Infinite 1-D Lattice II

<u>LAST TIME</u>:

$\mathbf{H}_2^+$ localization $\leftrightarrow$ tunneling: overlap
bonding and antibonding orbitals

R vs. $a_0 n^2$

distance below top of barrier

TIGHT-BINDING (Kronig-Penney) Model (see Baym pp. 116-122)

1-D ∞ lattice: 1 state per ion
tunneling only between nearest neighbors
∞ **H** matrix

$$\mathbf{H} = \begin{pmatrix} E_0 & -A & \ddots & 0 \\ -A & E_0 & \ddots & 0 \\ 0 & \ddots & \ddots & 0 \\ 0 & 0 & \ddots & \ddots \end{pmatrix}$$

$$\langle \nu_q | \mathbf{H} | \varphi \rangle = E \langle \nu_q | \varphi \rangle$$

$$|\varphi\rangle = \sum_{q=-\infty}^{\infty} c_q |\nu_q\rangle$$ Variational wavefunction. Minimize E.

$$0 = c_q (E_0 - E) - A(c_{q-1} + c_{q+1})$$ ∞ # of coupled equations

Usually solve for $\{c_q\}$ by setting determinant of coefficients = 0

and solving for E. Can't do this because determinant is ∞.

TRICK: expect equal probability of finding e^- on each lattice site by analogy to plane wave e^{ikx}, where probability density is uniform at all sites along x, try

$$c_q = e^{ikq\ell} \qquad x_q = q\ell$$

integer

distance between lattice sites

Notice that this is similar to free particle e^{ikx}, which seems rather strange because particle is never really free in "tight-binding" model.

$\left|c_q\right|^2 = 1$

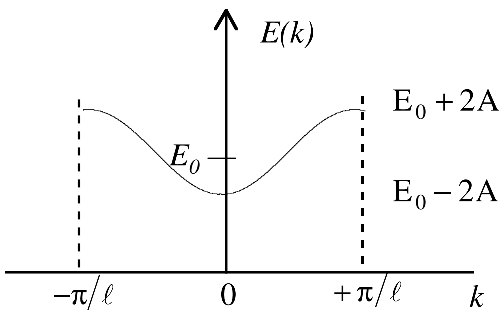
plug trial form for c_q into $0 = c_q(E_0 - E) - A(c_{q-1} + c_{q+1})$

$$0 = e^{ikq\ell}(E_0 - E) - Ae^{ikq\ell}\left(e^{-ik\ell} + e^{+ik\ell}\right)$$

divide through by $e^{ikq\ell}$

$0 = (E_0 - E) - A2\cos k\ell$

$$E(k) = E_0 - 2A\cos k\ell$$



E varies continuously over an interval 4A, where A is the adjacent site interaction strength or the "tunneling integral"

What happens when we look at k outside $-\pi/\ell \le k < \pi/\ell$
"1st Brillouin Zone"

$$c_k = e^{ikq\ell}$$

$$k' = k + \frac{2\pi}{\ell}$$ (one additional wavelength per lattice spacing ℓ)

$$c_{k'} = e^{i\left(k+\frac{2\pi}{\ell}\right)q\ell} = e^{ikq\ell}e^{i2\pi q} = e^{ikq\ell}$$

wavefunction is unchanged!

So if k goes outside 1st Brillouin Zone, get same ψ, so get same E

nothing new!

No point in allowing k to vary more widely than $-\pi/\ell \le k \le \pi/\ell$.

Unanswered Questions:

1. How many distinct orbitals are there in a band?

   N-atom periodic array. Periodic Boundary conditions:

   $$\left.\begin{array}{l}\text{longest } \lambda = \ell N \\ \text{shortest } \lambda = \ell\end{array}\right\} \text{N possible value of } \lambda = 2\pi / k$$

   $$\frac{2\pi}{\ell N} \leq |k| \leq \frac{2\pi}{\ell} \text{ in N steps}$$

   infinite lattice: $\frac{-\pi}{\ell} < k < \frac{\pi}{\ell}$ contains all the states generated from one state per atom.

2. What happens at $E > E_0 + 2A$?

   gap – no states allowed
   next higher state of each atom?
   free particle if E > work function

3. Orbitals not states! Two spin-orbitals per orbital.

   Antisymmetrization.
   Lowest band: all spins paired. No G term.
   $e^- - e^-$ repulsion raises overall E above that of single state of each atom
   Work function is smaller than single atom IP

4. How many e^- does each atom contribute to ψ?

   alkali: $1e^-$ ∅ half full band
   alkaline earth: $2e^-$∅ full band

Now take a closer look at $\varphi_k(x)$

$$\varphi(x) = \langle x | \varphi_k \rangle = \sum_{q=-\infty}^{+\infty} e^{ikq\ell} \underbrace{\langle x | v_q \rangle}_{v_q(x)}$$

$$v_q(x) = v_0(x - q\ell)$$ shift x by $-q\ell$ to get from site q to site 0

$$\varphi_k(x) = \sum_q e^{ikq\ell} v_0(x - q\ell)$$

translate entire φ by ℓ

$$\varphi_k(x+\ell) = \sum_q e^{ikq\ell} \underbrace{v_0(x - q\ell + \ell)}_{v_0(x-(q-1)\ell)}$$

$$= e^{ik\ell} \sum_q e^{ik(q-1)\ell} v_0(x - (q-1)\ell)$$

re-index summation

$$\varphi_k(x+\ell) = e^{ik\ell} \sum_q e^{ikq\ell} v_0(x - q\ell) = \underbrace{e^{ik\ell}}_{\text{translation of plane wave by } \ell} \varphi_k(x)$$

implies that it is possible to write $\varphi_k(x)$ in more general form

$$\boxed{\varphi_k(x) = e^{ikx} u_k(x)}$$ Bloch wave function

where $u_k(x+\ell) = u_k(x)$ perodicity of ℓ

e^{ikx} conveys translational symmetry of plane wave with wavevector k
$u_k(x)$ conveys translational symmetry of lattice with spacing ℓ

<u>Localized time dependent state :</u> wavepacket

We are gong to build intuitive insight by comparison to free particle.

Recall free particle:

$$\Psi(x,t) = (2\pi)^{-1/2} \int dk \underbrace{g(k)}_{\substack{\text{envelope}\\ \text{of k}\\ \text{centered}\\ \text{at } k_0}} e^{i[kx - \underbrace{E(k)t/\hbar}_{\omega t}]}$$

Group velocity: motion of stationary phase point (stationary with respect to k near k_0)

$$0 = \frac{d}{dk}[kx - Et/\hbar]\Big|_{k=k_0}$$

$$x_{center}(t) = \frac{dE}{dk}\Big|_{k_0} t/\hbar \qquad \text{take } \frac{d}{dt}$$

$$v_{center} = \frac{dE}{dk}\Big|_{k_0} \frac{1}{\hbar}$$

$$E = \frac{\hbar^2 k^2}{2m}$$

$$\frac{dE}{dk}\Big|_{k_0} = \frac{\hbar^2 k_0}{m}$$

$$v_{center} = v_G = \frac{1}{\hbar}\left[\frac{dE}{dk}\Big|_{k_0}\right] = \frac{\hbar k_0}{m}$$

free particle relationship between v_G and $\hbar k$,m

use this to understand motion in a periodic lattice

Up to here we have been analyzing the free particle.

for 1–D lattice

$$|\Psi(t)\rangle = (2\pi)^{-1/2}\int dk \underbrace{g(k)}_{\substack{\text{peak}\\ \text{at } k_0}} e^{-iE(k)t/\hbar}|\varphi_k\rangle$$

instead of asking for location of stationary phase point, ask for time dependent overlap of $\Psi(t)$ with specific lattice site $|\nu_q\rangle$.

$$\langle \nu_q|\Psi(t)\rangle = (2\pi)^{-1/2}\int dk\, g(k) e^{i[kq\ell - E(k)t/\hbar]}$$

because $|\varphi_k\rangle = \sum_{q=-\infty}^{\infty} e^{ikq\ell}|\nu_q\rangle$

$$\left(\text{same thing as } \phi_k(x) = \sum_{q=-\infty}^{\infty} e^{ikq\ell}\langle x\,|\,\nu_q\rangle\right)$$

We can use either state vector or wavefunction picture.

and $\langle \nu_q|$ picks out only the $e^{ikq\ell}$ term

because $\langle \nu_p|\nu_q\rangle = \delta_{pq}$

recall that $x = q\mathbf{l}$, so we can think of $\langle \nu_q|\Psi(t)\rangle$ as function of x,t

Overlap of $\Psi(t)$ with particluar lattice site $|\nu_q\rangle$. $\Psi(t)$ moves and sequentially overlaps succesive lattice sites.

meaningful only for regions of x near $q\ell$

$$\langle \nu_q|\Psi(t)\rangle = \chi(x,t) = (2\pi)^{-1/2}\int dk\, \underbrace{g(k)}_{\text{real part}}\, \underbrace{e^{i[kx - E(k)t/\hbar]}}_{\text{phase factor}}$$

ask for stationary phase factor (near $x = 0, \pm\ell, \pm 2\ell, \ldots$) with respect to k

$$0 = \frac{d}{dk}\left[kx - E(k)t/\hbar\right]$$

$$x_c(t) = \left.\frac{dE}{dk}\right|_{k_0} t/\hbar$$

wavepacket is created centered at $k=k_0$

$$v_G = \frac{dx_c}{dt} = \left.\frac{dE}{dk}\right|_{k_0} \frac{1}{\hbar}$$

Up to here, everything is identical for free particle and motion in a periodic lattice.

$$E(k) = E_0 - 2A\cos k\ell$$

Now use E×k relationship derived for periodic (tight binding) lattice.

$$\left.\frac{dE}{dk}\right|_{k_0} = 2A\ell \sin k_0\ell$$

$$v_G = \frac{2A\ell}{\hbar}\sin k_0\ell$$

quite different from plane wave result

$$V_G = \frac{\hbar k_0}{m}$$

Note that $v_G = 0$ when k_0 is at bottom ($k_0 = 0$) or top ($k_0 = \pm\pi/\ell$) of band.

Building of intuition:

* $v_G \propto A$ [as $|A|$ increases it becomes easier to take a step]

* $v_G \propto \ell$ (but $A\downarrow$ as $\ell\uparrow$)

(because tunneling rate decreases as ℓ increases) but if A is kept constant as ℓ increases, each step is longer so velocity will be higher

* $v_G = 0$ when $k_0 = 0$ and when $k_0 = \pm\pi/\ell$

bottom of band
Not a surprise because expect $k = 0 \varnothing v = 0$

top of band
Big surprise.
Use concept of "effective mass" to rationalize.

e^- cannot move if it is too close to edges of band

"Effective Mass:" free vs. lattice

$$v_G = \frac{\hbar k_0}{m} \qquad v_G = \frac{2A\ell \sin k_0\ell}{\hbar} \approx \hbar k_0\left[\frac{2A\ell^2}{\hbar^2}\right]$$

at small $k_0\ell \leftarrow$ near bottom of band

$\sin k_0\ell \approx k_0\ell$

compare the terms and identify reciprocal of the coefficient of $\hbar k_0$:

$$m_{eff} = \frac{\hbar^2}{2A\ell^2} \text{ at small } k_0\ell$$

* large interaction strength makes m_{eff} small
* large ℓ makes m_{eff} small (large jumps)

Next: How do we show that m_{eff} increases to ∞ at band edges ($k = \pm\pi/\ell$)?

When k_0 is near $\pm\pi/\ell$

$$k_0 = \pm\left(\frac{\pi}{\ell} - \varepsilon\right)$$

$$\sin k_0\ell = \sin\pm\left(\frac{\pi}{\ell} - \varepsilon\right)\ell \approx \pm\varepsilon\ell$$

$$v_G = \hbar k_0\left[\frac{2A\ell}{\hbar^2 k_0}\sin k_0\ell\right] \approx \pm\hbar k_0\left[\frac{2A\ell}{\hbar^2 k_0}\varepsilon\ell\right]$$

$$m_{eff} = \frac{\hbar^2 k_0}{2A\ell^2\varepsilon} \longrightarrow \infty \text{ as } \varepsilon \to 0$$

Full band: no e^- transport.

1/2 Full band: $m_{eff} = \frac{\sqrt{2}}{2}\frac{\hbar^2}{A\ell^2}$ (slightly heavier than at bottom of band)

Alternative approach to m_{eff}:

$E = p^2/2m$ for free particle

$\left(\frac{d^2E}{dp^2}\right)^{-1} = m$ Use this to define m_{eff}

$$E(k) = E_0 - 2A\cos k\ell$$

$$E(p) = E_0 - 2A\cos(p\ell/\hbar)$$

$$\frac{d^2E}{dp^2} = \left(2A\ell^2/\hbar^2\right)\cos k\ell \qquad \cos k\ell = 1 - \tfrac{1}{2}(k\ell)^2 + \ldots$$

at small $k\ell$ $\quad m_{eff} = \frac{\hbar^2}{2A\ell^2}$