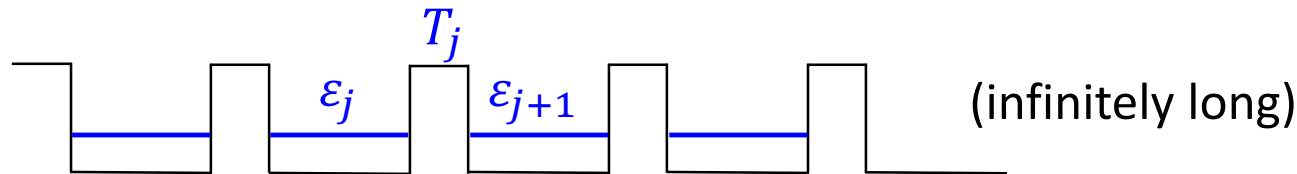


1D array of quantum wells (tight-binding model)

Works well for superlattices, the same idea in some other cases



Consider only one level in each well (can be generalized to several levels)

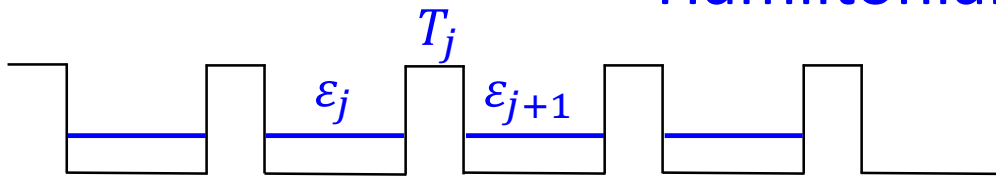
$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{tun}}$$

\hat{H}_0 → wells without tunneling, eigenstates $|\psi_j\rangle$ $\hat{H}_0|\psi_j\rangle = \epsilon_j|\psi_j\rangle$
 \hat{H}_{tun} → tunneling between wells (small perturbation)
 j → well number

Actually, not trivial to introduce tunneling Hamiltonian correctly, however quite clear physically: jumps between neighboring wells

Idea: Use basis $|\psi_j\rangle$ (without tunneling), energies ϵ_j (usually equal), and tunnelling matrix element $T_j = \langle \psi_j | \hat{H}_{\text{tun}} | \psi_{j+1} \rangle$ (has dimension of energy)

Hamiltonian



$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{tun}} \quad \hat{H}_0 |\psi_j\rangle = \varepsilon_j |\psi_j\rangle$$

$$T_j = \langle \psi_j | \hat{H}_{\text{tun}} | \psi_{j+1} \rangle$$

$$T_j = \frac{\hbar^2}{m} \left[\psi_{j+1}(x) \frac{d\psi_j^*}{dx} - \frac{d\psi_{j+1}}{dx} \psi_j^*(x) \right]_{x=x_{Bj}} \quad \text{usually } T_j < 0$$

Hamiltonian

$$\hat{H} = \sum_j \varepsilon_j |\psi_j\rangle \langle \psi_j| + \sum_j (T_j |\psi_j\rangle \langle \psi_{j+1}| + T_j^* |\psi_{j+1}\rangle \langle \psi_j|)$$

↖ reciprocity: jumps back
formally: because \hat{H} is Hermitian

$$\hat{H}_0 = \sum_j \varepsilon_j |\psi_j\rangle \langle \psi_j|, \quad |\psi_j\rangle \langle \psi_j| \text{ is projector onto state } |\psi_j\rangle, \quad \hat{H}_0 |\psi_j\rangle = \varepsilon_j |\psi_j\rangle$$

(Formally any Hamiltonian can be written via its eigenstates $|\psi_n\rangle$
and corresponding energies ε_n as $\hat{H} = \sum_n \varepsilon_n |\psi_n\rangle \langle \psi_n|$)

Another form for Hamiltonian (second quantization, will not use):

$$\hat{H} = \sum_j \varepsilon_j a_j^\dagger a_j + \sum_j (T_j a_j^\dagger a_{j+1} + T_j^* a_{j+1}^\dagger a_j)$$

Eigenstates of \hat{H} and corresponding energies

$$\hat{H} = \sum_j \varepsilon_j |\psi_j\rangle\langle\psi_j| + \sum_j (T_j |\psi_j\rangle\langle\psi_{j+1}| + T_j^* |\psi_{j+1}\rangle\langle\psi_j|)$$

Expand an eigenstate in the basis, $|\psi\rangle = \sum_j \alpha_j |\psi_j\rangle$

$$\begin{aligned} \hat{H}|\psi\rangle &= \sum_j \varepsilon_j \alpha_j |\psi_j\rangle + \sum_j (\alpha_j T_{j-1} |\psi_{j-1}\rangle + \alpha_j T_j^* |\psi_{j+1}\rangle) = \\ &= \sum_j (\varepsilon_j \alpha_j + T_j \alpha_{j+1} + T_{j-1}^* \alpha_{j-1}) |\psi_j\rangle = E \sum_j \alpha_j |\psi_j\rangle \quad (\text{TISE}) \end{aligned}$$

TISE gives infinite set of equations

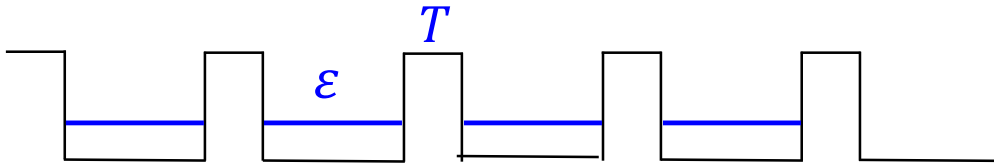
$$\boxed{\varepsilon_j \alpha_j + T_j \alpha_{j+1} + T_{j-1}^* \alpha_{j-1} = E \alpha_j} \quad \text{for any } j$$

Consider uniform case: $\varepsilon_j = \varepsilon$, $T_j = T$, then $(\varepsilon - E)\alpha_j + T\alpha_{j+1} + T^*\alpha_{j-1} = 0$

Assume $\alpha_j = A e^{iqj}$
 \leftarrow site (well) number
 \leftarrow some number (proportional to quasimomentum)
 i imaginary unit

$$(\varepsilon - E) + T e^{iq} + T^* e^{-iq} = 0 \quad \Rightarrow \quad E = \varepsilon + 2 \operatorname{Re}(T e^{iq})$$

Result for eigenstates and energies



$$E = \varepsilon + 2 \operatorname{Re}(T e^{iq})$$

For simplicity assume $T^* = T$ (actually, it should be $T < 0$)

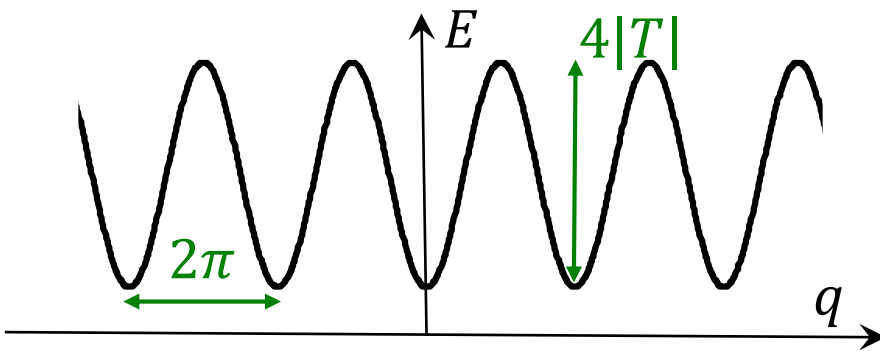
$$E = \varepsilon + 2 T \cos q$$

$$\alpha_j = A e^{iqj}, |\psi\rangle = \sum_j \alpha_j |\psi_j\rangle$$

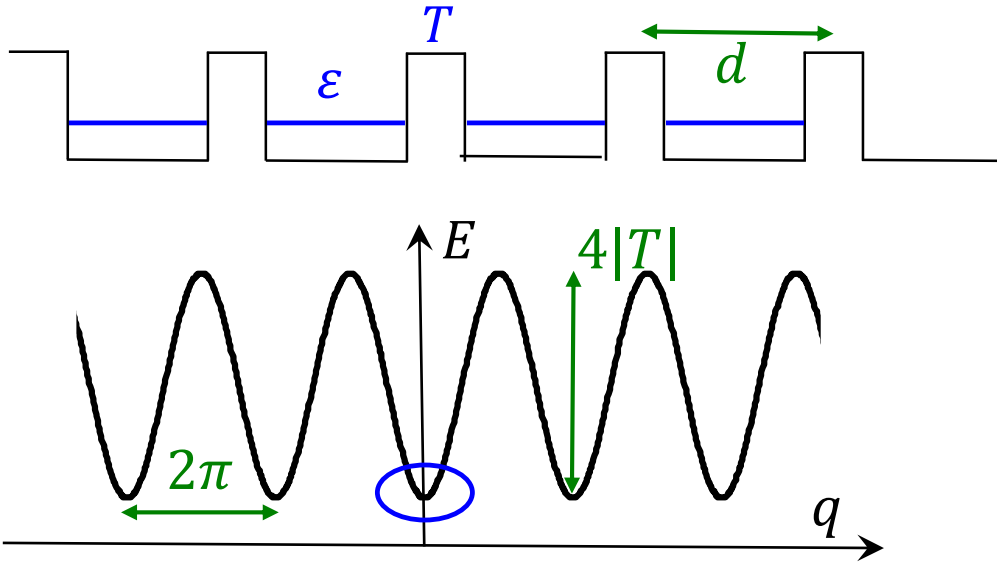
q : some real number

T : tunnel matrix element ($T < 0$)

This is a simple band (miniband in superlattices)



Effective mass



$$|\psi\rangle = \sum_j \alpha_j |\psi_j\rangle$$

$$\alpha_j = A e^{iqj}$$

$$E = \varepsilon + 2 T \cos q$$

q : some real number

T : tunnel matrix element ($T < 0$)

For lattice period d , we have $\alpha(x) = A e^{iqx/d}$

Since for quasimomentum K we should have $\alpha(x) \propto e^{iKx}$, then $q = Kd$

$$E = \varepsilon - 2 |T| \cos(Kd) \quad \text{Then for } |Kd| \ll 1 \quad E = \varepsilon - 2 |T| + \underbrace{2|T| \frac{K^2 d^2}{2}}_{\frac{\hbar^2 K^2}{2m_{\text{eff}}}}$$

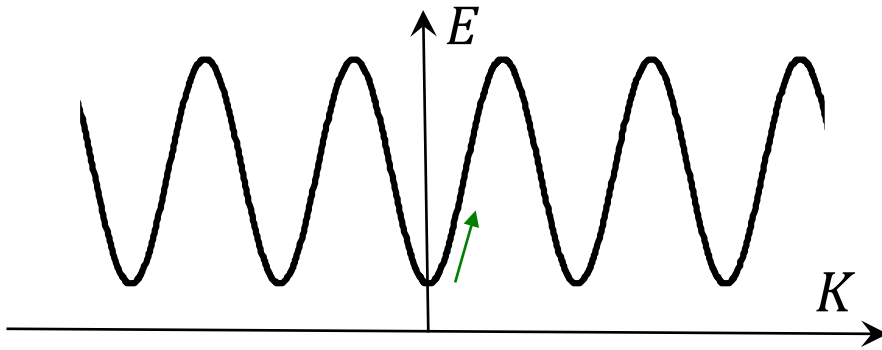
Therefore

$$m_{\text{eff}} = \frac{\hbar^2}{2|T|d^2}$$

Interesting that m_{eff} has no relation to actual electron mass.

Check dimension: $(\text{J s})^2 / (\text{J m}^2) = \text{kg}$ OK

Conductivity and Bloch oscillations



$$\frac{d}{dt}K = \frac{F}{\hbar} = \frac{-e\mathcal{E}}{\hbar}$$

velocity

$$v_{\text{gr}} = \frac{d\omega}{dk} \rightarrow v_{\text{gr}} = \frac{1}{\hbar} \frac{dE}{dK}$$

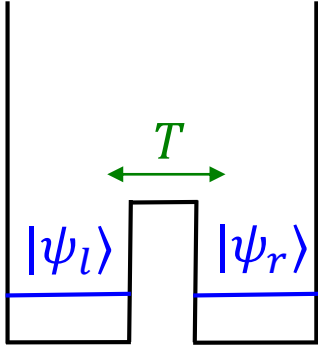
Usual conductivity: quasielectron scatters (loses K) well before the middle energy of the band is reached. Then conductivity is proportional to the scattering time.

Bloch oscillations In a very pure case (achieved in superlattices), quasielectron reaches the top of the band (there velocity is zero) and continues further, so that velocity becomes negative, then again positive, and so on (oscillations). This also leads to negative differential resistance (therefore can be used for amplification).

$$m_{\text{eff}} = \left[\frac{1}{\hbar^2} \frac{d^2 E}{dK^2} \right]^{-1}$$

Effective mass becomes negative in the upper half of the band, therefore positive force decreases velocity.

Two-level system



Similar system, with only two wells

$$\hat{H} = \hat{H}_0 + \hat{H}_{\text{tun}} \quad \hat{H}_0 |\psi_j\rangle = \varepsilon_j |\psi_j\rangle$$

$$T = \langle \psi_l | \hat{H}_{\text{tun}} | \psi_r \rangle$$

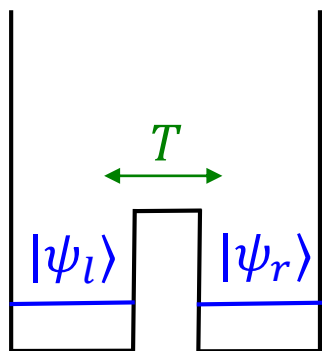
$$\hat{H} = \varepsilon_l |\psi_l\rangle\langle\psi_l| + \varepsilon_r |\psi_r\rangle\langle\psi_r| + T |\psi_l\rangle\langle\psi_r| + T^* |\psi_r\rangle\langle\psi_l|$$

$$|\Psi(t)\rangle = \alpha(t) |\psi_l\rangle + \beta(t) |\psi_r\rangle \quad \text{Evolution} \quad i\hbar \frac{d|\Psi\rangle}{dt} = \hat{H} |\Psi(t)\rangle$$

$$i\hbar \frac{d\alpha}{dt} |\psi_l\rangle + i\hbar \frac{d\beta}{dt} |\psi_r\rangle = \varepsilon_l \alpha |\psi_l\rangle + \varepsilon_r \beta |\psi_r\rangle + T \beta |\psi_l\rangle + T^* \alpha |\psi_r\rangle$$

$$\left[\begin{array}{l} i\hbar \frac{d\alpha}{dt} = \varepsilon_l \alpha + T \beta \\ i\hbar \frac{d\beta}{dt} = \varepsilon_r \beta + T^* \alpha \end{array} \right.$$

Eigenenergies and eigenstates



$$\hat{H} = \varepsilon_l |\psi_l\rangle\langle\psi_l| + \varepsilon_r |\psi_r\rangle\langle\psi_r| + T|\psi_l\rangle\langle\psi_r| + T^*|\psi_r\rangle\langle\psi_l|$$

$$|\Psi(t)\rangle = \alpha(t)|\psi_l\rangle + \beta(t)|\psi_r\rangle$$

$$i\hbar\dot{\alpha} = \varepsilon_l\alpha + T\beta, \quad i\hbar\dot{\beta} = \varepsilon_r\beta + T^*\alpha$$

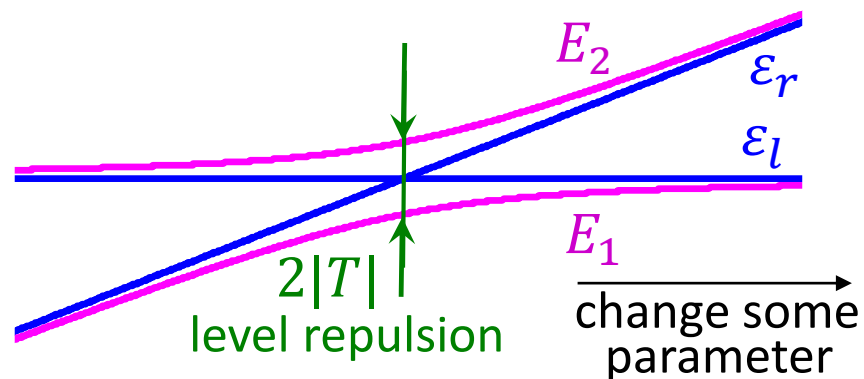
Find stationary states: $\hat{H} |\psi\rangle = E|\psi\rangle$ $\alpha(t) = \alpha_0 e^{-iEt/\hbar}$, $\beta(t) = \beta_0 e^{-iEt/\hbar}$

$$\begin{cases} \varepsilon_l\alpha_0 + T\beta_0 = E\alpha_0 \\ \varepsilon_r\beta_0 + T^*\alpha_0 = E\beta_0 \end{cases} \Rightarrow \begin{pmatrix} \varepsilon_l - E & T \\ T^* & \varepsilon_r - E \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \beta_0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

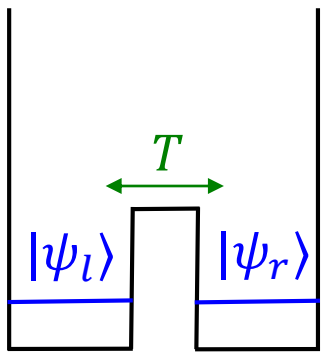
$$\Rightarrow \det(\dots) = 0 \quad \Rightarrow (\varepsilon_l - E)(\varepsilon_r - E) - |T|^2 = 0$$

$$E_{1,2} = \frac{\varepsilon_l + \varepsilon_r}{2} \mp \sqrt{\left(\frac{\varepsilon_l - \varepsilon_r}{2}\right)^2 + |T|^2}$$

Avoided level crossing



Symmetric case, $\varepsilon_l = \varepsilon_r = \varepsilon$



$$\begin{cases} \varepsilon_l \alpha + T \beta = E \alpha_0 \\ \varepsilon_r \beta + T^* \alpha = E \beta_0 \end{cases} \quad E_{1,2} = \frac{\varepsilon_l + \varepsilon_r}{2} \mp \sqrt{\left(\frac{\varepsilon_l + \varepsilon_r}{2}\right)^2 + |T|^2}$$

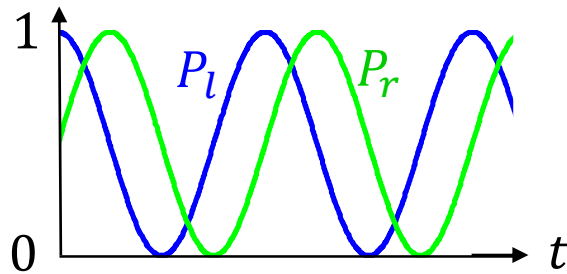
$$\begin{cases} |\Psi_1(t)\rangle = \frac{|\psi_l\rangle + |\psi_r\rangle}{\sqrt{2}} \exp\left(-i \frac{\varepsilon - |T|}{\hbar} t\right) & \text{ground state} \\ |\Psi_2(t)\rangle = \frac{|\psi_l\rangle - |\psi_r\rangle}{\sqrt{2}} \exp\left(-i \frac{\varepsilon + |T|}{\hbar} t\right) & \text{excited state} \end{cases}$$

If start in the left well, $|\Psi(0)\rangle = |\psi_l\rangle$, then superposition of $|\Psi_1\rangle$ and $|\Psi_2\rangle$

$$|\Psi(t)\rangle = \left[\cos\left(\frac{|T|}{\hbar} t\right) |\psi_l\rangle + \sin\left(\frac{|T|}{\hbar} t\right) |\psi_r\rangle \right] \exp\left(-i \frac{\varepsilon}{\hbar} t\right)$$

Quantum coherent (Rabi) oscillations – smoking gun for a qubit

$$\begin{cases} P_l = \cos^2(|T| t/\hbar) \\ P_r = \sin^2(|T| t/\hbar) \end{cases}$$



oscillation frequency

$$\omega = \frac{2|T|}{\hbar} = \frac{E_2 - E_1}{\hbar}$$

(similar to Larmor precession)