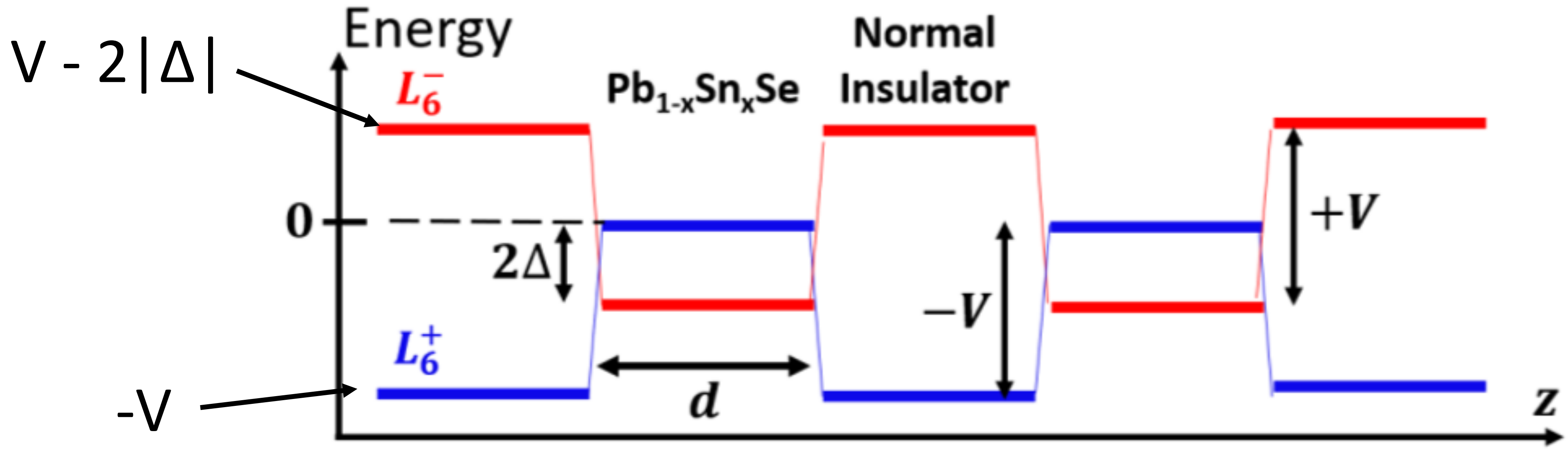
Numeric Solutions for the Eigenenergies of Topological Quantum Wells

Christian Bunker

Quantum Well Setup

- Band gap difference → potential barrier ±V (meV)
- Gap in the well is 2Δ (meV), negative due to inversion
- Assuming growth in z direction, d (nm) is well thickness



Hamiltonian

- Bulk k.p hamiltonian ($|L_6^+\uparrow\rangle$, $|L_6^+\downarrow\rangle$, $|L_6^-\uparrow\rangle$, $|L_6^-\downarrow\rangle$ basis)

$$\begin{pmatrix} \frac{\hbar^2 k_\perp^2}{2m^*} & 0 & \hbar v_z k_z & \hbar v_\perp (k_x - i k_y) \\ 0 & -\frac{\hbar^2 k_\perp^2}{2m^*} & \hbar v_\perp (k_x + i k_y) & -\hbar v_z k_z \\ \hbar v_z k_z & \hbar v_\perp (k_x - i k_y) & 2|\Delta| + \frac{\hbar^2 k_\perp^2}{2m^*} & 0 \\ \hbar v_\perp (k_x + i k_y) & -\hbar v_z k_z & 0 & -2|\Delta| - \frac{\hbar^2 k_\perp^2}{2m^*} \end{pmatrix}$$

Hamiltonian

- k_x, k_y are good quantum numbers which we set to 0
- k_z is not due to confinement in the z direction
- We can empirically determine the Dirac dispersion-like velocity v_z

Hamiltonian

- Heterostructure k.p hamiltonian ($|L_6^+\uparrow\rangle$,$|L_6^+\downarrow\rangle$,$|L_6^-\uparrow\rangle$,$|L_6^-\downarrow\rangle$ basis)

$$\begin{pmatrix} V_- & 0 & \hbar v_z k_z & \hbar v_\perp (k_x - i k_y) \\ 0 & V_- & \hbar v_\perp (k_x + i k_y) & -\hbar v_z k_z \\ \hbar v_z k_z & \hbar v_\perp (k_x - i k_y) & -2|\Delta| + V_+ & 0 \\ \hbar v_\perp (k_x + i k_y) & -\hbar v_z k_z & 0 & -2|\Delta| + V_+ \end{pmatrix}$$

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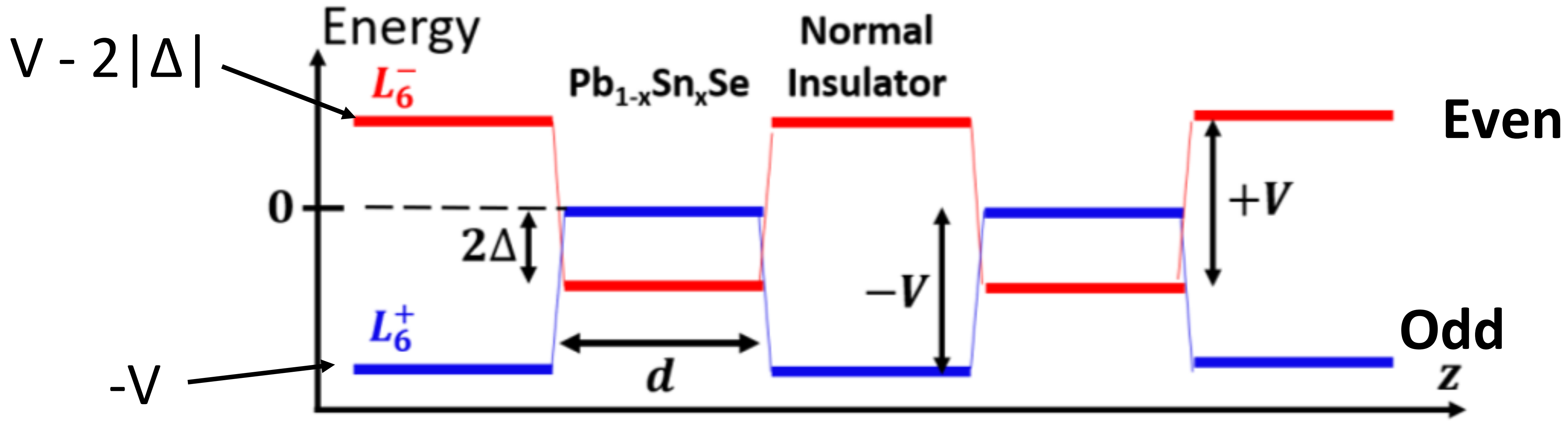

Hamiltonian

- Start by solving simpler case k_x, $k_y = 0 \rightarrow k_\perp = 0$
- Focus on z dependence which is where interesting physics is

Wavefunctions

- Consider $f(\mathbf{r})u_{\mathbf{k}}(\mathbf{r})$ where $u(\mathbf{r}) = u(\mathbf{r}+\mathbf{R}),\ V(\mathbf{r}) = V(\mathbf{r}+\mathbf{R})$
- Bloch basis: wavefunction obeys $\psi(\mathbf{r}) = \sum_l f_l^{A,B}(\mathbf{r})u_{l,\mathbf{k}}(\mathbf{r})$
- Want to find envelope functions $f_l^{A,B}(\mathbf{r})$

Wavefunctions

- Separate out the z dependence of envelope functions

$$f_l^{A,B}(\mathbf{r}_\perp, z) = \frac{1}{\sqrt{S}} e^{i\mathbf{k}_\perp \cdot \mathbf{r}_\perp} \chi_l^{A,B}(z)$$

- Chi functions obey Schrodinger-like differential equation which is even in z

Bound States

- Choosing z = 0 such that the well extends from z = -d/2 to z = d/2
- Since the “potential” is even in z around z = 0, solutions are guaranteed to be alternating even and odd in z [3]

$$\chi(z) = A\cos\left(k_z z\right), \;\; \chi(z) = A\sin\left(k_z z\right)$$

$$k_z = \sqrt{\frac{2m_A E}{\hbar^2}\left(1+\frac{E}{2|\Delta|}\right)} = \frac{1}{\hbar v_z}\sqrt{E(E+2|\Delta|)} \;\; \text{since } m_A = \frac{|\Delta|}{v_z^2}$$

$$k_z = i\kappa, \;\; \kappa = \frac{1}{\hbar v_z}\sqrt{-E(E+2|\Delta|)}$$

Bound States

- Choosing z = 0 such that the well extends from z = -d/2 to z = d/2
- Since the "potential" is even in z around z = 0, solutions are guaranteed to be alternating even and odd in z [3]
- Solutions are evanescent in the barrier

$$\chi(z) = Be^{-\rho(|z|-d/2)}$$

$$\rho = \frac{1}{\hbar v_z}\sqrt{(E+V)(-E-2|\Delta|+V)}$$

Eigenenergies

- Simplify the hamiltonian

$$\mathcal{H} = \begin{pmatrix} V_-(z) & -i\hbar v_z \frac{d}{dz} \\ -i\hbar v_z \frac{d}{dz} & -2|\Delta| + V_+(z) \end{pmatrix}, \mathcal{H}' = \begin{pmatrix} V_-(z) & i\hbar v_z \frac{d}{dz} \\ i\hbar v_z \frac{d}{dz} & -2|\Delta| + V_+(z) \end{pmatrix}$$

Hamiltonian

- Heterostructure k.p hamiltonian ($|L_6^+\uparrow\rangle$,$|L_6^+\downarrow\rangle$,$|L_6^-\uparrow\rangle$,$|L_6^-\downarrow\rangle$ basis)

$$\begin{pmatrix} V_- & 0 & \hbar v_z k_z & \hbar v_\perp (k_x - ik_y) \\ 0 & V_- & \hbar v_\perp (k_x + ik_y) & -\hbar v_z k_z \\ \hbar v_z k_z & \hbar v_\perp (k_x - ik_y) & -2|\Delta| + V_+ & 0 \\ \hbar v_\perp (k_x + ik_y) & -\hbar v_z k_z & 0 & -2|\Delta| + V_+ \end{pmatrix}$$

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$$\overrightarrow{\Psi_\mathrm{i}} = \begin{pmatrix} \mathrm{F}_1^{(i)} \\ \mathrm{F}_2^{(i)} \end{pmatrix} \text{ and } \overrightarrow{\varphi_\mathrm{i}} = \begin{pmatrix} \mathrm{F}_1^{(i)} \\ -\mathrm{F}_2^{(i)} \end{pmatrix}$$

$$\mathcal{H}\overrightarrow{\Psi_\mathrm{i}} = \mathrm{E_i}\overrightarrow{\Psi_\mathrm{i}}$$

$$\mathcal{H}'\overrightarrow{\varphi_\mathrm{i}} = \mathrm{E_i}\overrightarrow{\varphi_\mathrm{i}}$$

Wavefunctions

- Separate out the z dependence of envelope functions

$$f_l^{A,B}(\mathbf{r}_\perp, z) = \frac{1}{\sqrt{S}} e^{i\mathbf{k}_\perp \cdot \mathbf{r}_\perp} \chi_l^{A,B}(z)$$

- Chi functions obey Schrodinger-like differential equation which is even in z

Eigenenergies

- Potential is even so we are guaranteed even and odd solutions [3]
- In fact, for E > 0:

$$\tan\left(\frac{k_z d}{2}\right) = \frac{\rho}{k_z}\frac{E + 2|\Delta|}{E + 2|\Delta| - V} \qquad \textit{even case}$$

$$\mathrm{cotan}\left(\frac{k_z d}{2}\right) = -\frac{\rho}{k_z}\frac{E + 2|\Delta|}{E + 2|\Delta| - V} \qquad \textit{odd case}$$

$$k_z = \frac{1}{\hbar v_z}\sqrt{E(E + 2|\Delta|)}$$

$$\rho = \frac{1}{\hbar v_z}\sqrt{(E + V)(-E - 2|\Delta| + V)}$$

Eigenenergies

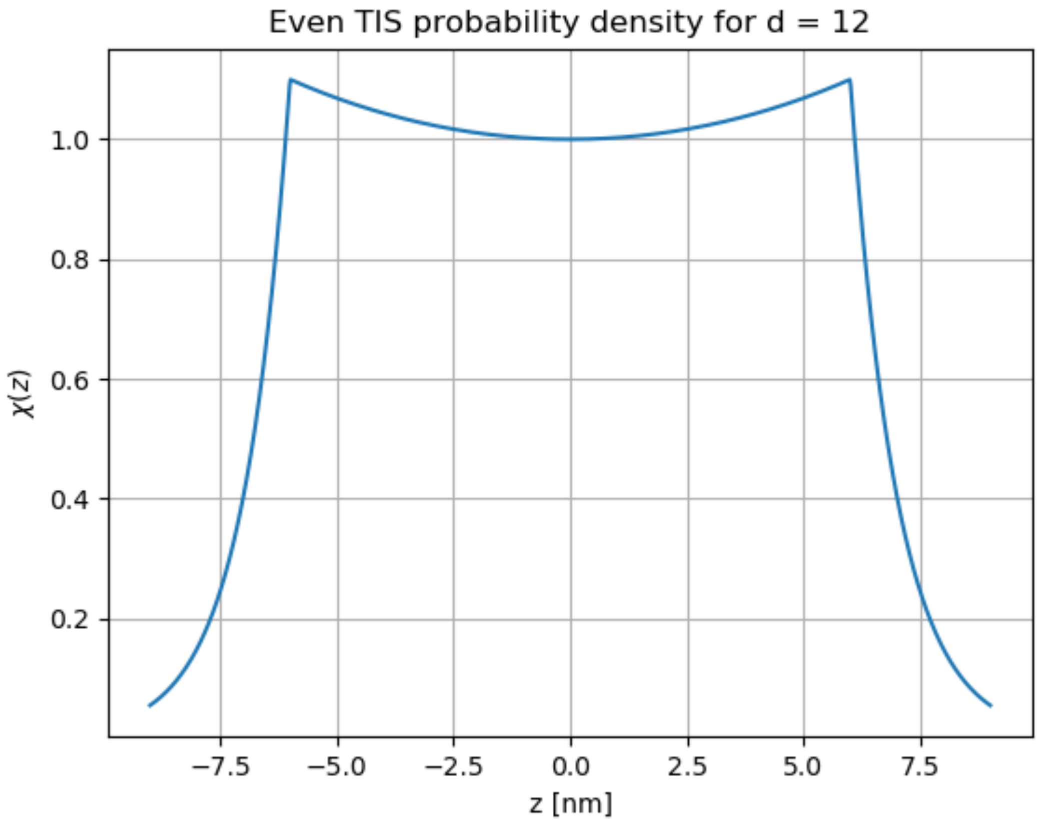
- In the regime $-2|\Delta| < E < 0$, k_z becomes imaginary, $k_z = i\kappa$

$$\tanh\left(\frac{\kappa d}{2}\right) = -\frac{\rho}{\kappa}\frac{E + 2|\Delta|}{E + 2|\Delta| - V} \qquad \textit{even case}$$

$$\operatorname{cotanh}\left(\frac{\kappa d}{2}\right) = -\frac{\rho}{\kappa}\frac{E + 2|\Delta|}{E + 2|\Delta| - V} \qquad \textit{odd case}$$

Topological Interface States

- The evanescent (imaginary k_z) regime $-2|\Delta| < E < 0$ is of special interest
- The cos/sin solutions become hyperbolic



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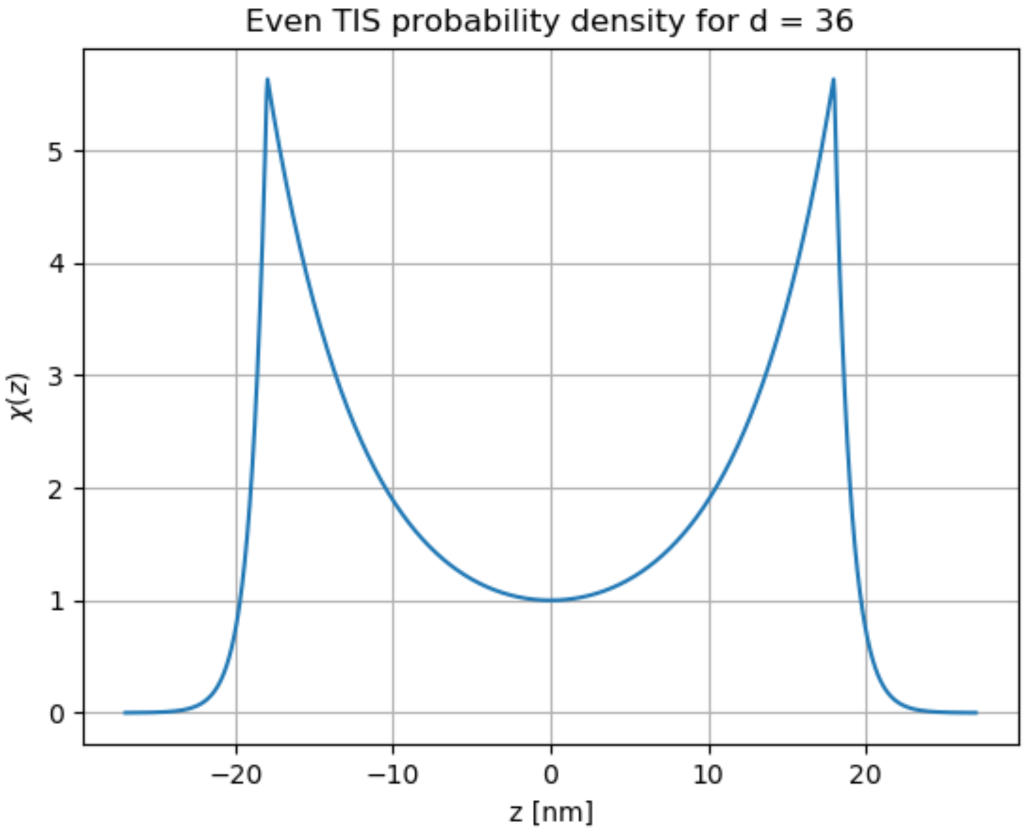
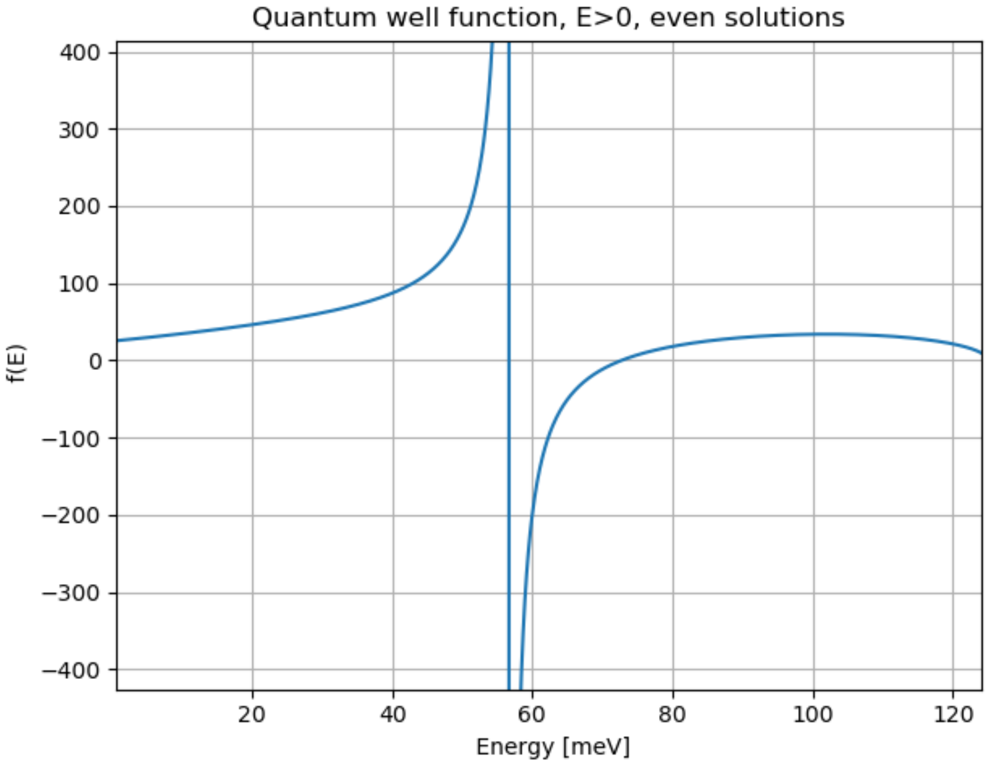


Numeric Solutions

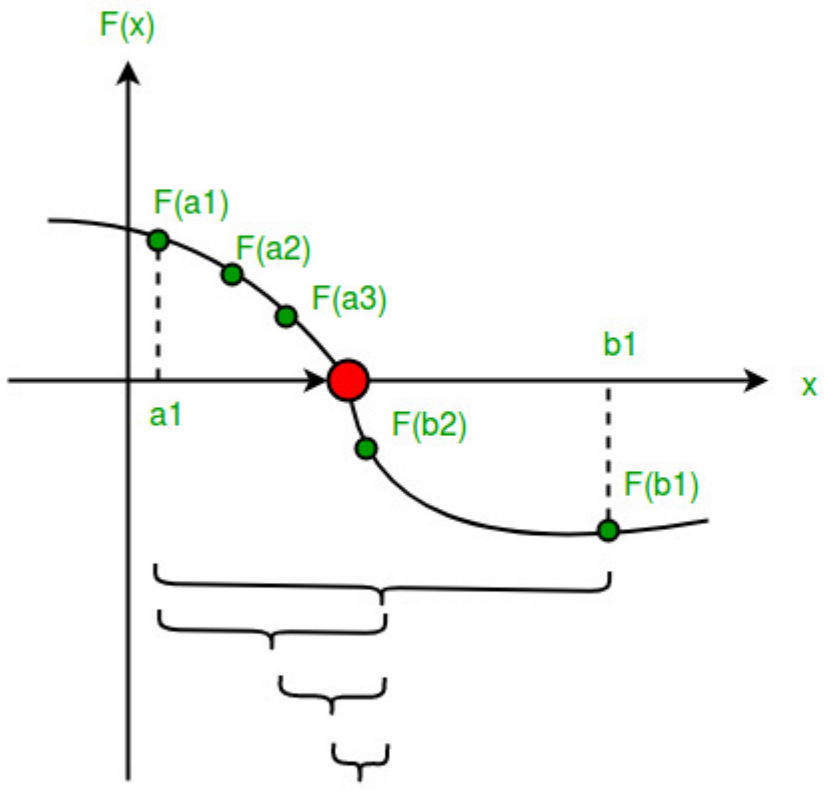
- Rearrange equations to remove (most) singularities

$$\rho(E+2|\Delta|) - k_z(E+2|\Delta|-V)\tan\left(\frac{k_z d}{2}\right) = 0$$

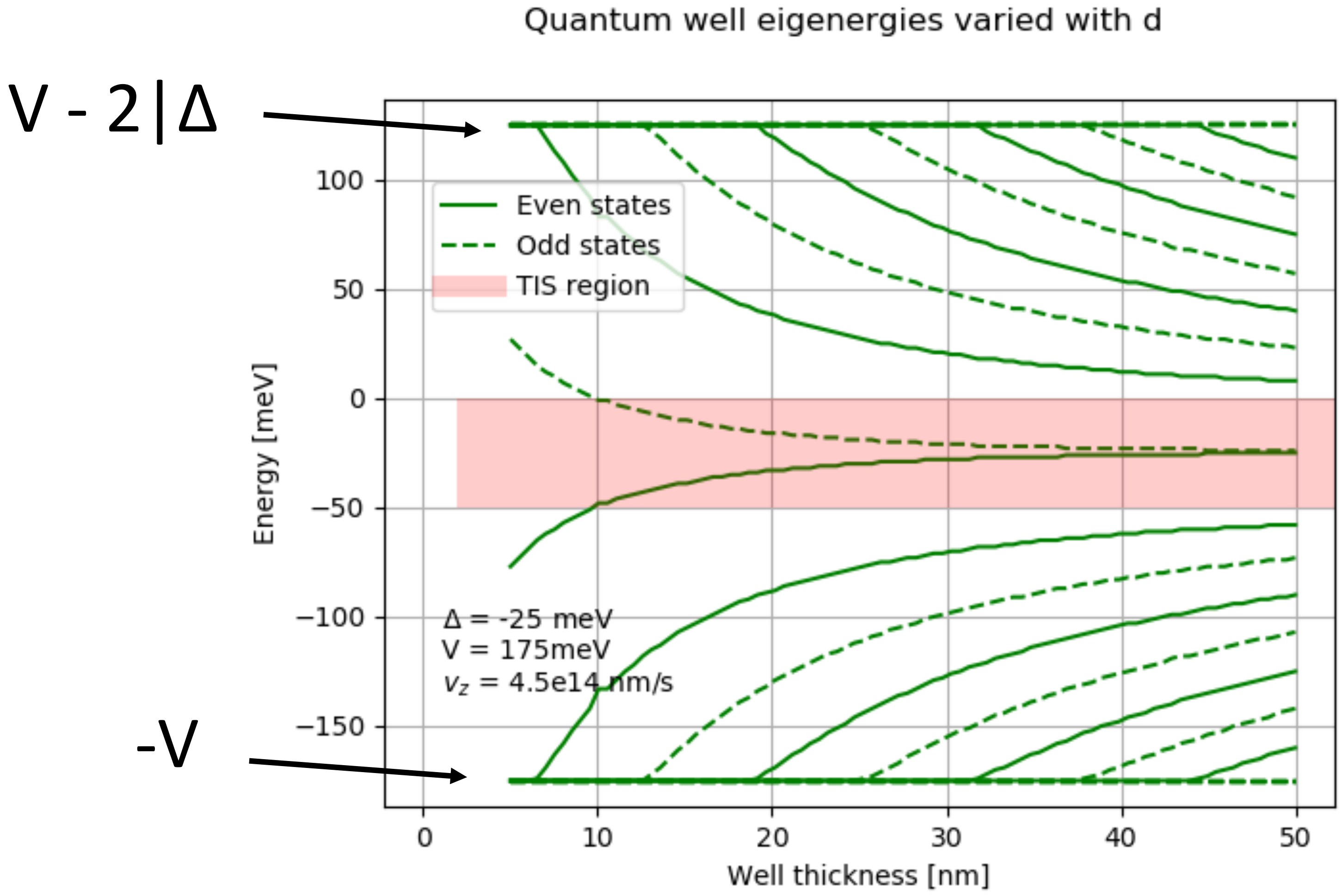


Solution Implementation

- Use the bisection method in Python

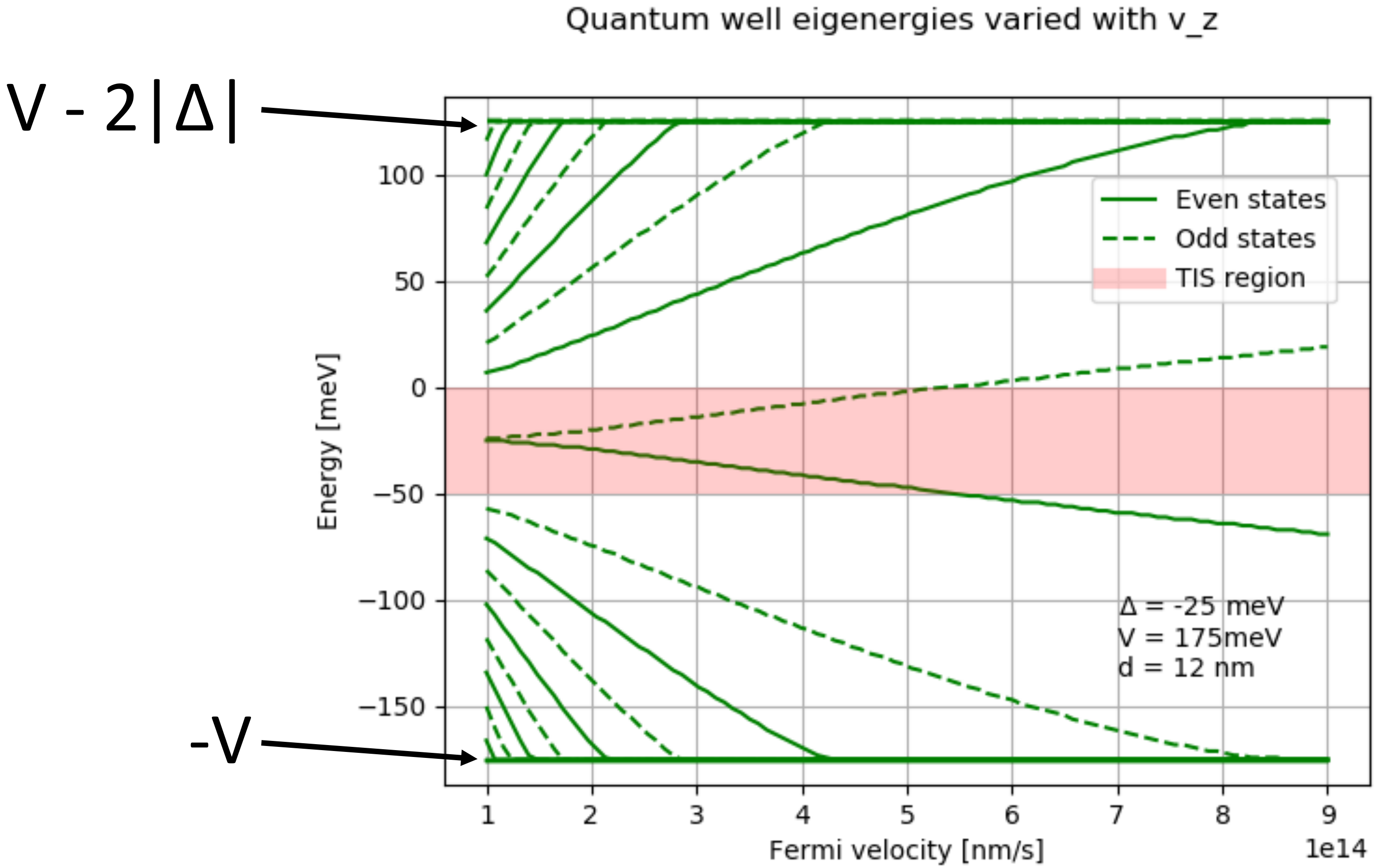


Solutions at $\mathbf{k}_\perp = 0$



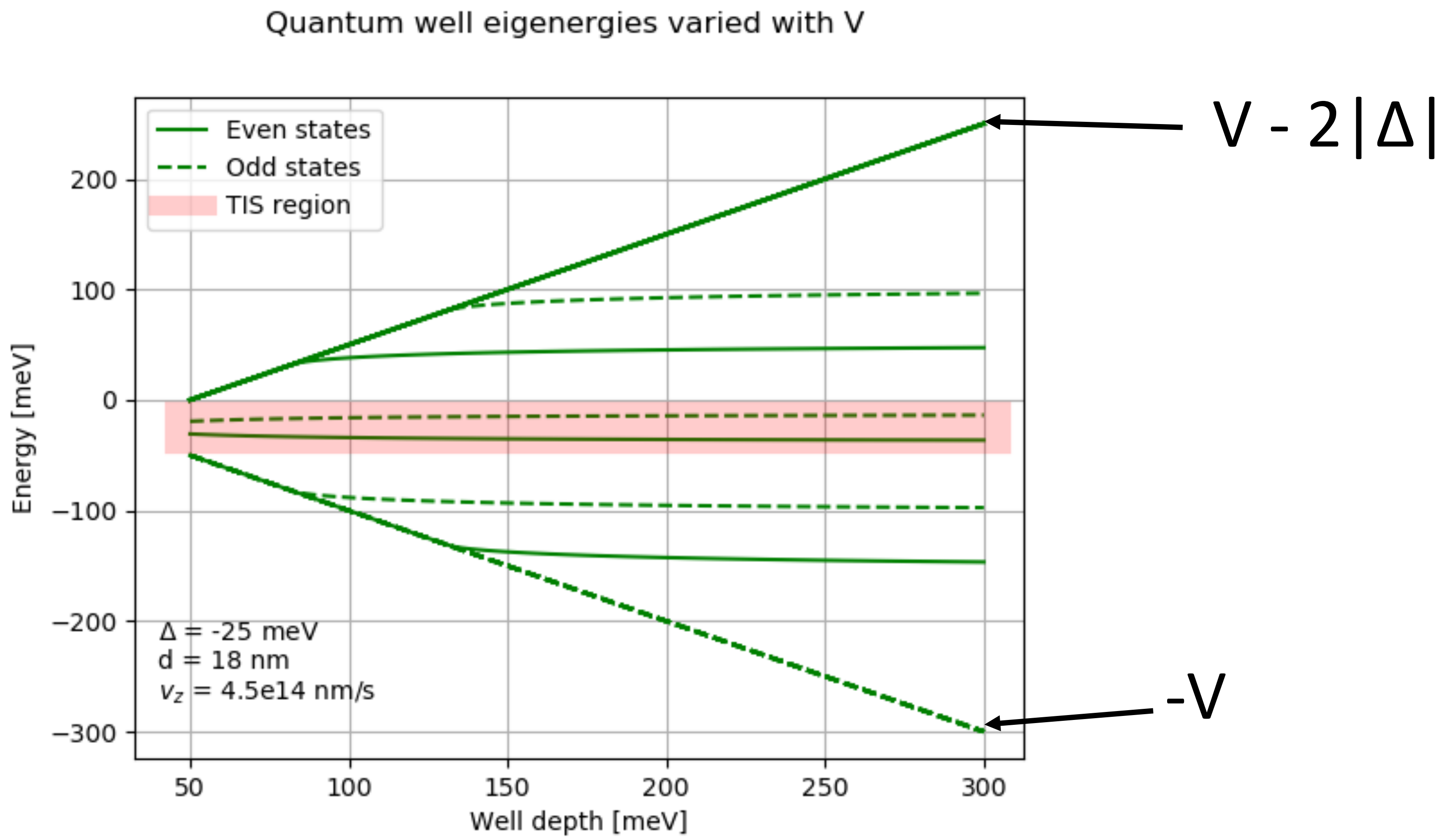
- New bound states are added with increasing well thickness

Solutions at $\mathbf{k}_\perp = 0$



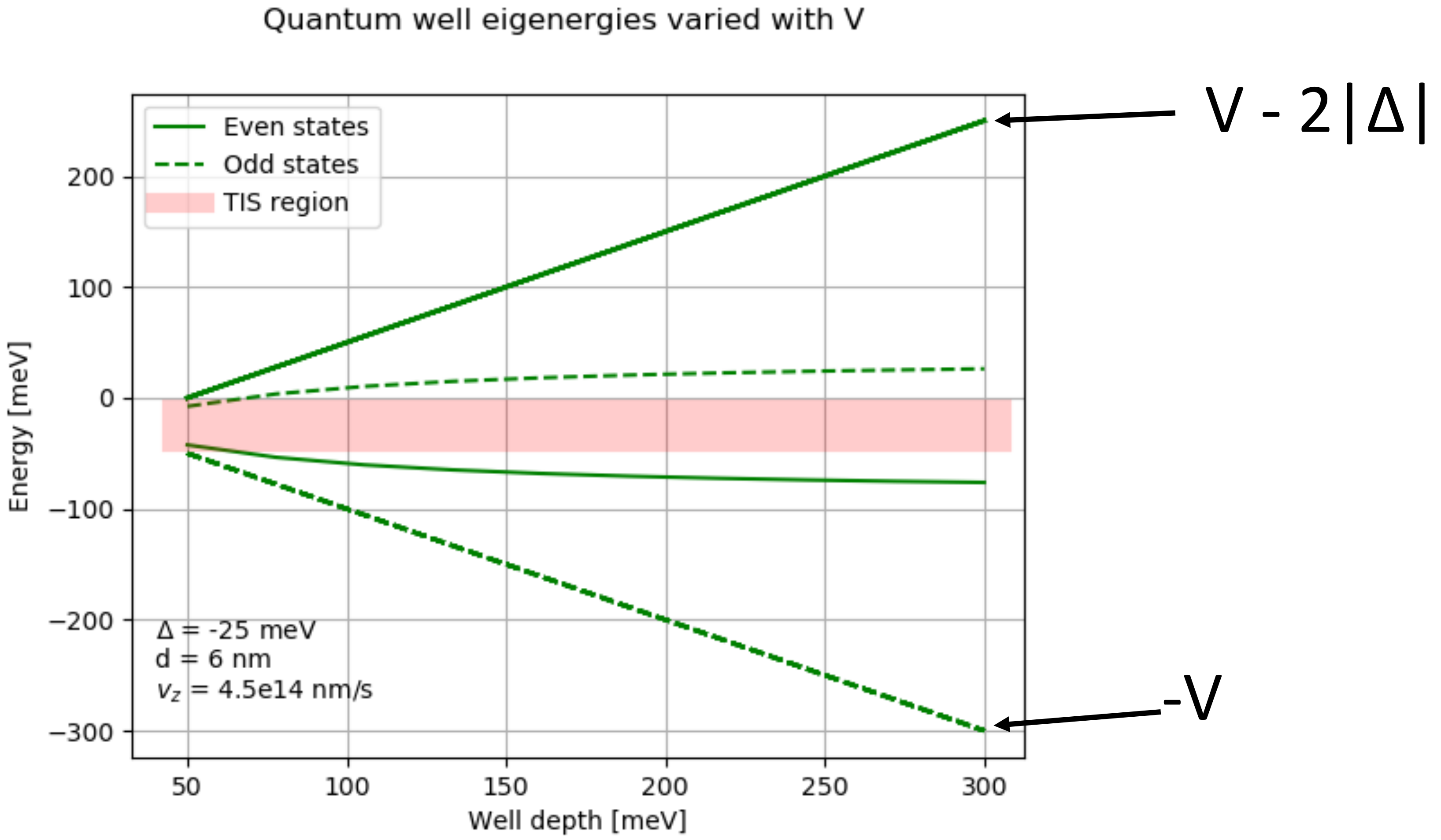
- Bound states escape at higher velocities

Solutions at $\mathbf{k}_\perp = 0$



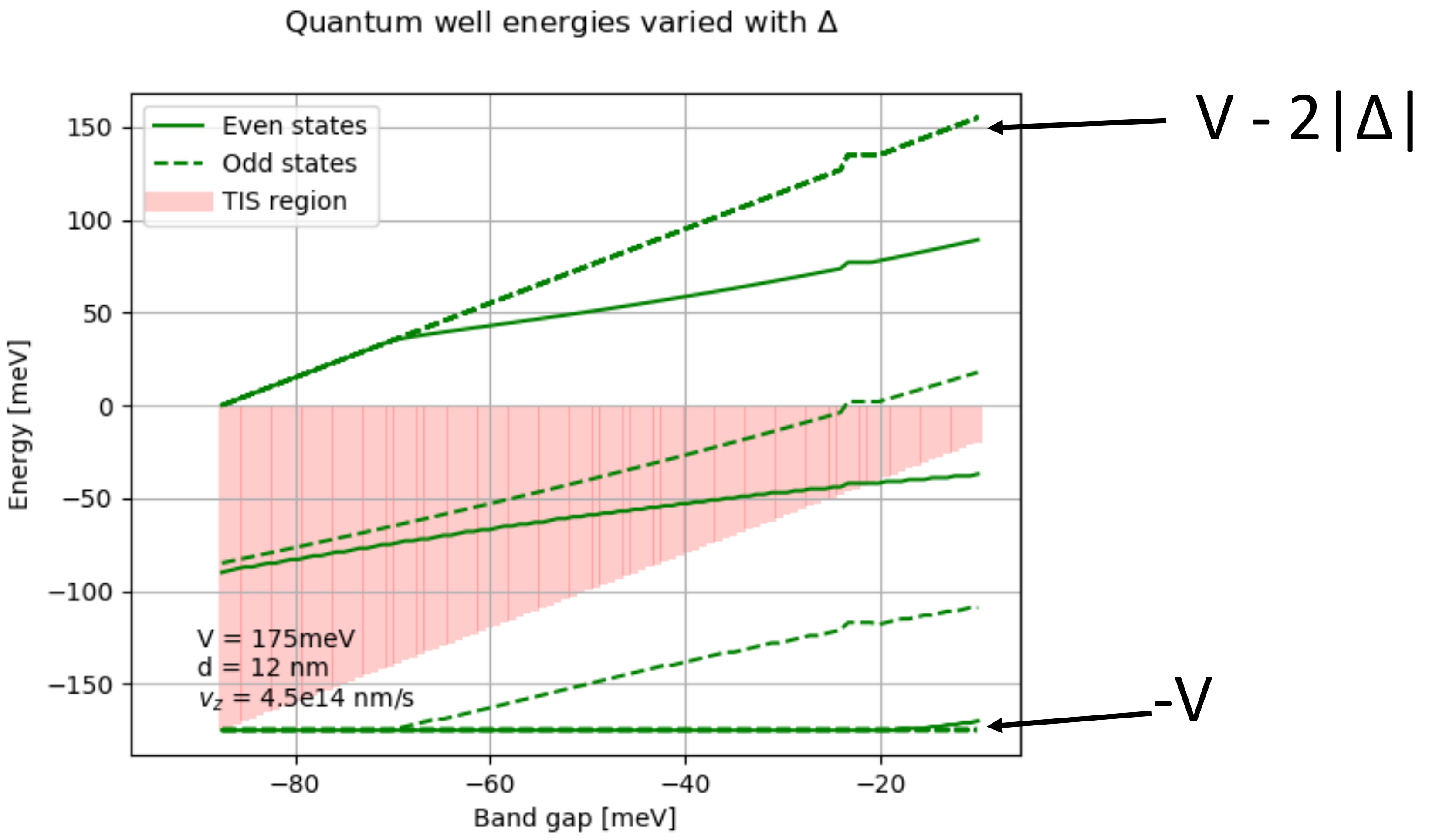
- New bound states unlocked as well gets deeper

Solutions at $\mathbf{k}_{\perp} = 0$



- TIS can escape under the right conditions

Solutions at $\mathbf{k}_\perp = 0$



- TIS region slowly shrinks

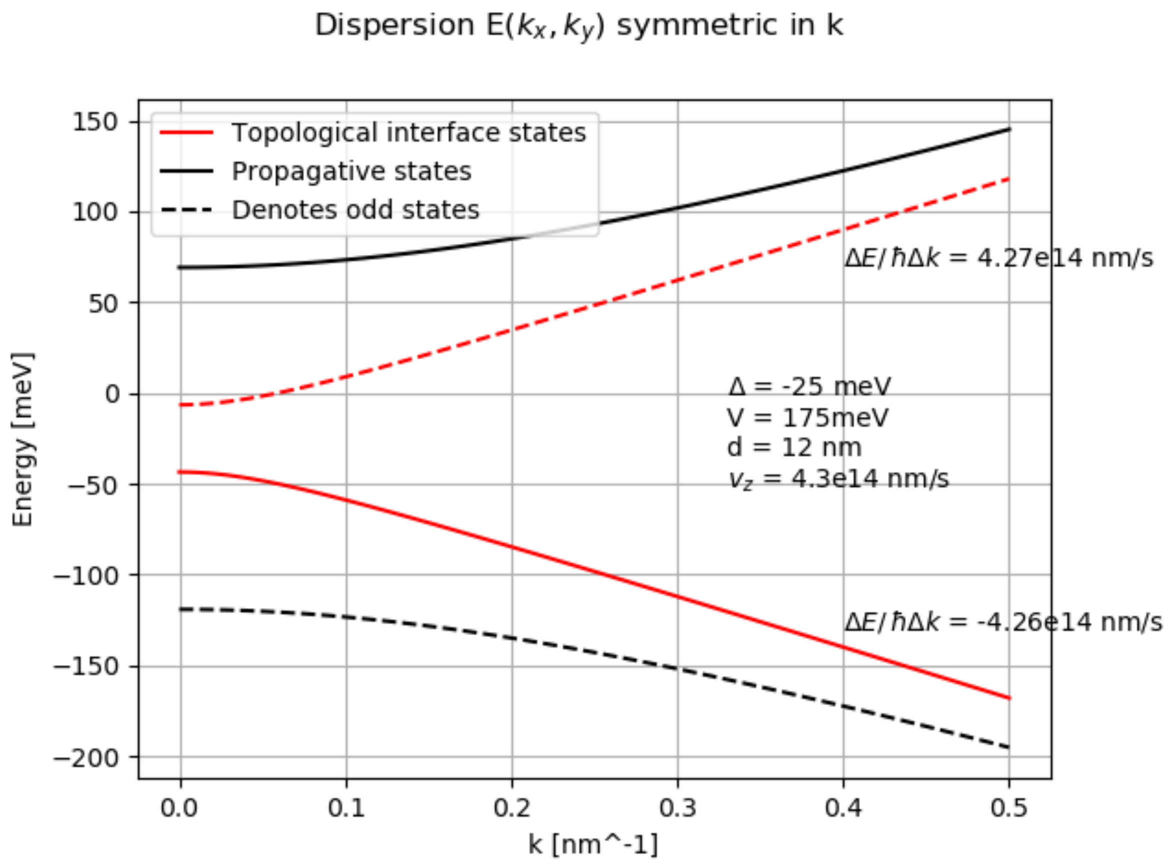
Solutions at $\mathbf{k}_{\perp} \neq 0$

- Must include hamiltonian elements dependent on k_x, k_y
- Eigenenergies are starting point for this eigenvalue problem

$$\tilde{H} = \begin{pmatrix} 0 & 0 & 0 & \frac{\hbar}{m_0} P(k_x - ik_y) \\ 0 & 0 & \frac{\hbar}{m_0} P(k_x + ik_y) & 0 \\ 0 & \frac{\hbar}{m_0} P(k_x - ik_y) & 0 & 0 \\ \frac{\hbar}{m_0} P(k_x + ik_y) & 0 & 0 & 0 \end{pmatrix}$$

Solutions at $\mathbf{k}_\perp \neq 0$

- All dispersion becomes linear at high k $E(\mathbf{k}_\perp) = \sqrt{(E(\mathbf{k}_\perp = 0))^2 + (\hbar v_z k_\perp)^2}$



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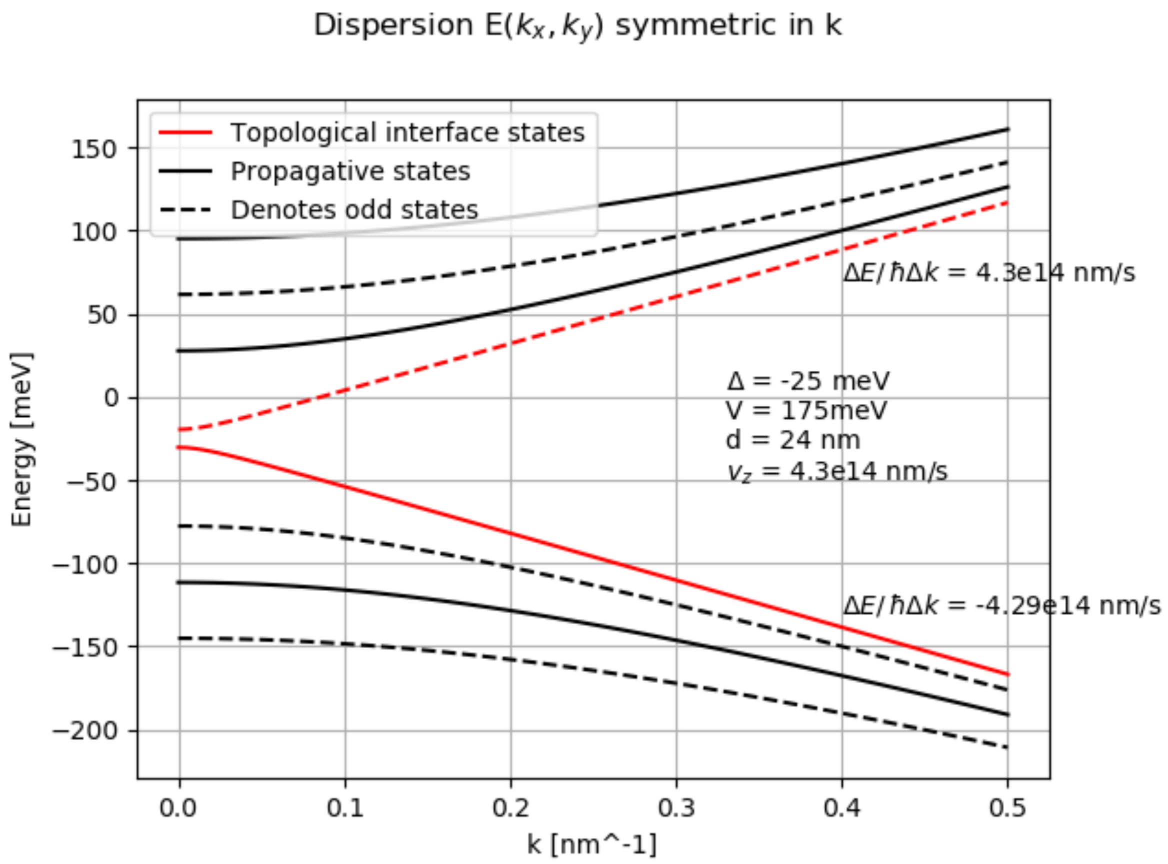

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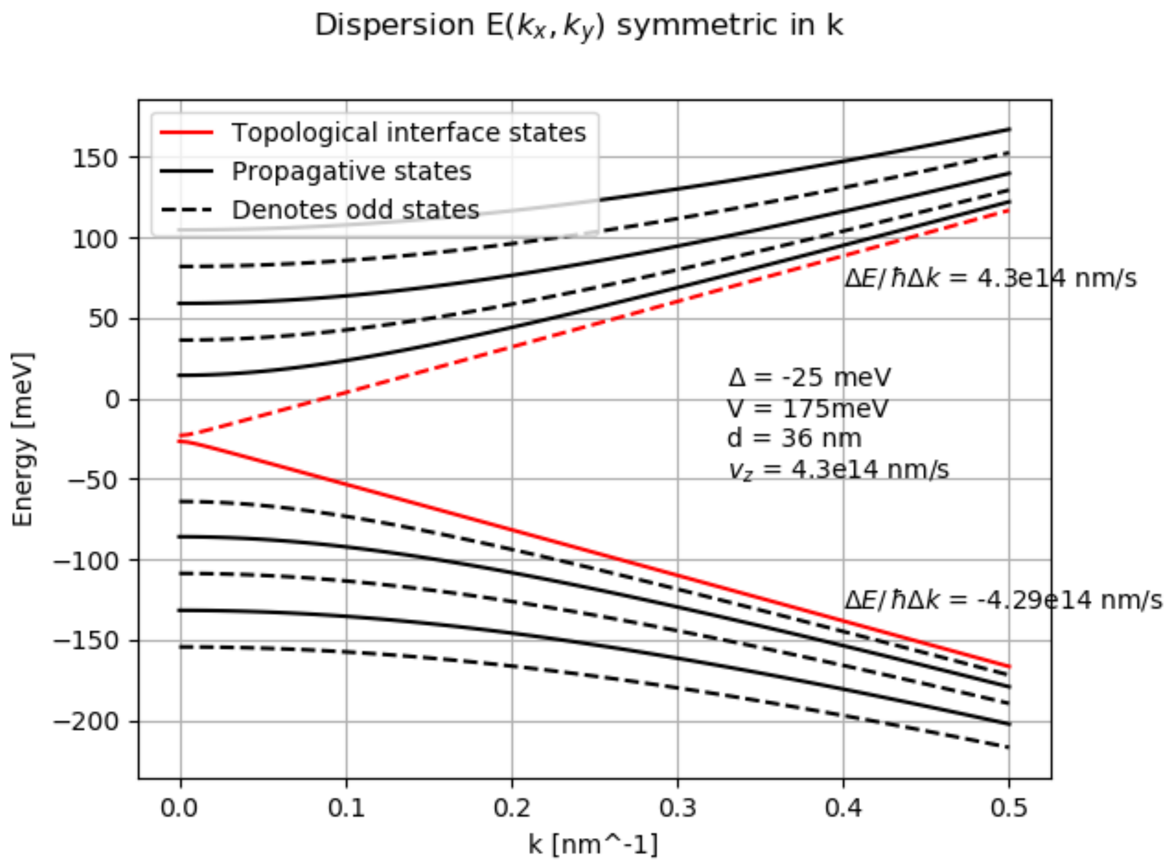

Next steps

- Fully treat $\mathbf{k}_\perp$ terms as a perturbation in $|\boldsymbol{\Psi}_m\rangle$, $|\boldsymbol{\varphi}_n\rangle$ basis

$$H = \begin{pmatrix} \begin{pmatrix} E_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & E_n \end{pmatrix} & \begin{pmatrix} \langle \overrightarrow{\Psi_1} | \widetilde{H} | \overrightarrow{\varphi_1} \rangle & \cdots & \langle \overrightarrow{\Psi_1} | \widetilde{H} | \overrightarrow{\varphi_n} \rangle \\ \vdots & \ddots & \vdots \\ \langle \overrightarrow{\Psi_m} | \widetilde{H} | \overrightarrow{\varphi_1} \rangle & \cdots & \langle \overrightarrow{\Psi_m} | \widetilde{H} | \overrightarrow{\varphi_n} \rangle \end{pmatrix} \\ \begin{pmatrix} \langle \overrightarrow{\varphi_1} | \widetilde{H} | \overrightarrow{\Psi_1} \rangle & \cdots & \langle \overrightarrow{\varphi_1} | \widetilde{H} | \overrightarrow{\Psi_m} \rangle \\ \vdots & \ddots & \vdots \\ \langle \overrightarrow{\varphi_n} | \widetilde{H} | \overrightarrow{\Psi_1} \rangle & \cdots & \langle \overrightarrow{\varphi_n} | \widetilde{H} | \overrightarrow{\Psi_m} \rangle \end{pmatrix} & \begin{pmatrix} E_1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & E_m \end{pmatrix} \end{pmatrix}$$

References

[1] G. Bastard, *Wave mechanics applied to semiconductor heterostructures.* 1988.

[2] G. Krizman, B. A. Assaf, G. Bauer, G. Springholz, R. Ferreira, G. Bastard, L.A. de Vaulchier, Y. Guldner, "Pb1-xSnxSe: a new tunable topological platform with terahertz band gap," Proc. SPIE 11124, Terahertz Emitters, Receivers, and Applications X, 111240R (6 September 2019); doi: 10.1117/12.2529335

[3] D. Griffiths, *Introduction to Quantum Mechanics*. 2015.

[4] G. Krizman, “Topological Phase Transition in Dirac Matter,” 2017.