Landau levels in bilayer quantum spin Hall systems

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Landau levels in the BHZ model

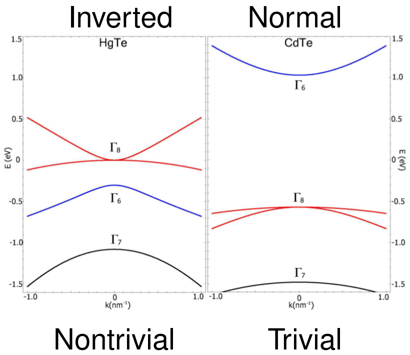
Materials of interest are HgTe/CdTe.

We want a simple model for the low energy limit.

Use the tetrahedral symmetry of the crystal.

Expand around the Γ-Point with $\boldsymbol{kp}$ perturbation theory
$\rightarrow$ 8x8 Kane Hamiltonian.

Neglect energetically distant split-off band Γ_7.



Bulk bandstructure near the neutrality point.

Bernevig, Hughes and Zhang (BHZ) model

To describe a quantum well, we use envelope instead of bloch functions and can obtain the BHZ model.

The basis of this 4x4 Hamiltonian is

$$|E1,\pm\rangle = \alpha\left|\Gamma_6,\pm\frac{1}{2}\right\rangle + \beta\left|\Gamma_8,\pm\frac{1}{2}\right\rangle \quad \text{and}$$

$$|H1,\pm\rangle = \left|\Gamma_8,\pm\frac{3}{2}\right\rangle .$$

The Hamiltonian is

$$H_{\mathrm{BHZ}}(\boldsymbol{k}) = \begin{pmatrix} h(\boldsymbol{k}) & \\ & h^*(-\boldsymbol{k}) \end{pmatrix},$$

$$h(\boldsymbol{k}) = \boldsymbol{d}\cdot\boldsymbol{\sigma} \equiv d_0\sigma_0 + d_1\sigma_1 + d_2\sigma_2 + d_3\sigma_3 \,,$$

$$\boldsymbol{d} = (C - D\boldsymbol{k}_\parallel^2, Ak_x, -Ak_y, M - B\boldsymbol{k}_\parallel^2)\,.$$

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Explicit form of $h(\boldsymbol{k})$ with $k_\pm = k_x \pm \mathrm{i}k_y$:

$$h(\boldsymbol{k}) = \begin{pmatrix} M - \frac{D+B}{2}(k_+k_- + k_-k_+) & Ak_+ \\ Ak_- & -M - \frac{D-B}{2}(k_+k_- + k_-k_+) \end{pmatrix} .$$

Use Peierl's substitution $\boldsymbol{k} \to \boldsymbol{\pi} = -\mathrm{i}\nabla + e\boldsymbol{A}$. With a symmetric gauge $\boldsymbol{A} = \mathcal{B}/2(-y, x, 0)$, we get

$$k_+ \to \pi_+ = k_+ + \mathrm{i}\frac{e\mathcal{B}}{2}(x + \mathrm{i}y)\,,$$
$$k_- \to \pi_- = k_- - \mathrm{i}\frac{e\mathcal{B}}{2}(x - \mathrm{i}y)\,.$$

By calculating the commutators we see that

$$a = \frac{l_B}{\sqrt{2}}\pi_- \quad \text{and} \quad a^\dagger = \frac{l_B}{\sqrt{2}}\pi_+$$

are bosonic ladder operators, where $l_B = 1/\sqrt{e\mathcal{B}}$.

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$$\Rightarrow h(\boldsymbol{k}) \to h_+ = \begin{pmatrix} M - \frac{2(D+B)}{l_B^2}(a^\dagger a + \frac{1}{2}) & \frac{\sqrt{2}A}{l_B} a^\dagger \\ \frac{\sqrt{2}A}{l_B} a & -M - \frac{2(D-B)}{l_B^2}(a^\dagger a + \frac{1}{2}) \end{pmatrix}$$

and $h^*(-\boldsymbol{k}) \to h_-$ with negative complex conjugate on the offdiagonal.

Ansatz which respects the position of ladder operators

$$|\psi_+\rangle = \begin{pmatrix} e_+ |n\rangle \\ h_+ |n-1\rangle \end{pmatrix} \quad \text{and} \quad |\psi_-\rangle = \begin{pmatrix} e_- |n-1\rangle \\ h_- |n\rangle \end{pmatrix}$$

leads to an easily solvable 2x2 matrix with eigenvalues:

$$E_\alpha^{1/2} = \frac{1}{l_B^2}(-\alpha B - 2Dn) \pm \sqrt{\left(M - \frac{2}{l_B^2}\left(nB + \alpha\frac{D}{2}\right)\right)^2 + \frac{2A^2 n}{l_B^2}}, \quad \alpha = \pm\,.$$

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Zero modes

$1/l_B^2 \propto \mathcal{B}, \quad e > 0$

For $n = 0$ we use

$$|\psi_+\rangle = \begin{pmatrix} |0\rangle \\ 0 \end{pmatrix} \quad \text{and} \quad |\psi_-\rangle = \begin{pmatrix} 0 \\ |0\rangle \end{pmatrix} ,$$

and obtain

$$E_\alpha^0 = \alpha M - \frac{(D + \alpha B)}{l_B^2} .$$

These lines cross if $E_+^0 - E_-^0 = 0$,

$$\Rightarrow \ \mathcal{B}_c = M/(Be)$$

For inverted layers $M/B > 0$, there is a finite crossing point.

Noninverted layers have positive mass M and show no crossing.

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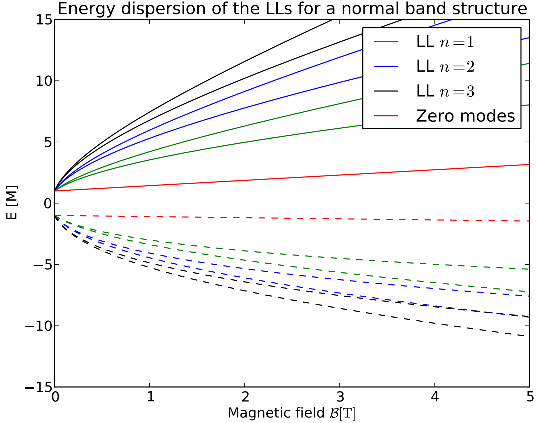
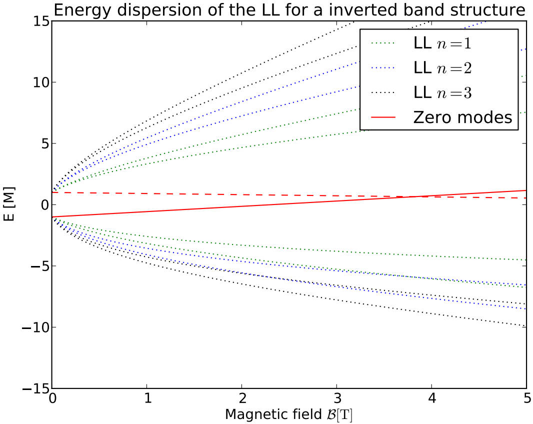
Energy dispersion of the Landau levels



Dashed (solid) represent H1 (E1). Quantum well is embedded in material with normal band structure. No edge channels if ϵ_F is in the gap.

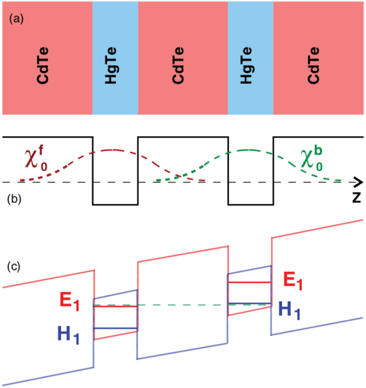
Phenomenology of the quantum spin Hall effect



Dotted lines correspond to strongly mixed states. Zero modes have to cross ϵ_F if $\mathcal{B} < \mathcal{B}_c \rightarrow$ Edgde channels for ($\boldsymbol{k} \uparrow$) and ($-\boldsymbol{k} \downarrow$).

Topologically nontrivial $\Rightarrow$ crossing of zero modes

Double quantum well



(a) Schematic representation of symmetric structure.
(b) Finite overlap of the envelope functions.
(c) Band inversion caused by potential.

Describe system with two BHZ models coupled by

$$H_T = +\frac{1}{2}(\boldsymbol{\Delta}\cdot\boldsymbol{\sigma})\mathcal{P}_1\,,$$
$$\boldsymbol{\Delta} = (\Delta_0, \alpha k_x, -\alpha k_y, \Delta_z)\,.$$

$\mathcal{P}_\alpha$ are Pauli matrices, correspond to layer pseudospin.

For spin up, we obtain

$$H^{\uparrow} = (\boldsymbol{d}\cdot\boldsymbol{\sigma})\,\mathcal{P}_0 + \frac{1}{2}(\boldsymbol{\Delta}\cdot\boldsymbol{\sigma})\,\mathcal{P}_1 + \frac{V}{2}\sigma_0\,\mathcal{P}_3$$
$$= \begin{pmatrix} \boldsymbol{d}\cdot\boldsymbol{\sigma} + \frac{V}{2}\,\sigma_0 & +\frac{1}{2}(\boldsymbol{\Delta}\cdot\boldsymbol{\sigma}) \\ +\frac{1}{2}(\boldsymbol{\Delta}\cdot\boldsymbol{\sigma}) & \boldsymbol{d}\cdot\boldsymbol{\sigma} - \frac{V}{2}\,\sigma_0 \end{pmatrix}.$$

An inversion of bands with E1 and H1 occurs at the Γ point for

$$V_c^2 = \frac{1}{4M^2}\left[\left(4M^2 - \frac{\Delta_0^2+\Delta_z^2}{2}\right)^2 - \frac{\left(\Delta_0^2-\Delta_z^2\right)^2}{4}\right]$$

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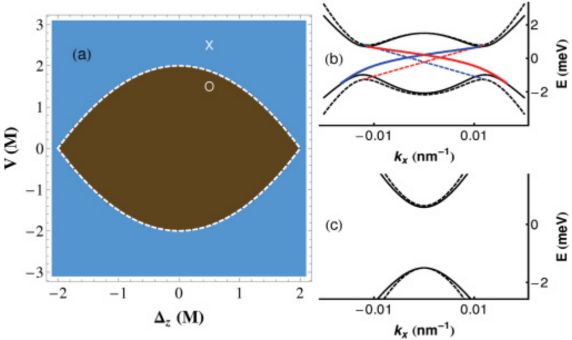

(a) Kramers Chern number for $\Delta_{H1H1} \approx 0$.
Black: topologically trivial. Blue: nontrivial.

(b) Edge state dispersion (blue, red) in the nontrivial regime.
Reduced two-band model is dashed.

(c) Conduction and valence band in trivial regime.

External magnetic field breaks time-reversal symmetry.
$\rightarrow$ We need both Kramer's blocks. Choice of basis:

$$\Big(|U, E1+\rangle\,, |U, H1+\rangle\,, |L, E1+\rangle\,, |L, H1+\rangle\,, \\ |U, E1-\rangle\,, |U, H1-\rangle\,, |L, E1-\rangle\,, |L, H1-\rangle \Big)\,.$$

The Hamiltonian

$$H_{\mathrm{DQW}}(\boldsymbol{k}) = \begin{pmatrix} H^{\uparrow}(\boldsymbol{k}) & \\ & H^{\downarrow}(\boldsymbol{k}) \end{pmatrix}\,,$$

$$H^{\downarrow}(\boldsymbol{k}) = H^{\uparrow}(-\boldsymbol{k})^{*}$$

preserves the expected symmetry: $T_{8\mathrm{x}8}\mathcal{H}_{\mathrm{DQW}}T_{8\mathrm{x}8}^{-1} = \mathcal{H}_{\mathrm{DQW}}$,
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Like before $h(\boldsymbol{k}) \to h_+$, $h^*(-\boldsymbol{k}) \to h_-$. Same substitutions yield

$$\boldsymbol{\Delta}(\boldsymbol{k}) \cdot \boldsymbol{\sigma} \to \Delta\sigma_+, \qquad \boldsymbol{\Delta}^*(-\boldsymbol{k}) \cdot \boldsymbol{\sigma} \to \Delta\sigma_-,$$

$$\Delta\sigma_+ = \begin{pmatrix} \Delta_{E1E1} & \frac{\sqrt{2}\alpha}{l_B} a^\dagger \\ \frac{\sqrt{2}\alpha}{l_B} a & \Delta_{H1H1} \end{pmatrix},$$

and $\Delta\sigma_-$ with negative complex conjugate on offdiagonal.

In total:

$$H_{DQW} \to \begin{pmatrix} H_+ & \\ & H_- \end{pmatrix},$$

where

$$H_\pm = \begin{pmatrix} h_\pm + V/2 & \Delta\sigma_\pm/2 \\ \Delta\sigma_\pm/2 & h_\pm - V/2 \end{pmatrix}.$$

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The ansatz for $n > 0$, respecting operator structure, is

$$|\psi_+\rangle = \begin{pmatrix} a_+ |n\rangle \\ b_+ |n-1\rangle \\ c_+ |n\rangle \\ d_+ |n-1\rangle \end{pmatrix} \quad \text{and} \quad |\psi_-\rangle = \begin{pmatrix} a_- |n-1\rangle \\ b_- |n\rangle \\ c_- |n-1\rangle \\ d_- |n\rangle \end{pmatrix} .$$

Leads to two algebraic 4x4 matrices. In general not analytically solvable. For $n = 0$, we use $\Delta_{\mathrm{H1H1}} \approx 0$.
$\rightarrow$ For spin down the layers are decoupled:

$$\left|\psi_-^U\right\rangle = \begin{pmatrix} 0 \\ |0\rangle \\ 0 \\ 0 \end{pmatrix} \quad \text{and} \quad \left|\psi_-^L\right\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ |0\rangle \end{pmatrix}$$

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Corresponding energies:

$$E_{-}^{U/L} = -M - \frac{D-B}{l_B^2} \pm \frac{V}{2} \,. \qquad \text{Degenerated for } V = 0.$$

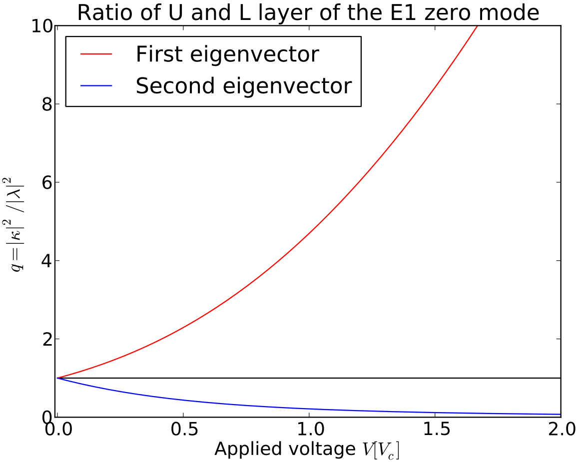
For spin up we need a relative phase between the layers:

$$|\psi_+\rangle = \begin{pmatrix} \kappa\,|0\rangle \\ 0 \\ \lambda\,|0\rangle \\ 0 \end{pmatrix}$$

This yields

$$E_{+}^{1/2} = M - \frac{D+B}{l_B^2} \pm \frac{\sqrt{V^2 + \Delta_{\mathrm{E1E1}}^2}}{2} \,.$$

Weight of the eigenvectors



For a barrier of $t = 5\,\mathrm{nm}$, $V_c = 10.23\,\mathrm{meV}$ is the inversion point. Layers decouple for increasing V.

Possible crossings are

$$\mathcal{B}_c^{1U/L} = \frac{4M \mp V - \sqrt{V^2 + \Delta_{E1E1}^2}}{4eB},$$
$$\mathcal{B}_c^{2U/L} = \frac{4M \mp V + \sqrt{V^2 + \Delta_{E1E1}^2}}{4eB}.$$

By using two noninverted layers, we have $B < 0$ and $M > 0$.
$\rightarrow$ $\mathcal{B}_c^{2U/L}$ has no positive value.
If $4M > \Delta_{\mathrm{E1E1}}$, only $\mathcal{B}_c^{1U}$ is left. By setting $\mathcal{B}_c^{1U} = 0$, we obtain

$$V_c = 2M - \frac{\Delta_{E1E1}^2}{8M}.$$

Same condition as inversion of bands at Γ point.

Crossing of zero modes

$E_+^{1/2} = M - \frac{D+B}{l_B^2} \pm \frac{\sqrt{V^2+\Delta^2_{\mathrm{E1E1}}}}{2}$ $\quad E_-^{U/L} = -M - \frac{D-B}{l_B^2} \pm \frac{V}{2}$ $\quad \frac{1}{l_B^2} \propto \mathcal{B}$ $\quad e > 0$

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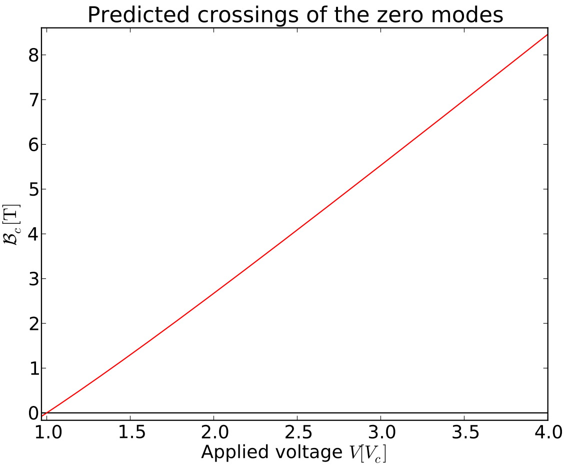
Tuning of crossing point $\mathcal{B}_c^{1U} = (4eB)^{-1}\left(4M - V - \sqrt{V^2 + \Delta_{E1E1}^2}\right)$

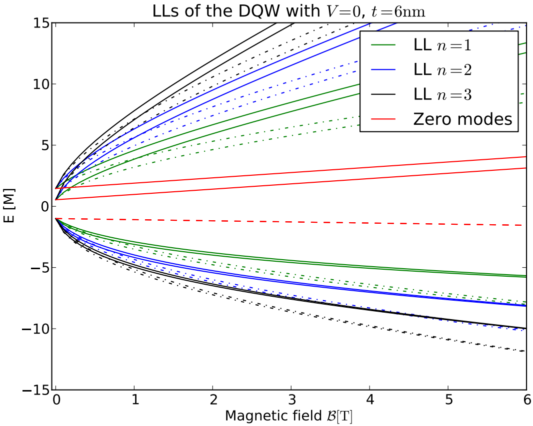


Depending on the applied voltage, the crossing point can be varied. Almost linear behaviour. Was only depending on material parameters for single layer.

Exploring the parameter space

Noninverted layers with reasonable coupling

$M \approx 6.5\,\mathrm{meV} \Leftrightarrow d = 5.7\,\mathrm{nm}$



No crossing without interlayer voltage. Ordinary insulator, if ϵ_F is in the gap. $E_-^{U/L}$ with H1 character fall together.

$\rightarrow$ Jump of two units in Hall conductivity.

Noninverted layers with reasonable coupling

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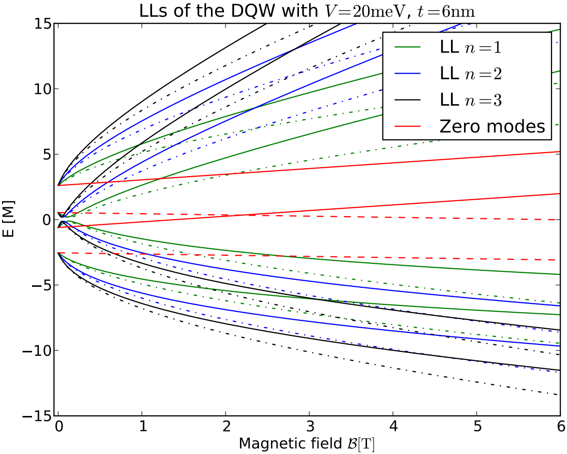


One crossing since $V > V_c$. Splitting of $E_-^{U/L}$. Topologically nontrivial system for $\mathcal{B} < \mathcal{B}_c$. Anti-crossing close to $\mathcal{B} = 0$.

Noninverted layers with strong coupling

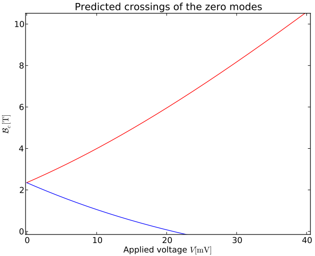
$M \approx 6.5\,\text{meV} \Leftrightarrow d = 5.7\,\text{nm}$

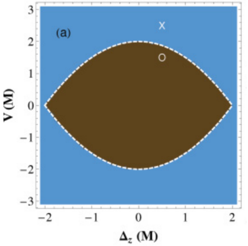
Strong coupling $4M \leq \Delta_{\text{E1E1}}$, corresponds to $t = 3\,\text{nm}$.

Second crossing (blue) appears.

Degenerated at $V = 0$ because of $E_{-}^{U/L}$.

Topologically nontrivial for all voltages.





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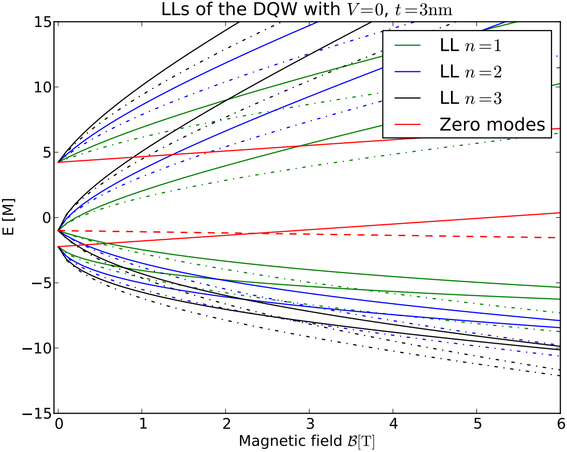

Double crossing is degenerated at first.

Noninverted layers with strong coupling

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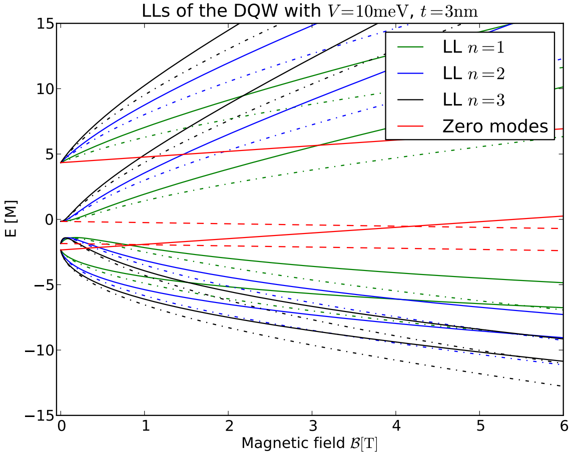

Second crossing is never in the bulk insulating gap. Doesn't change topology or correspond to second edge channel.

For $V \approx 2M$ the DQW can be described by a reduced low-energy Hamiltonian.

Works only if energy levels are seperated.

We can't expect good results for large fields.

Preserves topology $\rightarrow$ existence of crossing point is correctly predicted.

Can't reproduce the correct value of the full model.

Comparison with reduced model

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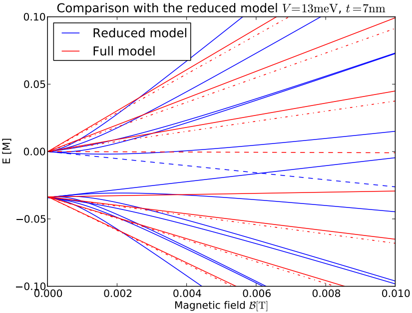
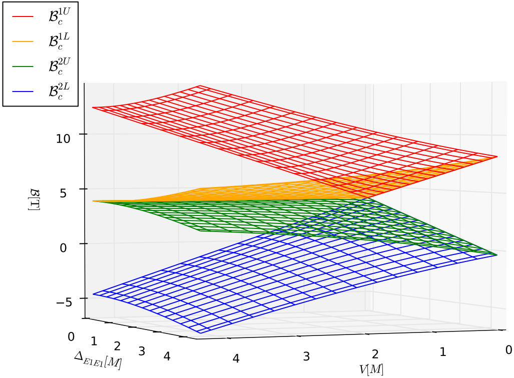
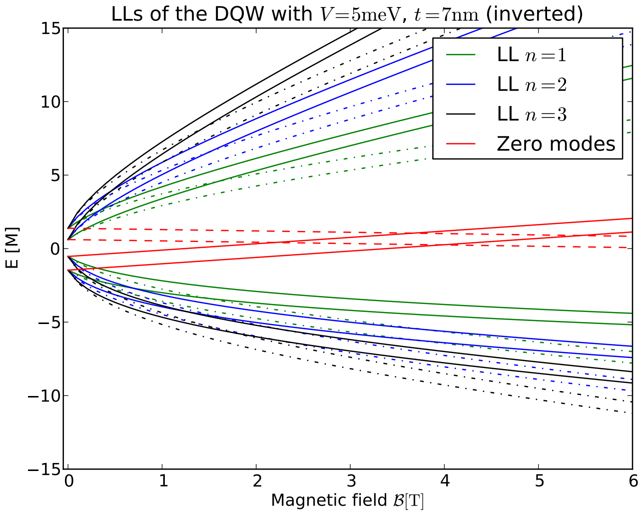


Negative mass allows for up to four crossings.

Topologically nontrivial without coupling or interlayer voltage.

Always at least two crossings. Inherited crossings of inverted single layer can be destroyed by voltage or coupling.





Resembles the dispersion of a single inverted layer.

- Crossing of zero-modes as visualization of inverted band structure.
- DQW can change it's topological insulator phase depending on the applied interlayer voltage.
- Interesting QH effect of the DQW can be expected. Easiest way to verify the change of the phase.
- Gapless systems are created for $V = V_c$. Not depending on the exact thickness of the layers.
- Experimental realization should be quite feasible.

Conclusion

- Crossing of zero-modes as visualization of inverted band structure.
- DQW can change it's topological insulator phase depending on the applied interlayer voltage.
- Interesting QH effect of the DQW can be expected. Easiest way to verify the change of the phase.
- Gapless systems are created for $V = V_c$. Not depending on the exact thickness of the layers.
- Experimental realization should be quite feasible.