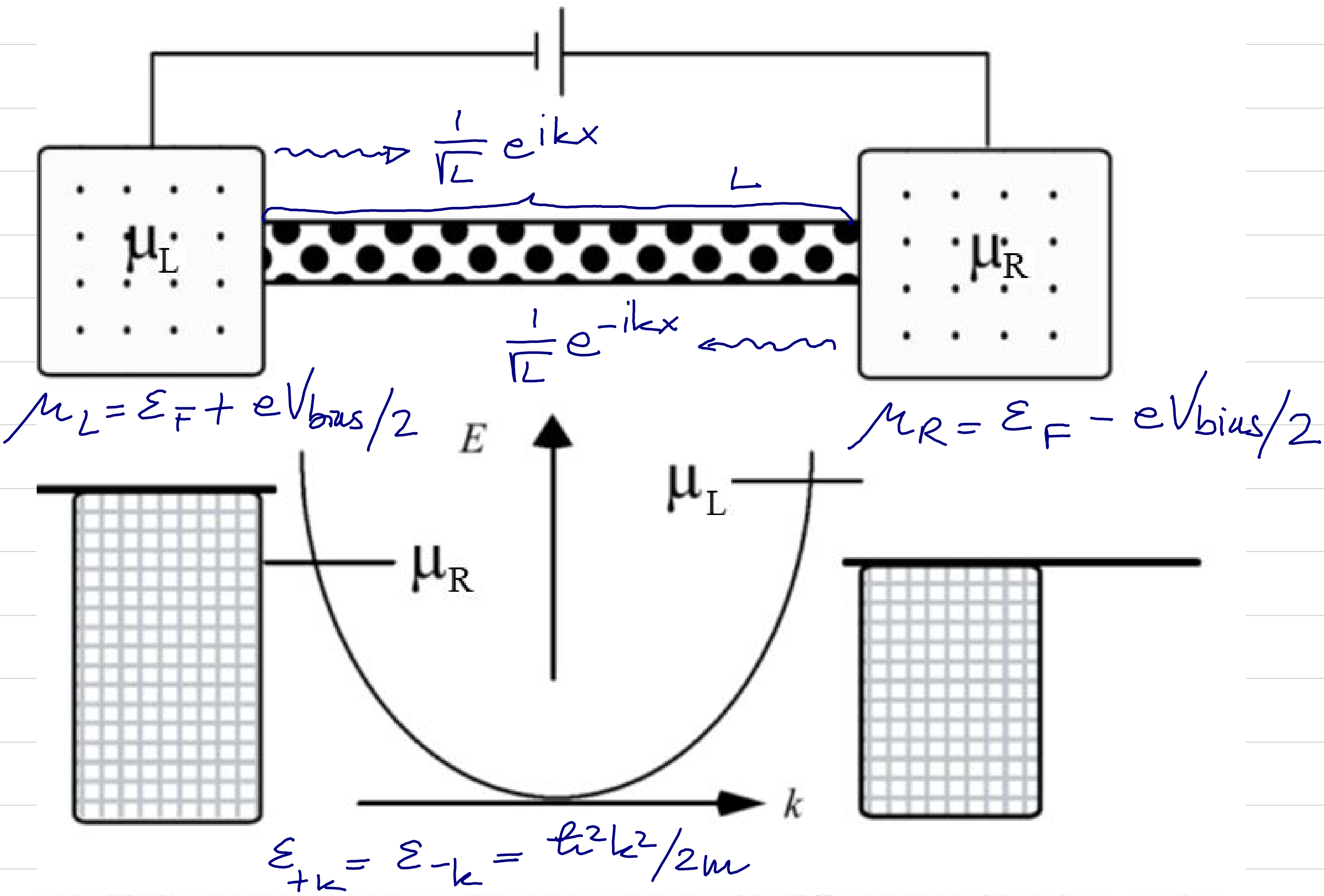
LECTURE 6: Landauer formula for ballistic quasi-1D nanowires with applications to edge state transport in topological insulators

1° Conductance of 1D ballistic nanowire

$$eV_{\text{bias}} = \mu_L - \mu_R$$



A ballistic conductor connected to two contacts with different Fermi levels μ_L and μ_R

$$\vec{j}(\vec{r}) = \frac{ei\hbar}{2m}\left[\Psi(\nabla\Psi^*) - \Psi^*(\nabla\Psi)\right], \quad \nabla = \frac{\partial}{\partial x}\vec{e}_x + \frac{\partial}{\partial y}\vec{e}_y + \frac{\partial}{\partial z}\vec{e}_z$$

$$j_{+k} = \frac{ei\hbar}{2m}\left[\frac{-ik}{L}\underbrace{e^{ikx}}_{\Psi}\underbrace{e^{-ikx}}_{\partial\Psi^*/\partial x} - \frac{ik}{L}\underbrace{e^{-ikx}}_{\Psi^*}\underbrace{e^{ikx}}_{\partial\Psi/\partial x}\right] = \frac{e\hbar k}{mL}$$

$$j_{-k} = -\frac{e\hbar k}{mL}$$

$\rightarrow$ how are these $+k$ & $-k$ states occupied?

■ despite complicated nature of interface between the left and right macroscopic reservoirs and wire, experiments suggest that:

- $+k$ states are occupied primarily by electrons coming from the left macroscopic reservoir
  $f_{+k}(\varepsilon) = f(\varepsilon - \mu_L)$
- $-k$ states are occupied primarily by electrons coming from the right macroscopic reservoir
  $f_{-k}(\varepsilon) = f(\varepsilon - \mu_R)$

$$\begin{array}{cc} +k & -k \end{array} \qquad \begin{array}{cc} +k & -k \end{array}$$
$$\underbrace{\begin{pmatrix} e\hbar k/mL & 0 \\ 0 & -e\hbar k/mL \end{pmatrix}} \qquad \underbrace{\begin{pmatrix} f_{+k} & 0 \\ 0 & f_{-k} \end{pmatrix}}$$

$$I = 2_s e \sum_{k>0} \left[j_{+k} f_{+k} + j_{-k} f_{-k} \right] = \mathrm{Tr}\left[\hat{J} \cdot \hat{\rho}_{neq} \right]$$

$$= 2_s e \sum_{k>0} \frac{\hbar k}{mL} \left[f(\varepsilon_k - \mu_L) - f(\varepsilon_k - \mu_R) \right]$$

using $\sum_k \mapsto \frac{L}{2\pi} \int_0^\infty dk$ and $\frac{\hbar k}{m} = v = \frac{1}{\hbar} \frac{\partial \varepsilon_k}{\partial k}$

$$= \frac{2_s e}{\hbar} \frac{\cancel{L}}{2\pi} \int dk \frac{1}{\cancel{L}} \frac{\partial \varepsilon_k}{\partial k} \left[f(\varepsilon_k - \mu_L) - f(\varepsilon_k - \mu_R) \right]$$

$$I = \frac{2_s e}{h} \int d\varepsilon \underbrace{\left[f(\varepsilon - \mu_L) - f(\varepsilon - \mu_R) \right]}_{eV_{bias} \cdot \left(-\frac{\partial f}{\partial \varepsilon} \right) \text{ for } eV_{bias} \ll \varepsilon_F} = \frac{2_s e^2}{h} V_{bias}$$

$$\boxed{G = \lim_{V_{bias} \to 0} \frac{I}{V_{bias}} = \frac{2e^2}{h}}$$

$\frac{2e^2}{h}$ → conductance quantum for spin-degenerate electrons

G ← linear-response conductance $= 1/R$ → resistance

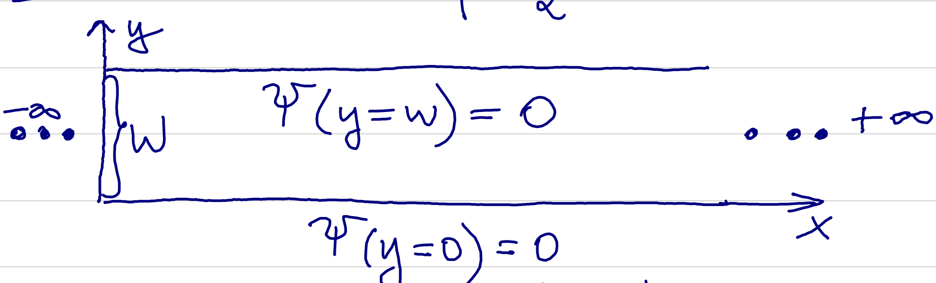
→ we could also perform calculations using linear combination of eigenstates, which are also eigenstates:

$$\psi_{c,k}(x) = \sqrt{\frac{2}{L}}\cos kx \qquad \psi_{s,k}(x) = \sqrt{\frac{2}{L}}\sin kx$$

$$I = 2_s \sum_{k>0} \left[j_{c,k} f_{c,k} + j_{s,k} f_{s,k} \right] \equiv 0$$

this is obviously WRONG!

2° Conductance of quasi-1D ballistic nanowire



↳ "hard wall" boundary conditions

i) Subband structure

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \hat{V}(y), \quad \hat{p}_x = -i\hbar\frac{\partial}{\partial x}, \quad \hat{p}_y = -i\hbar\frac{\partial}{\partial y}$$

$\hat{H}\psi(x,y) = \varepsilon\psi(x,y)$ is partial differential equation

→ instead of following mathematicians, use symmetry

$[\hat{H}, \hat{p}_x] = 0 \Rightarrow \hat{H}$ and $\hat{p}_x$ have common set of eigenvectors $\psi(x,y) = Ae^{ik_x x}\phi(y)$

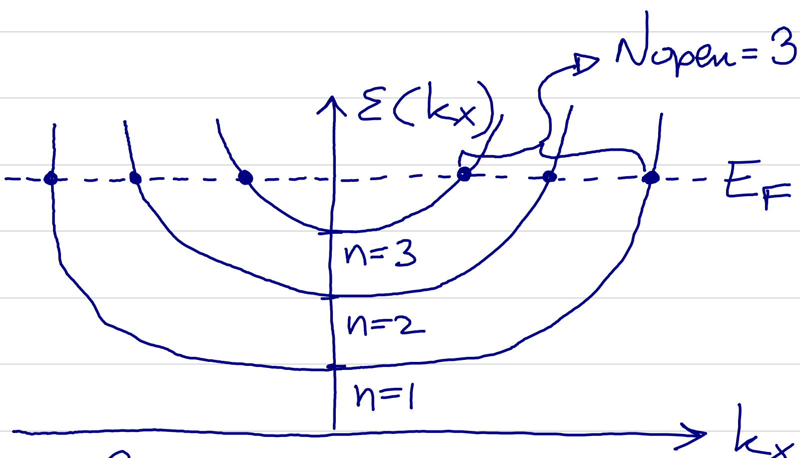
$$\hat{H}\Psi(x,y) = \frac{\hbar^2 k_x^2}{2m} A e^{ik_x x}\phi(y) + A e^{ik_x x}\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}\phi(y)\right] + \hat{V}(y) A e^{ik_x x}\phi(y)$$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \hat{V}(y) + \frac{\hbar^2 k_x^2}{2m}\right]\phi(y) = \underbrace{\varepsilon\,\phi(y)}$$

$$\phi(y) = \sqrt{\frac{2}{W}}\sin\frac{n\pi y}{W}$$
for hard wall $\hat{V}(y)$

$$\varepsilon - \frac{\hbar^2 k_x^2}{2m} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{W}\right)^2$$

$$\varepsilon(k_x) = \frac{\hbar^2}{2m}\left(\frac{n\pi}{W}\right)^2 + \frac{\hbar^2 k_x^2}{2m}$$ is subband energy – momentum dispersion



$$\Psi(x,y) = A e^{ik_x x}\sqrt{\frac{2}{W}}\sin\frac{n\pi y}{W}$$
is transverse propagating mode or "conducting channel"

ii) Conductance

$$I = 2_s e \sum_{k_x>0}\sum_{k_y}\left[J_{+k_x} f(\varepsilon-\mu_L) + J_{-k_x} f(\varepsilon-\mu_R)\right]$$

$$= 2_s e \sum_{k_y}\int_0^\infty dk_x \frac{1}{L}\frac{1}{\hbar}\frac{\partial\varepsilon}{\partial k_x}\left[f(\varepsilon-\mu_L) - f(\varepsilon-\mu_R)\right]$$

$$= \frac{2_s e}{h} N_{open}\int d\varepsilon \underbrace{\left[f(\varepsilon-\mu_L) - f(\varepsilon-\mu_R)\right]}_{\to\, eV_{bias}\left(-\partial f/\partial\varepsilon\right)} = N_{open}\frac{2_s e^2}{h}V_{bias}$$

$$G = \lim_{V_{bias}\to 0} I/V_{bias} = \frac{2e^2}{h}\cdot N_{open}$$

3° Conductance of edge states in 2D topological insulators

i) Quantum spin Hall insulator as 2D TI

Quantum Spin Hall Insulator State in HgTe Quantum Wells

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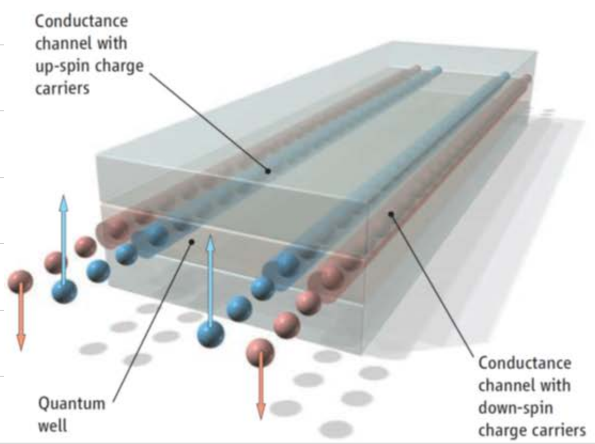
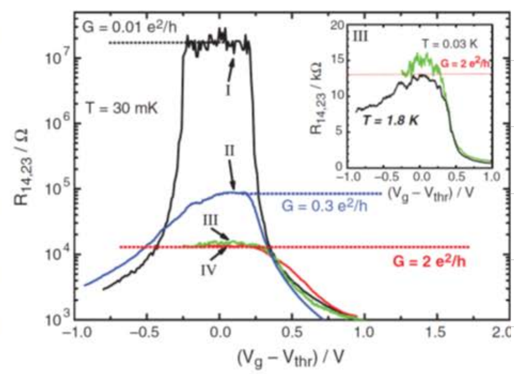
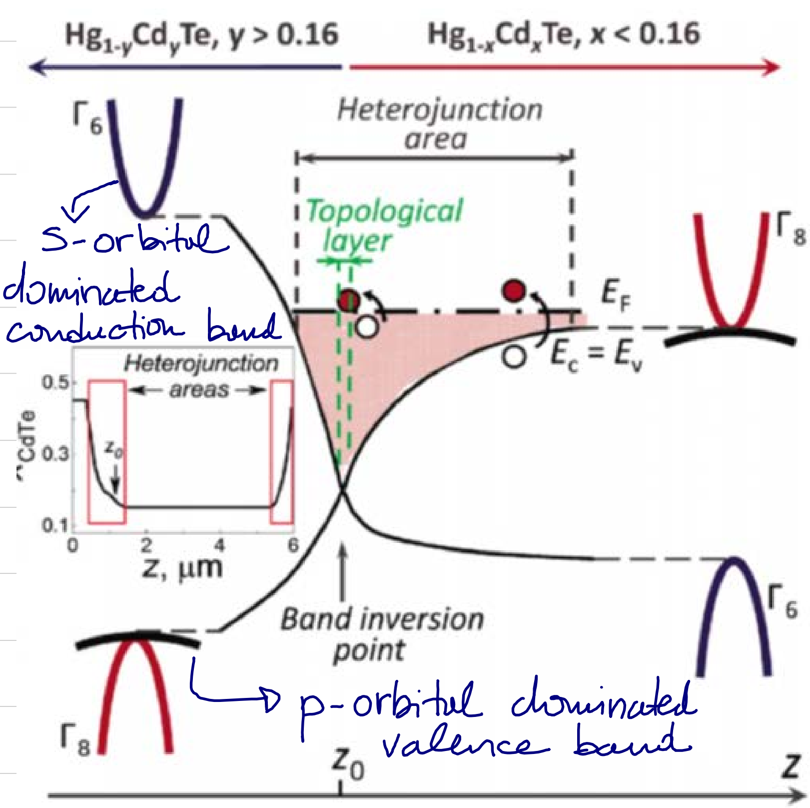


Fig. 4. The longitudinal four-terminal resistance, $R_{14,23}$, of various normal (d = 5.5 nm) (I) and inverted (d = 7.3 nm) (II, III, and IV) QW structures as a function of the gate voltage measured for B = 0 T at T = 30 mK. The device sizes are (20.0 × 13.3) μm^2 for devices I and II, (1.0 × 1.0) μm^2 for device III, and (1.0 × 0.5) μm^2 for device IV. The inset shows $R_{14,23}(V_g)$ of two samples from the same wafer, having the same device size (III) at 30 mK (green) and 1.8 K (black) on a linear scale.



→ band inversion by spin-orbit coupling generates 2DTI

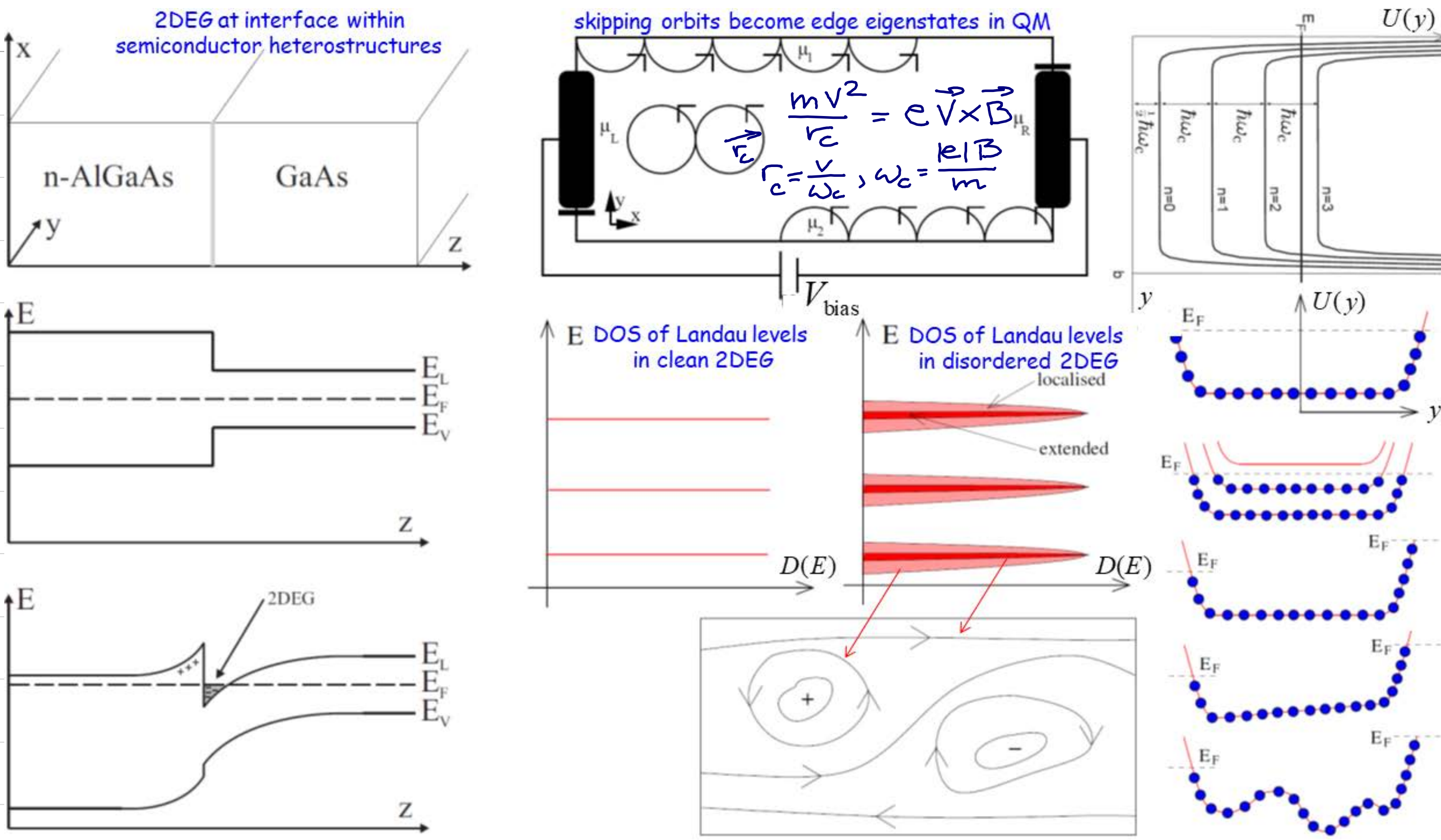


s-orbital dominated conduction band

→ p-orbital dominated valence band

FIG. 7. (a) The crystal structure of $Hg_{1-x}Cd_xTe$ is a zinc-blende type fcc structure of space group $F\bar{4}3m$, with Hg at (0, 0, 0) and Te at $(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$. (b) Band inversion occurs near the HgTe-CdTe interface of the quantum well. (c) HgTe-CdTe binary phase diagram shows the full solubility, and the liquid + solid mixture between the liquidus and solidus indicates that a strain energy is stored in the system. [Panel (b) is reproduced with permission from Galeeva *et al.*, Beilstein J. Nanotechnol. **9**, 1035 (2018); copyright 2018 Elsevier[27] and panel (c) is reproduced with permission from Moskvin *et al.*, J. Cryst. Growth **310**, 2617 (2008); copyright 2018 Elsevier.][28]

ii) Quantum Hall insulator as historically first 2D TI example



■ Landau levels in infinite 2DEG

$$\hat{H} = \frac{(\hat{\vec{p}} - e\vec{A})^2}{2m}, \quad \vec{B} = B\vec{e}_z \Rightarrow \vec{A} = -By\,\vec{e}_x; \quad \hat{\vec{p}} = \left(-i\hbar\frac{\partial}{\partial x}, -i\hbar\frac{\partial}{\partial y}\right)$$

$$\left[\frac{\hat{p}_y^2}{2m} + \frac{(p_x + eBy)^2}{2m}\right]\Psi(x,y) = E\,\Psi(x,y)$$

$$v = \frac{1}{\hbar}\frac{\partial E_n}{\partial k} = ?$$

$$[\hat{H}, \hat{p}_x] = 0 \Rightarrow \Psi(x,y) = \frac{1}{\sqrt{L}} e^{ikx}\chi(y)$$

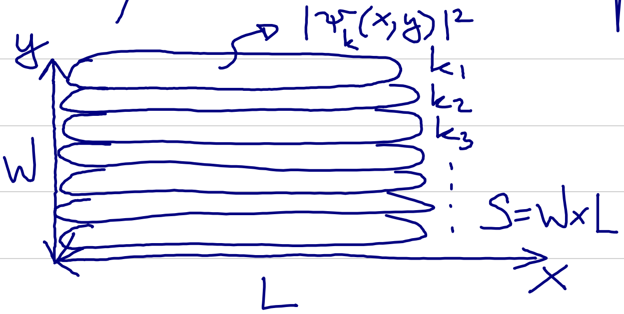
$$(p_x + eBy)^2\,\Psi(x,y) = (\hbar k + eBy)^2\,\Psi(x,y)$$

$$\left[\frac{\hat{p}_y^2}{2m} + \frac{1}{2}m\omega_c^2(y + y_k)^2\right]\chi(y) = E\,\chi(y) \quad \text{LHO} \Rightarrow E_n = \left(n + \frac{1}{2}\right)\hbar\omega_c$$

Hermite polynomial $\quad \hookrightarrow y_k = \hbar k / eB \qquad \chi_{n,k} = u_n(q + q_k)$

$$u_n(q) = e^{-q^2/2} H_n(q), \quad q = \sqrt{\frac{m\omega_c}{\hbar}}\,y, \quad q_k = \sqrt{\frac{m\omega_c}{\hbar}}\,y_k$$

→ spatial extent of each eigenfunction in the y-direction is $\approx \sqrt{\frac{\hbar}{m\omega_c}} = \frac{\sqrt{\hbar\omega_c/m}}{\omega_c} \to v/\omega_c$



which is radius of classical orbit for electron of energy $\hbar\omega_c/2$

→ they shift along the transverse coordinate y as we change wavevector k in the longitudinal x-direction

→ how many electrons can fit into one Landau level?

$$\Delta y_k = \frac{\hbar \Delta k}{|e|B} = \frac{2\pi\hbar}{|e|BL}, \quad \Delta k = 2\pi/L$$

→ spacing of eigenfunctions along the y-axis

$$N = 2_s \cdot \frac{W}{\Delta y_k} = \frac{|e|BS}{\pi\hbar} = \frac{mS}{\pi\hbar^2}\cdot\hbar\omega_c$$

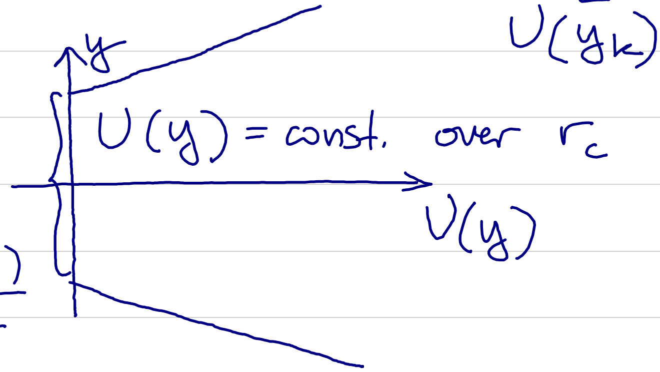
Landau levels in quasi-1DEG infinite wire

→ centered around $y_k = \frac{\hbar k}{eB}$

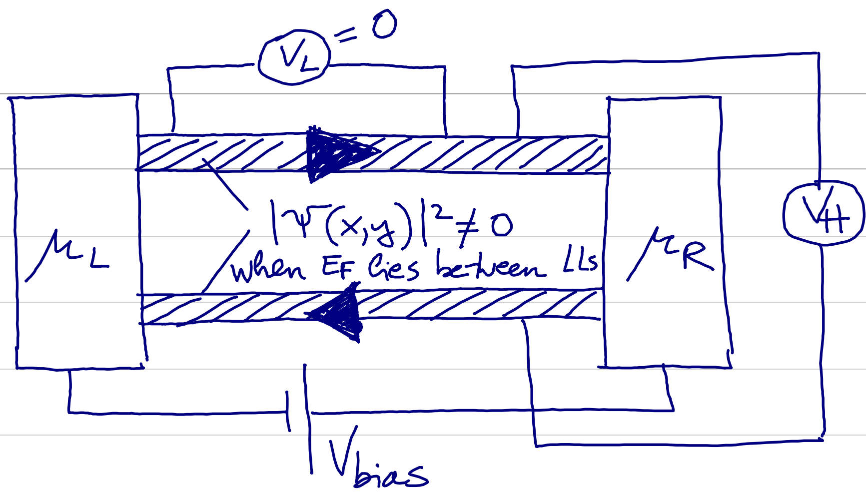
$$E_n(k) = \left(n+\frac{1}{2}\right)\hbar\omega_c + \langle n,k|U(y)|n,k\rangle = \left(n+\frac{1}{2}\right)\hbar\omega_c + U(y_k)$$

$$v = \frac{1}{\hbar}\frac{\partial E_n}{\partial k} = \frac{1}{\hbar}\frac{\partial U(y_k)}{\partial k}$$

$$= \frac{1}{\hbar}\frac{\partial U(y)}{\partial y}\frac{\partial y_k}{\partial k} = \frac{1}{eB}\frac{\partial U(y)}{\partial y}$$



→ changes sign at opposite edges



$$eV_H = \mu_L - \mu_R$$

$$R_L = \frac{V_L}{I} = 0$$

$$R_H = \frac{V_H}{I} = \frac{(\mu_L - \mu_R)/e}{\frac{2e}{h} N_{filled} (\mu_L - \mu_R)} = \frac{h}{2e^2 N_{filled}}$$

number of filled Landau levels in the bulk or, EQUIVALENTLY, number of edge states at E_F

→ when E_F is at the center of bulk Landau level, then extended states connect two edges and backscattering gives rise to maximum R_L

$$\boxed{R_H = \frac{25.8128\ \text{k}\Omega}{2 N_{fill}} \text{ is plateau whenever } E_F \text{ lies between two LLs; } N_{fill} \in \mathbb{N} \text{ decreases with increasing B-field}}$$