Fri. Nov. 09

- Due to limited time, we will only briefly describe an important result for electrons in a periodic potential, known as <u>Bloch's theorem</u>

- <u>Theorem</u>: the eigenstates of the one-electron Hamiltonian

$$H = \frac{-\hbar^2 \nabla^2}{2m} + V(\vec{r})$$

where $V(\vec{r}+\vec{R}) = V(\vec{r})$ for all $\vec{R}$ being lattice vectors can be chosen to have the form of a plane wave multiplied by a function $u(\vec{r})$ that has the periodicity of the lattice

$$\psi_{n,\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} u_{n,\vec{k}}(\vec{r}) \quad \Big\} \; n = \text{band index}$$

where $u_{n,\vec{k}}(\vec{r}+\vec{R}) = u_{n,\vec{k}}(\vec{r})$, for all $\vec{R}$

- let's look at $\psi(\vec{r}+\vec{R}) \rightarrow$ [assume $\psi = \psi_{n,\vec{k}}$ etc.]

$$\psi(\vec{r}+\vec{R}) = e^{i\vec{k}\cdot(\vec{r}+\vec{R})} u(\vec{r}+\vec{R})$$

$$= \underbrace{e^{i\vec{k}\cdot\vec{r}} u(\vec{r})}_{\psi(\vec{r})} e^{i\vec{k}\cdot\vec{R}}$$

$$\therefore \boxed{\psi(\vec{r}+\vec{R}) = \psi(\vec{r}) e^{i\vec{k}\cdot\vec{R}}}$$ $\rightarrow$ also a statement of Bloch's theorem

- a couple of observations about the theorem
- the eigenstates & eigen values are periodic functions of $\vec{k}$ in the reciprocal lattice

$$\psi_{n,\vec{k}+\vec{G}}(\vec{r}) = \psi_{n,\vec{k}}(\vec{r})$$

$$E_{n,\vec{k}+\vec{G}} = E_{n,\vec{k}}$$

- we already used this fact in band structure discussions

- an electron in a band 'n' and with wave vector $\vec{k}$ has an average velocity

$$\vec{V}_n(\vec{k}) = \frac{1}{\hbar} \nabla_k E_n(\vec{k})$$

- it might not be clear at first glance, but what the above equation implies is that electron speeds do not decay in time, i.e. they are time independent.

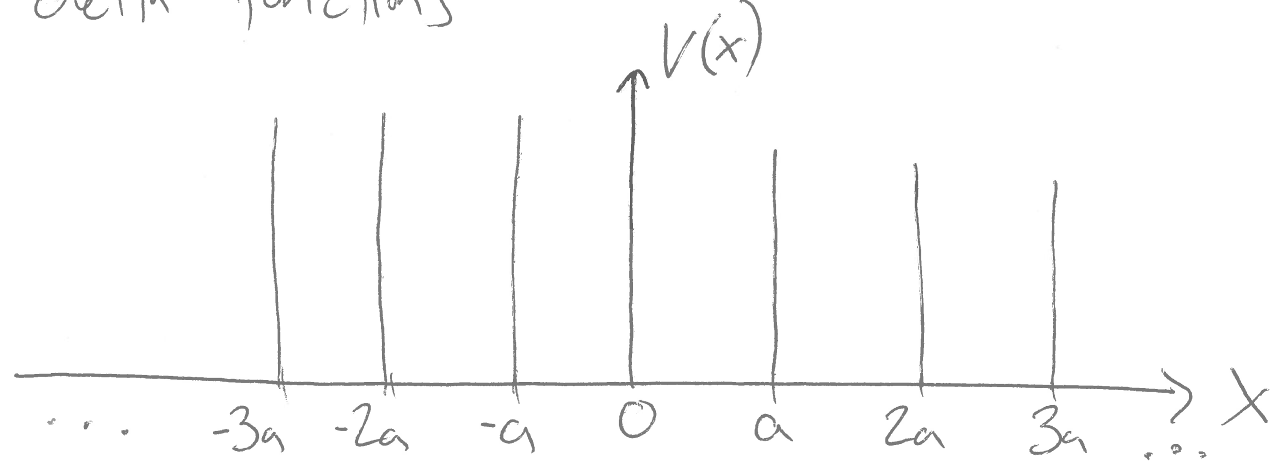
- compare this with Drude theory: recall that this classical theory predicts the momentum of a (charged gas) of electrons decays in time

$$\vec{p}(t) = \vec{p}_0 e^{-t/\tau}$$

resulting from collisions with the lattice

- remarkably, the electrons actually pass directly through the crystal unimpeded $\longrightarrow$ see slides

- This will be one of your HW problems, but we will get started on it today:
- let's solve for the energy of electrons in a "Dirac comb" $\rightarrow$ evenly spaced Dirac delta functions



- Clearly $V(x+a) = V(x)$
- Bloch's theorem tells us

$$\psi(x+a) = e^{iKa}\psi(x)$$

- the potential $$V(x) = \alpha \sum_{j=0}^{N-1} \delta(x - ja)$$

periodic b.c.'s

- for region $0 < x < a$, $V = 0$

$$\psi(x) = A\sin(qx) + B\cos(qx)$$

- note we use q as the wave # for the electron
- just to the left of $x=0$,

$$\psi(x) = e^{-ika}\left[A\sin q(x+a) + B\cos(x+a)q\right]$$

$$(-a < x < 0)$$

by Bloch's theorem

- at $x=0$, ψ is continuous
- but derivative has discontinuity $\propto \alpha$ prop. to alpha

$$\left.\frac{d\psi}{dx}\right|_{x=0^+} - \left.\frac{\partial\psi}{\partial x}\right|_{x=0^-} = \frac{-2m\alpha}{\hbar^2}\psi(0)$$

- putting these b.c.'s together,

$$\cos(ka) = \cos(qa) - \frac{m\alpha}{\hbar^2 q}\sin(qa)$$

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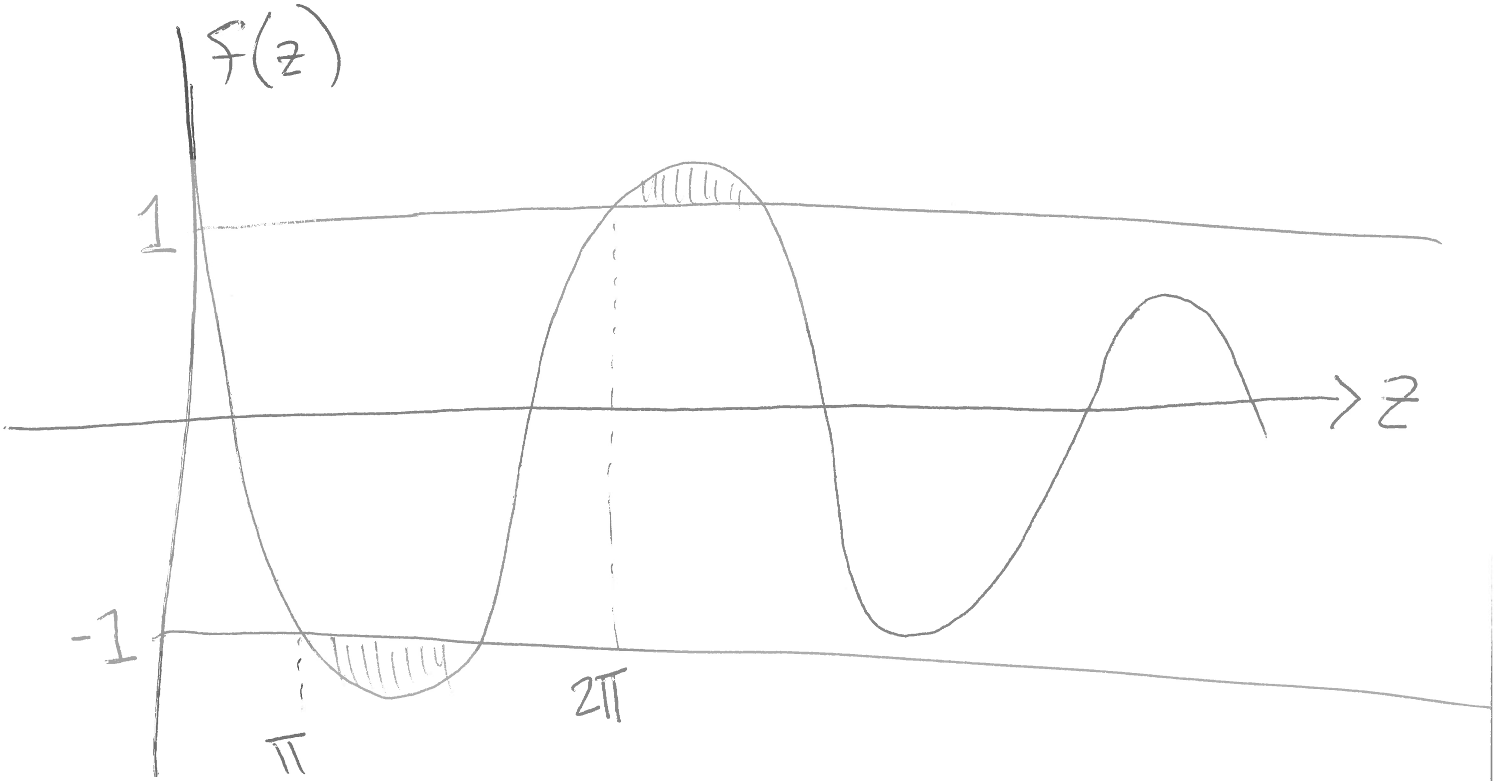
- let $z \equiv qa$ & $\beta \equiv \frac{m\alpha a}{\hbar^2}$

$$f(z) = \cos(z) - \frac{\beta \sin(z)}{z} = \cos(ka)$$



$$f(z) = \cos(ka), \text{ but } |\cos(ka)| \leq 1$$

- the shaded regions are gaps in values of q that are not possible → correspond to bands of energy