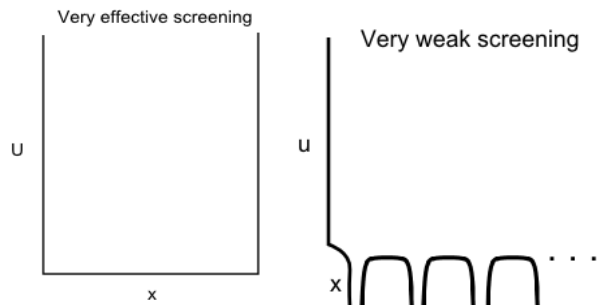


Topic 8-4: Screening

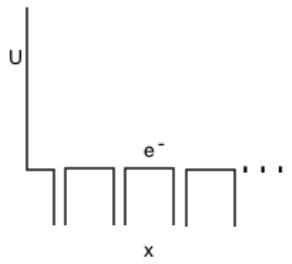
Summary: In this video we discuss why the constant potential box is a good model for solids. We describe a concept known as screening which is the reason behind the free electron model's applicability to solids. We also look at the effects of creating a perturbation in our potential box and develop an expression for how screening changes because of this perturbation.

- So far we have assumed that there is one electron in our system and it is just in a constant potential box
 - How does this simple model work so well for solids
- Screening is why this model works so well
- Screening is how an electron doesn't "see" the nucleus because all the core and valence electrons are in the way
- Example: Helium
 - Has two protons and two electrons
 - An incoming, third electron would not feel the nucleus until it can get past the two electrons helium has

- Screening in solids



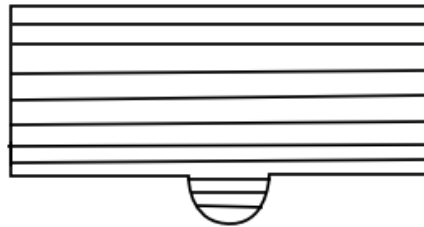
- With the square well we are assuming that screening is so effective there is no spatial variation in the potential within the solid
 - Graph on the right is weak screening which gives a $1/r$ coulombic potential for the nuclei
- Reality in a metal



- Screening is highly effective unless the electron is really close to the nuclei
- Need to figure out how close an electron can get to a nucleus in a metal before screening breaks down
- Invoke that the local internal chemical potential $\mu(x)$ is a function of the local electron concentration
- At equilibrium $\mu(x)$ is constant throughout the free electron gas
- When there is no electrostatic contribution to μ :

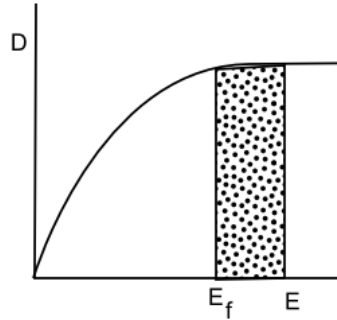
$$\mu = E_f^0 = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3} \quad [1]$$

- n is the electron charge density
- This gives a direct connection between chemical potential and electron charge density
- Create a local change in electrostatic potential (a positive charge, aka a nucleus)



- Lines are energy levels
- Bump is the perturbation in potential from the nucleus and is equal to $-e\delta V$
- There is increased local charge density $n(x)$ at the perturbation
- *The positive charge screens itself from far away electrons by piling up charge nearby*
- A local change in potential needs to be self-consistent with the change in electron density
 - $-e\delta V(\vec{r}) \rightarrow \delta n(\vec{r})$
- Away from the perturbation the density of states is what you would expect with filled states to the Fermi level

- At the perturbation the density of states graph just shifts by the charge time del V



- Can figure out $\delta n(\vec{r}) = D(E_f) \cdot e\delta V(\vec{r})$
 - Using rectangle approach as before
- **Derivation approach:** We're going to play around with E&M and the expressions above to ultimately set up a differential equation in terms of $\delta V(\vec{r})$. We'll solve this differential equation for $\delta V(\vec{r})$ to determine the perturbation in the potential from a positively charged nucleus.

- Start with Maxwell's equation:

$$\nabla \cdot E = \frac{\rho}{\epsilon_0} \quad [2]$$

- E is the electric field, ρ is the charge density, ϵ_0 is the dielectric constant and V is the electric potential

$$E = -\nabla \cdot V \quad [3]$$

$$-\nabla \cdot (-\nabla V) = \frac{\rho}{\epsilon_0} \quad [4]$$

- Combining the above two expressions yields:

$$\nabla^2 V = -\frac{\rho}{\epsilon_0} \quad [5]$$

- We are interested in δV
 - The charge density and number density is trivially related by the electric charge:
 $\delta\rho=e\delta n$
 - As stated above, $\delta n = D(E_f)e\delta V$
- Switching from V and ρ to δV and $\delta\rho$, inserting expression for δn gives us the differential equation we were looking for:

$$\nabla^2 \delta V = \frac{-e\delta n}{\epsilon_0} = \frac{-e^2 D(E_f) \delta V}{\epsilon_0} \quad [6]$$

- Solving the differential equation we get $\delta V(\vec{r}) = \frac{e}{4\pi\epsilon_0} \frac{e^{-r/r_{TF}}}{r}$
 - $r_{TF} = \sqrt{\frac{\epsilon_0}{e^2 D(E_f)}}$
 - r_{TF} comes from Thomas Fermi
- r_{TF} is related to how close an electron has to get to the nucleus before it feels a non-zero potential gradient
- $r_{TF} \rightarrow \infty$ our expression for $\delta V(\vec{r})$, the perturbation, goes to the unscreened potential $1/r$
- $r_{TF} \rightarrow 0$ the perturbation is almost a delta function which is equivalent to very strong screening
- **Physical interpretation:** We have an expression for how the potential changes with screening; let's highlight the critical terms:
- $r_{TF} \propto \frac{1}{\sqrt{D(E_f)}}$ and $D(E_f) = \frac{3}{2} \frac{n}{E_f}$; a large density of states at E_f leads to a small r_{TF} and thus good screening.
- Increasing n leads to a shorter r_{TF} (screening length); this makes sense – greater electron density provides screening of the nucleus, decreasing the impact of the nucleus on the potential $V(r)$.
- Going back to solids, one of the reasons the free electron model works so well is because the electrons are screened by from the nucleus by other electrons.
- Example: phase transition
 - Large $n \rightarrow$ small n
 - Small $r_{TF} \rightarrow$ large r_{TF} and screening suddenly fails
 - This will allow the free electrons to see the atomic nuclei much more strongly
 - We call this a Mott transition, Wikipedia has a nice writeup
http://en.wikipedia.org/wiki/Mott_transition