

ECE 659 Quantum Transport: Atom to Transistor

Lecture 11: Semi classical Dynamics

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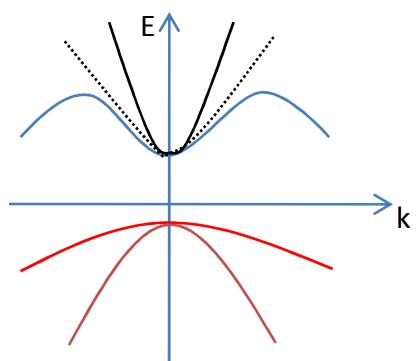
Newton's Law:

$$\frac{dx}{dt} = v$$

$$\frac{dp}{dt} = F$$

Bandstructure

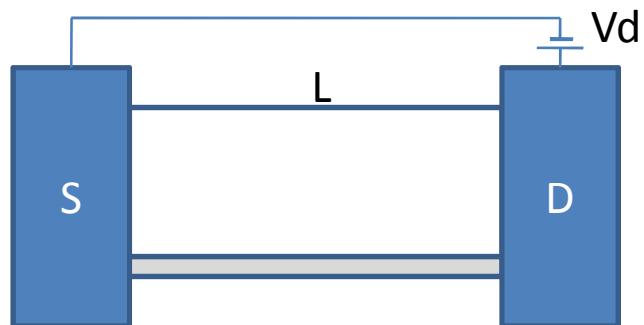
$$E = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$



Hamilton's form of Newton's Law:

$$\frac{dx}{dt} = \frac{\partial E}{\partial p}$$

$$\frac{dp}{dt} = -\frac{\partial E}{\partial x}$$



$$\frac{df^+}{dz} = \frac{df^-}{dz} = -\frac{(f^+ - f^-)}{\lambda}$$

$$E = \frac{p^2}{2m} + U(x)$$

$$\frac{dx}{dt} = \frac{p}{m}, \quad \frac{dp}{dt} = -\frac{\partial U}{\partial x}$$

Schrodinger Equation:

$$i\hbar \frac{d\psi}{dt} = \left(\left(i\hbar \frac{d}{dx} \right)^2 + U(x) \right) \psi$$

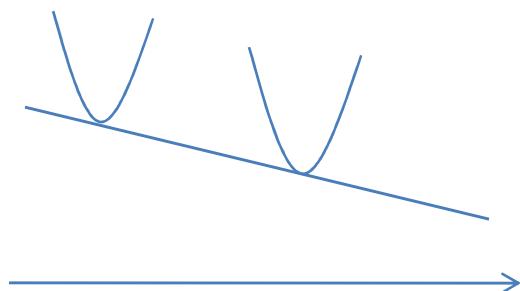
If $U(x)$ is constant, we can solve this by:

$$\psi \sim e^{-iEt/\hbar} e^{ikx}$$

If U is space variant (say in x) but time invariant:

$$\psi \sim e^{-iEt/\hbar} e^{i \int dx' k(x')}$$

$$E = \frac{\hbar^2 k^2}{2m} + U(x)$$



$$\frac{dx}{dt} = \frac{1}{\hbar} \frac{\partial E}{\partial k} \quad -A$$

$$\frac{dk}{dt} = -\frac{1}{\hbar} \frac{\partial E}{\partial x} \quad -B$$

eqn. B can be shown to be true in the following way:

$$\frac{dE(x, k)}{dt} = 0$$

$$\frac{\partial E}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial E}{\partial k} \frac{\partial k}{\partial t} = 0$$

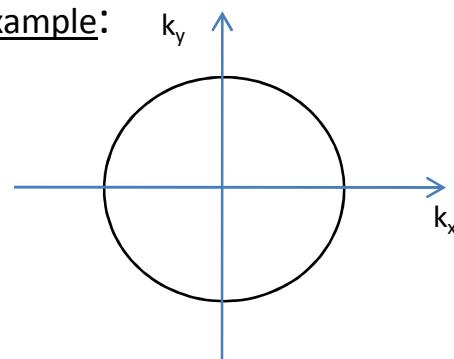
$$v \left(\frac{\partial E}{\partial x} + \hbar \frac{\partial k}{\partial t} \right) = 0$$

In 3D:

$$\frac{d\vec{x}}{dt} = \frac{1}{\hbar} \nabla_k E$$

$$\frac{d\vec{k}}{dt} = -\frac{1}{\hbar} \nabla E$$

Example:

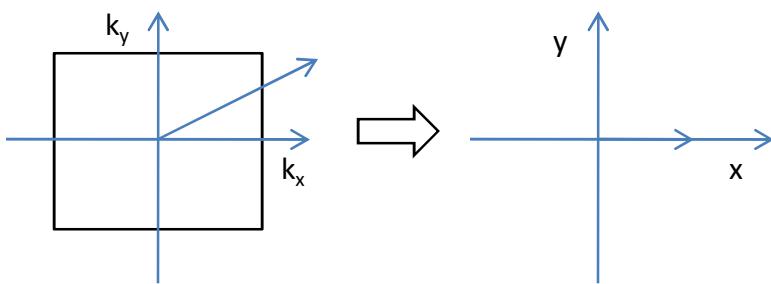


$$E = \frac{\hbar^2 (k_x^2 + k_y^2)}{2m}$$

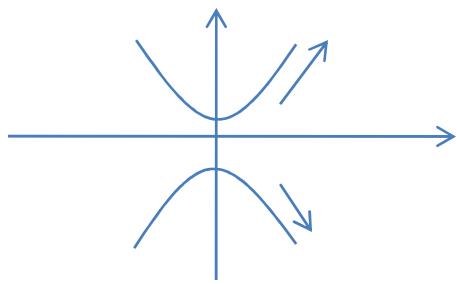
$$\text{Which gives: } \frac{d\vec{x}}{dt} = \frac{\hbar \vec{k}}{m}$$

Hence, v and k are collinear

Example:



k and v are collinear depending upon E-k diagram
If E goes down with k (e.g. in valence band) v will
be in opposite direction



Effect of Magnetic Field

$$E = \frac{\hbar^2 k^2}{2m} + \underbrace{qV}_{U}$$

$$\bar{\xi} = -\nabla V$$

$$\bar{B} = \nabla \times \bar{A}$$

$$E = \frac{(\hbar\vec{k} - q\vec{A}) \cdot (\hbar\vec{k} - q\vec{A})}{2m} + qV$$

$$B_y = \frac{\partial A_x}{\partial z} - \frac{\partial A_z}{\partial x}$$

$$A_x = B_y z$$

$$A_z = -B_y x$$

$$E = \frac{(\hbar k_x - qA_x)^2 + (\hbar k_z - qA_z)^2}{2m}$$

$$\frac{d\vec{x}}{dt} = \frac{\hbar\vec{k} - q\vec{A}}{m} = \frac{\hbar\vec{k}'}{m}$$

$$\hbar \frac{dk_x}{dt} = \underbrace{\frac{\hbar k_z - qA_z}{m}}_{v_z} \cdot q \frac{\partial A_z}{\partial x}$$

We can show: $\hbar \frac{d\vec{k}'}{dt} = q(\vec{v} \times \vec{B})$

Hence: $\frac{d\vec{x}}{dt} = \frac{\hbar\vec{k}'}{m}$

$$\hbar \frac{d\vec{k}'}{dt} = q(\vec{v} \times \vec{B})$$