In QFT the result that $\sigma_{xy} = \frac{1}{2} \frac{\text{sgn}(m)}{2\pi} \frac{e^2}{h}$ per fermionic species is known as the <u>parity anomaly</u>. Analogs of this anomaly occur in <u>odd</u> space-time dimensions (0+1, 2+1, 4+1, ...)

II <u>Topological Invariant</u>

This is a generalization of TKNN to a two-band model. The formulation that I give here follows the work of X.L. Qi, Y.S. Wu and S.C. Zhang, 2006, ~~and~~

~~by QR, the~~

As we saw, in general σ_{xy} is defined as

$$\sigma_{xy} = \lim_{\omega \to 0} \frac{i}{\omega} \lim_{\vec{Q} \to 0} \Pi_{xy}(\omega, \vec{Q})$$ (notice the order of limits!)

For a free fermion system the current correlator is

$$\Pi_{xy}(\omega, \vec{Q}=0) = \int_{BZ} \frac{d^2k}{(2\pi)^2} \int \frac{d\Omega}{2\pi}\, \mathrm{tr}\left[J_x(\vec{k})\, G(\vec{k}, \omega+\Omega)\, J_y(\vec{k}) \right]$$

$G(\vec{k}, \Omega)$

$$\mathcal{H}(\vec{k}) = h_0(\vec{k})\, \mathbb{1} + \vec{h}(\vec{k}) \cdot \vec{\sigma}$$

one-particle H.

$$\Rightarrow \cancel{\vec{J}_\ell(\vec{k}) = \frac{\partial \mathcal{H}(\vec{k})}{\partial k_\ell}} \qquad E_\pm(\vec{k}) = h_0(\vec{k}) \pm \|\vec{h}(\vec{k})\|$$

$$\vec{J}(\vec{k}) = \frac{\partial \mathcal{H}(\vec{k})}{\partial \vec{k}} = \frac{\partial h_0(\vec{k})}{\partial \vec{k}}\, \mathbb{1} + \frac{\partial h_a(\vec{k})}{\partial \vec{k}}\, \sigma_a$$

<u>Propagator</u>

$$G(\vec{k}, \omega) = \left(\omega \mathbb{1} - \mathcal{H}(\vec{k}) + i\epsilon \right)^{-1}$$

$$= \frac{\mathbb{P}_+(\vec{k})}{\omega - E_+(\vec{k}) + i\epsilon} + \frac{\mathbb{P}_-(\vec{k})}{\omega - E_-(\vec{k}) + i\epsilon}$$

$$\mathbb{P}_\pm(\vec{k}) = \frac{1}{2}\left(\mathbb{1} \pm \hat{h}_a(\vec{k})\, \sigma_a \right)$$

$$\hat{h}_a(\vec{k}) = \frac{\vec{h}(\vec{k})}{\|\vec{h}(\vec{k})\|}$$

unit vector

norm

$\Rightarrow$

$$\sigma_{xy} = \frac{e^2}{2} \int_{BZ} \frac{d^2k}{(2\pi)^2} \varepsilon_{abc} \frac{\partial \hat{h}_a(\vec{k})}{\partial k_x} \frac{\partial \hat{h}_b(\vec{k})}{\partial k_y} \hat{h}_c(\vec{k})$$

$(n_+(\vec{k}) - n_-(\vec{k}))$

$n_\pm(\vec{k})$ are Fermi functions (at $T=0$)

Since $E_+(\vec{k}) - E_-(\vec{k}) = 2\|\vec{h}(\vec{k})\| > 0$

$\Rightarrow \exists$ a finite energy gap between

$\min_{BZ}(E_+(\vec{k}))$ and $\max_{BZ}(E_-(\vec{k}))$

conduction band　　　valence band

Put E_F in the gap $\Rightarrow$ the valence band is full $n_-(\vec{k})=1$ and the conduction band is empty, $n_+(k)=0$

(for all $\vec{k} \in BZ$)

$$\Rightarrow \sigma_{xy} = -\frac{e^2}{8\pi^2} \int_{BZ} d^2k \; \varepsilon_{abc} \hat{h}_a(\vec{k}) \frac{\partial \hat{h}_b(\vec{k})}{\partial k_x} \frac{\partial \hat{h}_c(\vec{k})}{\partial k_y}$$

(see also Yakovenko 1990)

The BZ is a 2-torus (in $d=2$ dimensions!)

The unit vectors $\hat{\vec{h}}(\vec{k})$ satisfy

$$\hat{\vec{h}}(\vec{k})^2 = 1 \quad (\text{they are unit vectors})$$

$\Rightarrow$ $\hat{\vec{h}}(\vec{k})$ label points of a 2-sphere S_2

$\Rightarrow$ The quantity

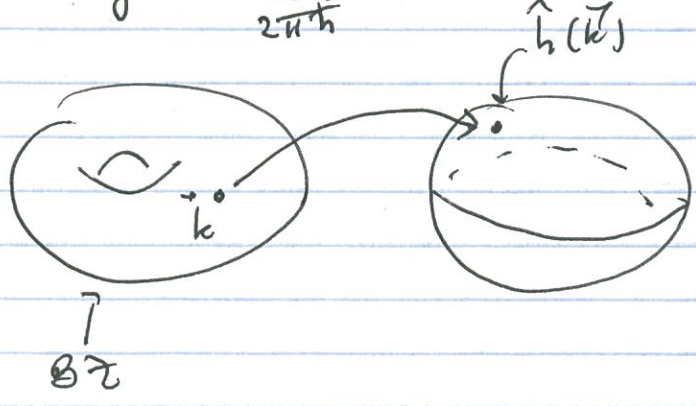
$$Q = \frac{1}{4\pi} \int_{BZ} d^2k \; \varepsilon_{abc} \, \hat{h}_a(\vec{k}) \, \frac{\partial \hat{h}_b(\vec{k})}{\partial k_x} \, \frac{\partial \hat{h}_c(\vec{k})}{\partial k_y}$$

is a topological invariant (Pontryagin index)

$\Rightarrow$ $Q \in \mathbb{Z}$ that counts the # of times S_2 is swept as $\vec{k}$ varies on the BZ.

In standard units

$$\sigma_{xy} = -\frac{e^2}{2\pi\hbar} Q$$



topological charge

In the non-linear σ-model this is the skyrmion charge

What about the Dirac theory?

For each Dirac fermion, the one-particle Hamiltonian is a 2×2 matrix (2D)

$$h(\vec{p}) = \vec{\alpha}\cdot\vec{p} + \beta m \equiv \vec{h}(\vec{p})\cdot\vec{\sigma}$$

when $\vec{h}(p) = (p_x, p_y, m)$

$$\Rightarrow \|\vec{h}(p)\| = \sqrt{\vec{p}^{\,2}+m^2} \equiv E(\vec{p})$$

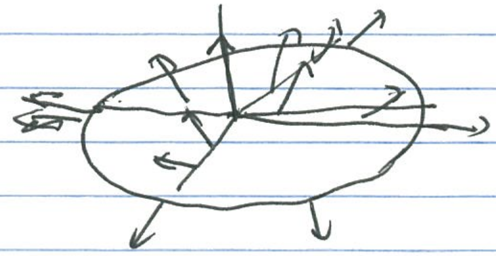
$$\Rightarrow \hat{h}(\vec{p}) = \frac{\vec{h}(\vec{p})}{\|\vec{h}(\vec{p})\|} = \frac{1}{E(\vec{p})}(p_x, p_y, m)$$

$$\lim_{|p|\to\infty} \hat{h}(\vec{p}) = \frac{1}{|\vec{p}|}(p_x, p_y, 0)$$

meron!

$$\lim_{|\vec{p}|\to 0} \hat{h}(\vec{p}) = \operatorname{sgn}(m)\ (0,0,1)$$

$m>0$



This is ½ of a skyrmion!

It ~~..~~ sweeps ½ of ~~...~~ the sphere $\Rightarrow 2\pi$

$$\Rightarrow Q = -\frac{1}{2}\,\operatorname{sgn}(m)$$

$\Rightarrow$ The Berry curvature is concentrated near $\vec{p}=0$!

The Quantum Spin Hall Effect

(C. Kane & E. Mele 2005; A. Bernevig, T. Hughes, S.C. Zhang 2006)

Expt.: König, Wiedmann, Brüne, Roth, Buhmann, Molenkamp, Qi, Zhang (2007)

Review: König, Buhmann, Molenkamp, Hughes, Liu, Qi, Zhang, J. Phys. Soc. Japan 2008

It is closely related to the AQHE except that it involves the spin current.

It was discovered in 2DEG HgTe/CdTe heterostructures (2008)

First: What is the spin current and when may the QSH effect occur?

Fundamental difference between the charge current J_μ (generator of global U(1) gauge transf.) and the spin current $\vec{J}_\mu$ (generators of the global SU(2) invariance of spin rotations)

J_μ^a, $a=1,2,3$ (or x,y,z), $\mu=0,1,2,\dots,d$

U(1): abelian, SU(2): non-abelian.

The spin conductivity is well defined only if $SU(2)$ is broken down to its $U(1)$ (diagonal) subgroup, e.g. J^3_μ is conserved by J^1_μ and J^2_μ are not. This requires that the spin-orbit interaction be present (and large enough to be significant) so that lattice effects couple to the spin.

However the QSH effect can occur even if $SU(2)$ is broken to a $\mathbb{Z}_2$ (discrete) subgroup. In this case there is no bulk spin conductance but there is spin transport on the edges.

I) The Kane-Mele model (2005)

Kane and Mele (KM) suggested that the QSHE may be observed in graphene but the SO interaction is negligible in that case ⟹ no QSH but it is a simple model.

KM considered a tight binding model of the form of Haldane's but for free fermions with spin and with SO coupling

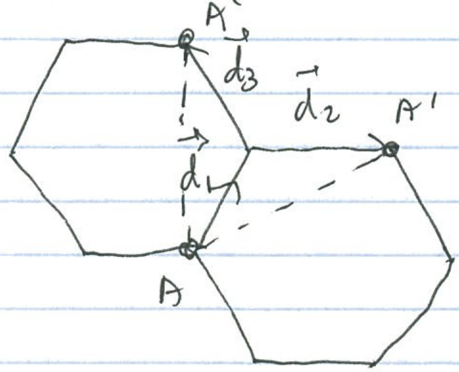
$$H_{KM} = t_1 \sum_{\vec{r}_A} \sum_{\substack{i=1,2,3 \\ \sigma=\uparrow,\downarrow}} \left[\psi^\dagger_\sigma(\vec{r}_A)\, \chi_\sigma(\vec{r}_A + \vec{d}_i) + h.c. \right]$$

$$+ t_2 \sum_{\langle \vec{r}_A, \vec{r}_A' \rangle} \sum_{\sigma,\sigma'=\uparrow,\downarrow} \left[i\, \psi^\dagger_\sigma(\vec{r}_A)\, \nu(\vec{r}_A, \vec{r}_A')\, S^z_{\sigma\sigma'}\, \psi_{\sigma'}(\vec{r}_A') + h.c. \right]$$

$$+ t_2 \sum_{\langle \vec{r}_B, \vec{r}_B' \rangle} \sum_{\sigma,\sigma'=\uparrow,\downarrow} \left[i\, \chi^\dagger_\sigma(\vec{r}_B)\, \nu(\vec{r}_B, \vec{r}_B')\, S^z_{\sigma\sigma'}\, \psi_{\sigma'}(\vec{r}_B') + h.c. \right]$$

$S_z \equiv \sigma_3$ and $\nu[\vec{r}_A, \vec{r}_A'] = \pm 1$ depending on the orientation of two n.n. bonds $\vec{d}_i$ and $\vec{d}_j$ which the electron traverses in going from $\vec{r}_A$ to $\vec{r}_A'$ (same for $\vec{r}_B$ and $\vec{r}_B'$) s.t.

$\nu(\vec{r}_A, \vec{r}_A') = +1\ (-1)$ if the electron makes a left (right) turn on the 2nd traversed bond



$\Rightarrow$ this amplitude is

$$i\, \vec{d}_i \times \vec{d}_j \cdot \vec{S}$$

$\uparrow$ spin

(this comes from SO)

This construction is equivalent to <u>two</u> Haldane models with $\phi = \pi/2$ for $\uparrow$ spin and $\phi = -\pi/2$ for $\downarrow$ spin.

Eff. Low Energy Theory

Dirac theory with two bispinors each with a flavor (spin) index $I = 1, 2$

$$\mathcal{H} = -i\hbar v_F \underbrace{\Psi^\dagger(x)}_{\text{bispinor}} (\alpha_1 \partial_x + \alpha_2 \partial_y) \Psi(x) + \Delta_{SO} \Psi^\dagger(x) \beta \underbrace{S^z}_{\text{two signs!}} \Psi(x)$$

$\Delta_{SO} = 3\sqrt{3}\, t_2$

$$\Psi_{1,\sigma} = \begin{pmatrix} \psi_{K,\sigma} \\ \chi_{K,\sigma} \end{pmatrix}, \quad \Psi_{2,\sigma} = \underbrace{\begin{pmatrix} -i\chi_{K',\sigma} \\ i\psi_{K',\sigma} \end{pmatrix}}_{\text{change of basis for } K'}$$

This model is Time-Reversal Invariant

$$\Rightarrow \sigma_{xy} = \sigma_{xy}^{\uparrow} + \sigma_{xy}^{\downarrow} = \frac{e^2}{h} - \frac{e^2}{h} = 0 \Rightarrow \underline{\text{insulator}}$$

$$\vec{J}_{spin} = \frac{\hbar}{2e}(\vec{J}_\uparrow - \vec{J}_\downarrow) = \frac{\hbar}{2e} \sum_{I=1,2} \Psi_I^\dagger S^z \vec{\alpha}\, \Psi_I$$

$$= \frac{\hbar}{2e} \sum_{I=1,2} \bar{\Psi}_I S_z \vec{\gamma}\, \Psi_I$$

An external electric field will generate equal and opposite currents for electrons with ↑ and ↓ spins

$$\Rightarrow \sigma^{spin}_{xy} = \frac{\hbar}{2e}\left(\sigma^{\uparrow}_{xy} - \sigma^{\downarrow}_{xy}\right) = \frac{e}{2\pi} \qquad \text{QSH!}$$

In the presence of an $\vec{E}$ field (or a substrate) graphene also admits a Rashba coupling

$$H_R = i\lambda_R \sum_{\vec{r}_A, i} \psi^\dagger(\vec{r}_A)\left(\vec{\sigma} \times \vec{d}_i\right)_z \chi(\vec{r}_A + \vec{d}_i) + h.c.)$$

this term breaks $z \to -z$ (mirror symmetry) and breaks the spin conservation law but it is TR invariant ($\mathbb{Z}_2$).

$\Rightarrow$ the conductivity cannot be defined as before

$$\mathcal{H}_R = \lambda_R \sum_{I=1,2} \Psi^\dagger_I(x)\left(\vec{\sigma} \times \vec{S}\right)_z \Psi_I$$

If $\lambda_R < \Delta_{SO}$ it remains a Top. Insulator.

QSH in Quantum Wells

(Bernevig, Hughes, Zhang, 2006) (BHZ)

SO coupling is very weak in graphene but not in several narrow-gap semiconductors (e.g. CdTe ~~β~~ and HgTe). BHZ showed that a CdTe/HgTe/ CdTe quantum well can harbor the QSHE.

CdTe and HgTe ~~have~~ have a narrow gap at the Γ point of the BZ. The bands that nearly cross ~~at~~ at the Γ point are the s-band Γ_6 and a higher energy band Γ_7 with $J = 1/2$ $(\vec{J} = \vec{L} + \vec{S})$

In HgTe the Γ_8 band lies above Γ_6 and in CdTe the order is reversed. BHZ derived an effective model near the Γ point $(\vec{k} = 0)$ for the 2 bands labelled $|E1, m_J = 1/2\rangle$, $|H1, m_J = 3/2\rangle$ $|E1, m_J = -1/2\rangle$ and $|H1, m_J = -3/2\rangle$

(These are l.c. of Γ_6 and Γ_8)

$$H_{eff} = \begin{pmatrix} h(\vec{k}) & 0 \\ 0 & h^{*}(-\vec{k}) \end{pmatrix}$$

$$h(\vec{k}) = \varepsilon(\vec{k})\,\mathbb{1} + \vec{d}(\vec{k})\cdot\vec{\sigma}$$

$\mathbb{1} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $\vec{\sigma}$: Pauli matrices

$$d_1 \pm i d_2 = A(k_x \pm i k_y) + \cdots$$

$$d_3 = M - B\vec{k}^2 + \cdots$$

$$\varepsilon(\vec{k}) = C - D\vec{k}^2 + \cdots$$

$A, B, C, D > 0$; M opens a single particle gap.

Time Reversal exchanges the two blocks $\Rightarrow$ model is TRI. These two pairs have opposite parity.

Close similarity with KM model.

SO $\Rightarrow$ only the z projection is a good quantum #.

$$\vec{m}_\uparrow \equiv \vec{d}_\uparrow(\vec{k}) = \frac{1}{\sqrt{\vec{k}^2+M^2}}(+k_x, k_y, M)$$

$$\vec{m}_\downarrow(\vec{k}) \equiv \vec{d}_\downarrow(\vec{k}) = \frac{1}{\sqrt{\vec{k}^2+M^2}}(-k_x, k_y, M)$$

$(k_x, k_y, -M)$

after a rotation by $e^{i\frac{\pi}{2}\sigma_2}$

(here I rescaled $\vec{k}$ by $1/A > 0$)

$$\Rightarrow \lim_{\vec{k}\to 0} \vec{m}_\uparrow(\vec{k}) = \mathrm{sgn}(M)\,(0,0,1)$$

and $$\lim_{|\vec{k}|\to\infty} m_\uparrow(\vec{k}) = \frac{1}{|\vec{k}|}(k_x, k_y, 0)$$

meron with $Q = -\frac{1}{2}\mathrm{sgn}(M)$

$$\Rightarrow \lim_{\vec{k}\to 0} m_\downarrow(\vec{k}) = -\mathrm{sgn}(M)(0,0,1)$$

$$\lim_{|\vec{k}|\to\infty} m_\downarrow(\vec{k}) = \frac{1}{|\vec{k}|}(k_x, k_y, 0)$$

meron with $Q = +\frac{1}{2}\mathrm{sgn}(M)$

This suggests that we could proceed as in the KM model but now we have a four band model and we need to be more careful.

The solution is to write a tight binding model near Γ that reduces to the block H

BHZ replaced each 2×2 block H with a lattice model on a square lattice with

$$H = \sum_{\vec{r}} \Big\{ \big[\mp c^\dagger(\vec{r}+\hat{e}_x)\,\sigma_x\, c(\vec{r}) - i\, c^\dagger(\vec{r}+\hat{e}_y)\,\sigma_y\, c(\vec{r}) + h.c. \big]$$
$$+ \big[c^\dagger(r+e_x)\,\sigma_z\, c(\vec{r}) + c^\dagger(\vec{r}+\hat{e}_y)\,\sigma_z\, c(\vec{r}) + h.c. \big]$$
$$+ (M-2)\, c^\dagger(\vec{r})\,\sigma_z\, c(\vec{r}) \Big\}$$

This is essentially the same as a Wilson fermion.

$$H = \int_{BZ} \frac{d^2k}{(2\pi)^2} \sum_{\alpha,\beta=1,2} \Big[c^{\dagger}_{\alpha,\uparrow}(\vec{k})\, \vec{d}_{\uparrow}(\vec{k}) \cdot \vec{\sigma}_{\alpha\beta}\, c_{\beta,\uparrow}(\vec{k})$$
$$+ c^{\dagger}_{\alpha,\downarrow}(\vec{k})\, \vec{d}_{\downarrow}(\vec{k}) \cdot \vec{\sigma}_{\alpha\beta}\, c_{\beta,\downarrow}(\vec{k}) \Big]$$

$|k_x| \le \pi, \quad |k_y| \le \pi$

$$\vec{d}_{\pm}(\vec{k}) = \left(\pm \sin k_x,\ \sin k_y,\ M + \cos k_x + \cos k_y - 2 \right)$$

$+$ for $\uparrow$ and $-$ for $\downarrow$.

$\Rightarrow$ the two bands have opposite parities

since $\vec{d}_{\downarrow}(\vec{k}) \cdot \vec{\sigma} = \vec{d}_{\uparrow}(-\vec{k}) \cdot \vec{\sigma}^{*}$

Four special points in the BZ

$$\vec{Q} = (0,0),\ (\pi,0),\ (0,\pi),\ (\pi,\pi)$$

$$\vec{k} = \vec{Q} + \vec{q}$$

$\cancel{\vec{d}_{\uparrow,(0,0)}(\vec{q}) \approx (q_x, q_y, M)}$

$$\vec{d}_{\uparrow,(0,0)}(\vec{q}) = (q_x, q_y, M) \quad , \quad \vec{d}_{\downarrow,(0,0)}(\vec{q}) = (-q_x, q_y, M)$$

$$\vec{d}_{\uparrow,(\pi,0)}(\vec{q}) = (-q_x, q_y, M-2) \quad , \quad \vec{d}_{\downarrow,(\pi,0)}(\vec{q}) = (q_x, q_y, M-2)$$

$$\vec{d}_{\uparrow,(0,\pi)}(\vec{q}) = (q_x, -q_y, M-2) \quad , \quad \vec{d}_{\downarrow,(0,\pi)}(\vec{q}) = (-q_x, -q_y, M-2)$$

$$\vec{d}_{\uparrow,(\pi,\pi)}(\vec{q}) = (-q_x, -q_y, M-4) \quad , \quad \vec{d}_{\downarrow,(\pi,\pi)}(\vec{q}) =$$

$$= (q_x, -q_y, M-4)$$

$\Rightarrow$ near Γ $((0,0))$ $\vec{d}_\uparrow$ and $\vec{d}_\downarrow$ have opposite parities $\Rightarrow$ breaks TRI.

Topological Charges

$$Q^\pm(0,0) = \mp \frac{1}{2}\,\mathrm{sgn}(M)$$

$$Q^\pm(\pi,0) = \pm \frac{1}{2}\,\mathrm{sgn}(M-2)$$

$$Q^\pm(0,\pi) = \pm \frac{1}{2}\,\mathrm{sgn}(M-2)$$

$$Q^\pm(\pi,\pi) = \mp \frac{1}{2}\,\mathrm{sgn}(M-4)$$

$$Q^\pm_T = Q^\pm(0,0) + Q^\pm(0,\pi) + Q^\pm(0,\pi) + Q^\pm(\pi,\pi)$$

$$\Rightarrow Q^\pm_T = \begin{cases} 0 , & M<0 \\ \pm 1 , & 0<M<2 \\ \pm 1 , & 2<M<4 \\ 0 , & 4<M \end{cases}$$ AQH for each band

As M increases from $M<0 \rightarrow M>0$ the gap closes and opens at ~~k~~ $(0,0) \Rightarrow$ the Chern # of each band. At $M=2$ the gaps close and open at $(0,\pi)$ and $(\pi,0)$, and at $M=4$ it happens at (π,π).

Total topological charge ~~of~~ of the 4-band model is $Q = Q_T^{\uparrow} + Q_T^{\downarrow} = 0 \Rightarrow \sigma_{xy} = 0$

But the spin Hall conductivity

$$\sigma_{xy}^{QSH} = \sigma_{xy}^{\uparrow} - \sigma_{xy}^{\downarrow} = -\frac{e^2}{h}\left(Q_T^{\uparrow} - Q_T^{\downarrow}\right)$$

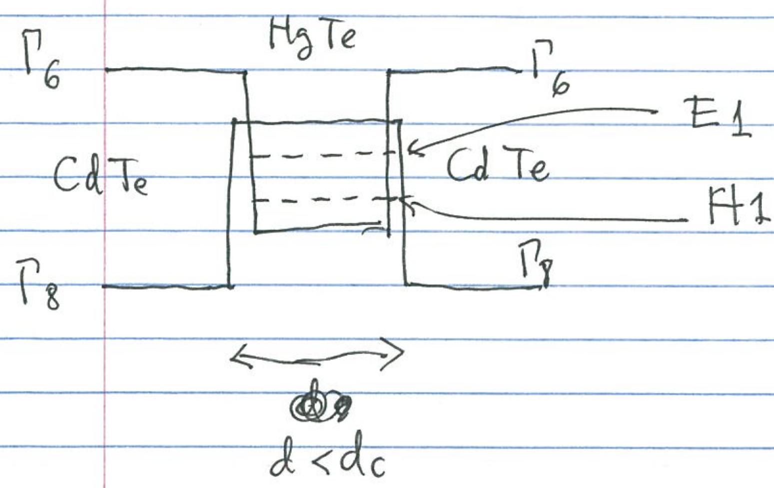
$$\Rightarrow \sigma_{xy}^{QSH} = \begin{cases} 0 & M<0 \\ 2\frac{e^2}{h} & 0<M<2 \\ -2\frac{e^2}{h} & 2<M<4 \\ 0 & 4<M \end{cases}$$

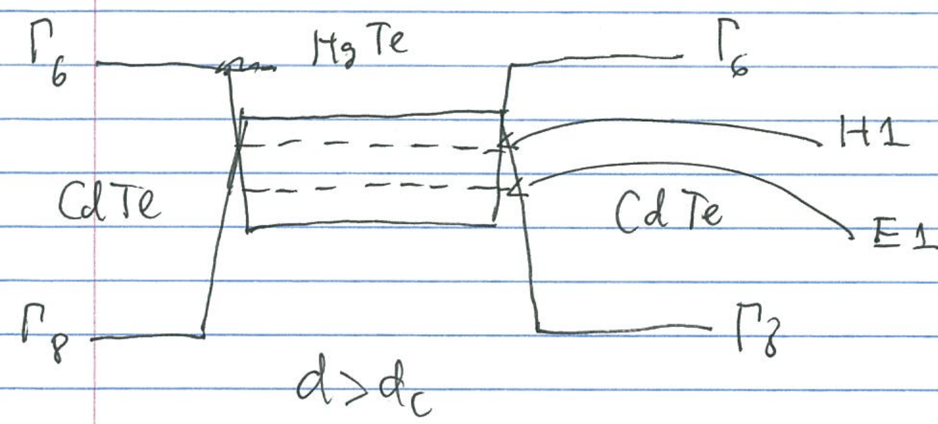
In the heterostructure the sign of M changes as a function of the thickness $\underline{d}$ from $M<0$ (E1 below H1) to $M>0$ (E1 above H1)

as in bulk CdTe

~~cha~~ band inversion.

States in the CdTe | HgTe | CdTe heterostructures





band inversion for $d < d_c$