

**The road to the
quantum spin Hall effect.**

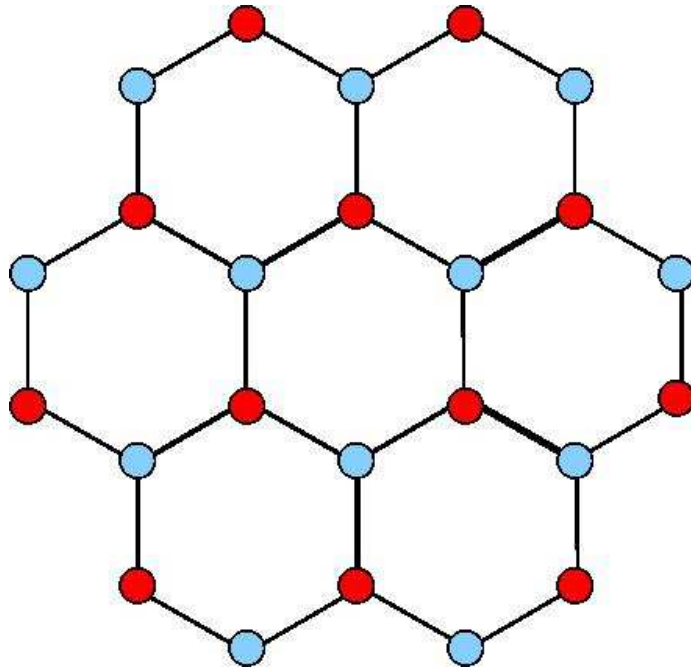
Haldane: Hall conductance with zero flux.



Duncan Haldane



2016



Spinless fermions in a
Graphene-like lattice
model (two triangular
sublattices)

F.D.M. Haldane,
Phys. Rev. Lett. 61, 2015 (1988)

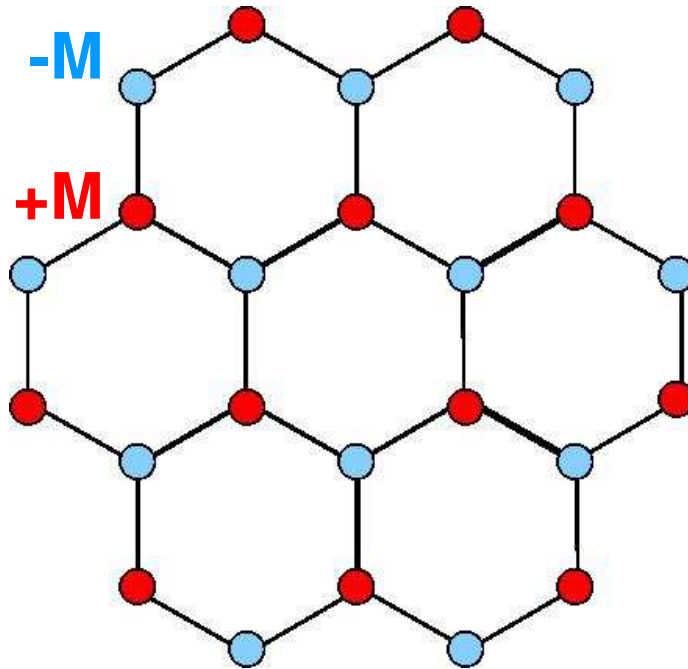
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Spinless fermions in a
Graphene-like lattice
model (two triangular
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Each sublattice has a
different “mass term”:
Inversion symmetry
breaking.

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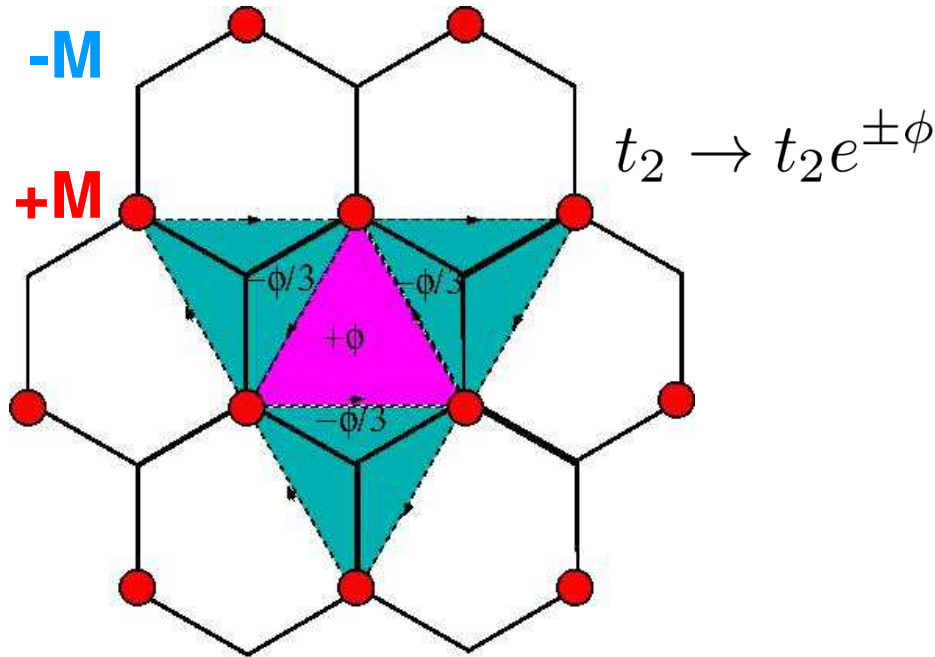
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Spinless fermions in a Graphene-like lattice model (two triangular sublattices)

Each sublattice has a different “mass term”: Inversion symmetry breaking.

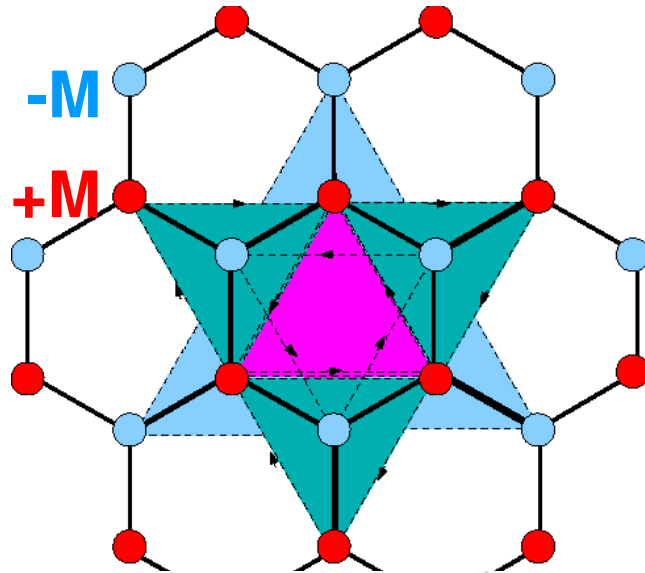
Space-varying $B(r)$ with **ZERO NET FLUX**: Time reversal symmetry breaking.

F.D.M. Haldane,
Phys. Rev. Lett. 61, 2015 (1988)

$$\hat{H}_{\text{Haldane}} = -t_1 \sum_{\langle i,j \rangle} c_i^\dagger c_j - t_2 \sum_{\langle\langle i,j \rangle\rangle} e^{i\phi_{ij}} c_i^\dagger c_j + M \sum_i \epsilon_i c_i^\dagger c_i$$

https://topocondmat.org/w4_haldane/haldane_model.html

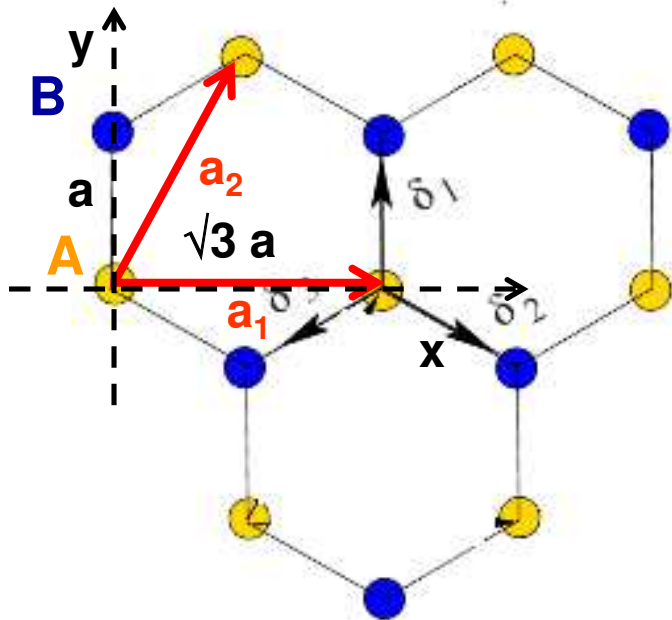
Haldane model: eigenvalues



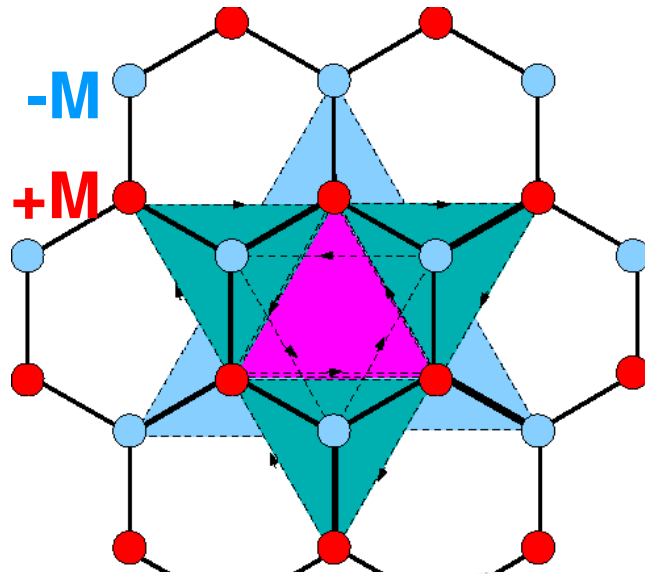
$$\frac{\mathcal{H}_{\mathbf{q}}}{N} = \begin{pmatrix} M + 2t_2 f(\mathbf{q}, \phi) & t_1 \gamma_{\mathbf{q}} \\ t_1 \gamma_{\mathbf{q}}^* & -M + 2t_2 f(\mathbf{q}, -\phi) \end{pmatrix}$$

$$\gamma_{\mathbf{q}} = 1 + e^{i\mathbf{q} \cdot \mathbf{a}_2} + e^{i\mathbf{q} \cdot (\mathbf{a}_2 - \mathbf{a}_1)}$$

$$f(\mathbf{q}, \phi) = \cos(\mathbf{q} \cdot \mathbf{a}_1 + \phi) + \cos(\mathbf{q} \cdot \mathbf{a}_2 - \phi) + \cos(\mathbf{q} \cdot (\mathbf{a}_2 - \mathbf{a}_1) + \phi)$$



Tarefa 21: Haldane model



$$\frac{\mathcal{H}_{\mathbf{q}}}{N} = \begin{pmatrix} M + 2t_2 f(\mathbf{q}, \phi) & t_1 \gamma_{\mathbf{q}} \\ t_1 \gamma_{\mathbf{q}}^* & -M + 2t_2 f(\mathbf{q}, -\phi) \end{pmatrix}$$

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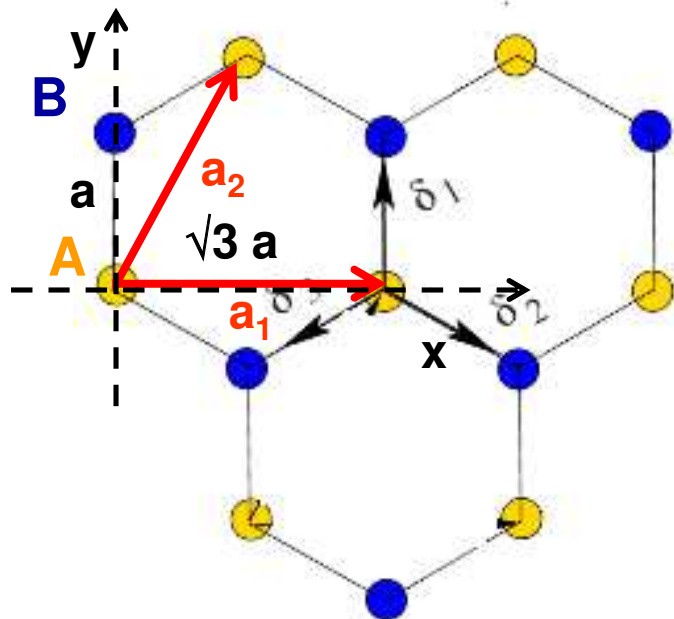
Consider: $t_1=1$, $\phi=\pi/2$, and \mathbf{a}_1 and \mathbf{a}_2 as in the left.

1) Calculate the Hamiltonian matrix for the Brillouin zone vertices $\mathbf{q}=\mathbf{K}$ and $\mathbf{q}=\mathbf{K}'$. (remember Lista 03!)

2) Show that the gap *vanishes* for

$$t_2 = \pm M / (3\sqrt{3})$$

but not in \mathbf{K} and \mathbf{K}' at the same time!



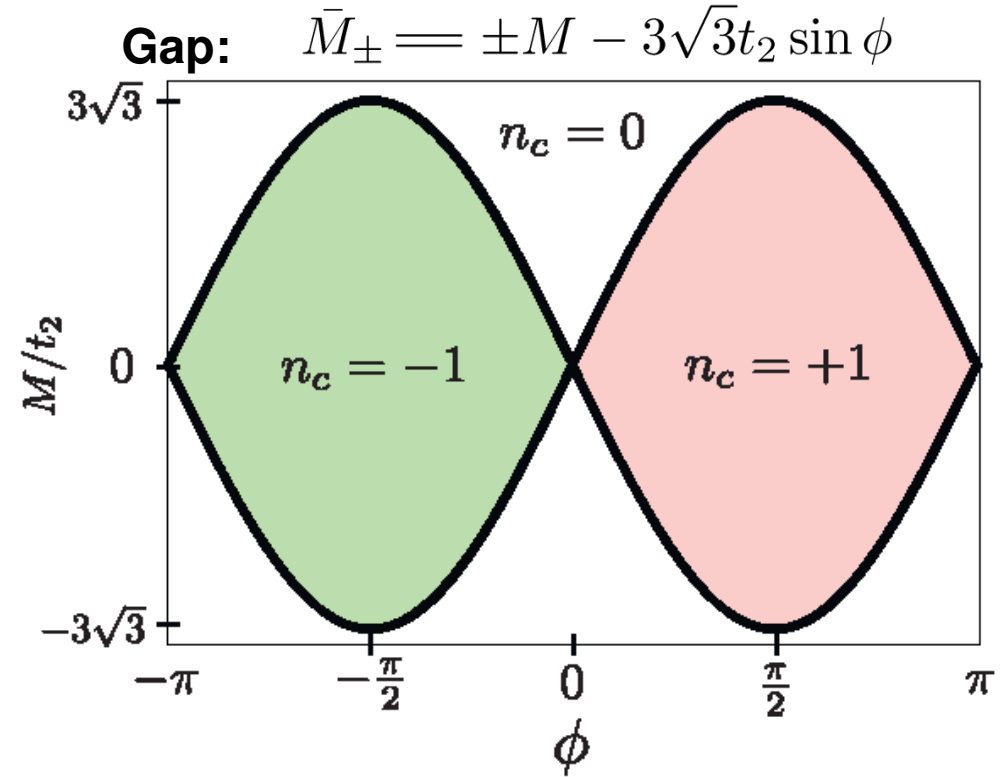
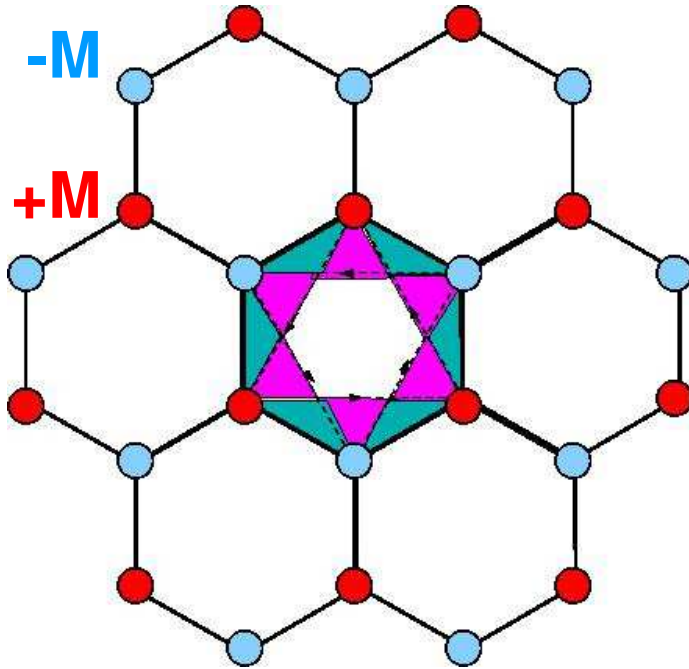
Haldane: Hall conductance with zero flux.



Duncan Haldane



2016



F.D.M. Haldane,
Phys. Rev. Lett. 61, 2015 (1988)

Hall conductance also given by a
Chern number:

$$n_c = \frac{1}{2} [\text{sgn}(\bar{M}_+) + \text{sgn}(\bar{M}_-)]$$

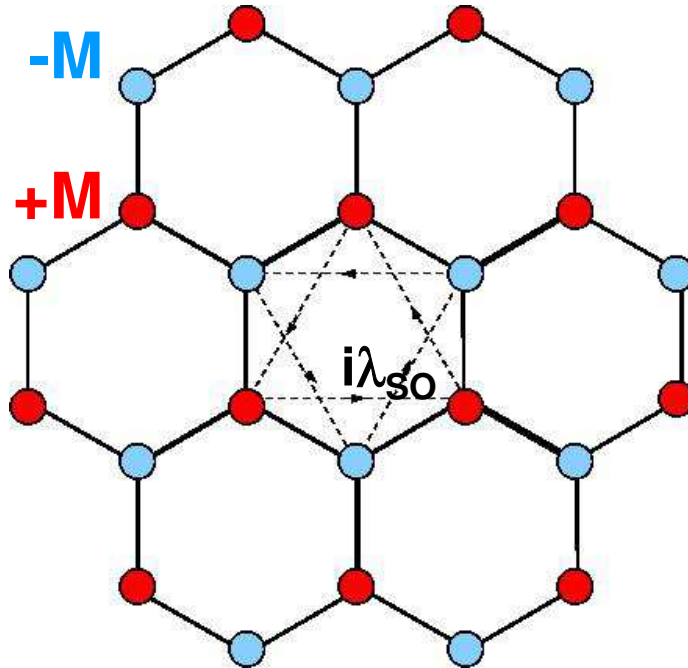
$$\sigma_{xy} = n_c \frac{e^2}{h}$$

$n_c = \pm 1$: **Topological phases**

Kane and Mele: Quantum Spin Hall effect.



Charles Kane



Spinful fermions in a Graphene-like lattice model: 4-band model.

Inversion symmetry breaking (not really needed.)

Spin orbit term connecting sites in the same sublattice!

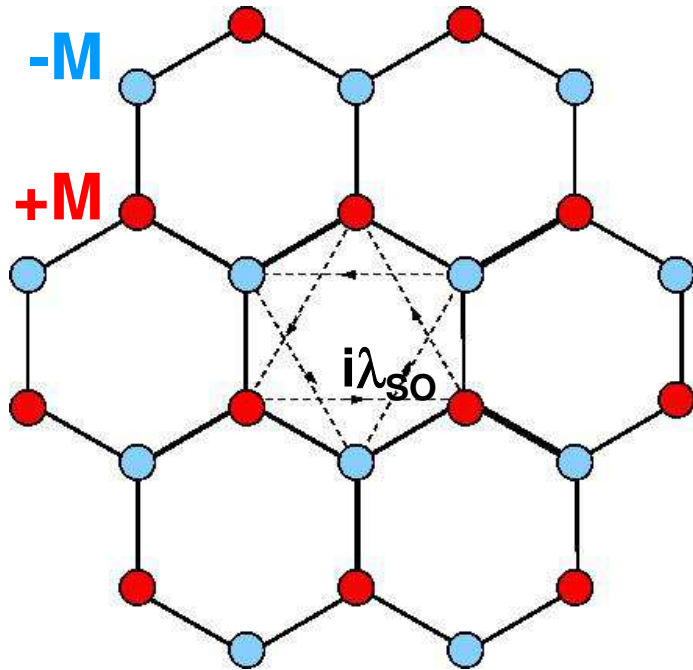
Hamiltonian obeys **time-reversal symmetry**.

A **Rashba spin orbit coupling** term can be added (results are qualitatively the same!)

C. L. Kane, E. J. Mele
Phys. Rev. Lett. 95, 146802 (2005)
Phys. Rev. Lett. 95, 226801 (2005).

https://topocondmat.org/w5_qshe/fermion_parity_pump.html

Kane and Mele model (no Rashba SOC)



Spin \uparrow : essentially the Haldane model with $\phi=\pi/2$

$$\frac{\mathcal{H}_{\mathbf{q}}^{\uparrow}}{N} = \begin{pmatrix} M + 2\lambda_{SO}f(\mathbf{q}, \frac{\pi}{2}) & t_1\gamma_{\mathbf{q}} \\ t_1\gamma_{\mathbf{q}}^* & -M + 2\lambda_{SO}f(\mathbf{q}, -\frac{\pi}{2}) \end{pmatrix}$$

$$\gamma_{\mathbf{q}} = 1 + e^{i\mathbf{q}\cdot\mathbf{a}_2} + e^{i\mathbf{q}\cdot(\mathbf{a}_2-\mathbf{a}_1)}$$

$$f(\mathbf{q}, \phi) = \cos(\mathbf{q}\cdot\mathbf{a}_1 + \phi) + \cos(\mathbf{q}\cdot\mathbf{a}_2 - \phi) + \cos(\mathbf{q}\cdot(\mathbf{a}_2 - \mathbf{a}_1) + \phi)$$

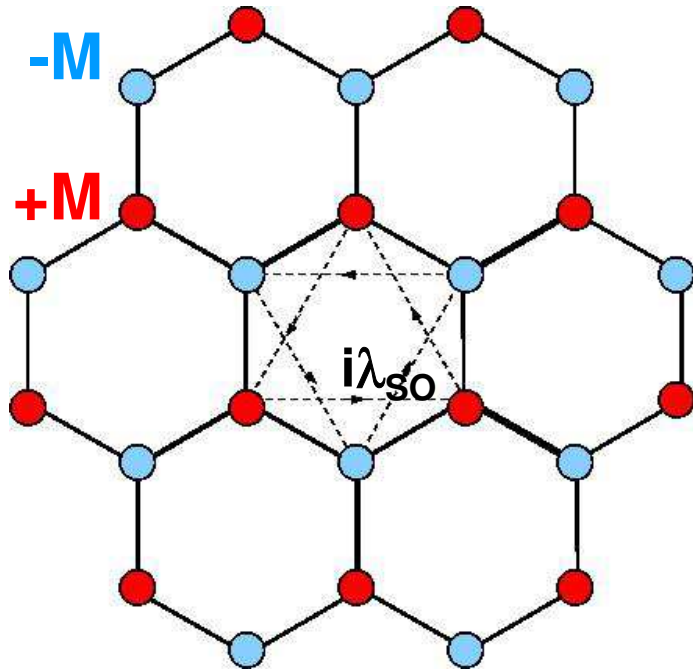
Time-reversal symmetry: $\mathcal{H}_{\mathbf{q}}^{\downarrow} = \left(\mathcal{H}_{-\mathbf{q}}^{\uparrow}\right)^*$

$$\left\{ \begin{array}{l} (\gamma_{-\mathbf{q}})^* = \gamma_{\mathbf{q}} \\ f(-\mathbf{q}, \phi) = f(\mathbf{q}, -\phi) \end{array} \right.$$

Spin \downarrow : Haldane model with $\phi=-\pi/2$

$$\frac{\mathcal{H}_{\mathbf{q}}^{\downarrow}}{N} = \begin{pmatrix} M + 2\lambda_{SO}f(\mathbf{q}, -\frac{\pi}{2}) & t_1\gamma_{\mathbf{q}} \\ t_1\gamma_{\mathbf{q}}^* & -M + 2\lambda_{SO}f(\mathbf{q}, \frac{\pi}{2}) \end{pmatrix}$$

Kane and Mele: Quantum Spin Hall effect.



Gap: $|6\sqrt{3}\lambda_{SO} - 2M|$

Topological phase : $M < 3\sqrt{3}\lambda_{SO}$

Chern number
(in the top. phase) $n_s = \text{sgn}(s\lambda_{SO})$

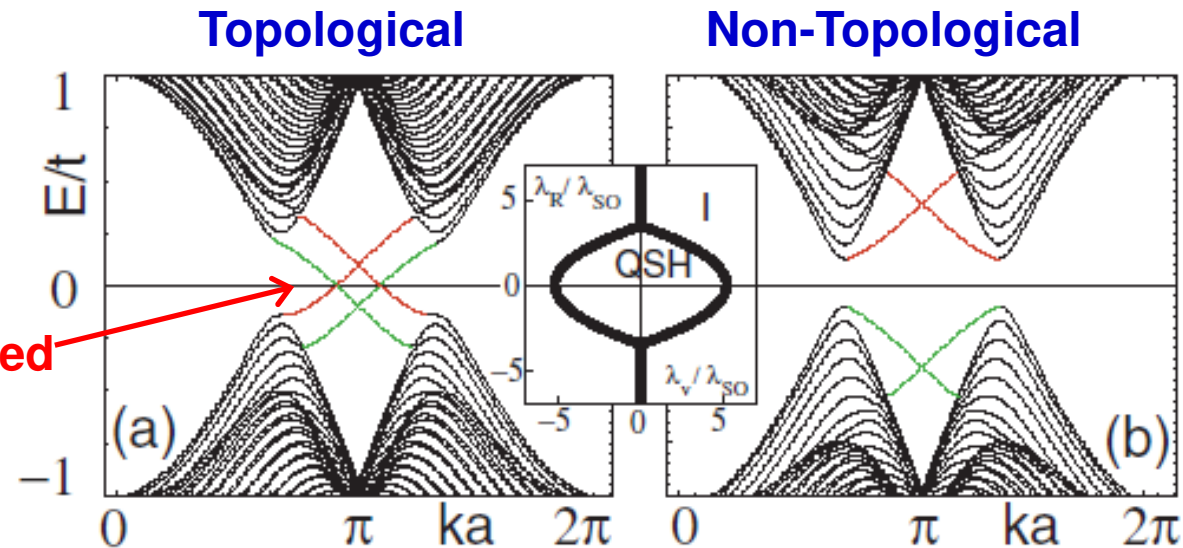
Z_2 invariant $\nu = \frac{1}{2}(n_{\uparrow} - n_{\downarrow}) = \pm 1$

New ingredients:

- Particles with spin s .
- Spin-Orbit coupling λ_{SO} (TRS preserved)
- Assuming no Rashba SO.

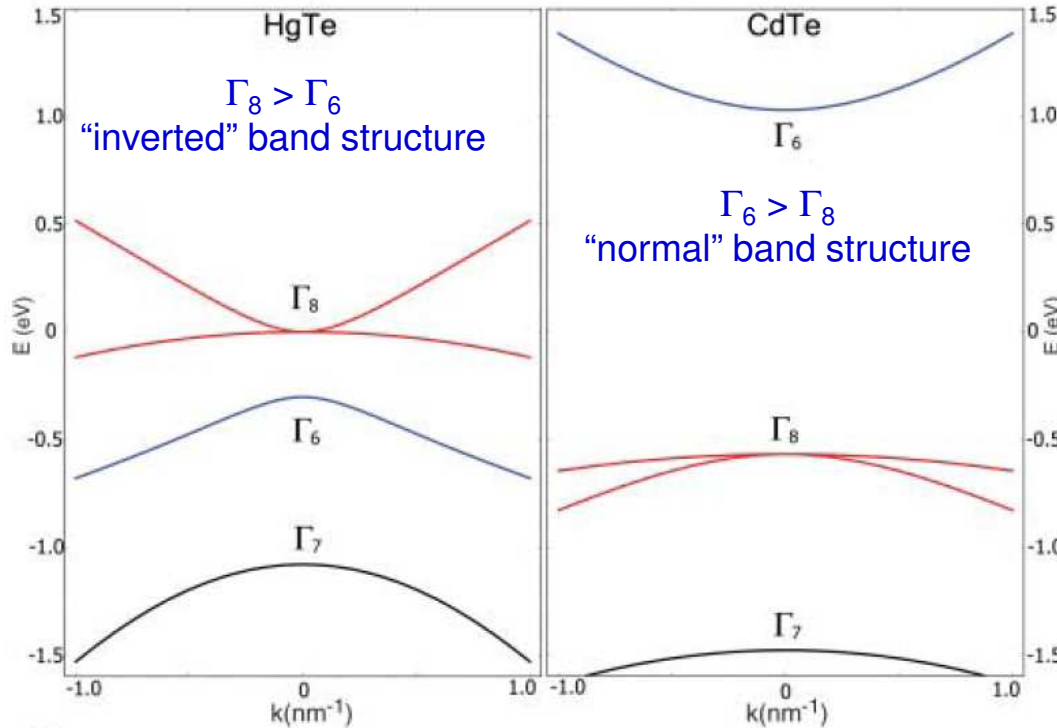
C. L. Kane, E. J. Mele
Phys. Rev. Lett. 95, 146802 (2005)
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Spin-polarized
Edge states

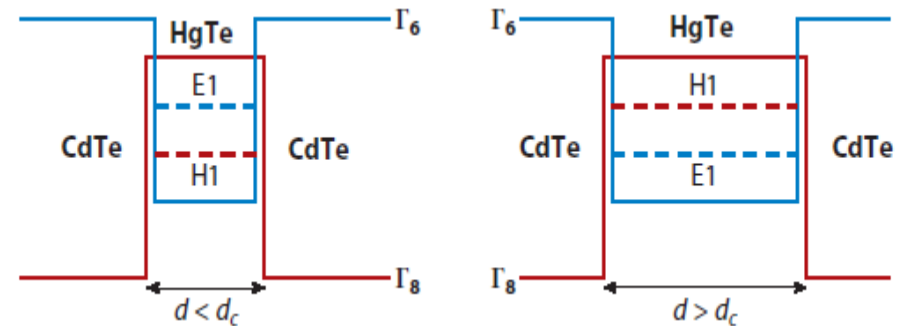
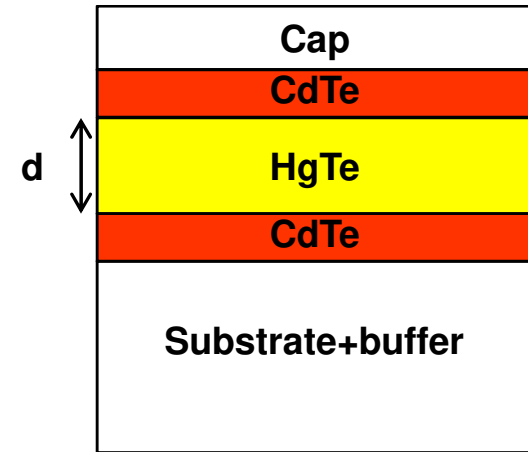


https://topocondmat.org/w5_qshe/fermion_parity_pump.html

HgTe Quantum Wells: “inverted” bands



HgTe quantum wells



Gap: $M \equiv E_{E1} - E_{H1}$

$d < d_c \Rightarrow M > 0$ $d > d_c \Rightarrow M < 0$

$d_c = 6.3 \text{ nm}$

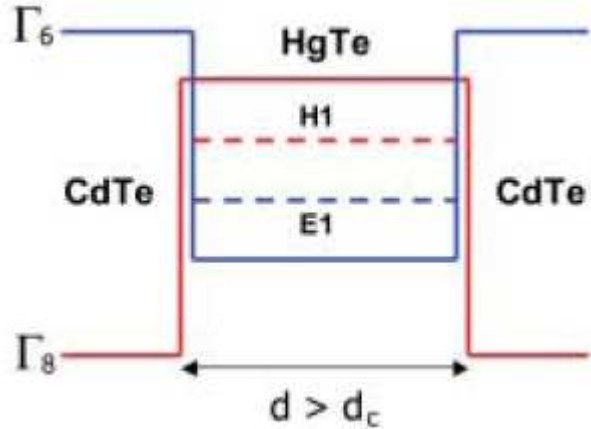
“ Γ_6 ”: s-type (s orbitals) $S=1/2$

“ Γ_8 ”: p-type (p orbitals) $J=3/2$
 (“light and heavy holes”)

HgTe: “zero gap” semiconductor.

Effective model for HgTe QWs (BHZ).

Bernevig, Hughes, Zhang, *Science* 314, 1757 (2006)



Basis: $\left\{ \begin{array}{l} |E+\rangle \\ |H+\rangle \\ |E-\rangle \\ |H-\rangle \end{array} \right.$

Basis functions: $\left\{ \begin{array}{l} \Psi_{\mathbf{k}}^{E+}(\mathbf{r}) \\ \Psi_{\mathbf{k}}^{H+}(\mathbf{r}) \\ \Psi_{\mathbf{k}}^{E-}(\mathbf{r}) \\ \Psi_{\mathbf{k}}^{H-}(\mathbf{r}) \end{array} \right.$

Hamiltonian (low energy from $\mathbf{k}\cdot\mathbf{p}$ theory):

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} h_+(\mathbf{k}) & 0 \\ 0 & h_+^*(-\mathbf{k}) \end{pmatrix}$$

$$h_+(k_x, k_y) = \begin{pmatrix} \epsilon(k) + \mathcal{M}(k) & Ak_- \\ Ak_+ & \epsilon(k) - \mathcal{M}(k) \end{pmatrix}$$

$$\begin{cases} \epsilon(k) & = & C - Dk^2 \\ \mathcal{M}(k) & = & M - Bk^2 \\ k_{\pm} & = & k_x \pm ik_y \end{cases}$$

d (Å)	A (eV)	B (eV)	C (eV)	D (eV)	M (eV)
58	-3.62	-18.0	-0.0180	-0.594	0.00922
70	-3.42	-16.9	-0.0263	0.514	-0.00686

$d < d_c$
 $d > d_c$

Table 1: Parameters for $\text{Hg}_{0.32}\text{Cd}_{0.68}\text{Te}/\text{HgTe}$ quantum wells.

Quantum Spin Hall effect in HgTe QWs.



Shoucheng Zhang

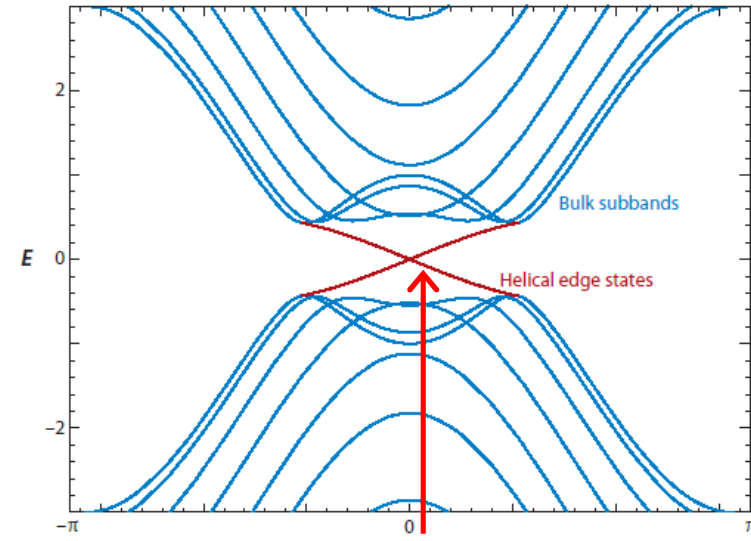
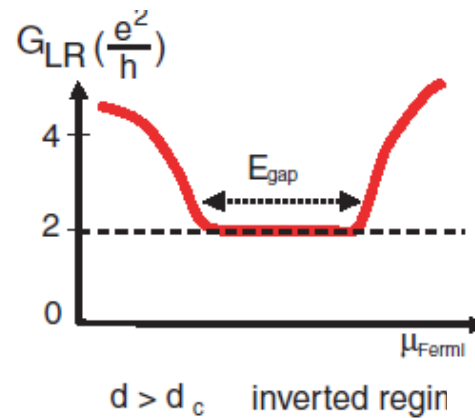
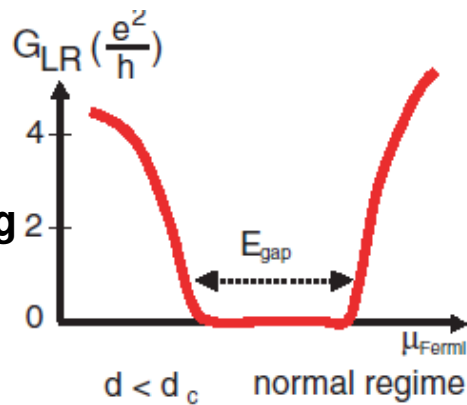


Andrei Bernevig

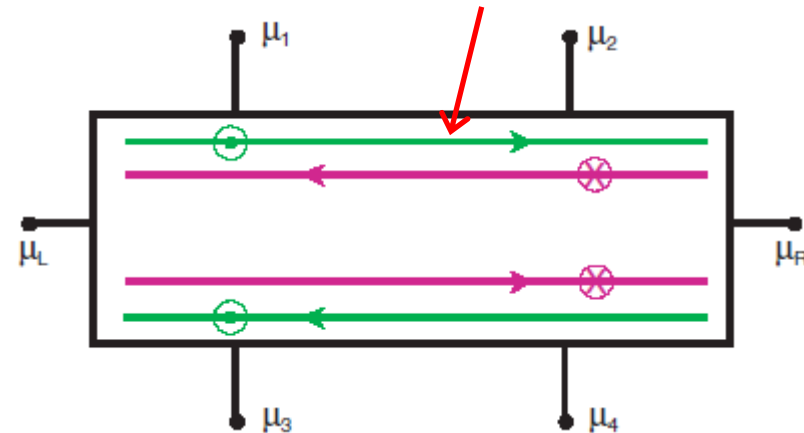
Gap: $|E_{E1} - E_{H1}| \equiv |M|$

Chern number

$$n_s = \text{sgn}(M)$$



Spin-polarized Edge states

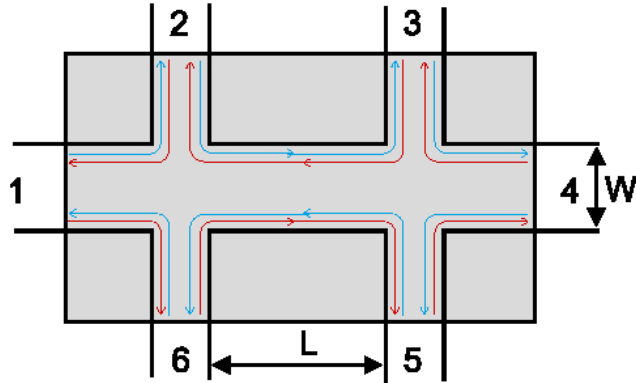


$$\Delta\sigma_{xy} = 2\frac{e^2}{h}$$

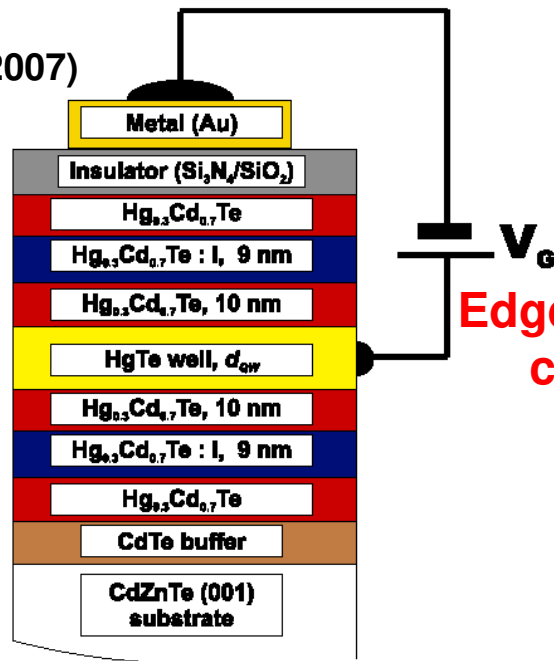
QSH effect in HgTe QWs: Experiment



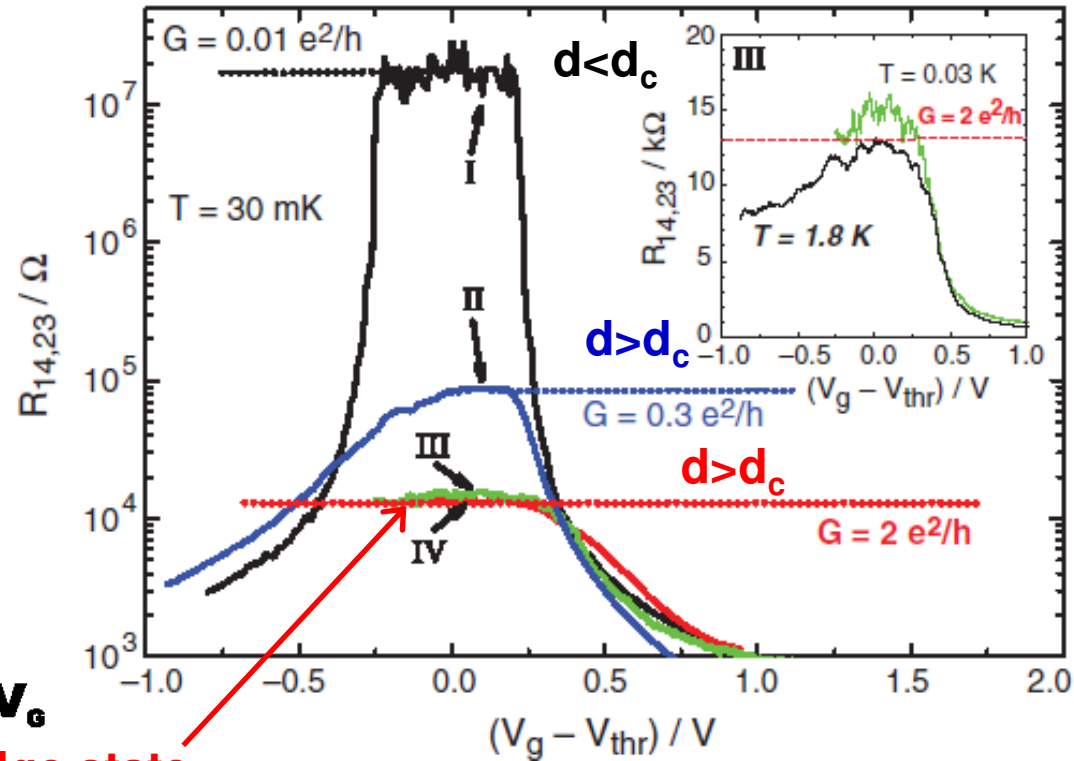
Laurens Molenkamp



König et al, *Science* 318, 766 (2007)



Edge state
conductance



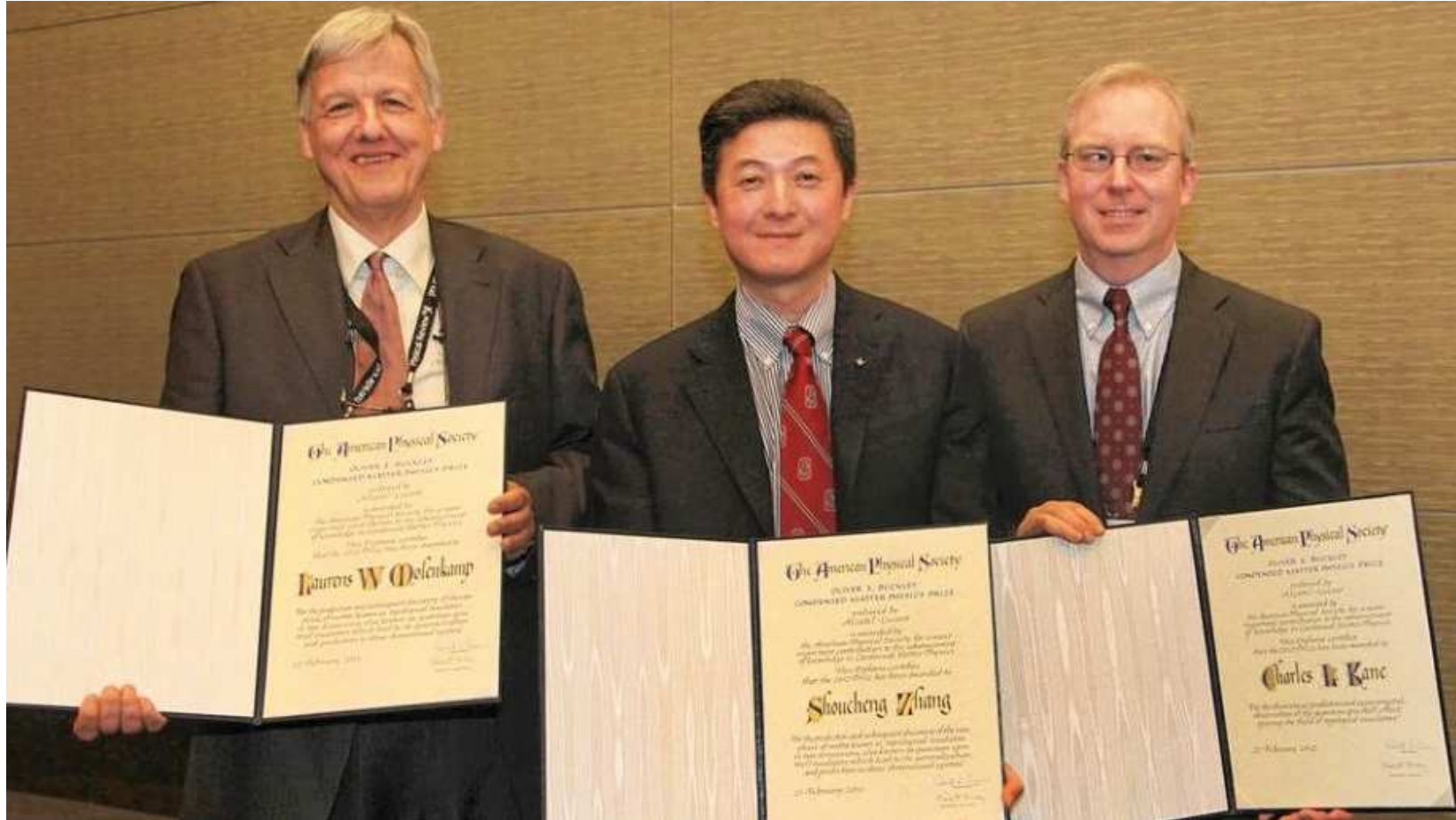
I- $L=20\ \mu\text{m}$ $W=13\ \mu\text{m}$ ($d < d_c$)

II- $L=20\ \mu\text{m}$ $W=13\ \mu\text{m}$ ($d > d_c$)

III- $L=1\ \mu\text{m}$ $W=1\ \mu\text{m}$ ($d > d_c$)

IV- $L=1\ \mu\text{m}$ $W=0.5\ \mu\text{m}$ ($d > d_c$)

A future Nobel Prize?



Physics Frontiers Prize 2013

also: APS Buckley Prize 2012

Tarefa 22: BHZ model

$$\mathcal{H}(k_x, k_y) = \begin{pmatrix} \epsilon(k) + \mathcal{M}(k) & Ak_- & 0 & 0 \\ Ak_+ & \epsilon(k) - \mathcal{M}(k) & 0 & 0 \\ 0 & 0 & \epsilon(k) + \mathcal{M}(k) & -Ak_+ \\ 0 & 0 & -Ak_- & \epsilon(k) - \mathcal{M}(k) \end{pmatrix}$$

$$\begin{cases} \epsilon(k) = C - Dk^2 \\ \mathcal{M}(k) = M - Bk^2 \\ k_{\pm} = k_x \pm ik_y \end{cases}$$

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$d < d_c$
 $d > d_c$

Table 1: Parameters for $\text{Hg}_{0.32}\text{Cd}_{0.68}\text{Te}/\text{HgTe}$ quantum wells.

- 1) Show that 2 of the 4 bands are always degenerate independently of the parameters.
- 2) Calculate the value of M such that the energy gap *vanishes* at $\mathbf{k}=(0,0)$.