A *possible* half-integer Quantum Hall Effect: RQED bulk perspective and more

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Overview

Mixed-dimensional QED: QFT model for $2D$ materials

Mass gaps and material realization

Reduced QED: better QFT model for $2D$ materials

Generalized Coleman-Hill theorem and half-integer anomalous Quantum Hall Effect

"Half-topology" in the bulk

Edge perspective

Honeycomb-like materials

- We are a priori interested in graphene-like $2D$ materials, built from 2 triangular Bravais (A, B) lattices. Tight binding model, ignoring higher order interactions. Electron creation/annihilation operators $a^\dagger, a, b^\dagger, b$ per sublattice, ordered into a 4-spinor (per spin s)

$$\Psi_s = \begin{pmatrix} \Psi_{s,+} \\ \Psi_{s,-} \end{pmatrix} = \begin{pmatrix} a_s^\dagger \\ b_s^\dagger \\ b_s^- \\ a_s^- \end{pmatrix}$$

The $\pm$ are valley indices referring to $K_\pm$.

Honeycomb-like materials

- In the continuum limit:

$$\mathcal{L} = \sum_s \bar{\Psi}_s \left(i\gamma^0 \hbar D_t + i\hbar v_F \gamma^x D_x + i\hbar v_F \gamma^y D_y \right) \Psi_s .$$

  with $D_\alpha = \partial_\alpha - (ie/\hbar c) A_\alpha$. A_α is the gauge field associated to the electromagnetic interaction and v_F is the Fermi velocity. Mixed-dimensional theory: planar fermions and bulk EM. We work in the Weyl basis,

$$\gamma^0 = \begin{pmatrix} 0 & \mathbb{1}_2 \\ \mathbb{1}_2 & 0 \end{pmatrix}, \gamma^i = \begin{pmatrix} 0 & \sigma^i \\ -\sigma^i & 0 \end{pmatrix}, \gamma^5 = \begin{pmatrix} -\mathbb{1}_2 & 0 \\ 0 & \mathbb{1}_2 \end{pmatrix}.$$

- Excellent review: Gusynin, Sharapov, Carbotte, Int.J.Mod.Phys.B 21 (2007)

Honeycomb-like materials

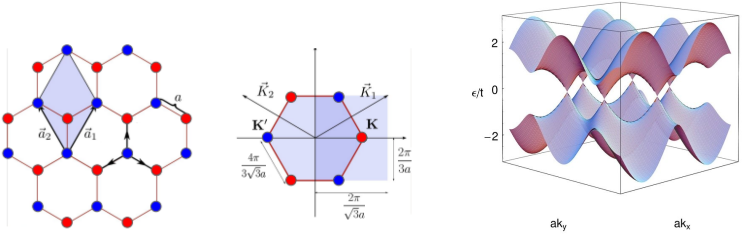

Figure: (Left) Lattice structure Mizher et al, Eur.Phys.J.C 78 (2018) (Right) Energy dispersion. The $K^{\pm}$ are the 2 inequivalent "touching points".

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The band (gap) structure we are after

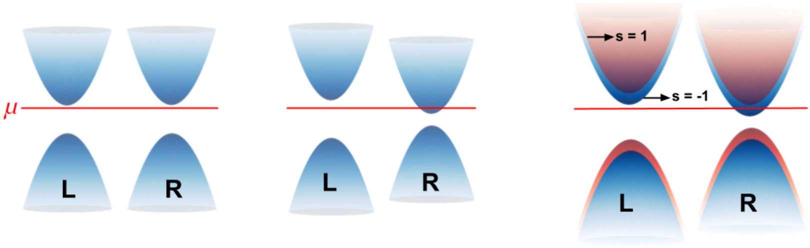

Figure: (Left) Dirac cones with simple gap; (Middle) Valley asymmetry corresponding to imbalance in “chirality”; (Right) Schematic representation of the band structure when a spin split is present besides valley asymmetry. The chemical potential μ is fine-tuned to “cut” one (and only one) of the cones. This can be achieved by a suitable electrostatic potential.

The reason for all of this will soon become clear.

Two types of (inequivalent) mass gaps

- A T-even mass term $\sim m_e \bar{\Psi}\gamma^3\Psi$
- A T-odd mass term $\sim m_o \bar{\Psi}\gamma^3\gamma^5\Psi$

  (corresponds to Haldane mass Phys.Rev.Lett. 61 (1988))

Gapped Lagrangian

- We introduce the chiral projectors $P_5^{\pm} = \frac{1}{2}(1 \pm \gamma_5)$, after which

$$\mathcal{L} = \sum_{s,\chi=\pm} \bar{\Psi}_{\chi,s}[i\gamma^0\hbar\partial_t + \mu\gamma^0 + i\hbar v_F\gamma^x D_x + i\hbar v_F\gamma^y D_y + m_{s,\chi}\gamma^z]\Psi_{\chi,s},$$

where we included the chemical potential, μ, and $m_{s,\pm} = m_{s,e} \pm m_{s,o}$. $\chi = L/R = \pm$ refers to the valley index (“chirality”), while

$$\Psi_{s,+} = \begin{pmatrix} 0 \\ \psi_{s,+} \end{pmatrix}, \qquad \Psi_{s,-} = \begin{pmatrix} \psi_{s,-} \\ 0 \end{pmatrix}$$

- In 2-spinor language, we get for the mass sector (s suppressed):

$$S_{\mathrm{mass}} = \int d^3x\,(\bar{\psi}_+(\mu\sigma^z + m_+)\psi_+ + \bar{\psi}_-(\mu\sigma^z - m_-)\psi_-)\,,$$

Where can such mass gaps come from?

- Including spin-orbit couplings and anti-ferromagnetic order due to different spin per sublattice $\rightarrow$ inequivalent sublattices, split by gap $\sim m_e$, next to Haldane mass $\sim m_o$.
- In concreto, using original valley 2-spinors ($\tau \rightarrow$ valley, $\sigma \rightarrow$ sub-lattice):

  $$\delta\tau_z \otimes \sigma_z, \qquad \Delta\tau_0 \otimes \sigma_z$$

  leading to

  $$m_{s,\pm} = s(\Delta \pm \delta)$$

  Notice the different sign per spin s!
- Alleviate —spin— degeneracy via (induced) Zeeman effect $\rightarrow$ doping material to induce a net magnetization.

  Additional (theoretical) background: see Levrouw, KU Leuven MSc thesis (2022), Li et al, PNAS110 (10) (2013), Wu et al, J.Phys.D Appl.Phys.53 (2020).

Do such materials exist? Dudal et al, Sci.Rep. 12 (2022)

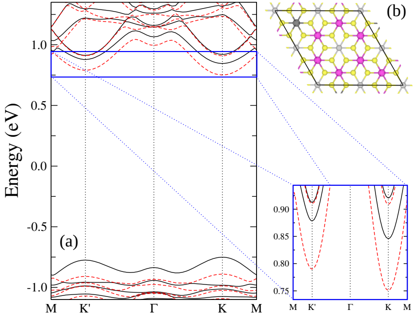

Figure: Evidence from Density Functional Theory simulations of Zn-doped $MnPSe_3$ (manganese chalcogenophosphate) via `VASP`. (a) DFT band structure. Spin up (down) bands are represented by straight (dashed) black (red) lines. The inset shows the conduction band region in detail. (b) Unit cell of Zn-doped $MnPSe_3$ with pink, dark gray, yellow and gray spheres representing Mn, Zn, Se, and P, respectively. There is a spin up (down) valley splitting of 33 (40) meV and a spin splitting of 89 (93) meV at the K' (K) point.

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Mixed-dimensional QED $\rightarrow$ Reduced QED

Consider mixed-dimensional QED, written as (no fermion dynamics for now)

$$\mathcal{S}_{\mathrm{QED}_4} \quad = \quad \int d^4x \left[-\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + \frac{1}{2\xi} (\partial \cdot A)^2 + j_\mu A^\mu \right] .$$

with

$$j^\mu \quad = \quad \begin{cases} i\bar{\psi}\gamma^\mu \psi \delta(x_3) & \text{for } \mu = 0,1,2\,, \\ 0 & \text{for } \mu = 3\,, \end{cases} \quad ,$$

with linear covariant gauge fixing. We can integrate out the $(3+1)D$ gauge field to end up with a fully $(2+1)D$ fermion theory

$$\mathcal{S}_{eff} \quad = \quad \int d^3p \left[\hat{j}^\mu \hat{\mathcal{D}}^T_{\mu\nu}(\vec{p}) \hat{j}^\nu \right] .$$

which can be put in QED-like format again (in $(2+1)D$) introducing a new gauge field

$$\mathcal{S}_{\mathrm{RQED}_3} = \int d^3x \left[\frac{1}{2} F^{\mu\nu} \frac{1}{\sqrt{-\partial^2}} F_{\mu\nu} + \bar{\psi}(i\not{D})\psi + \frac{1}{2\zeta} (\partial \cdot A)^2 \right] ,$$

defining Reduced QED (or Pseudo-QED). See also Marino, Nucl.Phys.B 408 (1993), Gorbar et al, Phys.Rev.D 64 (2001) and talk of Raya.

Reduced QED: some fait divers

- Reduced QED attracted quite some attention recently from people working on "CFTs with defects/boundaries", e.g. Herzog, Huang JHEP 10 (2017); Karch, Sato, JHEP 07 (2018).

$\rightarrow$ Indeed, ultrarelativistic RQED ($v_F \rightarrow c$) is scale invariant, $\beta(e^2) \equiv 0$. All-order proof given in Dudal et al, Phys.Rev.D 99 (2019).

Careful: for $v_F < c$, this is no longer true, see for instance Vozmediano, Phil.Trans.Roy.Soc.Lond.A 369 (2011) for one-loop anomalous dimensions.

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Comments about $(2+1)D$ QED

- In case of an odd number of 2-spinors (with mass $m_f \to 0$), there is room for a parity anomaly Redlich, Phys.Rev.D 29 (1984), Semenoff, Phys.Rev.Lett. 53 (1984).

$\to$ Dynamical Chern-Simons term in the action

$$\propto \sum_{\text{fermions } f} e^2 \frac{|m_f|}{m_f} \varepsilon^{\mu\rho\nu} A_\mu \partial_\rho A_\nu$$

Origin is the $(2+1)D$ Dirac algebra for which $\mathrm{Tr}(\gamma^\mu\gamma^\rho\gamma^\nu) \propto \varepsilon^{\mu\rho\nu}$.

- The Coleman-Hill theorem Coleman, Hill, Phys.Lett.B 159 (1985) ensures that the zero momentum limit of the Chern-Simons term is one-loop exact. In $(2+1)D$ this generates the so-called "topological photon mass" $\propto e^2$ (which has mass dimension).

- In RQED, e^2 is still the dimensionless $(3+1)D$ EM coupling $\to$ room for CS term, but different interpretation (no photon mass)

$(2+1)D$ RQED

- Coleman, Hill, Phys.Lett.B 159 (1985) presented a combinatorial/ diagrammatic proof.
- In Dudal et al, Phys.Rev.D 98 (2018), we generalized the Coleman-Hill theorem to RQED, based on the Slavnov-Taylor identity and a careful analysis of its low-momentum expansion at the level of the self-energy aka. current correlator aka. polarization tensor. Our proof is valid both for the relativistic case $v_F = c$ and non-relativistic case $v_F < c$.

  In other words: a massive two-spinor fermion generates a Chern-Simons term in the RQED case as well, with its zero momentum limit one-loop exact.

$(2+1)D$ RQED

- A concrete computation Dudal et al, Sci.Rep. 12 (2022) gives for the RQED photon self-energy a v_F-independent T-odd contribution, $\tilde{\Pi}^{ij}(\vec{p}) = \varepsilon^{ijk} p_k \pi(p)$

$$\pi(\vec{p}) = \begin{cases} \frac{e^2}{2\pi}\frac{|m|}{p}\mathrm{ArcCot}\left(2\frac{|m|}{|p|}\right) & \text{if } m^2 \geq \mu^2 \\ \frac{e^2}{2\pi}\frac{|m|}{p}\mathrm{ArcCot}\left(2\frac{|\mu|}{\sqrt{4m^2-4\mu^2+\vec{p}^2}}\right) & \text{if } m^2 < \mu^2, \vec{p}^2 > 4\mu^2 - 4m^2 \\ 0 & \text{otherwise.} \end{cases}$$

or

$$\tilde{\Pi}^{yx}(\vec{p}) = -\frac{m}{|m|}\frac{e^2}{4\pi}\theta(m^2-\mu^2)\varepsilon^{yx0}\omega + \mathcal{O}(p^2)$$

- Coupling a background $\vec{E} = E\vec{e}_y$-field to RQED is a bit tricky, but after a careful analysis, the known Kubo relation for the (anomalous) quantum Hall effect—$\langle \vec{j} \rangle = \sigma_{xy} E\vec{e}_x$ — remains valid,

$$\sigma_{xy} = \lim_{\omega\to 0}\frac{1}{\hbar\omega}\left\{\int_0^\infty d\tau e^{i\omega\tau}\langle 0|\left[j_y(0), j_x(\tau)\right]|0\rangle\right\}$$

Half-integer anomalous Quantum Hall effect

- We are now ready to bring everything together, first assuming a single massive 2-spinor

$$\sigma_{xy} = \lim_{\omega\to 0} \frac{1}{\hbar\omega}\Pi^{yx} = \frac{e^2}{4\pi\hbar}\frac{m}{|m|}\theta(m^2-\mu^2)$$

- and then for our case, also summing over the spins

$$\sigma_{xy} = \sum_s \frac{e^2}{4\pi}\left[\frac{m_{s,+}}{|m_{s,+}|}\theta(m_{s,+}^2-\mu^2) - \frac{m_{s,-}}{|m_{s,-}|}\theta(m_{s,-}^2-\mu^2)\right],$$

- To avoid a net cancellation due to different mass sign per spin, we need a spin split (see before). Furthermore, we had, for the contributing spin, $m_+ > 0$, $m_- > 0$ and $m_-^2 < \mu^2 < m_+^2$, so our main prediction is

$$\sigma_{xy} = \frac{e^2}{2h}$$

  which corresponds to a half-integer anomalous quantum Hall conductivity (at least from the bulk QFT perspective).

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Topological nature of the Quantum Hall conductivity

- The Kubo relation can be “massaged” into the TKNN formula Thouless et al, Phys.Rev.Lett. 49 (1982)

$$\sigma_{xy} = \frac{2e^2}{\hbar} \mathrm{Im} \sum_{\alpha} \int_{T^2} \frac{d^2 p}{(2\pi)^2} \left\langle \partial_{p_y} u^{\alpha}_{\vec{p}} | \partial_{p_x} u^{\alpha}_{\vec{p}} \middle| \partial_{p_y} u^{\alpha}_{\vec{p}} | \partial_{p_x} u^{\alpha}_{\vec{p}} \right\rangle = \frac{e^2}{h} \sum_{\alpha} \mathcal{C}_{\alpha}$$

  where the sum runs over filled bands, and $\mathcal{C}_{\alpha}$ is the (integer) Chern number of the band.

- Careful: we chose μ in the gap between the 2 Dirac points $\rightarrow$ “cutting” of the respective band! So are we looking at something topological or not?

Topological nature of the $\frac{1}{2}$ Quantum Hall conductivity?

- Our underlying low energy effective Hamiltonian per valley per spin is of the type

$$H(\vec{p}) = h_0(\vec{p})\mathbb{1}_2 + h_i(\vec{p})\sigma_i$$

- In Sticlet et al, Phys. Rev. B85 (2012), it was shown that, in general, each massive Dirac point (cone) contributes with $\pm\frac{1}{2}$ "topological charge". If a full (smooth) band is taken into account for a double cone system $\rightarrow$ integer Chern number and thence $\sigma = \pm\frac{e^2}{h}, 0$ as possible conductivities.

  Due to our fine-tuned μ in the finite intervalley gap between the K and K' Dirac points, we are effectively cutting away part of that band and only a single cone will contribute to the conductivity.

Topological nature of the $\frac{1}{2}$ Quantum Hall conductivity?

- Denoting with α' all completely filled bands and singling out that "partially cut" band (the encircled piece), we actually have

$$\sigma_{xy} = \underbrace{\frac{e^2}{h}\sum_{\alpha'} C_{\alpha'}}_{\text{integer}} \pm \frac{e^2}{h}\frac{1}{2},$$

  where the encircled piece is only there for the spin projection that is partially filled.
- Small perturbations of the band geometry will preserve the fact that only a single Dirac point contributes with $\frac{1}{2}$ to the Berry curvature integral.

  The cutting of the band is a non-smooth operation, leading to a non-smooth integration zone, explaining why strictly speaking, we dot not find a topological integer, but the $\frac{1}{2}$ is still "topologically" safe from small perturbations.
- This nicely matches with one-loop exactness from QFT analysis.

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Bulk-edge correspondence

- Usually, the topological nature of the (A)QHE current/conductivity is understood from a bulk-edge correspondence: when edges (boundaries) are introduced, the integer nature of the conductivity also follows from the contribution of (massless) edge modes. Equivalence of both topological arguments on a lattice: Hatsugai, Phys. Rev. Lett. 71 (1993).

  (Equivalence not carved in stone though: Büttiker et al, Phys. Rev. B82 (2010).)

- Can we understand (or not) the $\frac{1}{2}$ AQHE from an edge perspective?
- As common in literature, we may follow the intuitive physical reasoning of Büttiker, Physical Review B38 (1988), a mathematically rigorous source is Gruber, Leitner, Letters in Mathematical Physics 75 (2006).
- Based on work in progress and Levrouw, KU Leuven MSc thesis (2022)

Potential caveats in our bulk (QFT) analysis

- Perhaps a continuum QFT description is not always 100% appropriate to describe lattice based materials?

$\rightarrow$ Are we overlooking something?

- Strictly speaking, the integral defining the Chern number should run over a compact space ($\rightarrow$ Brillouin torus), but in the continuum limit, this becomes the plane $\mathbb{R}^2$ $\rightarrow$ requires adding $p^2 = \infty$ to compactify, but this "UV completion" is not always uniquely defined Volovik, Int.Ser.Monogr.Phys. 117 (2006).
- Proper compactification can be acquired by e.g. adding (no matter how small) p^2-corrections to effective Hamiltonian, which can influence the Chern integral.
- Downside: the QFT model is less "nice", and (yet) unclear how the induced CS term will be influenced by such corrections.

  (for the record: these p^2-corrections are rarely considered in general, and usually put in by hand in models. Proper NLO expansion in lattice size a of tight-binding models leads to several different p^2-terms.)

Our model on the half-space

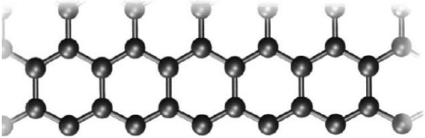

Figure: We add a boundary at $x = 0$. Prize to pay: the Hamiltonian needs to be supplemented with boundary conditions to ensure a Hermitian setup. Crucial role played by these boundary conditions, also for topology (which can depend on the boundary), see e.g. Tanhayi Ahari et al, American Journal of Physics 84 (2016). Shown here is a zigzag-edge, with the lattice terminating on either the A or B sublattice.

Our model on the half-space: boundary condition

- Hermitian extension: $j_x|_{x=0} = 0$.
- For a single 2-spinor ψ, this amounts to $\psi_2 = i\zeta\psi_1$, with $\zeta \in \mathbb{R}\bigcup\pm\infty$. Setting $\zeta = \tan\frac{\phi}{2}$, one gets

$$\psi \sim \begin{pmatrix} \cos\frac{\phi}{2} \\ i\sin\frac{\phi}{2} \end{pmatrix}$$

- $\zeta = 0$ corresponds to *zigzag A* edge, $\zeta = \pm\infty$ to *zigzag B* edge. sgn(ζ) does not play a role here it seems, the density at terminating *A* or *B* edge depends on $|\zeta|$.

Our model on the half-space: edge spectrum

- We then search for (real) modes, located at the edge, via solutions with energy E of

$$H_{\pm} = -\mu \pm (-\partial_i \sigma^i) + m_{\pm} \sigma^3$$

- Zero modes ($E = 0$) interest us the most. Only possible for $\mu^2 < m_{\pm}^2$. Only $m_+ > 0$ can support a zero edge mode in our setup!
- For a 1D mode with momentum κ along the edge ($\varepsilon = E + \mu$):

$$\begin{aligned} \varepsilon &= \kappa \sin\phi + m_+ \cos\phi \\ 0 &\leq -\kappa \cos\phi + m_+ \sin\phi \end{aligned}$$

and

$$\begin{aligned} \varepsilon &= -\kappa \sin\phi + m_- \cos\phi \\ 0 &\leq \kappa \cos\phi - m_- \sin\phi \end{aligned}$$

Our model on the half-space: edge conductivity

- One then finds

$$\sigma_{\text{edge}} = \begin{cases} -\text{sgn}(\zeta)\frac{e^2}{h} & \text{if} \quad \text{sgn}(\zeta) = \text{sgn}(m_+) \\ 0 & \text{otherwise} \end{cases}$$

- The topological stability of this result under small perturbations was shown in Gruber, Leitner, Letters in Mathematical Physics 75 (2006).

What do we get?

- Depending on $\text{sgn}(\zeta)$, keeping in mind that $m_+ > 0$, we either find $\sigma_{\text{edge}} = 0$ or $\sigma_{\text{edge}} = \frac{e^2}{h}$. So no $\frac{1}{2}$ conductivity, but also not a clear picture. Indeed, e.g. $\zeta \to 0^\pm$ corresponds to *zigzag A*, but gives different result depending if right-or left-limit is taken. The (physical) meaning of $\text{sgn}(\zeta)$ is unclear.
- One can interpret the $\frac{1}{2}$ as the mean value of the 2 (equivalent?) results. Using a different edge study, a similar statement can be found in Ando, Journal of the Physical Society of Japan 84 (2015).

Our model on the half-space: edge disorder?

- A bit unsatisfactory finding.
- For the record, also the TKNN result crucially depends on taking an average over boundary conditions (fluxes), see e.g. Tong, arXiv:1606.06687 [hep-th] or Fradkin, Field Theories of Condensed Matter Physics (2013).
- "Just arithmetically averaging" looks a tad suspicious here, a more interesting avenue to potentially understand the physical meaning (or not) of the $\frac{1}{2}$ might come from averaging taking into proper account a disordered edge, where sampling over ζ becomes part of the deal Walter et al, Phys. Rev. Lett. 121 (2018).

Concluding outlook

- Add (zigzag) edges in DFT simulation(s) (next to `VASP`, also `OpenMX` or `ATOMOS`). and confirm (or not!?) the $\frac{1}{2}$ AQHE from an edge perspective for Zn doped $MnPSe_3$ (that is, next to band structure, also probe the (edge) current).
- If numerically confirmed: try to understand better the edge dynamics from the analytical viewpoint. Also here: lattice vs. continuum viewpoint?
- Search for other interesting materials with similar gap structure. Options are e.g. heterojunctions of different $2D$ materials such as $MnPSe_3/CrBr_3$, $MnPSe_3/MoS_2$ or WS_2/h-VN, next to using (substrated) dichalcogenides like $NbSe_2$ and WS_2.
- Long run: allow for a thickness δ. $2D$ materials are never really planar, with δ related to the extension of the $2p_z$ orbitals (Mecklenburg & Regan, Phys. Rev. Lett. 106, 116803 (2011), etc.).
- The 3rd dimension might allow to also couple a $\vec{B}$ to the anomaly, in search of a quasi-$2D$ version of the chiral magnetic effect Fukushima et al, Phys.Rev.D 78 (2008), the original motivation for the presented work Mizher et al, Int.J.Mod.Phys.B 30 (2015), Eur.Phys.J.C 78 (2018).
- ...

O fim!

Muito obrigado!