Section II: Band Structures.

4-17-2017

Phys 175

Outline

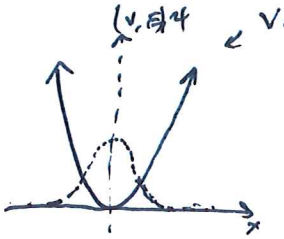
- Hand wavy B.S.
  (made up from single atom potentials)
- Calculate for "simple" potential
- Some practical notes about reading B.S. plots.

Questions?

So to try to get further intuition about the band structure of solids (w/ periodic potentials) we will again (as in class w/ Markus) start w/ a single particle in a single well.

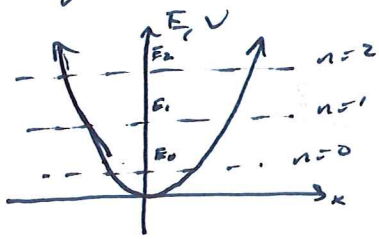
1-Well

Imagine we have a single harmonic well



these wells have E's related to the Hermite polynomials & gaussians.

Energies in the well

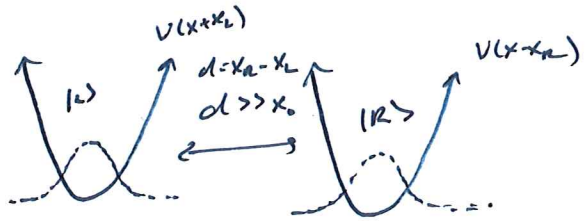


↑ energies of vibrational states in H.O.

So lowest state is E_0

$\Delta E = E_1 - E_0$

2-wells



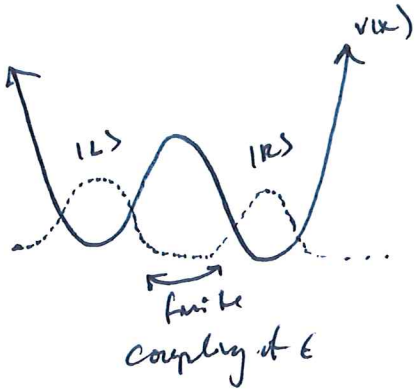
Now we have still 1-particle, but 2-wells. What do the eigenstates look like w/ no coupling?

In the case $d \to \infty$ the two wells are completely decoupled & Means the eigenstates can be a superposition of the two wells w/ a phase degree of freedom $|L\rangle + e^{i\phi}|R\rangle = E_0$ for all ϕ

Now if we make the wells at some finite distance apart they can have some ϵ coupling that breaks this degeneracy. (We will assume we're in the lowest vibrational states)

Now not any arbitrary $|L\rangle + e^{i\phi}|R\rangle$ is an eigenstate.
So for our small coupling we'll draw this potential as a double-well.

Double-Well



You would probably, and correctly, just naively say the e-states are $|+\rangle = |L\rangle + |R\rangle$ & $|-\rangle = |L\rangle - |R\rangle$

We can formally find this effect by asking how does $\hat{H}$ act on

So, in a matrix form then we see we diagonalize $|L\rangle$ or $|R\rangle$ and we see it couples

$$\begin{pmatrix} E_0 & \epsilon \\ \epsilon & E_0 \end{pmatrix} = \hat{H}$$

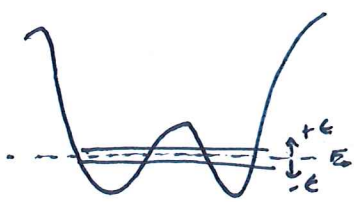
$\langle R|H|L\rangle \sim \epsilon$ also like asking $|x_i\rangle \to |R\rangle$

define $|L$-offset $= E_0$ $\to \epsilon\,|L\rangle$

$(\lambda - E_0)^2 - \epsilon^2 = 0$

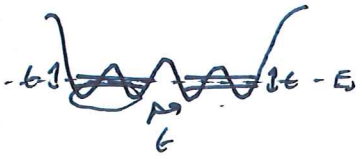
$\lambda_\pm = \pm\epsilon + E_0$ eigenenergies of $\pm\epsilon$

& $|\Omega_+\rangle = |L\rangle + |R\rangle$



So now we split the degenerate ground states about E_0 by their coupling ϵ! This is the most rudimentary way to get to the band structure.

To extend this concept consider now coupling two double wells



We again split the values by ϵ big around E_0

$$\begin{pmatrix} E_0 & \epsilon & 0 \\ \epsilon & E_0 & \epsilon \\ 0 & \epsilon & E_0 \end{pmatrix}$$

can also set $E_0 = 0$? solve:

$$\rightsquigarrow \quad \begin{aligned} E_1 &\approx 1.6\,\epsilon \\ E_1 &\approx 0.6\,\epsilon \\ E_{-1} &\approx -0.6\,\epsilon \\ E_{-2} &\approx -1.6\,\epsilon \end{aligned}$$

~~Obviously~~ doing this sort of ladder sequence I can do this to infinite second in that case

$$\boxed{-2\epsilon \le E_0 \le 2\epsilon}$$

So the splitting of this bottom band eventually approaches a width of $4\cdot\epsilon$.

Typically this is called the "band width".

The type of diagonalization problem we just did is called the "tight-binding" model. Which is a practical way to get to the eigen energies & band structure, but you need to look at each $|\psi_i\rangle$ eigen function to understand what the wavefunction looks like.

This is similar for the higher bands where we see some hybridization about energies $E_1, E_2, \ldots$ with their respective couplings ϵ_i

There is, of course, a more formal solution that can be taken to be able to easily write the eigenfunctions of the periodic system or get to the "dispersion curve".

Also our previous argument holds for cases when our vibrational energies are much larger than our coupling "ϵ" such that these are well defined gaps of $\omega_i >> \epsilon$.

~~More formal calculation~~

Hand-wavy explanation from other extreme,

(Nearly free e^-)

So imagine a shallow potential that is periodic.

$|k\rangle$ ~ free particle

$V = 2\epsilon \cos(k_x x)$

Just comes from:

$$\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi + 0 = E\psi$$

$$\Rightarrow \psi_k = e^{i k\cdot x}; \quad E_k = \frac{\hbar^2}{2m}k^2$$

We define our free electron as $\psi_k(r) = e^{ikx}$

Now we add a very small potential $V(x) = 2\epsilon\cos(k_x x)$

$$= \epsilon\left[e^{ik_x x} + e^{-ik_x x}\right]$$

From this type of potential we could guess that $|k\rangle$'s written as standing waves $(\psi_k + e^{i\phi}\psi_{-k})$ would give time-independent eigenstates.

So we'll pick $|\psi_k\rangle \approx \frac{1}{2}\left(e^{ikx} + e^{i\phi} e^{-ikx}\right)$

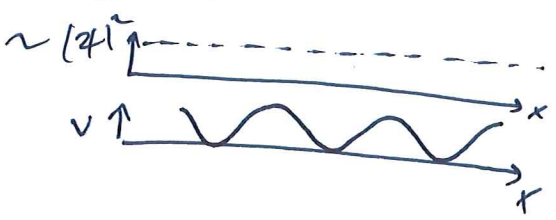
$$\frac{1}{2} e^{-i\phi/2}\left(e^{ikx - i\phi/2} + e^{-(ikx - i\phi/2)}\right)$$

$$\Rightarrow e^{i\phi/2}\left(\cos(kx - \phi/2)\right)$$

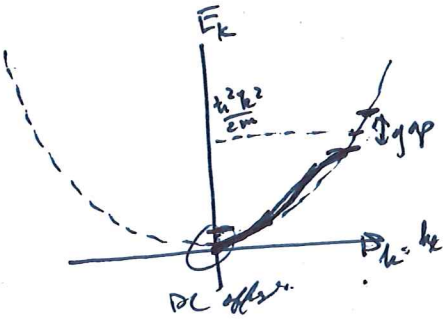
which gives solutions for $|\psi\rangle$ as standing waves or wave functions w/ periodic density probabilities of k compared to the k_a of the lattice.

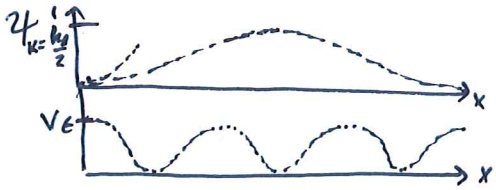
----- free e^-

as $k \to 0$

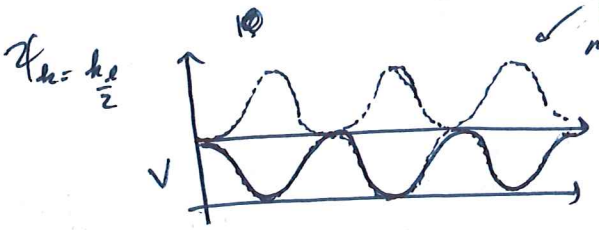


} translationally invariant! who cares what ϕ is. → gives some offset in k



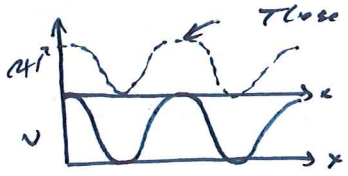


} some translational variation but slight.

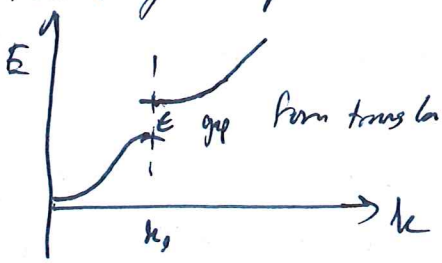


v.s. $\phi_0 = \pi$

equally valid $|\psi_k\rangle$ w/ wave vectors $k = k_a$



There is most definitely then a difference in energy between these two wave functions. This is attributed as the origin of the energy gap at $k = k_a$



Okay so enough hand waviness, let's do some math

Solve for periodic potential

$$V(x) = 2V_0 \cos(k_0 x)$$

The general approach for these problems, as we know periodic structures is to go into the Fourier domain and solve in terms of k-vectors & assume WFs that are periodic. These Ψs are called block functions,

$$\Psi_k = u_k(x)\, e^{ikx}$$ where also $u_k(x)$ has a periodicity of the lattice $\Rightarrow$ $u_k(x) = u_k(x+T)$

T = translation vector of the lattice.

Theorists at Purdue tend to just assume that is also a "ring" structure where the boundary conditions are just what when you repeat back into itself. This is also useful for normalizing the wave function.

periodic

Okay so let's ignore the ~~dead~~ wiggles the

$$\frac{-\hbar^2}{2m}\frac{d^2}{dx^2}\psi + 2V_0\cos(\hbar g x)\psi = E\psi$$

$$\psi = \sum_h a_h e^{ihx}$$

$$\sum_h \frac{-\hbar^2}{2m}(-h)^2 a_h e^{ihx} + 2V_0\left(e^{igx}+e^{-igx}\right)a_h e^{ihx} = \sum_{a_h} E a_h e^{ihx}$$

$$\sum_h \frac{\hbar^2 h^2}{2m} a_h e^{ihx} + 2V_0\left(e^{i(h+g)x} + e^{-i(h-g)x}\right)a_h$$

$$= \sum_h a_h E e^{ihx}$$

We require the integral

$$\psi' = \frac{1}{Nd}\int_{-\frac{Nd}{2}}^{\frac{Nd}{2}} e^{iq'x}\,dx$$

is normalized.

$$\frac{\hbar^2 h^2}{2m}\cdot\frac{1}{Nd}\int_{-\frac{Nd}{2}}^{\frac{Nd}{2}} a_h e^{iq'x} e^{ihx}\,dx + \cdots$$

$\delta(h-q)$

$$\frac{1}{Nd}\int_{-Nd/2}^{Nd/2} dx\, e^{-ig'x}\sum_k\left[\frac{\hbar k^2}{2m}a_k e^{ikx} + V_0 a_k e^{i(k+g)x} + V_0 a_k e^{-i(k-g)x} = \sum_k a_k E_n e^{ikx}\right]$$

$$\frac{\hbar^2 g^2}{2m}a_g + V_0 a_{g-g} + V_0 a_{g+g} = E a_g$$

so restricting my k's now to be in $-\frac{\pi}{d} < k \le \frac{\pi}{d}$

$k = g + lg$ $\quad \pm g/2 \quad \pm g/2$

mean d always factor out the contributions of

mod (2π) from several reciprocal lattice vectors.

It is useful to compare these energy scales to

what is called the "Recoil energy". $E_r = \frac{\hbar^2 g^2}{2m}$

$$\tilde{g} = g/g \quad ; \quad V/E_r = \tilde{V}$$

$$\underbrace{\frac{\hbar^2 g^2}{2m}}_{E_r}\left[\frac{g^2}{g^2}a_g + \tilde{V}a_{g-g} + \tilde{V}a_{g+g}\right] = E a_g$$

now think of the $\tilde{q} \Rightarrow k = g(\tilde{q} + l)$

$$a_l^{(\tilde{q})} = a_{k = g(\tilde{q}+l)}$$

↑ for how a's couple to their vector reciprocal lattice amplitude,

$$E_r\left[(\tilde{q}+l)a_l^{(\tilde{q})} + \tilde{V}a_{l-1}^{(\tilde{q})} + \tilde{V}a_{l+1}^{\tilde{q}}\right] = E_r(\tilde{E})\, a_l^{\tilde{q}}$$

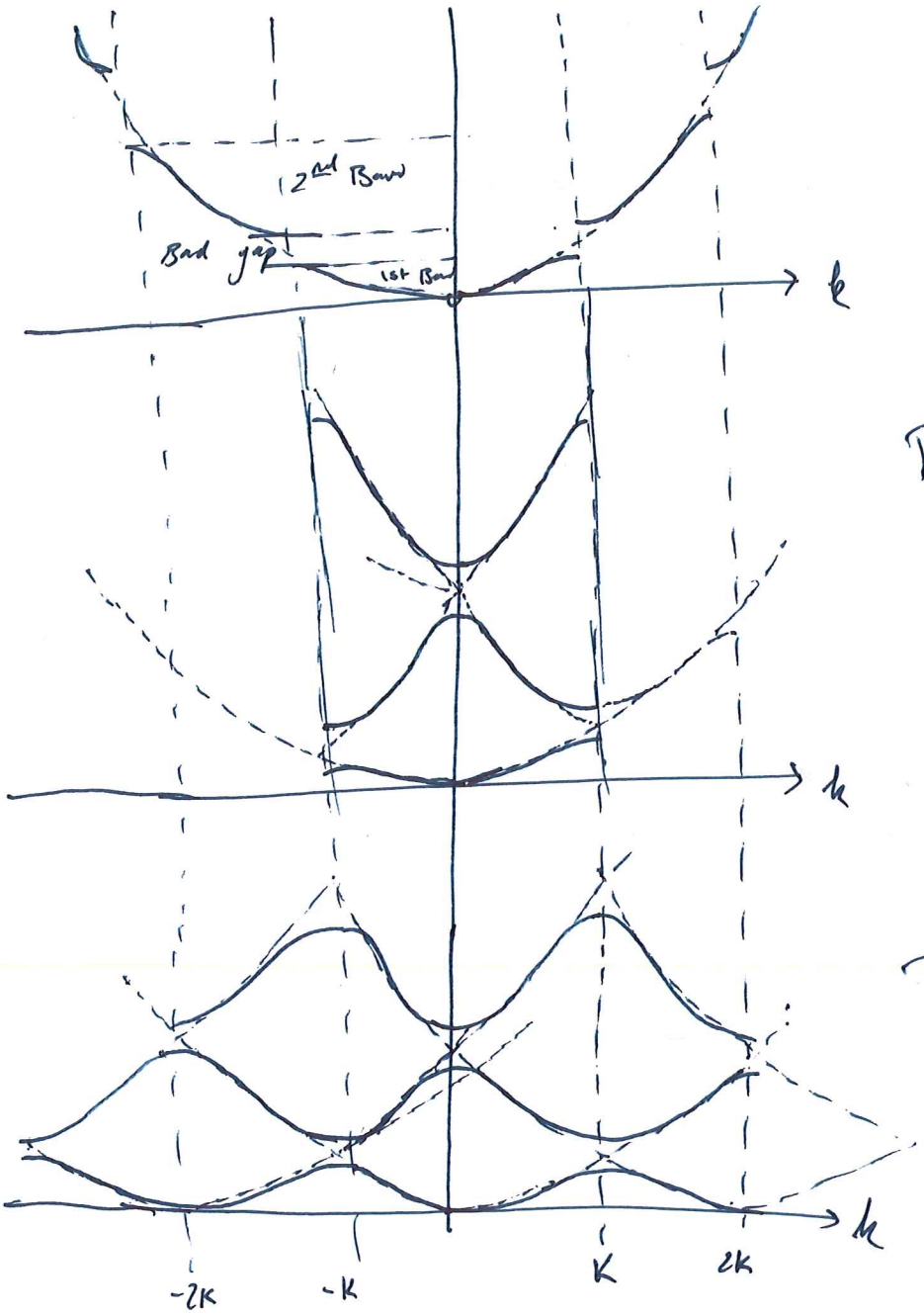
We do this so we can evaluate the matrix / diagonalize in this tridiagonal basis. for any given $\tilde{q}$

$$H\psi = E_\ell \begin{pmatrix} \ddots & & & & \\ & (\tilde{q}+(\ell+1))^2 & \tilde{V} & 0 & \cdots \\ \cdots & \tilde{V} & (\tilde{q}+\ell)^2 & \tilde{V} & 0 \\ & 0 & \tilde{V} & (\tilde{q}+(\ell-1))^2 & \tilde{V} \\ & & 0 & \tilde{V} & \ddots \\ & 0 & & & \end{pmatrix} \begin{pmatrix} \vdots \\ a^{\tilde{q}}_{\ell+1} \\ a^{\tilde{q}}_{\ell} \\ a^{\tilde{q}}_{\ell-1} \\ \vdots \end{pmatrix}$$

this matrix is strictly infinite in index ℓ for any $\tilde{q}$, but, as it turns out we can evaluate a finite # of elements $(-\ell_{max} \le \ell \le \ell_{max})$ to get nearly the exact answer for a # of bands near ℓ_{max}. There is an argument for energy why this too where based on $\tilde{V}$ only so many bands are "bound" so check when $\frac{\hbar^2(\ell\ell)^2}{2mR^2} \approx V_0$

So let's look at some code where I do this numerically. MATLAB code attached.

Some further comments about how band structure is typically drawn.



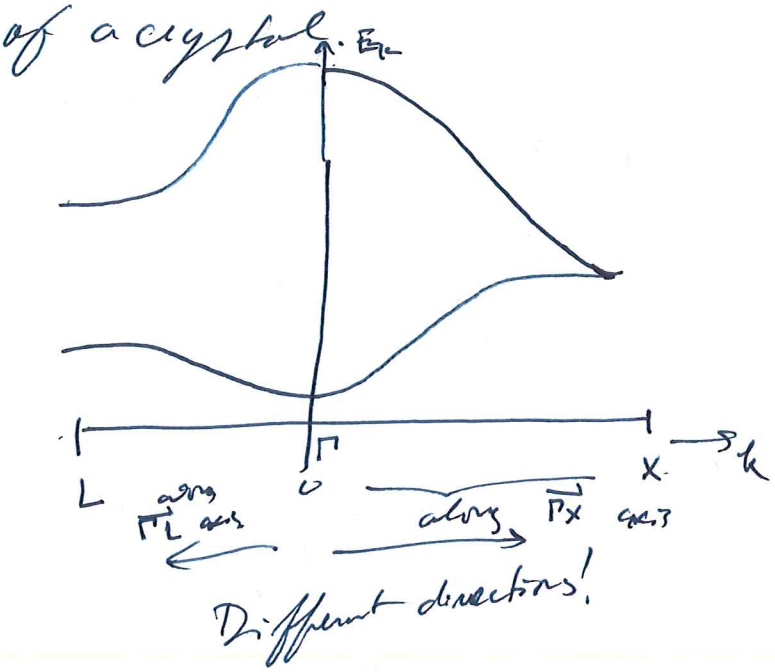
(I) Extended Zone Scheme

(II) Reduced Zone Scheme.

(III) Periodic Zone Scheme.

These are 3 different but identical ways to show this. (II) is the most common.

Just as a word of caution, this was all done for 1-D systems. Since condensed matter typically cares about real crystals which are 3-D, they sometimes draw them for many cross sections of a crystal.



$H \begin{pmatrix} a_N^{(k)} \\ \vdots \\ a_0^{(k)} \\ a_{-1}^{(k)} \\ \vdots \\ a_{-N}^{(k)} \end{pmatrix} \Rightarrow$ $H =$

$$\begin{pmatrix} \frac{\hbar^2(k+Ng)^2}{2m} & u & & & & \\ u & \frac{\hbar^2(k+(N-1)g)^2}{2m} & u & & & \\ & u & \ddots & u & & \\ & & u & \frac{\hbar^2(k+g)^2}{2m} & u & \\ & & & u & \frac{\hbar^2 k^2}{2m} & u \\ & & & & u & \frac{\hbar^2(k-g)^2}{2m} \ddots \\ & & & & & u \end{pmatrix}$$

restrict $k < \frac{\pi}{d}$

$$u \begin{pmatrix} \frac{\hbar^2}{2m}(k+Ng)^2 & \tilde{N} & & & \\ \tilde{N} & \frac{\hbar^2}{2m}(k+g)^2 & \tilde{N} & & \\ & \tilde{N} & \frac{\hbar^2}{2m}k^2 & \tilde{N} & \\ & & \tilde{N} & \frac{\hbar^2}{2m}(k-g)^2 & \tilde{N} \\ & & & \tilde{N} & \frac{\hbar^2}{2m}(k-Ng)^2 \end{pmatrix} \begin{pmatrix} a_2^k \\ a_1^k \\ a_0^k \\ a_{-1}^k \\ a_{-2}^k \end{pmatrix} = E \begin{pmatrix} a_2 \\ a_1 \\ a_0 \\ a_{-1} \\ a_{-2} \end{pmatrix}$$

$x = \frac{\hbar^2}{2m}\frac{1}{u}$

at some point the K.E. is much more than V and you can set the amplitudes for those $a_k^l \to 0$

$$\frac{u}{\left(\frac{\hbar^2 q^2}{2m}\right)} = \tilde{V}$$

$(x-1)^2 - (x)^2$ $\quad -2xN + N^2$
$+ 2(N-1)x + (N-1)^2$
$-2xN + 2x$
$+2xN + 2x - N^2$
$+ 2N + 1$
$-(2x + 2N + 1)$

$(x-N)^2 - (x-N+1)^2 \quad x^2$
$(x^2 - 2xN + N^2) - (x^2 - 2(N+1)x + (N-1)^2)$