BAND STRUCTURE

We considered free electron in a box explaining 6(\pi^2) = \pi^2\hbar^2.

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

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

\[ V(\vec{r}) = \sum \frac{\psi^2(\vec{r} - \vec{R}_n)}{R_n} \]

nuclear positions

2) Creation/destruction operator approach

Analogy to SHO in QM course

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

\(D\) change of variables

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

diff eqn for \(f(x)\)

power series soln

recursion reln

demand \(f(x)\) not oscillates in \(-\frac{cx^2}{2}\)

DIVOGA

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

Also can treat \( V(r) \) perturbatively.

2. Raising lowering (aka creation destruction operators)

\[
\hat{X} = \sqrt{\frac{\hbar}{2m}} \left( a + a^+ \right) \quad q = \sqrt{\frac{\mu}{2\hbar}} \hat{X} + i \sqrt{\frac{1}{2m\hbar}} \hat{P}
\]

\[
\hat{P} = i \sqrt{\frac{\hbar}{2m}} \left( a^+ - a \right) \quad \hat{a}^+ = \sqrt{\frac{\mu}{2\hbar}} \hat{X} - i \sqrt{\frac{1}{2m\hbar}} \hat{P}
\]

\[
[a, a^+] = -\frac{i}{\hbar} \left[ \hat{X}, \hat{P} \right] + \frac{i}{\hbar} \left[ \hat{P}, \hat{X} \right] = 1
\]

\[
\frac{\hat{a}}{\hbar} - \frac{\hat{a}^+}{\hbar} \quad aa^+ = a^+ a = 1
\]

\[
\hat{H} = \frac{\hbar^2}{2m} \hat{X}^2 + \frac{1}{2m} \hat{P}^2
\]

\[
= \frac{\hbar^2}{2m} \left( a^2 + aa^+ + a^+ a + a^+ a^2 \right) - \frac{\hbar}{2m} \frac{\mu}{2} \left( a^2 - a^+ a - aa^+ + a^2 \right)
\]

\[
= \frac{1}{4} \hbar \mu \left( a^2 + aa^+ + a^+ a + a^2 - a^2 + a + a^+ + a^2 \right)
\]

\[
= \frac{1}{2} \hbar \mu (aa^+ + a^+ a) = \hbar \mu (a^+ a + \frac{1}{2})
\]
Given eigenstate of \( H \): \( \hat{H} |\phi\rangle = E |\phi\rangle \)

\( |\alpha\rangle \) is also an eigenstate.
\[ q^+ q = q q^+ = 1 \]

\[ \hat{H} |\alpha\rangle = \hbar \omega (q^+ q + \frac{1}{2}) |\alpha\rangle \]

\[ q q^+ = 1 + q^+ q \]

\[ \hat{H} |\alpha\rangle = \hbar \omega (q q^+ - 1 + \frac{1}{2}) |\alpha\rangle \]

\[ |\alpha\rangle = \hbar \omega a \left( \frac{E}{\hbar \omega} - 1 \right) |\phi\rangle \]

\[ |\alpha\rangle = (E - \hbar \omega) a |\phi\rangle \]

\[ \Rightarrow \text{Eigenstate eigenvalue } E - \hbar \omega \]

Similarly \( a^+ |\phi\rangle \) 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 \( \phi \)

\[ |\phi_0\rangle = \frac{1}{\sqrt{\pi}} e^{-\frac{m \omega x^2}{2\hbar}} \]

Proof:

\[ e^{\frac{m \omega x^2}{2 \hbar}} \left( \frac{1}{2m \omega \hbar} \frac{d}{dx} + \frac{i}{2m \omega \hbar} \right) \]

\[ \hat{p} = \left( \sqrt{\frac{m \omega}{2 \hbar}} x + \frac{\hbar}{\sqrt{2m \omega \hbar}} \right) e^{-\frac{m \omega x^2}{2 \hbar}} \]
We ultimately denote
\[ |n\rangle \quad \text{as state} \quad \hat{N} |n\rangle = (n+\frac{1}{2})\hbar \omega |n\rangle \]
\( P \)
\[ a^\dagger |0\rangle = |1\rangle \quad (\text{vacuum or two-point energy}) \]
\[ a^\dagger |1\rangle = |2\rangle |2\rangle \]
\( \text{and thought of } n \text{ as } \# \text{ of particles/quantum present,} \]
\( \text{(Also } a |0\rangle = 0) \)

\[ \Rightarrow \text{We will follow a similar strategy here. We will write } \hat{N} \text{ in terms of creation/annihilation operators,} \]
\[ \text{for } e^- \text{ in lattice} \]
\[ |0\rangle \text{ } \text{ } \text{no } e^- \text{ present} \]
\[ \text{of ions} \]
\[ (a^\dagger |0\rangle = |1\rangle \text{ } \text{ } \text{\# 1 electron present} \]

\[ \begin{align*}
|0\rangle \rightarrow e^\dagger |1\rangle & \neq |0\rangle \quad \text{Pauli} \\
& \text{put 2 electrons} \\
& \text{in same state} \\
& \text{Pauli}
\end{align*} \]

Phonon pro

1 oscillator \( \xrightarrow{p} \) many oscillators \( x \) \( \rightarrow \) Normal modes

\[ \hat{H} = \sum_{q} \hbar \omega_q (\hat{a}_q^\dagger \hat{a}_q + \frac{1}{2}) \]

We treated this classically
\[ F = \vec{ma} \quad \text{for} \quad \omega^2 = \frac{2K}{m} \left[ 1 - \cos \theta \right] \]
all the masses
Normal modes

But if we had used \( q m \)
all that would have happened is collection of oscillators with frequencies \( \omega_q \).
\[ 0 \quad \mathbf{2} \quad c^+ \rightarrow c^+_n \]

Create a (quantum) particle on the ion at location \( R_n \)

States \( |0\rangle \rightarrow |0\ 0\ 0\ 0\ 0\rangle \) no electron on any of the ions.

\[
\begin{align*}
|c^+ |0\ 0\ 0\ 0\ 0\rangle &= |1\ 0\ 0\ 0\ 0\rangle \\
|c^+_3 |0\ 0\ 0\ 0\ 0\rangle &= |0\ 0\ 1\ 0\ 0\rangle \\
\end{align*}
\]

e tc.

Hamiltonian \( \hat{H} = -t \sum_{\ell} (c^+_\ell c_{\ell+1} + c^+_\ell c_{\ell+1}) \)

Can derive this from \( \hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \)

In fact \( t = \langle \phi_0(r+R) | \hat{H} | \phi_0(r+R') \rangle \)

\[ \sum_n \frac{1}{n} \psi(x-R_n) \]

In some way as derive \( \hat{H} = t w (\delta_{a\ell} + \delta_{a\ell'}) \)

from \( \hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{1}{2} \mu w^2 x^2 \)
\[ |00000...0\rangle = \phi \] because destruction operators act and no particles present.

\[ \hat{H} |0010...0\rangle = \hat{H} c^+_3 |00000...0\rangle \]

\[ \hat{H} = \sum_{\alpha \beta} \epsilon_{\alpha \beta} c^+_\alpha c_\beta + \epsilon_{e11} e^+ e^- \]

Terms in \( e^+ e^- \) do not involve \( \phi = 3 \) will vanish.

\[ e^+_5 e^+_4 c^+_3 |00000...0\rangle = \phi \]

no \( e^- \) present on site 4 → 0\( \phi \)

But \[ c^+_4 c^+_3 c^+_3 |00000...0\rangle \]

\[ = c^+_4 c^+_3 |0010...0\rangle \]

\[ = c^+_4 |00000...0\rangle \]

\[ = |00010...0\rangle \]

A very reasonable intuitively,

\( e^- \) "hops" from site \( R_3 \)

to site \( R_4 \)

(adjacent nucleus)
In general, the nucleus $i$:

\[ H |000\ldots010\ldots0\rangle = -t |000\ldots100\ldots0\rangle - t |000\ldots001\ldots0\rangle \]

\[ \begin{array}{cccc}
  0-t & -t & 0-t & 0-t \\
  -t & 0-t & 0-t & 0-t \\
  0-t & -t & 0-t & 0-t \\
  0-t & 0-t & 0-t & 0 \\
\end{array} \]

Matrix for $|U\rangle$:

\[ \begin{array}{cccc}
  A & B & & \\
  B & A & B & \\
  B & A & B & \\
  B & & & \\
\end{array} \]

HW:

\[ \lambda = A + 2B \cos q \]
So energy band is

\[ \lambda_2 = \lambda g = -2t \cos q \]

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

\[
\begin{pmatrix}
    E - t \\
    -t & E - t \\
    -t & E - t
\end{pmatrix}
\]

\[ H = \sum \limits_{\ell} E \psi_{\ell} \psi_{\ell}^\dagger - t \sum \limits_{\ell} \left( \psi_{\ell+1}^\dagger \psi_{\ell} + \psi_{\ell} \psi_{\ell+1} \right) \]
Where does this come from

\[ \text{EC}_3^+ | 00100 \ldots > \]

\[ = \text{EC}_3^+ | 00000 \ldots > \]

\[ = E | 00100 \ldots > \]

So \( \text{EC}_3^+ \) does not change state (\( e^- \) location).

It appears as diagonal of matrix.