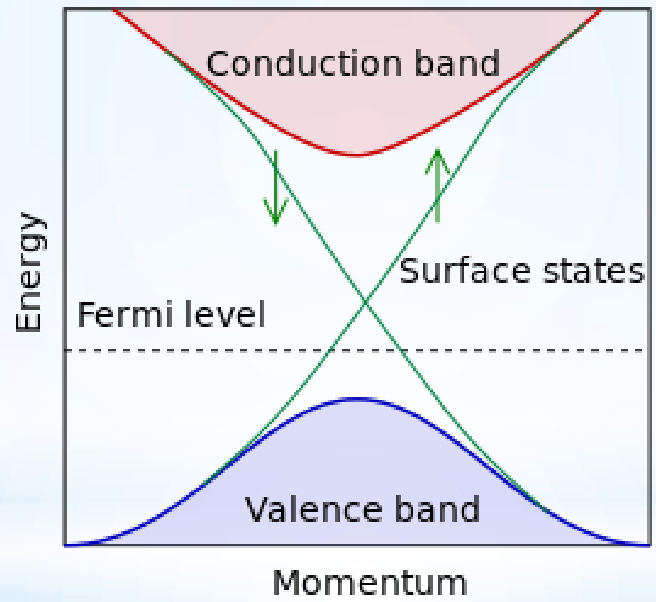
Diagrammatic Monte-Carlo

[Prokof'ev, Svistunov, van Houcke, Pollet, …]

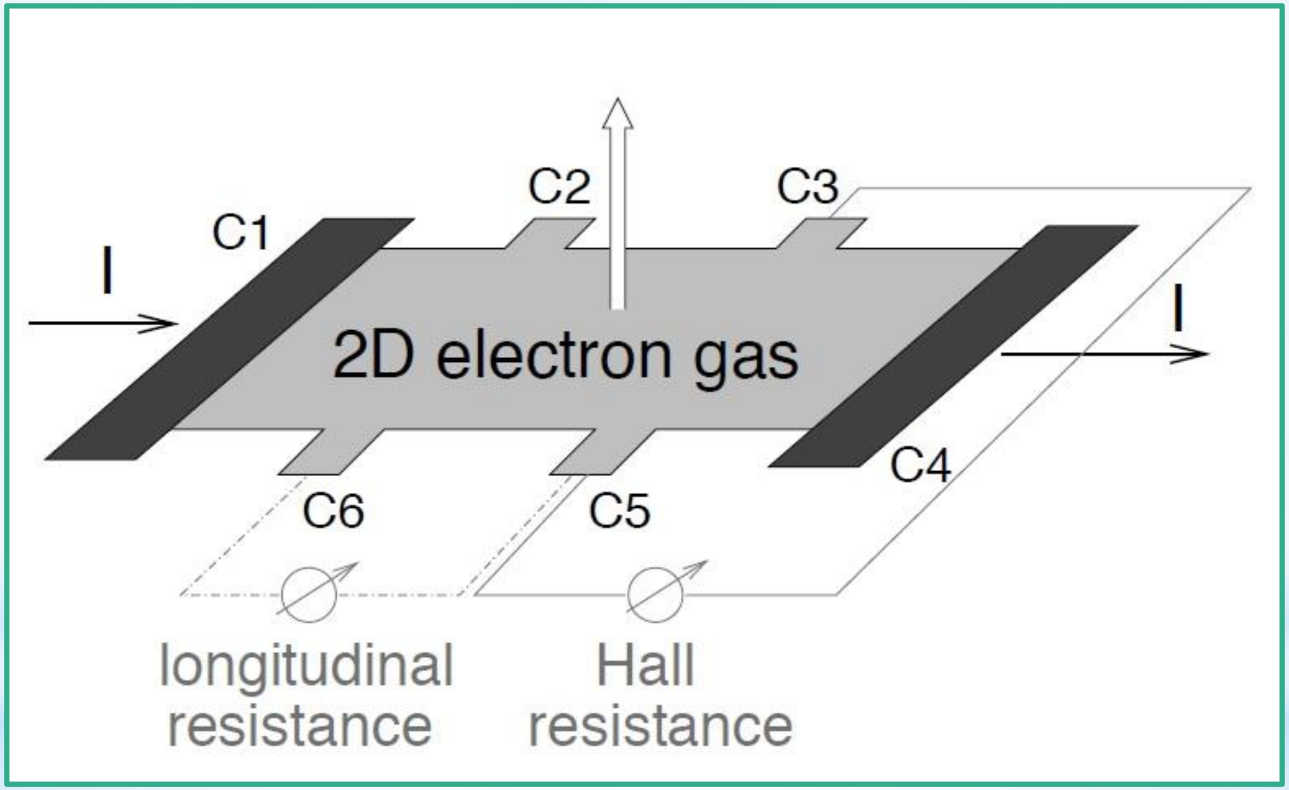
- Factorially growing number of Feynman diagrams from combinatorics
- Divergent series for bosons (Dyson argument)
- Sign blessing for fermions:
- Finite answer from PT series despite divergent number of diagrams
- Massive sign cancellations
- Polynomial complexity due to fast series convergence [R. Rossi, N. Prokof'ev, B. Svistunov, K. Van Houcke, F. Werner, 1703.10141]



Topological insulators



Hall effect



Classical treatment

Dissipative motion for point-like particles (Drude theory)

$$\dot{\mathbf{p}} = -e\left(\mathbf{E} + \frac{\mathbf{p}}{m} \times \mathbf{B}\right) - \frac{\mathbf{p}}{\tau}$$

Steady motion

$$\begin{aligned} eE_x &= -\frac{eB}{m}p_y - \frac{p_x}{\tau}, \\ eE_y &= \frac{eB}{m}p_x - \frac{p_y}{\tau}, \end{aligned}$$

Classical Hall effect

Cyclotron frequency

$$\omega_c = \frac{eB}{m} \,,$$

Drude conductivity

$$\sigma_0 = \frac{n_{el} e^2 \tau}{m} \,,$$

Current

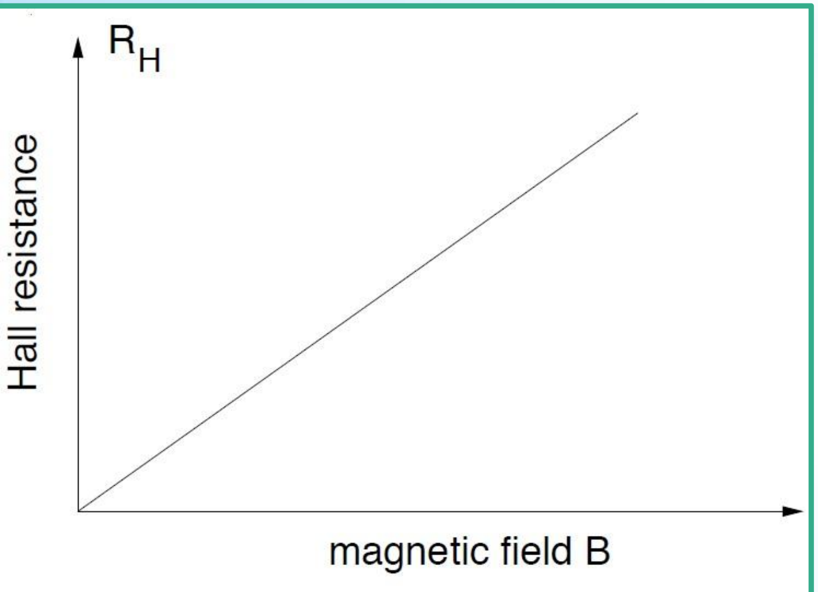
$$\mathbf{j} = -e n_{el} \frac{\mathbf{p}}{m} \,.$$

Resistivity tensor

$$\begin{aligned} \sigma_0 E_x &= -e n_{el} \frac{p_x}{m} - e n_{el} \frac{p_y}{m} \omega_c \tau, \\ \sigma_0 E_y &= e n_{el} \frac{p_x}{m} \omega_c \tau - e n_{el} \frac{p_y}{m}. \end{aligned}$$

$$\begin{pmatrix} E_x \\ E_y \end{pmatrix} = \frac{1}{\sigma_0} \begin{pmatrix} 1 & w_c \tau \\ -w_c \tau & 1 \end{pmatrix} \begin{pmatrix} j_x \\ j_y \end{pmatrix}$$

Hall resistivity (off-diag component of resistivity tensor)



$$\rho_H = \frac{\omega_c \tau}{\sigma_0} = \frac{eB}{m} \tau \times \frac{m}{n_{el} e^2 \tau} = \frac{B}{e n_{el}}$$

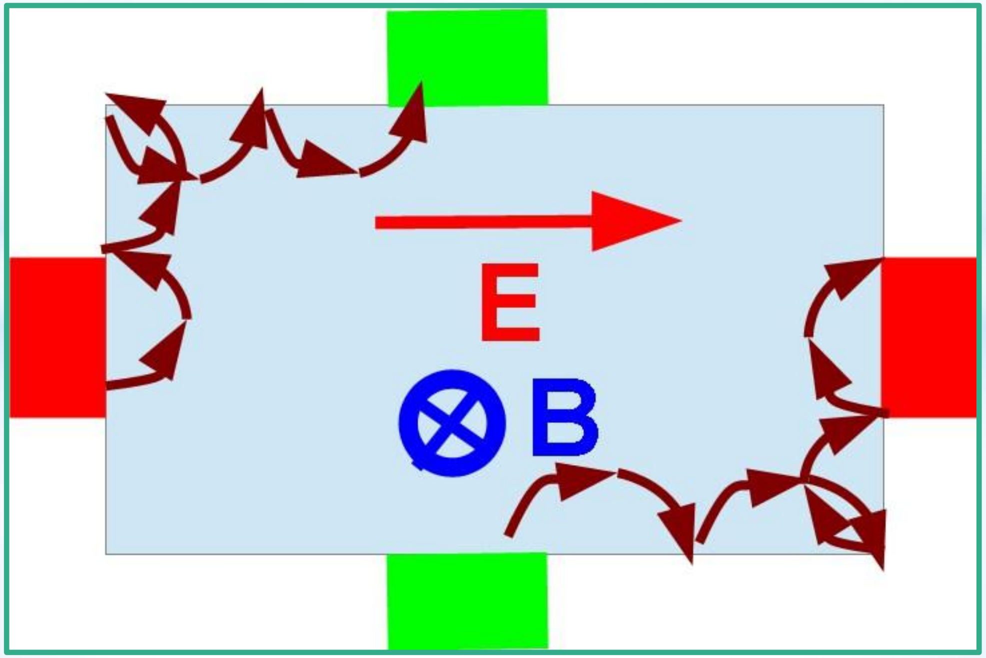
- Does not depend on disorder
- Measures charge/density of electric current carriers
- Valuable experimental tool

Classical Hall effect: boundaries

Clean system limit: INSULATOR!!!
Importance of matrix structure

$$\rho = \begin{pmatrix} 0 & \frac{B}{en_{el}} \\ -\frac{B}{en_{el}} & 0 \end{pmatrix} \qquad \sigma = \begin{pmatrix} 0 & -\frac{en_{el}}{B} \\ \frac{en_{el}}{B} & 0 \end{pmatrix}$$

Naïve look at longitudinal components:
INSULATOR AND CONDUCTOR SIMULTANEOUSLY!!!



Conductance happens exclusively due to boundary states!
Otherwise an insulating state

Quantum Hall Effect

Non-relativistic Landau levels $E_n = \hbar w_c (n + 1/2)$

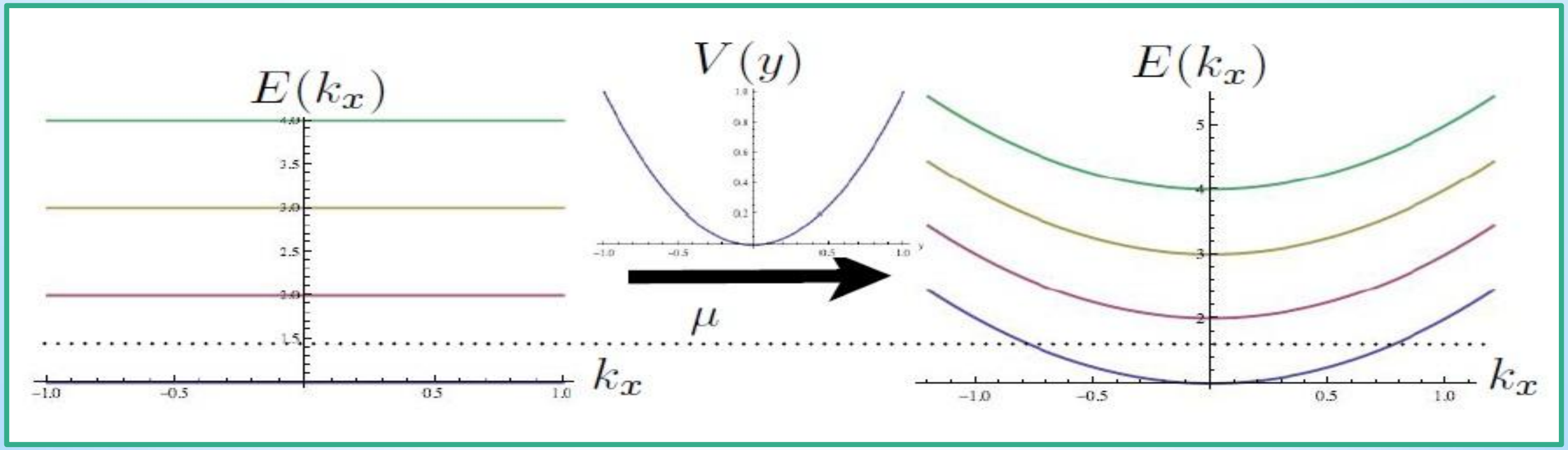
$$\hat{H} = -\frac{(\partial_x - iBy)^2}{2m} - \frac{\partial_y^2}{2m} = -\frac{\partial_y^2}{2m} + \frac{B^2}{2m}(y - k_x/B)^2$$

Model the boundary by a confining potential ***$V(y) = mw^2y^2/2$***

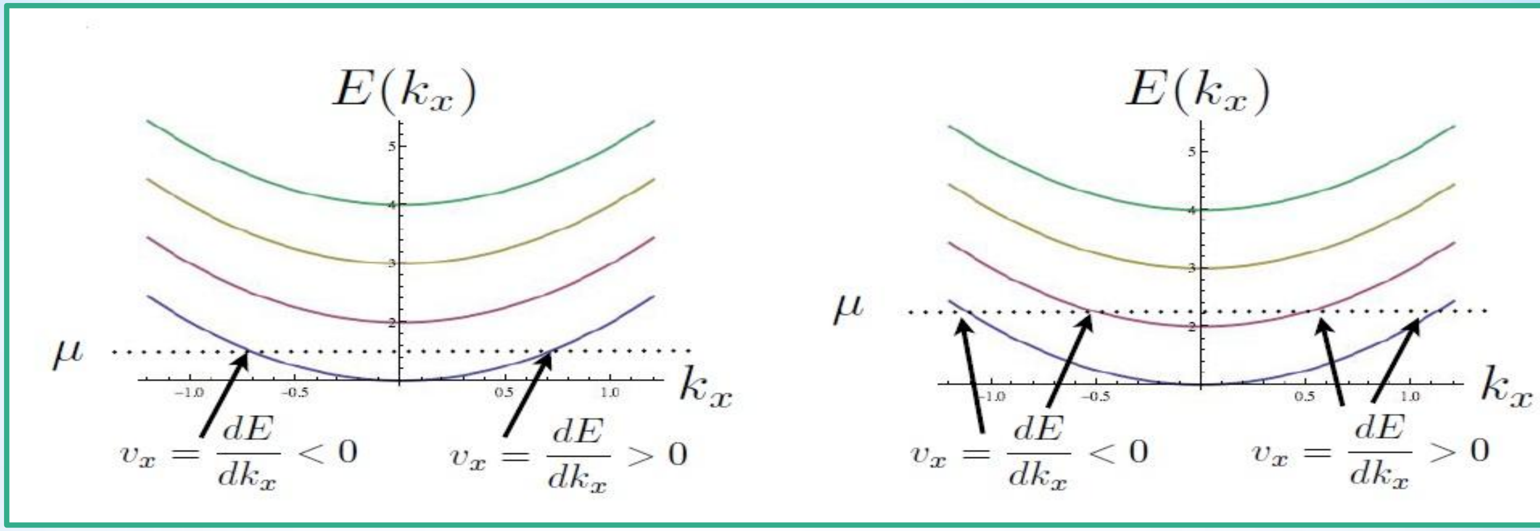
$$\hat{H} = -\frac{\partial_y^2}{2m} + \frac{mw_c^2}{2}(y - k_x/B)^2 + \frac{m^2w^2y^2}{2} =$$

$$= -\frac{\partial_y^2}{2m} + \frac{m\left(w^2 + w_c^2\right)}{2}\left(y - \frac{w_c^2}{w^2 + w_c^2}\frac{k_x}{B}\right)^2 + \frac{mw_c^2k_x^2}{2B^2}\frac{w^2}{w^2 + w_c^2}$$

$$E_n = \hbar\sqrt{w^2 + w_c^2}(n + 1/2) + \frac{mw_c^2k_x^2}{2B^2}\frac{w^2}{w^2 + w_c^2}$$

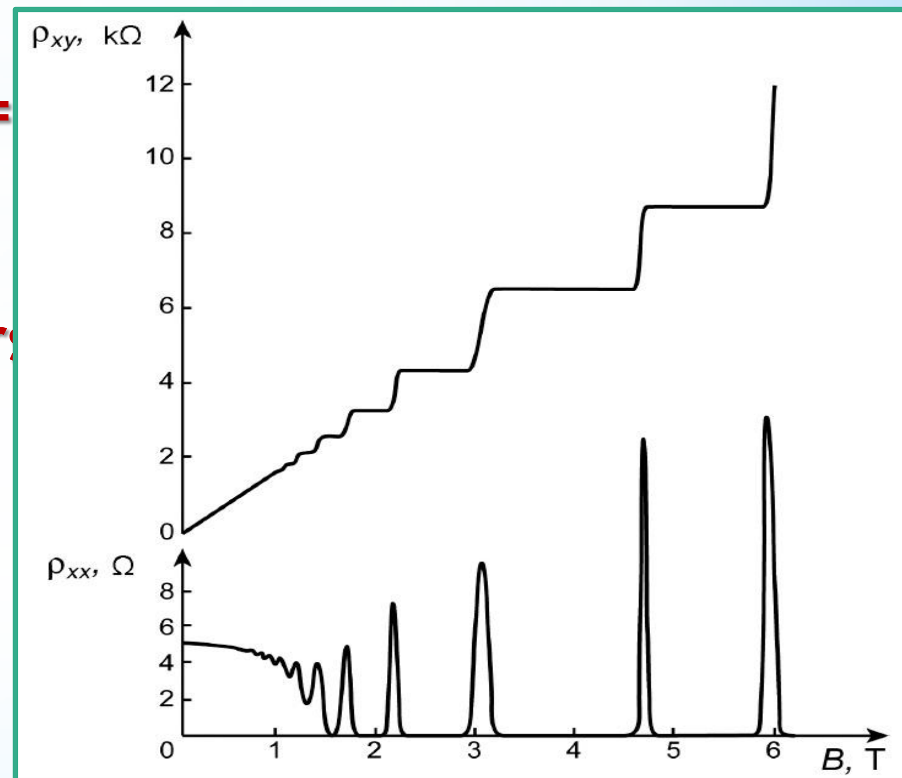


Quantum Hall Effect



- **Number of conducting states = no of LLs below *Fermi level***
- ***Hall conductivity σ ~ n***
- ***Pairs of right-* and left- movers *on the "Boundary"***

NOW THE QUESTION:
Hall state without magnetic Field???

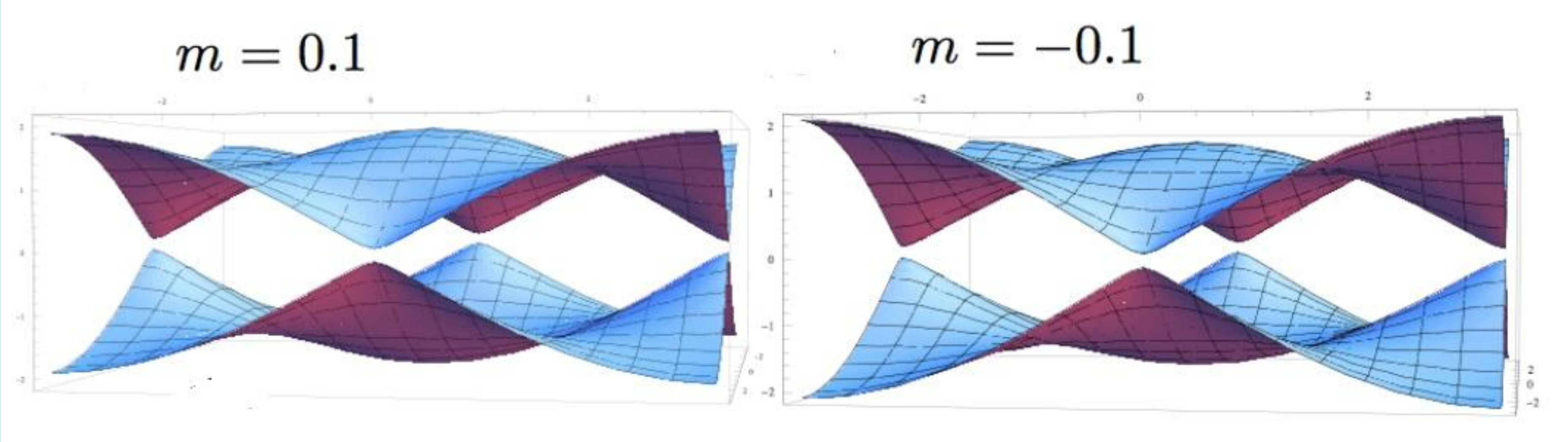


Chern insulator [Haldane'88]

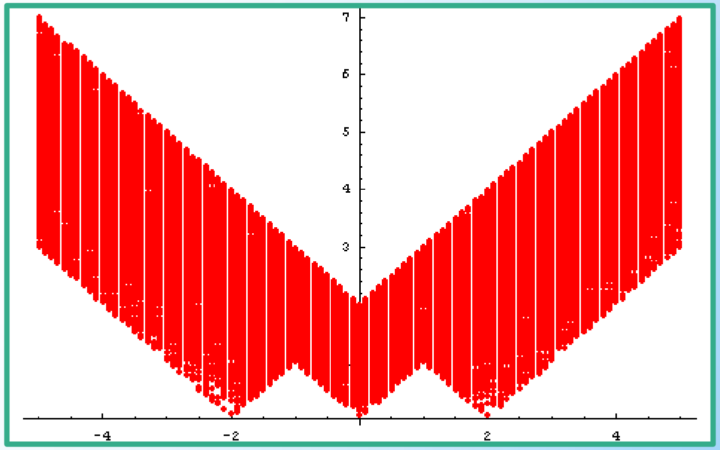
Originally, hexagonal lattice, but we consider square

$$H = \sigma_x \sin(k_x) + \sigma_y \sin(k_y) + \sigma_z \left(m + \cos(k_x) + \cos(k_y)\right)$$

Two-band model, similar to Wilson-Dirac [Qi, Wu, Zhang]



Phase diagram



m=2 Dirac point at kx,ky=±π

m=0 Dirac points at (0, ±π), (±π,0)

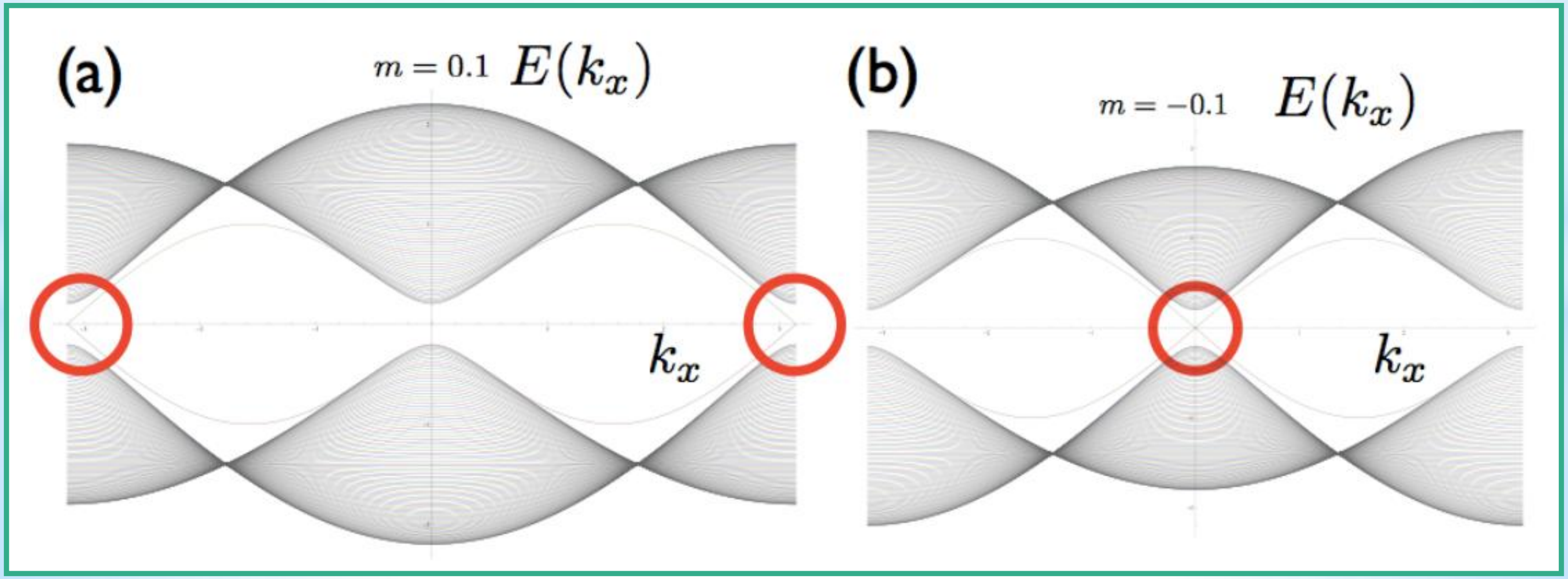
m=-2 Dirac point at kx,ky=0

Chern insulator [Haldane'88]

Open B.C. in y direction, numerical diagonalization

$$\mathcal{H}(k_x) = \sum_y \Psi_y^\dagger(k_x)(m + \sin k_x + \cos k_x)\Psi_y(k_x) + \sum_y \left(\Psi_y^\dagger(k_x)\frac{\sigma_z + i\sigma_y}{2}\Psi_{y+1}(k_x) + \text{h.c.}\right)$$

$$H(k_x = 0, y) = -i\partial_y\sigma_y + \delta m(y)\sigma_z$$



$$\Phi_+(y) \propto \phi_+ e^{\int_0^y \delta m(y')dy'} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{\int_0^y \delta m(y')dy'}$$

$$H^{1d}(k_x) = \phi_+^T H(k_x, y=0)\phi_+ = k_x$$

Electromagnetic response and effective action

Along with current, also charge density is generated

$$
\begin{aligned}
j_i &= \sigma_H \epsilon^{ij} E_j \\
&\Rightarrow \frac{\partial \rho}{\partial t} = -\nabla \cdot \mathbf{j} = -\sigma_H \nabla \times \mathbf{E} = \sigma_H \frac{\partial B}{\partial t} \\
&\Rightarrow \rho(B) - \rho_0 = \sigma_H B
\end{aligned}
$$

Response in covariant form

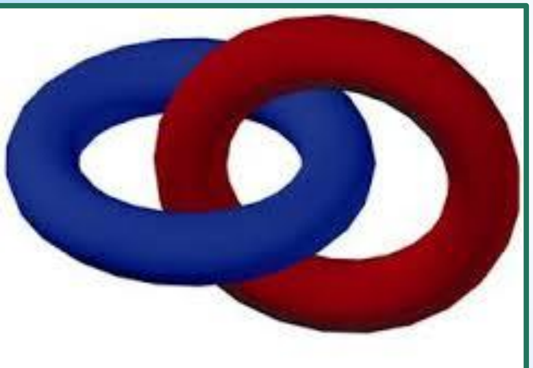
$$j^\mu = \frac{C_1}{2\pi} \epsilon^{\mu\nu\tau} \partial_\nu A_\tau$$

Effective action for this response

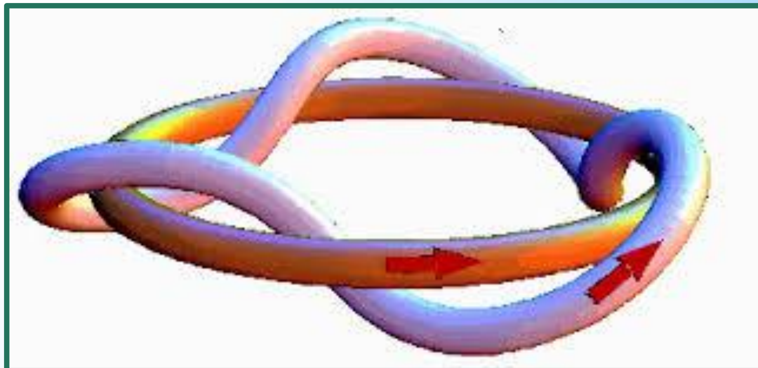
$$S_{\text{eff}} = \frac{C_1}{4\pi} \int d^2x \int dt A_\mu \epsilon^{\mu\nu\tau} \partial_\nu A_\tau$$

Electromagnetic Chern-Simons = Magnetic Helicity

Winding of magnetic flux lines



$$\mathbf{K} \equiv \int \mathbf{A}\cdot\mathbf{B}\, dV = 2\phi\psi$$

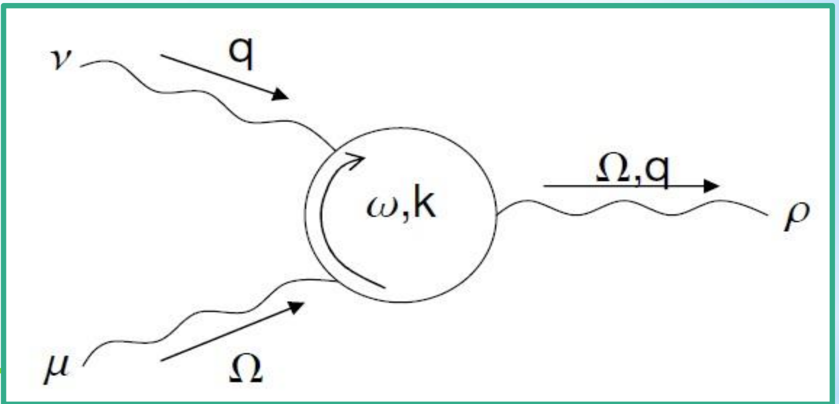


(4+1)D Chern insulators
(aka domain wall fermions)

Consider the 4D single-particle hamiltonian *h(k)*

Similarly to *(2+1)D* Chern insulator, electromagnetic response

$$j^\mu = \frac{C_2}{8\pi^2}\epsilon^{\mu\nu\rho\sigma\tau}\partial_\nu A_\rho \partial_\sigma A_\tau$$



C_2 is the "Second Chern Number"

$$C_2 = \frac{1}{32\pi^2}\int d^4k\, \epsilon^{ijk\ell}\,\mathrm{tr}\left[f_{ij} f_{k\ell}\right]$$

$$f_{ij}^{\alpha\beta} = \partial_i a_j^{\alpha\beta} - \partial_j a_i^{\alpha\beta} + i\left[a_i, a_j\right]^{\alpha\beta}$$

$$a_i^{\alpha\beta}(\mathbf{k}) = -i\left\langle \alpha, \mathbf{k}\right| \frac{\partial}{\partial k_i}\left|\beta, \mathbf{k}\right\rangle$$

Effective EM action

$$S_{\text{eff}} = \frac{C_2}{24\pi^2}\int d^4x\, dt\, \epsilon^{\mu\nu\rho\sigma\tau} A_\mu \partial_\nu A_\rho \partial_\sigma A_\tau$$

Parallel E and B in 3D generate current along 5th dimension

(4+1)D Chern insulators: Dirac models

In continuum space

$$H = \int d^4x \left[\psi^\dagger(x)\Gamma^i\left(-i\partial_i\right)\psi(x) + m\psi^\dagger\Gamma^0\psi\right]$$

Five (4 x 4) Dirac matrices: $\{\Gamma_\mu , \Gamma_\nu\} = 2\,\delta_{\mu\nu}$

Lattice model = (4+1)D Wilson-Dirac fermions

$$H = \sum_{n,i}\left[\psi_n^\dagger\left(\frac{c\Gamma^0 - i\Gamma^i}{2}\right)\psi_{n+\hat{i}} + h.c.\right]$$

In momentum space

$$H = \sum_{\mathbf{k}}\psi_{\mathbf{k}}^\dagger\left[\sum_i \sin k_i\Gamma^i + \left(m + c\sum_i \cos k_i\right)\Gamma^0\right]\psi_{\mathbf{k}}.$$

$$H = \sum_{\mathbf{k}}\psi_{\mathbf{k}}^\dagger d_a(\mathbf{k})\Gamma^a\psi_{\mathbf{k}}$$

$$d_a(\mathbf{k}) = \left(\left(m + c\sum_i \cos k_i\right), \sin k_x, \sin k_y, \sin k_z, \sin k_w\right)$$

Effective EM action of 3D TRI topinsulators

Dimensional reduction from (4+1)D effective action

$$S_{3D} = \frac{G_3(\theta_0)}{4\pi} \int d^3x dt \epsilon^{\mu\nu\sigma\tau} \delta\theta \partial_\mu A_\nu \partial_\sigma A_\tau$$

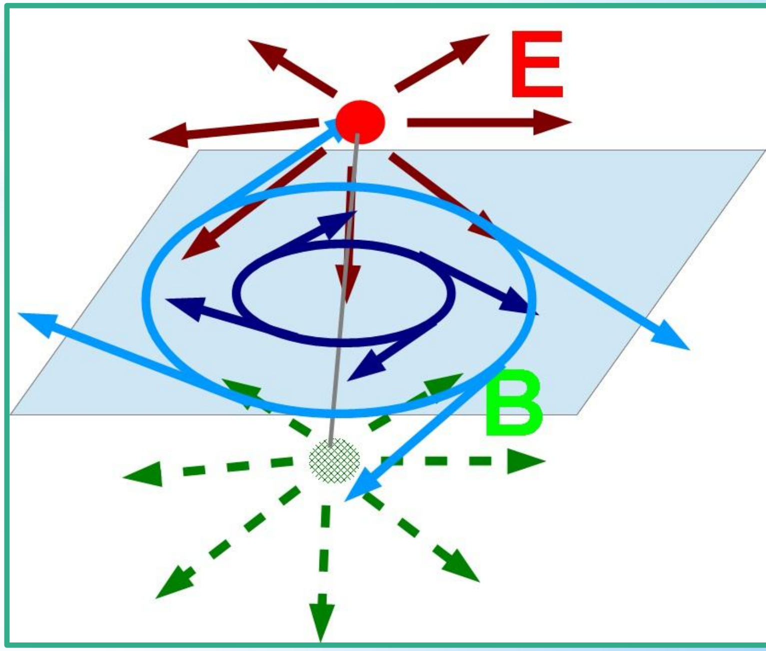
$$S_{3D} = \frac{1}{4\pi} \int d^3x dt \epsilon^{\mu\nu\sigma\tau} P_3(x,t) \partial_\mu A_\nu \partial_\sigma A_\tau$$

Electric current responds to the gradient of *A5 = Θ = p3* polarization

$$\partial_z P_3 \sim \delta(z)$$

$$j^\mu = \frac{1}{2\pi} \epsilon^{\mu\nu\sigma\tau} \partial_\nu P_3 \partial_\sigma A_\tau .$$

- Spatial gradient of P3: Hall current
- Time variation of P3: current || B
- P3 is like "axion" (TME/CME)



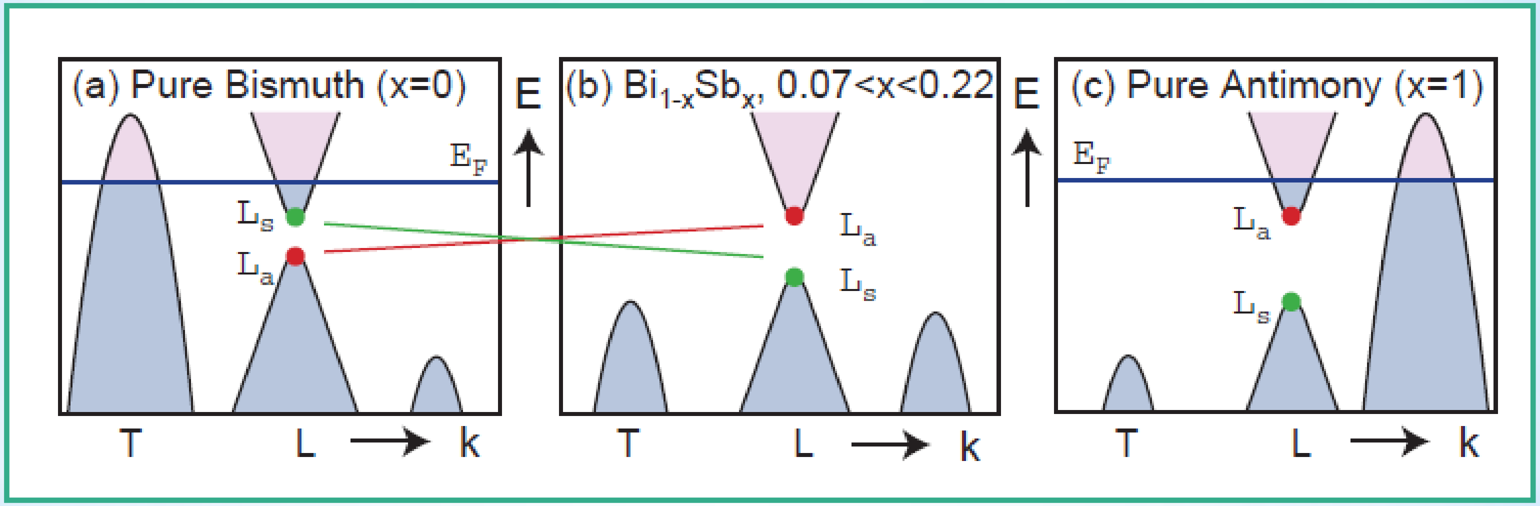
Response to electrostatic field near boundary

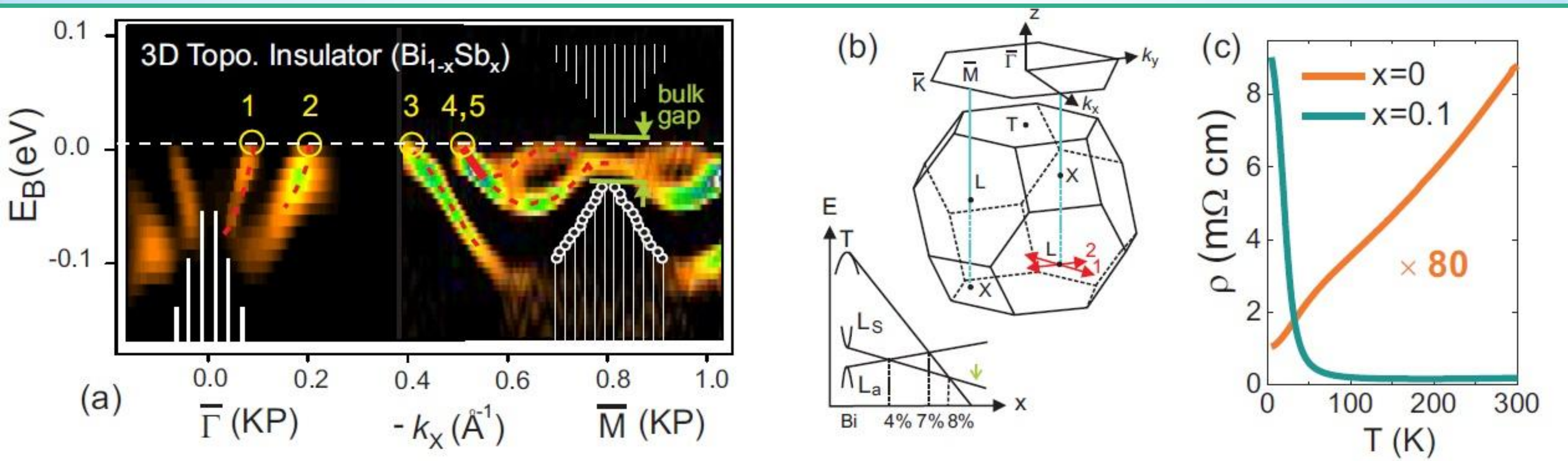
$$j_\alpha \sim \epsilon_{\alpha\beta} \partial_\beta \phi$$

Electrostatic potential A_0

Real 3D topological insulator: $Bi_{1-x}Sb_x$

Band inversion at intermediate concentration





Kramers theorem

Time-reversal operator for Pauli electrons $\boxed{\theta^2 = -1}$

$$\theta = -is_z K = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} K \qquad \theta \begin{pmatrix} \psi_\uparrow \\ \psi_\downarrow \end{pmatrix} = \begin{pmatrix} -\bar{\psi}_\downarrow \\ \bar{\psi}_\uparrow \end{pmatrix}$$

Anti-unitary symmetry $\langle \theta\psi | \, |\theta\chi\rangle = \langle \chi | \, |\psi\rangle$

Single-particle Hamiltonian in momentum space

$$h_{xy} = \sum_k e^{ik(x-y)} h(k)$$

(Bloch Hamiltonian)

If *[h,θ]=0* $h(k) = \theta h(-k)\theta^{-1}$

Consider some eigenstate $h(k)\,|u_k\rangle = \epsilon_k\,|u_k\rangle$

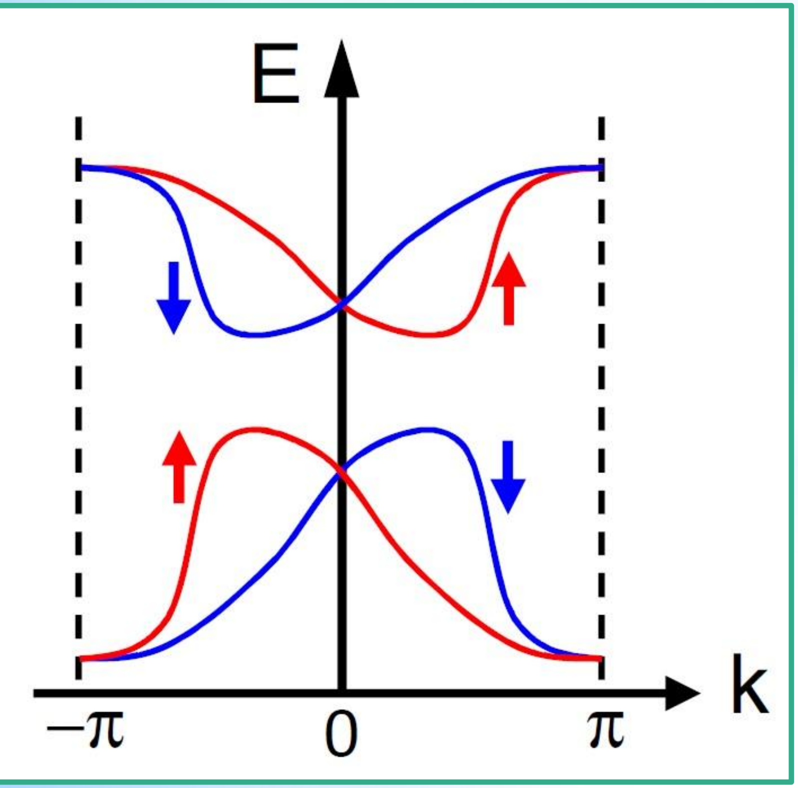
$$\begin{aligned} \theta h(-k)\theta^{-1}\,|u_k\rangle &= \epsilon_k\,|u_k\rangle \\ h(-k)\,|\theta u_k\rangle &= \epsilon_k\,|\theta u_k\rangle \end{aligned}$$

Kramers theorem

Every eigenstate $\boxed{|u_k\rangle}$ has a partner $\boxed{|\theta u_k\rangle}$ at (-k)

With the same energy!!!

Since θ changes spins, it cannot be $\boxed{|u_{-k}\rangle}$



Example: <u>TRIM</u>

(Time Reversal Invariant Momenta)

-k is equivalent to k

For 1D lattice, unit spacing

TRIM: k = {±π, 0}

Assume

$$\begin{aligned} \theta\,|u_k\rangle &= \alpha\,|u_k\rangle \\ \theta^2\,|u_k\rangle &= \theta\alpha\,|u_k\rangle = \\ &= \bar{\alpha}\theta\,|u_k\rangle = |\alpha|^2\,|u_k\rangle \neq -|u_k\rangle \end{aligned}$$

States at TRIM are always doubly degenerate

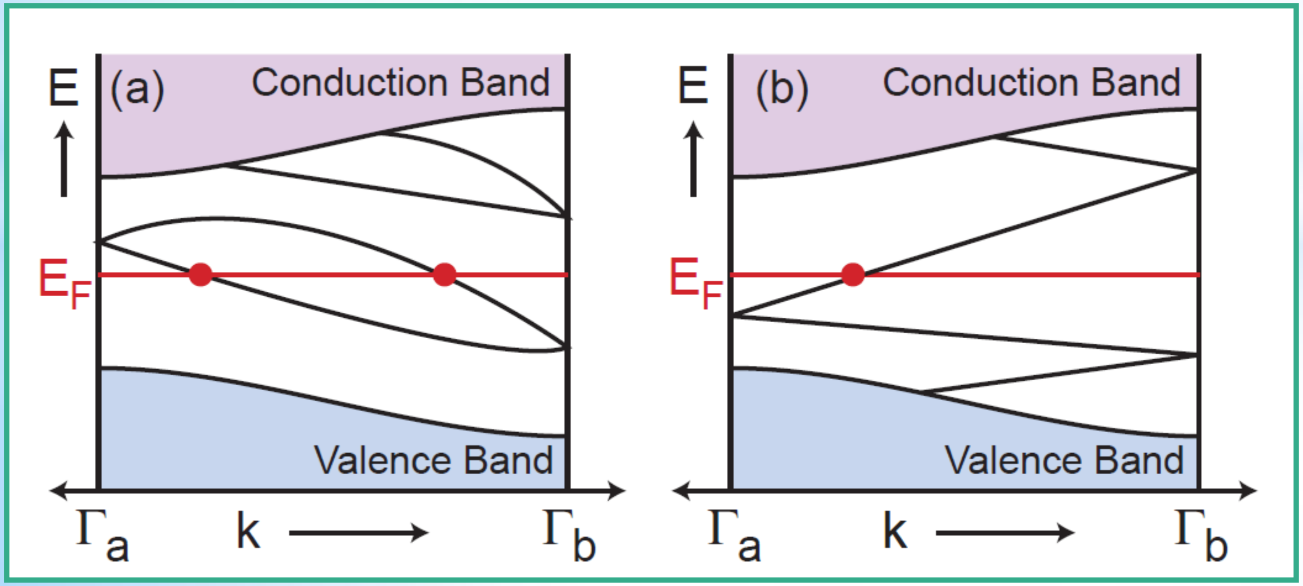
<u>Kramers degeneracy</u>

Time-reversal invariant TI

- Contact || x between two (2+1)D Tis
- k_x is still good quantum number
- There will be some midgap states crossing zero
- At $k_x = 0, \pi$ (TRIM) ➡ double degeneracy
- Even or odd number of crossings ➡ Z2 invariant

$$w_{mn}(\mathbf{k}) = \langle u_m(\mathbf{k})|\Theta|u_n(-\mathbf{k})\rangle$$

$$\delta_a = \mathrm{Pf}[w(\Lambda_a)]/\sqrt{\mathrm{Det}[w(\Lambda_a)]} = \pm 1$$

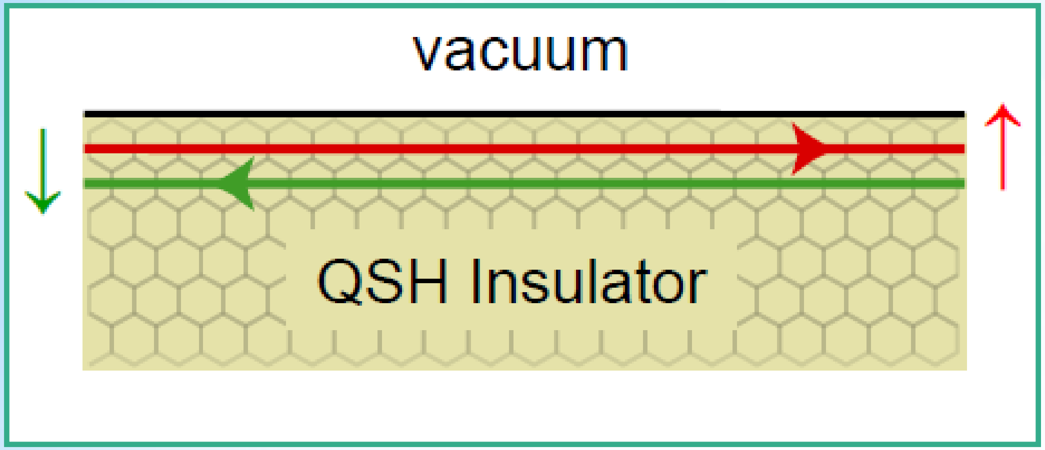


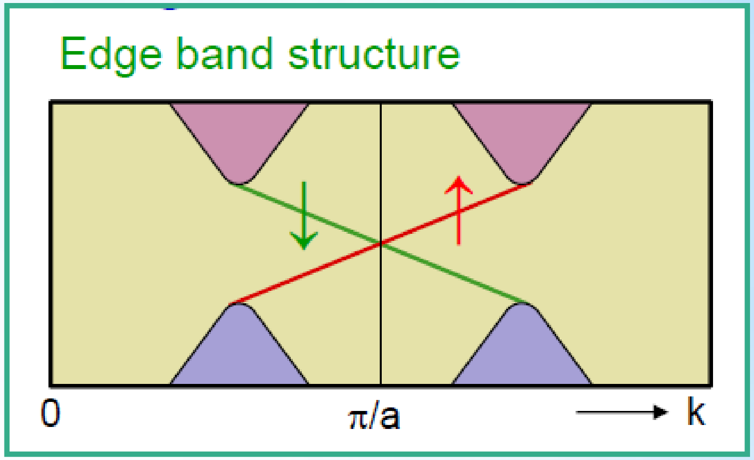
$$(-1)^\nu = \prod_{a=1}^{4} \delta_a$$

- Odd number of crossings = odd number of massless modes
- Topologically protected (no smooth deformations remove)

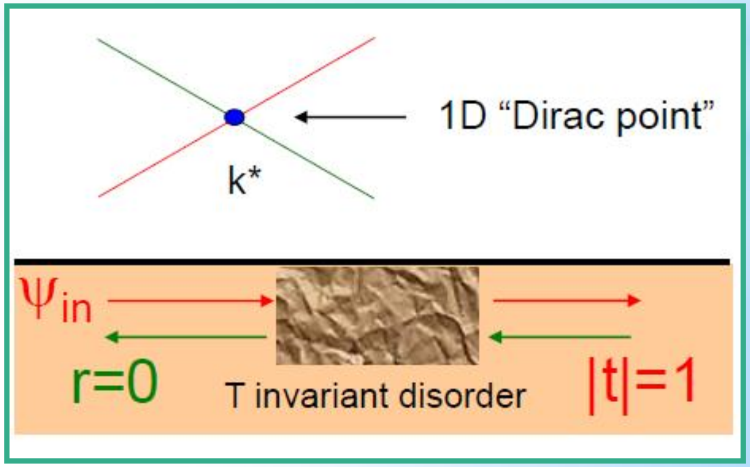
Spin-momentum locking

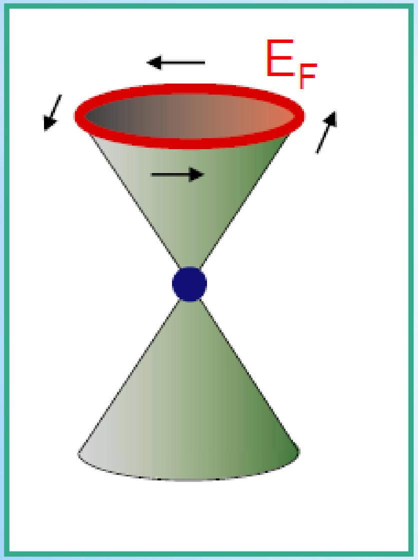
Two edge states with opposite spins: left/up, right/down





Insensitive to disorder as long as T is not violated





Magnetic disorder is dangerous

$$\Delta H_{SO} \sim \frac{1}{r}\partial_r U\left(r\right)\vec{L}\cdot\vec{S} \sim \left(\vec{\partial}U \times \vec{p}\right)\cdot\vec{S}$$

Some useful references

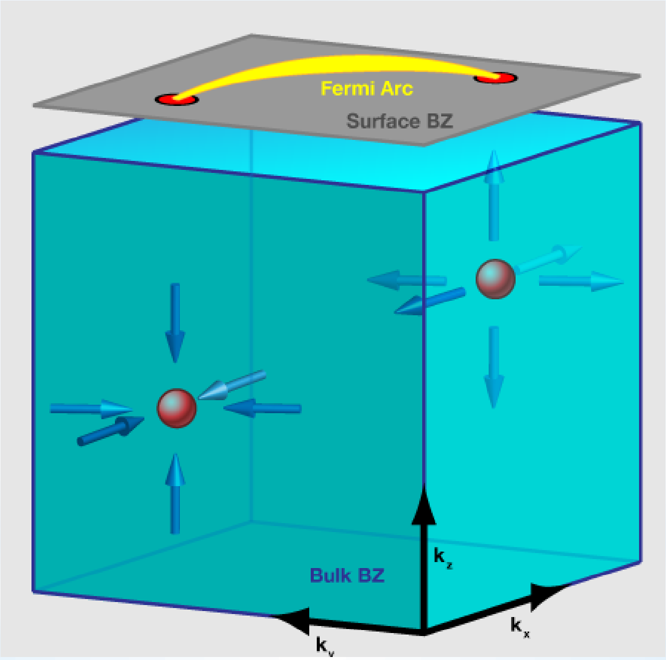
(and sources of pictures/formulas for this lecture :-)

- "Primer on topological insulators", A. Altland and L. Fritz

- "Topological insulator materials", Y. Ando, ArXiv:1304.5693

- "Topological field theory of time-reversal invariant insulators", X.-L. Qi, T. L. Hughes, S.-C. Zhang, ArXiv:0802.3537

Weyl/Dirac semimetals



Simplest model of Weyl semimetals

Dirac Hamiltonian
with time-reversal/parity-breaking terms

$$H = \alpha_i \nabla_i + m\gamma_0 + b_i \gamma_5 \alpha_i + \mu_A \gamma_5$$

Breaks time-reversal **Breaks parity**

γ_0	$even$
γ_5	$even$
γ_i	odd
$\alpha_i = \gamma_0 \gamma_i$	odd
$\alpha_i \gamma_5$	odd

γ_0	$even$
γ_5	odd
γ_i	odd
α_i	odd
$\gamma_5 \alpha_i$	$even$

Nielsen, Ninomiya and Dirac/Weyl semimetals

Axial anomaly on the lattice?

Axial anomaly =

= non-conservation of Weyl fermion number

BUT: number of states is fixed on the lattice???

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THE ADLER–BELL–JACKIW ANOMALY AND WEYL FERMIONS IN A CRYSTAL

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and

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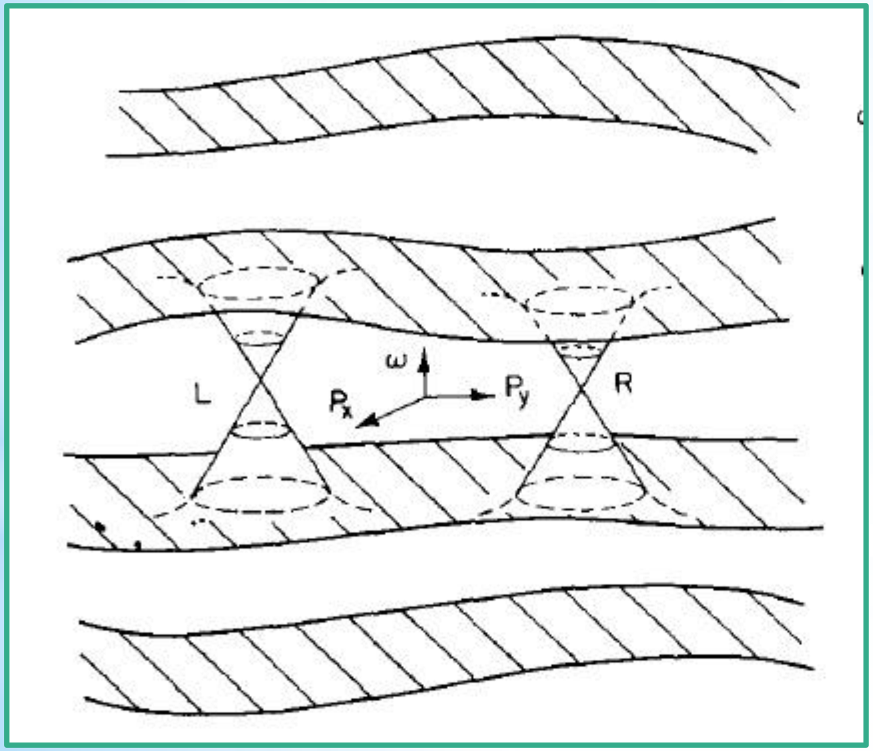
Nielsen, Ninomiya and Dirac/Weyl semimetals



Weyl points separated in momentum space

In compact BZ, equal number of right/left handed Weyl points

Axial anomaly = flow of charges from/to left/right Weyl point

Nielsen-Ninomiya and Dirac/Weyl semimetals

5. We assume that we have found a parity non-invariant zero-gap semiconductors which can be simulated by a Weyl fermion theory with a dispersion law $\epsilon^2 = v^2 P^2$. The effect analogous to the ABJ anomaly gives rise to a peculiar behavior of the conductivity of the electric current in the presence of the magnetic field. It is enough to consider one conduction band

Enhancement of electric conductivity along magnetic field

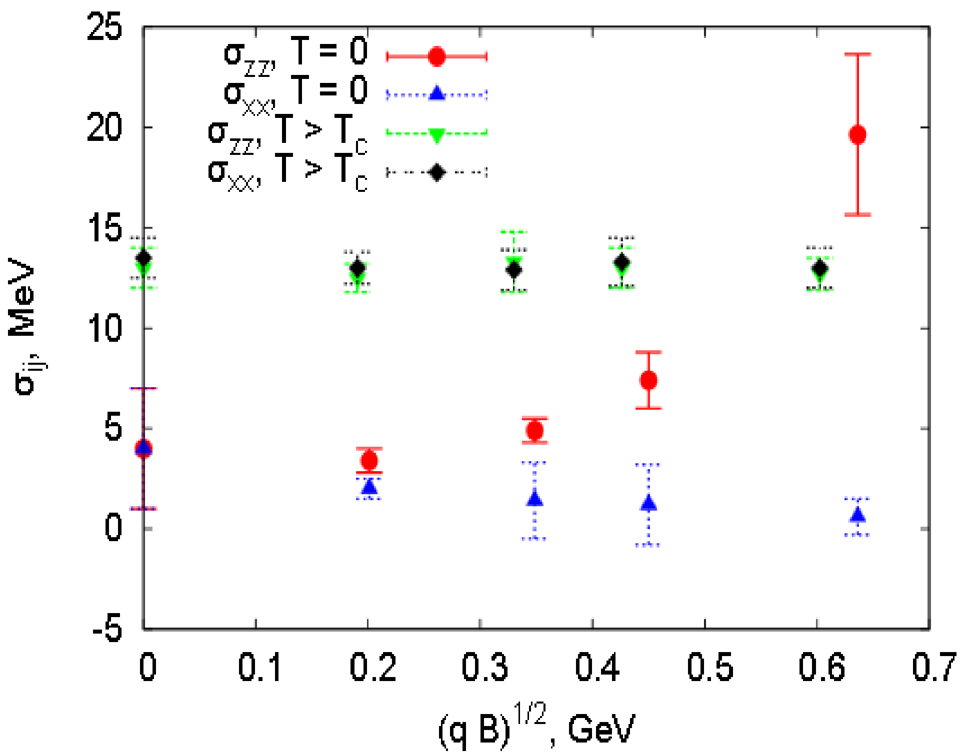
Intuitive explanation: no backscattering for 1D Weyl fermions

Negative magnetoresistance

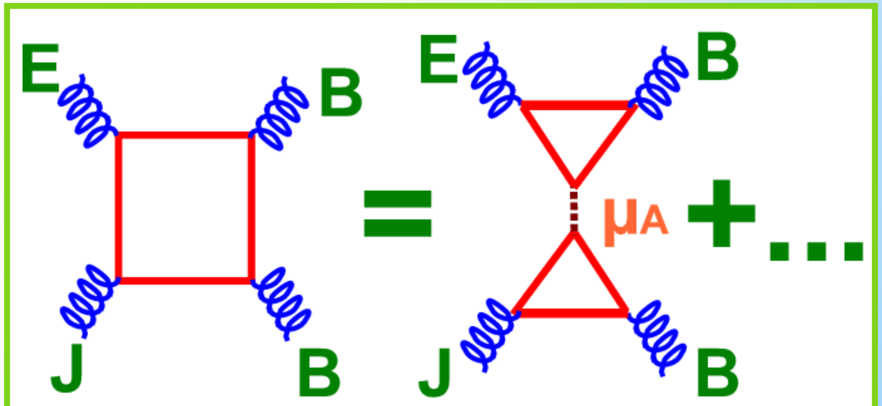
$$\partial_t Q_A \sim \vec{E}\cdot\vec{B}$$ $$\mu_A = \chi_A^{-1} Q_A$$ $$\vec{j} = \frac{\mu_A}{2\pi^2}\vec{B}$$

Electric conductivity in magnetic field

$$\vec{j} \sim \vec{B}\left(\vec{B}\cdot\vec{E}\right)$$



Lattice QCD data
[PB et al.,1003.2180]
NMR at low T

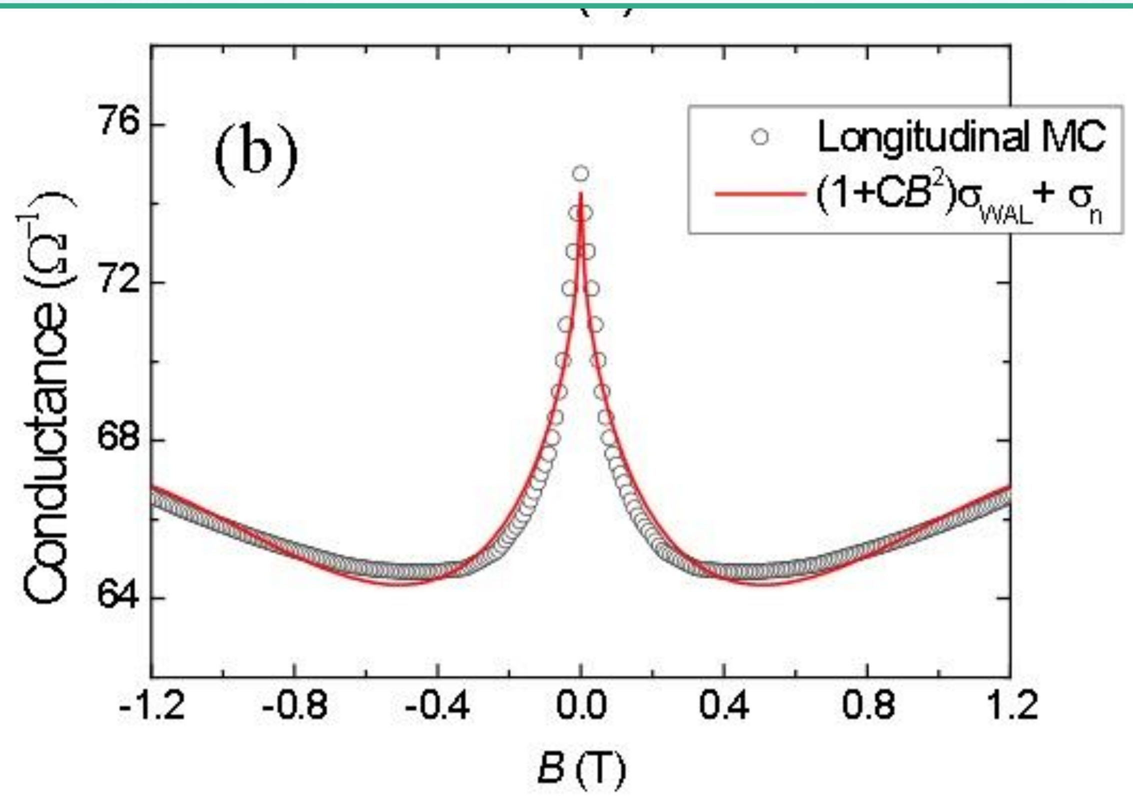


NMR in Dirac/Weyl semimetals

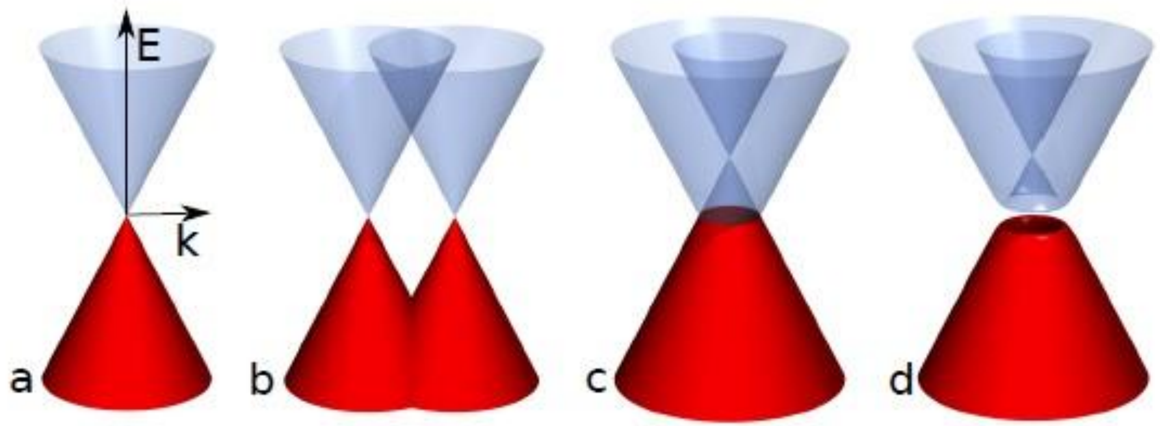
PRL **111,** 246603 (2013) PHYSICAL REVIEW LETTERS week ending 13 DECEMBER 2013

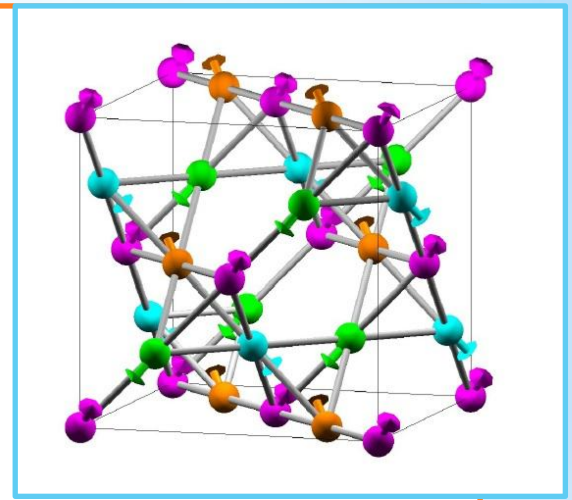
Dirac versus Weyl Fermions in Topological Insulators: Adler-Bell-Jackiw Anomaly in Transport Phenomena

Heon-Jung Kim,[1,*] Ki-Seok Kim,[2,3,†] J.-F. Wang,[4] M. Sasaki,[5] N. Satoh,[6] A. Ohnishi,[5] M. Kitaura,[5] M. Yang,[4] and L. Li[4]

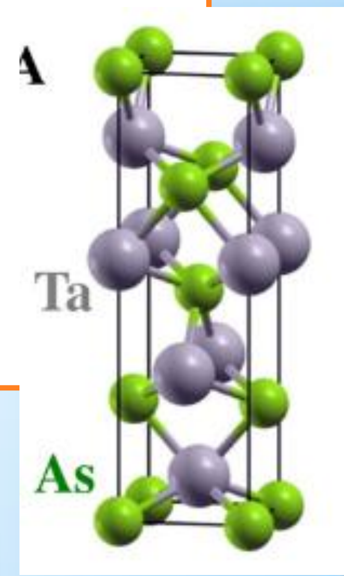


Weyl semimetals





- Take Dirac semi-metal/topological insulator
- Break $\mathcal{T}$ime reversal (e.g. magnetic doping) $\delta_H \sim \vec{b} \cdot \vec{\Sigma}$, $\vec{\Sigma}$ is the spin operator
- Break $\mathcal{P}$arity (e.g. chiral pumping) $\delta H \sim \gamma_5 \mu_A$
- $\Rightarrow$ Weyl fermions split, Dirac point $\Rightarrow$ Weyl points
- Broken $\mathcal{T}$: spatial shift, broken $\mathcal{P}$: energy shift



Weyl points survive ChSB!!!

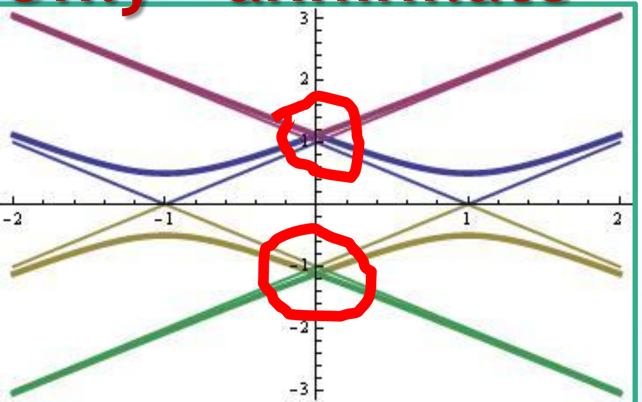
Topological stability of Weyl points

Weyl Hamiltonian in momentum space:

$$\boxed{H = k_i \sigma_i + \mu}$$

Full set of operators for 2x2 hamiltonian
Any perturbation (transl. invariant)
= just shift of the Weyl point

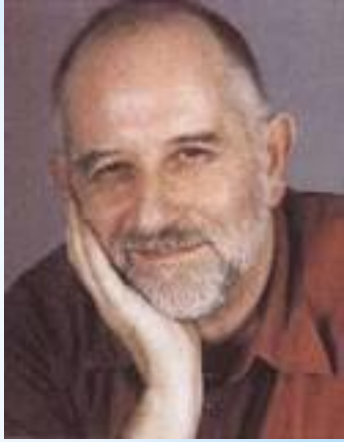
Weyl point are topologically stable
Only "annihilate" with Weyl point of another chirality



E.g. ChSB by mass term:

$$\boxed{\epsilon_{s,\sigma}\left(\vec{k}\right) = s\sqrt{\left(|\vec{k}| - \sigma\mu_A\right)^2 + m^2}}$$

Weyl points as monopoles in momentum space



Classical regime: neglect spin flips = off-diagonal terms in a_k

Classical action

$$S = \int d\tau \left(\vec{p} \cdot \dot{\vec{x}} - |\vec{p}| - (\vec{a}_p)_{11} \cdot \dot{\vec{p}} \right)$$

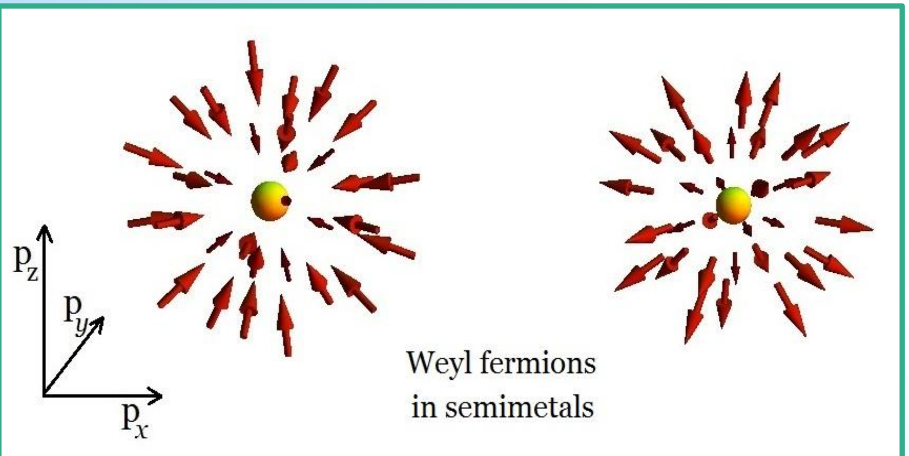
$(a_p)_{11}$ looks like a field of Abelian monopole in momentum space

Berry flux

$$\Phi_B = \int d\vec{S} \cdot \vec{b}, \quad \vec{b} = \vec{\partial}_p \times (\vec{a}_p)_{11}$$

Topological invariant!!!

$$\vec{b} = \frac{\vec{p}}{2p^3}$$



Fermion doubling theorem: In compact Brillouin zone only pairs of monopole/anti-monopole

Electromagnetic response of WSM

Anomaly: chiral rotation has nonzero Jacobian in *E* and *B*

Additional term in the action $\sim \frac{1}{2\pi^2}\int d^3x dt\, \theta(x)\, \vec{E}\cdot\vec{B}$

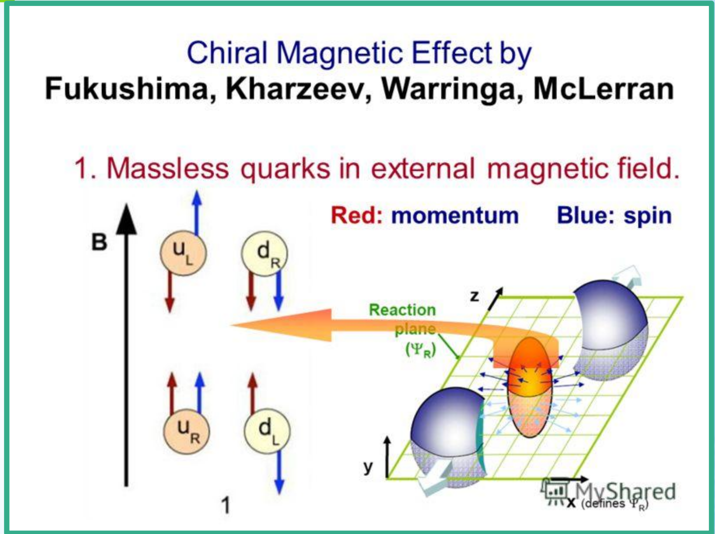
$$S_{eff} = \frac{1}{8\pi^2}\int d^4x\, \theta\, F_{\mu\nu}\tilde{F}_{\mu\nu} = \frac{1}{2\pi^2}\int d^4x\, \epsilon^{\alpha\beta\mu\nu}\, \partial_\alpha\theta\, A_\beta \partial_\mu A_\nu$$

Spatial shift of Weyl points: $\theta(\vec{x}) = \vec{b}\cdot\vec{x}$

Anomalous Hall Effect: $\vec{j} = \frac{1}{2\pi^2}\vec{b}\times\vec{E}$

Energy shift of Weyl points $\theta \sim \mu_A t$

Non-stationary state:
chirality pumping
and
chiral magnetic effect



Brief summary

In some (quite few) cond-mat systems inter-electron interactions are important, for example:

- Graphene
- High-Tc superconductors (Hubbard model)
- Frustrated systems

We can try to study them using (lattice) quantum field theory techniques

Physics of “topological materials” very similar to lattice fermions in QCD:

- Doublers, Nielsen-Ninomiya theorem
- Axial anomaly
- Domain-wall chiral fermions