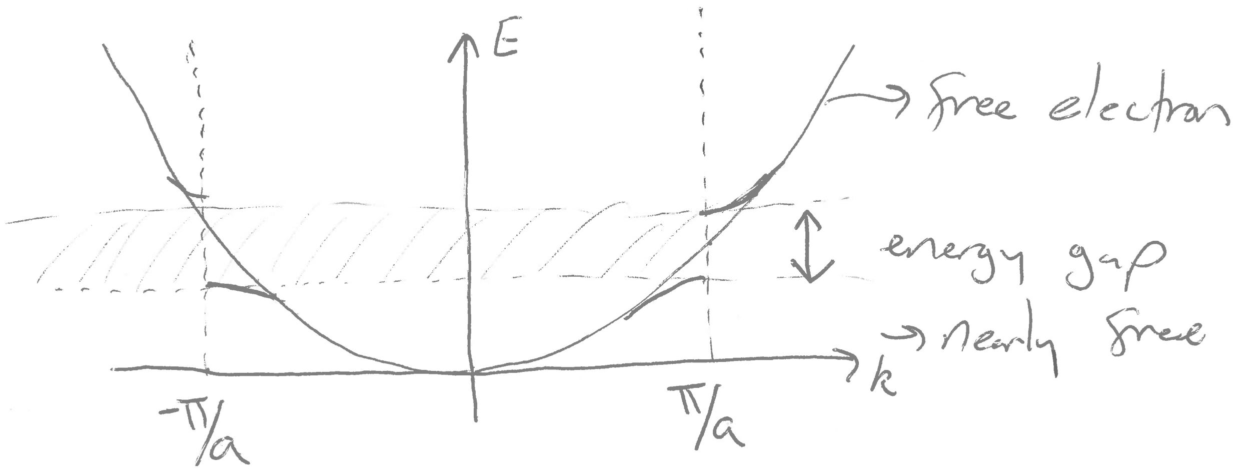
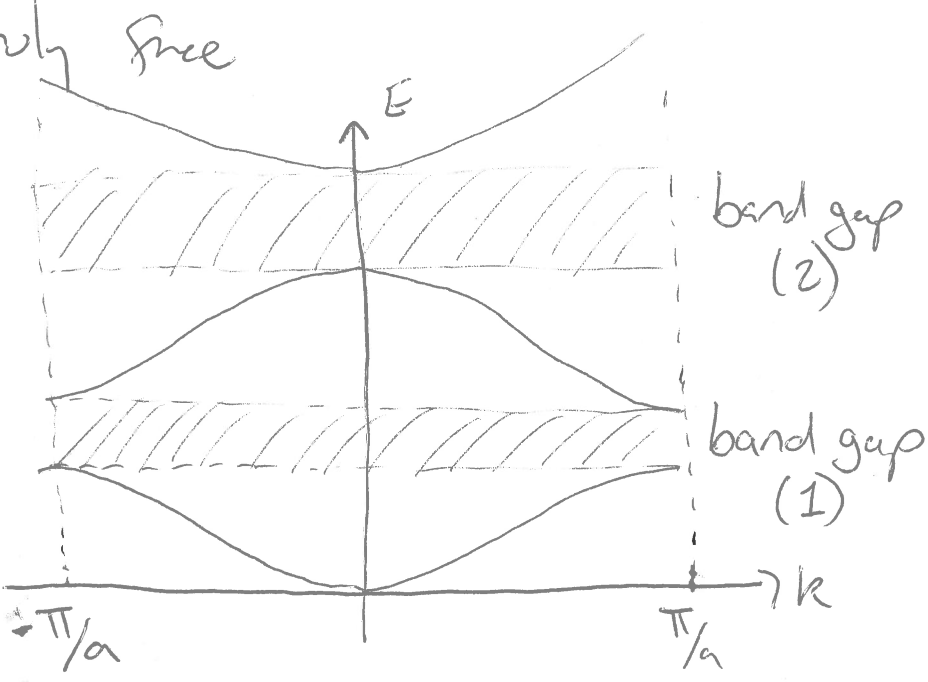
Wed. Nov. 07

- We've been working on the "nearly free electron" model
  - without specifying the form of the potential for the interaction between the electrons + the ions, we still find modification of the dispersion relation



- an important aspect of this model is that the overall behavior is almost the same as if the electrons were truly free
- reduced zone scheme



- recall the gaps opening up around the zone boundaries result from the wavelength of the electrons fulfilling the Bragg condition where they reflect from the lattice like a diffraction grating

- let's try to make this idea a bit more quantitative using perturbation theory

- Start with the solution to a known problem with a known solution to approximate desired solution

$$H^0 \psi_n^0 = E_n^0 \psi_n^0 \qquad \text{(known)}$$

$$H \psi_n = E_n \psi_n \qquad \text{(unknown)}$$

- the Hamiltonian with a perturbation, H'

$$H = H^0 + \lambda H' \quad (\lambda \rightarrow \text{strength parameter})$$

gives energy eigenstates

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \ldots$$

$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle$ is the expectation value of the perturbation in the unperturbed state

- For our problem, electrons are in a periodic potential

$$V(x) = V(x+a) \quad [\text{in 1D}]$$

- For band with index '1' * 'n' corresponds to band index

$$E_1(k) = E_1^0(k) + \langle \psi_{1,k}^0 | V | \psi_{1,k}^0 \rangle$$

→ first order correction

& '0' indicates the empty lattice model

- the perturbation in our case takes

$$V = 0 \longrightarrow V = V(x) \text{ : empty to weak potential}$$

& so we want to calculate

$$\langle \psi_{1,k}^0 | V(x) | \psi_{1,k}^0 \rangle$$

$$\langle \psi^0_{1,k} | V(x) | \psi^0_{1,k} \rangle$$

$$= \frac{1}{L} \int_0^L e^{-ikx} V(x) e^{ikx} \, dx \; ; \; \psi^0_{1,k} = \frac{1}{\sqrt{L}} e^{ikx} \text{ (free electron)}$$

- Since $V(x)$ is periodic, we can see

$$\frac{1}{L} \int_0^L V(x) \, dx = \text{some constant}$$

(does not depend upon 'k')

- so dispersion relation resulting from perturbation

$$E_1(k) = E_1^0(k) + \text{constant}$$

does not change shape so we can set constant $= 0$ without losing information

- we see a second order correction is required

$$\sum_{(n,k') \neq (1,k)} \frac{|\langle \psi^0_{n,k'} | V(x) | \psi^0_{1,k} \rangle|^2}{E_1^0(k) - E_n^0(k')}$$

$n \rightarrow$ band
$k \rightarrow$ state

we are evaluating state $1, k$, so exclude these states from sum

- We assume only adjacent bands couple, e.g., for band 1, we only see coupling to band 2 ($n=1$ + $n=2$)
- by Fourier analysis, any 1D potential can be written as

$$V(x) = \sum_{k} V_k e^{ikx}$$

where $V_k = \frac{1}{L}\int_0^L V(x) e^{-ikx}\,dx$ is the Fourier coefficient.

- as we have seen in the past $V_k = 0$ for $k \neq G$, where G = recip. lattice point
- thus $V(x) = \sum_G V_G e^{iGx}$

+ $\langle \psi^{\circ}_{n,k'} | V(x) | \psi^{\circ}_{1,k} \rangle = V_{k'-k} = V_G = V_{2\pi/a}$

→

- let's show $\langle \psi^{0}_{n,k'} | V(x) | \psi^{0}_{1,k} \rangle = V_G$
- as before, let's only look at coupling between first ($n=1$) + second ($n=2$) bands

$$\langle \psi^{0*}_{2,k'} | V(x) | \psi^{0}_{1,k} \rangle$$

$$= \int \psi^{0*}_{2,k'} \left[\sum_G V_G e^{iGx} \right] \psi^{0}_{1,k} \, dx$$

$$= \frac{1}{L} \int e^{-ik'x} \left[\sum_G V_G e^{i 2\pi/a \, x} \right] e^{ikx}$$

$$= \frac{1}{L} \int e^{-i(k'-k)x} \sum_G V_G e^{i 2\pi/a \, x}$$

- for $n=1$ + $n=2$, $\sum_G V_G e^{i 2\pi/a \, x} = V_{2\pi/a} e^{i 2\pi/a \, x}$

$$+ \; e^{-i(k'-k)x} = e^{-i 2\pi/a \, x}$$

$$\Rightarrow \langle \psi^{0}_{2,k'} | V(x) | \psi^{0}_{1,k} \rangle = V_{2\pi/a}$$

- so we have

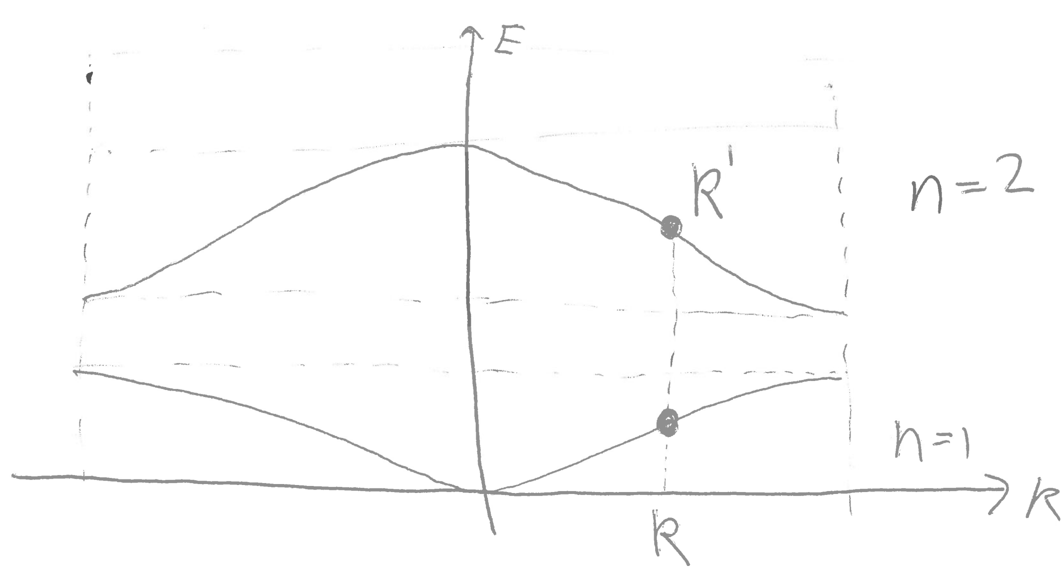
$$E_1(k) \approx E_1^0(k) + \frac{|V_G|^2}{E_1^0(k) - E_2^0(k)}$$

- for $E_1^0(k)$, we have the result for the free electron

$$E_1^0(k) = \frac{\hbar^2 k^2}{2m} \quad ; \quad n=1, \text{ first band}$$

- for $E_2^0(k)$, we have shifted by $2\pi/a$ to the right along the k-axis

$$E_2^0(k) = \frac{\hbar^2 (k - 2\pi/a)^2}{2m} \quad ; \quad n=2, \text{ second band}$$



- We see far from the zone boundaries

$$E_1(k) \approx E_1^0(k)$$

or little to no perturbation is present

- as we approach $k = \pm \pi/a$ the term

$$\frac{|V_G|^2}{E_1^0(k) - E_2^0(k)} \rightarrow \infty$$

- We must "lift" the degeneracy at the boundary using degenerate perturbation theory

$$E_\pm(k) = \frac{1}{2}\left[E_1^0 + E_2^0 \pm \left((E_2^0 - E_1^0)^2 + 4|V_G|^2\right)^{1/2}\right]$$

(−) altered lower band

(+) altered upper band

with gap width @ $k = \pm \pi/a$

$$E_g = 2|V_G|$$

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