Questions of the day:

(1) Is solid Lithium an insulator, metal or semiconductor

Please justify $Li = 3e^-$, $1s^2 2s^1$

Slides $\rightarrow$

(2) What are LCAO amplitude (eigenvector) for the lowest energy of 5-quantum well system?

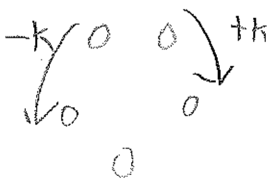
i. how would this change for periodic boundaries?

$$\lambda = (5+1)\times 2a = 12a, \quad k_1 = \frac{\pi}{6a}$$

	1	2	3	4	5
c_n	$e^{i\pi/6}$	$e^{i\pi/3}$	$e^{i\pi/2}$	$e^{i2\pi/3}$	$e^{i5\pi/6}$

$$|\psi_k\rangle = \sum_{n=1}^{5} e^{ikna} |n\rangle$$

Periodic boundaries: N sites $\Rightarrow$ $c_1 = c_{N+1}$



$$c_1 = e^{ikNa} c_1$$

$$1 = e^{ikNa}$$

$$Nka = q\, 2\pi$$

5 sites, both clockwise & counterclockwise

or $k = \frac{q}{N}\frac{2\pi}{a}$

$0 .. \frac{\pi}{a} \rightarrow -\frac{\pi}{a} ... \frac{\pi}{a}$

for periodic boundary conditions

i.e. $\lambda = \frac{Na}{q}$ $\rightarrow$ in the index of w.f. normal mode.

Ring Dance N=10 SHOW ME YOUR WAVEFUNCTION

1) Dance step #1: show me tunnelling

2) Dance step #2: $\lambda_1 = \frac{10a}{q}$, $q=1$ $\quad K = \pm\frac{\pi}{5a}$

$\lambda_{10} = a$ $\quad q=5$ $\quad K = \pm\frac{\pi}{a}$

$\Delta K = k_q - k_{q-1} = \frac{2\pi}{Na}$, the small $\Delta k = \frac{2\pi}{\ldots} \ll \frac{2\pi}{a}$

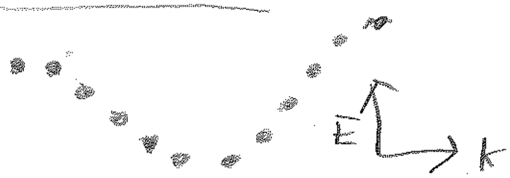
(See slides)

Metal:

$E = E_0 \sin \omega t$
↳ light frequency

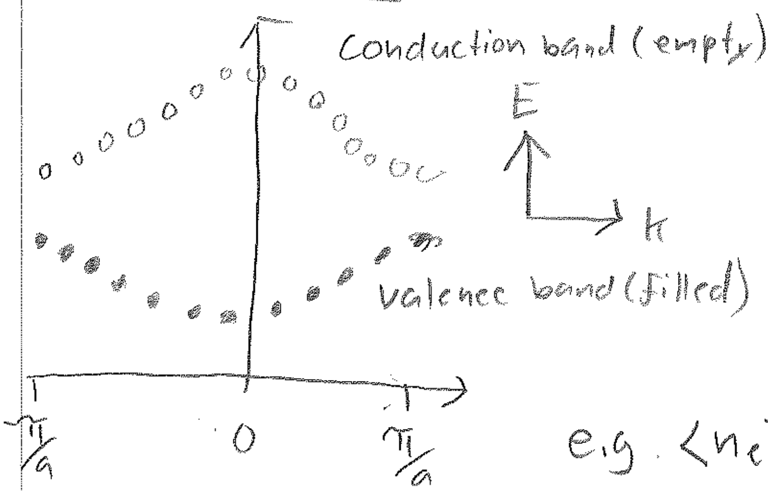
electrons us unoccupied k-states to move electrons back/forth. this screen the E-field & light is reflected (metals are shiny)

Insulators:



No net movement of charge possible when coupling with E-field. → Insulators are generally transparent

Semiconductors



if E_{gap} is small enough (~1eV) some electrons have enough energy to populate the conduction band at T=300K

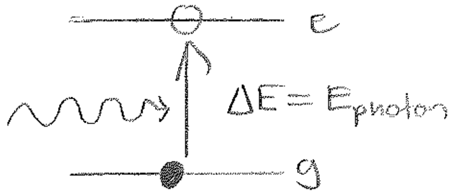
$$\text{e.g. } \langle n_e \rangle = \frac{1}{e^{E/k_BT} + 1}$$

$$\simeq e^{-E/k_BT} = e^{-40}$$

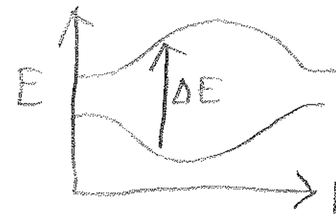
(small probability, poor conductor.

Slide 4 of day

Atomic solid



Periodic System



ΔE must match an occupied and un-occupied eigenstate and conserve K

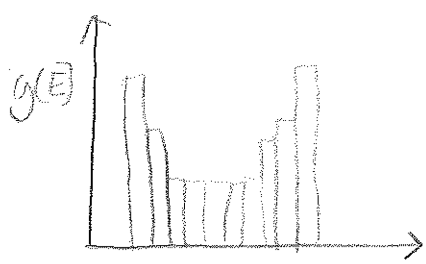
Semiconductors are further classified as direct vs. indirect

Direct gap materials are optically emissive

Worksheet: within a band are the energies evenly spaced?

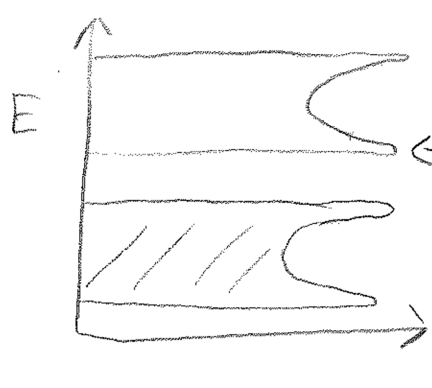
100 atom worksheet, construct a histogram

Band structure simulation



$g(E)dE$ is the number of eigenstates from E to $E+dE$

$$g(E) = L/\pi \left(dE/dk\right)^{-1}$$

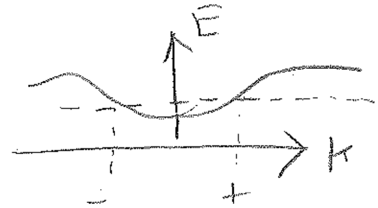


conduction band

← higher state density

valence band

$g(E)$ has units of inverse energy, $g(E) \propto \Delta E^{-1}$



crosses $E(k)$ twice
spin up & spin down
$\Rightarrow$ factor of 4

$$g(E) = \frac{4}{\Delta E}$$

$$= \frac{4}{\left(\frac{dE}{dk}\Delta k\right)}$$

$$= \frac{4}{\frac{dE}{dk}\left(\frac{2\pi}{L}\right)}, \quad \Delta k = \frac{2\pi}{L} \rightarrow \text{smallest possible } k\text{, for a system of "length" } L.$$

$$= \frac{2L}{\pi}\left(\frac{dE}{dk}\right)^{-1}$$

Problem set evaluate for a free-electron,
note $g(E)$ must not directly depend on k,
can depend on energy only.

Problem 15.7: evaluate $g(E)$ for $E = \frac{\hbar^2 k^2}{2m_e}$

Problem 15.6 is more difficult!
In general we may use $g(E)$ to calculate

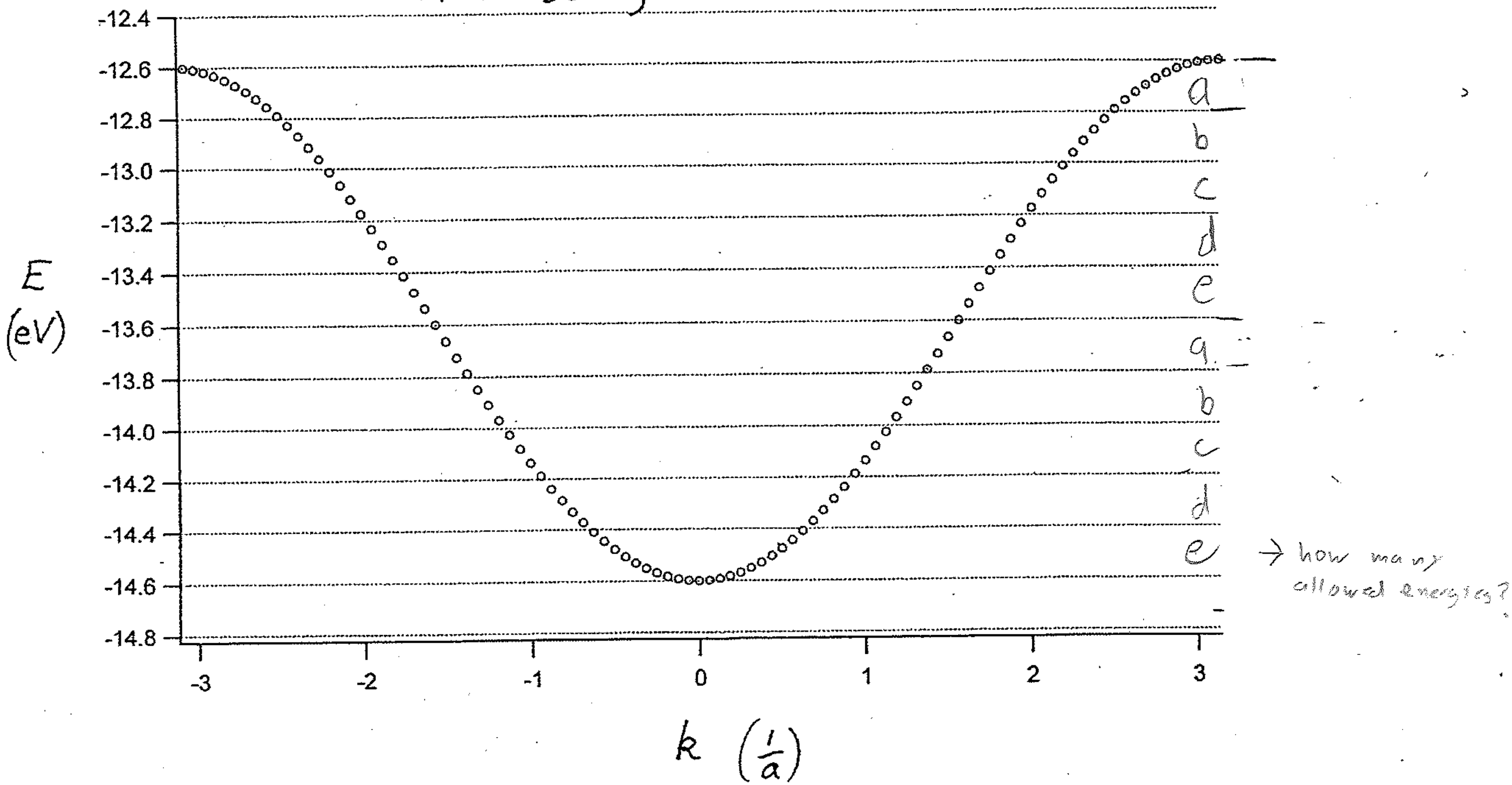
① total states in a band $= \int_{E_{min}}^{E_{max}} g(E)\,dE = N_{tot}$

② sum of all energies in the band $= \int_{E_{min}}^{E_{max}} E\,g(E)\,dE = E_{tot}$

in 15.17, use 15.45 that $g(E) = \frac{L}{2\pi\beta a \sin ka}$, $L = Na$

find $E_{tot} = \int_{\alpha+2\beta}^{\alpha-2\beta} E\,g(E)\,dE$

PH427 Density of states worksheet



This graph shows the LCAO eigenstates formed from the atomic gnd states of 100 hydrogen atoms in a 1d periodic structure (periodic B.Cs)