project:

B-1

BAND STRUCTURE

We considered free e^- in a box explaining $C(T) = \gamma T$

Q: What are energy levels of electrons when we include the periodic potential of nuclei?

[Still ignoring interactions of e^- with each other]

Two ways to proceed: (1) Attempt to solve

$$\left[-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r}) \right] \psi(\vec{r}) = E\,\psi(\vec{r})$$

$$V(r) = \sum_{R_n} v(\vec{r} - \vec{R}_n)$$

$\vec{R}_n$: nuclear positions

(2) Creation/destruction operator approach

Analogy to SHO in QM course

(1) $$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 \psi(x) \right] = E\psi(x)$$

→ change of variables

extract asymptotic behavior $\psi(x) = f(x)e^{-cx^2}$

diff eqn for $f(x)$

power series soln

recursion reln

demand $f(x)$ not overwhelm e^{-cx^2}

Hermite polynomials

...

project:

B-2

Can imagine 3D problem with many $\vec{R}_n$ will be quite challenging. There are some general theorems one can prove (Bloch's theorem) based on periodicity of $V(\vec{r})$

Also can treat $V(r)$ perturbatively.

(2) Raising/Lowering (aka creation destruction operators)

$$\hat{x} = \sqrt{\frac{\hbar}{2m\omega}}\,(a + a^\dagger) \qquad q = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + i\sqrt{\frac{1}{2m\omega\hbar}}\,\hat{p}$$

$$\hat{p} = i\sqrt{\frac{\hbar m\omega}{2}}\,(a^\dagger - a) \qquad a^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} - i\sqrt{\frac{1}{2m\omega\hbar}}\,\hat{p}$$

$$[a, a^\dagger] = -i\frac{1}{2\hbar}[\hat{x},\hat{p}] + i\frac{1}{2\hbar}[\hat{p},\hat{x}] = 1$$

$[\hat{x},\hat{p}] = i\hbar$; $[\hat{p},\hat{x}] = -i\hbar$

$$aa^\dagger = a^\dagger a = 1$$

$$\hat{H} = \frac{1}{2}m\omega^2\hat{x}^2 + \frac{1}{2m}\hat{p}^2$$

$$= \frac{1}{2}m\omega^2\frac{\hbar}{2m\omega}\left(a^2 + aa^\dagger + a^\dagger a + a^{\dagger 2}\right) - \frac{1}{2m}\frac{\hbar m\omega}{2}\left(a^{\dagger 2} - a^\dagger a - aa^\dagger + a^2\right)$$

$$= \frac{1}{4}\hbar\omega\left(a^2 + aa^\dagger + a^\dagger a + a^{\dagger 2} - a^{\dagger 2} + a^\dagger a + aa^\dagger - a^2\right)$$

$$= \frac{1}{2}\hbar\omega\left(aa^\dagger + a^\dagger a\right) = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right)$$

project:

B-3

Given eigenstate - of $\hat{H}$: $\hat{H}|\phi\rangle = E|\phi\rangle$

$\hat{a}|\phi\rangle$ is also an eigenstate!

$a^\dagger a = aa^\dagger - 1$

$aa^\dagger = 1 + a^\dagger a$

$$\hat{H}\hat{a}|\phi\rangle = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \tfrac{1}{2}\right)\hat{a}|\phi\rangle$$

$$= \hbar\omega\left(\hat{a}\hat{a}^\dagger - 1 + \tfrac{1}{2}\right)\hat{a}|\phi\rangle$$

$$= \hbar\omega\,\hat{a}\left(\hat{a}^\dagger\hat{a} + \tfrac{1}{2} - 1\right)|\phi\rangle \qquad \hbar\omega\left(a^\dagger a + \tfrac{1}{2}\right)|\phi\rangle = E|\phi\rangle$$

$$= \hbar\omega\,\hat{a}\left(\frac{E}{\hbar\omega} - 1\right)|\phi\rangle$$

$$= (E - \hbar\omega)\,\hat{a}|\phi\rangle$$

$\therefore$ Eigenstate eigenvalue $E - \hbar\omega$

Similarly $a^\dagger|\phi\rangle$ Eigenstate eigenvalue $E + \hbar\omega$

So can build up collection of eigenstates given only 1 of them.

Find $a|\phi_0\rangle = 0|\phi_0\rangle$ eigenstate eigenvalue 0

$$|\phi_0\rangle = \pi^{-1/4} e^{-m\omega x^2/2\hbar}$$

proof: $\left[\sqrt{\frac{m\omega}{2\hbar}}\,\hat{x} + \frac{i}{\sqrt{2m\omega\hbar}}\,\frac{\hbar}{i}\frac{d}{dx}\right] e^{-m\omega x^2/2\hbar}$

$\hat{p}$

$$= \left(\sqrt{\frac{m\omega}{2\hbar}}\,x + \frac{\hbar}{\sqrt{2m\omega\hbar}}\left(\frac{-m\omega x}{\hbar}\right)\right) e^{-\frac{m\omega x^2}{2\hbar}}$$

$\sqrt{}\sqrt{}$

we ultimately denoted

$|n\rangle$ as state $\quad \hat{H}|n\rangle = (n+\frac{1}{2})\hbar\omega\,|n\rangle$

↑ $\qquad |0\rangle$ ← no quanta/particles present

Integer $n = 0, 1, 2, \ldots \qquad a^+|0\rangle = |1\rangle \qquad$ ($\frac{1}{2}\hbar\omega$ is "vacuum or zero-point energy")

$a^+|1\rangle = \sqrt{2}\,|2\rangle$

and thought of n as # of particles/quanta present,

(Also $a|0\rangle = 0$)

$\Rightarrow$ We will follow a similar strategy here, we will

write $\hat{H}$ in terms of creation/destruction operators

↑ $\qquad |0\rangle$ ← no e^- present

for e^- in a lattice

of ions $\qquad c^+|0\rangle = |1\rangle$ ← 1 electron present

Clarify 2 points

① → $c^+|1\rangle = \phi$ ← !! Cannot put 2 electrons in same state PAULI

Phonon pro

1 oscillator x → many oscillators x_ℓ → Normal modes

$$\hat{H} = \sum_q \hbar\omega_q \left(\hat{a}_q^+ \hat{a}_q + \tfrac{1}{2}\right)$$

↑

We treated this classically

$\vec{F} = m\vec{a}$ for all the masses

→ $\omega_q^2 = \frac{2k}{m}\left[1 - \cos q\right]$

Normal modes

But if we had used qm all that would have happened is collection of oscillators with frequencies ω_q.

So (2) $c^+ \rightarrow c_n^+$

↑ create e^- (quantum / particle) on the ion at location $\vec{R}_n$

States $|0\rangle \rightarrow |0\,0\,0\,0\,0\ldots 0\rangle$ no e^- on any of the ions.

$$c_1^+ |0\,0\,0\,0\,0,\ldots 0\rangle = |1\,0\,0\,0\,0\ldots 0\rangle$$

$$c_3^+ |0\,0\,0\,0\,0,\ldots 0\rangle = |0\,0\,1\,0\,0\ldots 0\rangle$$

etc.

Hamiltonian $\hat{H} = -t \sum_l (c_l^+ c_{l+1} + c_{l+1}^+ c_l)$

can derive this from $\hat{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$

In fact $t = \underset{RR'}{} \langle \phi(r+R) | \hat{H} | \phi(r+R') \rangle$

$V(x) = \sum_n v(x - R_n)$

in same way as derive $\hat{H} = \hbar\omega(a^+a + 1/2)$

from $\hat{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$

$\hat{H}|00000\ldots0\rangle = \phi$ because destruction operators act and no particles present

$\hat{H}|0010\ldots0\rangle$

$= \hat{H}\, c_3^\dagger |00000\ldots0\rangle$ terms in $\hat{H} = -t\sum_\ell (c_\ell^\dagger c_{\ell+1} + c_{\ell+1}^\dagger c_\ell)$ not involving $\ell = 3$ will vanish

$=$

$c_5^\dagger c_4 c_3^\dagger |00000\ldots0\rangle = \phi$

no e^- present on site 4 $\rightarrow \phi$

BUT $c_4^\dagger c_3 c_3^\dagger |00000\ldots0\rangle$

$= c_4^\dagger c_3 |0010\ldots0\rangle$

$= c_4^\dagger |0000\ldots0\rangle$

$= |0001\ldots0\rangle$ ← very reasonable intuitively.

e^- "hops" from site $\vec{R}_3$ to site $\vec{R}_4$ (adjacent nucleus)

In general — nucleus j

$$\hat{H}\,|000\ldots010\ldots0\rangle$$

$$= -t\,|000\ldots100\ldots0\rangle - t\,|000\ldots001\ldots0\rangle$$

nucleus $j-1$ — nucleus $j+1$

MATRIX FOR $\hat{H}$:

$$\begin{bmatrix} 0 & -t & & & & & \\ -t & 0 & -t & & & & \\ & -t & 0 & -t & & & \\ & & -t & 0 & -t & & \\ & & & -t & 0 & -t & \\ & & & & -t & 0 & \\ & & & & & & \ddots \end{bmatrix}$$

$$\begin{bmatrix} A & B & & & B \\ B & A & B & & \\ & B & A & B & \\ & & & & \\ B & & & & \end{bmatrix}$$

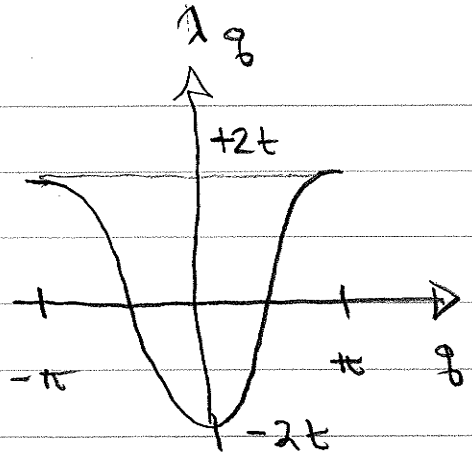
HW:

$$\lambda = A + 2B\cos q$$

So energy band is

$$\lambda_1 = \lambda_q = -2t \cos q$$

↗ more usual notation



Actually, to better connect with our original description we might expect

$$E - 2t \cos q$$

↗ original atomic level out of which band develops

$$\begin{pmatrix} E & -t & & \\ -t & E & -t & \\ & -t & E & -t \\ & & & \end{pmatrix}$$

↑

$$H = \sum_\ell E c_\ell^+ c_\ell - t \sum_\ell \left(c_\ell^+ c_{\ell+1} + c_{\ell+1}^+ c_\ell \right)$$

Where does this come from

$$E C_3^+ C_3 \,|00100\ldots\rangle$$

$$= E C_3^+ \,|00000\ldots\rangle$$

$$= E\,|00100\ldots\rangle$$

So $E C_3^+ C_3$ does not change state (e^- location)

It appears on diagonal of matrix,