PH 575 Spring 2014

Lecture #7
2 and 3 dimensions: Sutton Ch. 4 pp 74 -> 80

Space lattice formed by the combination of unit cells.
Summary: 1-D Chain, n-n, PBC

\[
\Psi_m = \sum_{j=1}^{N} \frac{1}{\sqrt{N}} e^{i j \frac{2\pi m}{N}} |j\rangle \\
\Psi_k = \sum_{j=1}^{N} \frac{1}{\sqrt{N}} e^{i j k a} |j\rangle
\]

\[
E^{(m)} = \alpha + 2\beta \cos \left( \frac{2m\pi}{N} \right) \\
E(k) = \alpha + 2\beta \cos(ka)
\]
MgO - an ionic crystal

Density of states

Dispersion relation

Fermi energy

www.crystal.unito.it/tutojan2004/tutorials/G_properties/}
img47.gif&imgrefurl=http://www.crystal.unito.it/tutojan2004/
tutorials/G_properties/properties_tut.html
The 2-dimensional square lattice:
① Band structure (dispersion relation)
② Wave functions (electron density)
③ Brillouin zone
④ Fermi surface

① Band structure (dispersion relation)

1-D to 2-D

\[ x \rightarrow \vec{r} \]
\[ k \rightarrow \vec{k} \]
\[ |j\rangle \rightarrow |\vec{R}\rangle \]
\[ |\Psi_m\rangle \rightarrow |\Psi_{\vec{k}}\rangle \]
\[ c_j^{(m)} \rightarrow c_{\vec{k}}(\vec{R}) \]
\[ |\Psi_{\vec{k}}\rangle = \sum_{\vec{R}} c_{\vec{k}}(\vec{R}) |\vec{R}\rangle \quad \text{MO made from AOs} \]

By analogy with 1D (you should prove it …)

\[ c_{\vec{k}}(\vec{R}) = \frac{1}{\sqrt{N}} e^{i\vec{k} \cdot \vec{R}} \]

This form ensures

1. Normalization
2. Periodicity in electron density
3. Appropriate translational symmetry of the wave function (PH grads, you should study this and ask me about it)

\[ \langle \vec{r} + \vec{T} | \Psi_{\vec{k}} \rangle = e^{i\vec{k} \cdot \vec{T}} \langle \vec{r} | \Psi_{\vec{k}} \rangle \]

\[ \Psi_{\vec{k}}(\vec{r} + \vec{T}) = e^{i\vec{k} \cdot \vec{T}} \Psi_{\vec{k}}(\vec{r}) \]

\( T \) is any lattice vector. \( R \) is a special lattice vector that starts from the origin. \( N \) is the number of atoms (lattice sites).
\[ |\Psi_{\bar{k}}\rangle = \frac{1}{\sqrt{N}} \sum_{\bar{R}} e^{i\bar{k} \cdot \bar{R}} |\bar{R}\rangle \]

Apply Schrödinger equation: \( \hat{H} |\Psi_{\bar{k}}\rangle = E(\bar{k}) |\Psi_{\bar{k}}\rangle \)

\[ \sum_{\bar{R}} e^{i\bar{k} \cdot \bar{R}} \hat{H} |\bar{R}\rangle = E(\bar{k}) \sum_{\bar{R}} e^{i\bar{k} \cdot \bar{R}} |\bar{R}\rangle \]

Project onto the other atomic orbitals \( |\bar{R}'\rangle \)

\[ \sum_{\bar{R}} e^{i\bar{k} \cdot \bar{R}} \langle \bar{R}' | \hat{H} | \bar{R}\rangle = E(\bar{k}) \sum_{\bar{R}} e^{i\bar{k} \cdot \bar{R}} \langle \bar{R}' | \bar{R}\rangle \]

\[ \sum_{\bar{R}} e^{i\bar{k} \cdot \bar{R}} \langle \bar{R}' | \hat{H} | \bar{R}\rangle = E(\bar{k}) e^{i\bar{k} \cdot \bar{R}'} \]

This is the dispersion relation (3D also) - but we need the Hamiltonian matrix!

\[ E(\bar{k}) = \sum_{\bar{R}} e^{i\bar{k} \cdot (\bar{R} - \bar{R}')} \langle \bar{R}' | \hat{H} | \bar{R}\rangle \]
\[ E(\vec{k}) = \sum_R e^{i\vec{k} \cdot (\vec{R} - \vec{R}')} \langle \vec{R}' | \hat{H} | \vec{R} \rangle \]

\[ \langle \vec{R}' | \hat{H} | \vec{R} \rangle = \begin{cases} 
\alpha & \text{if } \vec{R} = \vec{R}' \\
\beta & \text{if } \vec{R} \text{ and } \vec{R}' \text{ are n.n} \\
0 & \text{otherwise}
\end{cases} \]

Pick any \( R' \) to evaluate \( E(k) \) - all give same result. Choose \((0,0)\).

\[ E(\vec{k}) = \sum_R e^{i\vec{k} \cdot \vec{R}} \langle \vec{0} | \hat{H} | \vec{R} \rangle \]

\[ E(k_x, k_y) = \alpha + \beta e^{ik_x a} + \beta e^{-ik_x a} + \beta e^{ik_y a} + \beta e^{-ik_y a} \]

\[ E(k_x, k_y) = \alpha + 2\beta \cos(k_x a) + 2\beta \cos(k_y a) \]
\[ E(k_x,k_y) = \alpha + 2\beta \left[ \cos(k_x a) + \cos(k_y a) \right] \]

What values can \( k_x \) and \( k_y \) take?

Unique solutions for (PBC)

\[
\begin{align*}
-\frac{N_x}{2} & \leq m_x \leq \frac{N_x}{2} \\
-\frac{N_y}{2} & \leq m_y \leq \frac{N_y}{2}
\end{align*}
\]

\[ k_x \equiv \frac{2\pi m_x}{N_x a} ; k_y \equiv \frac{2\pi m_y}{N_y a} \]

\[ -\frac{\pi}{a} \leq k_x , k_y \leq \frac{\pi}{a} \]
$$E(k_x, k_y) = \alpha + 2\beta \left[ \cos(k_x a) + \cos(k_y a) \right]$$

How to represent this in a plot? What values can $k_x$ and $k_y$ take?

Unique solutions for

$$-\frac{\pi}{a} \leq k_x, k_y \leq \frac{\pi}{a}$$

$$\alpha = 1$$
$$\beta = -0.3$$
$$a = 1$$
\[ E(k_x, k_y) = \alpha + 2\beta \left[ \cos(k_x a) + \cos(k_y a) \right] \]
Simple cubic lattice

Dispersion relation?

\[ E(k) = \alpha + 2\beta \left( \cos(k_xa) + \cos(k_ya) + \cos(k_za) \right) \]

<table>
<thead>
<tr>
<th></th>
<th>Band width</th>
<th>#n.n.</th>
</tr>
</thead>
<tbody>
<tr>
<td>1D</td>
<td>4\beta</td>
<td>2</td>
</tr>
<tr>
<td>2D</td>
<td>8\beta</td>
<td>4</td>
</tr>
<tr>
<td>3D</td>
<td>12\beta</td>
<td>6</td>
</tr>
</tbody>
</table>
Reciprocal lattice of a square lattice is also square, but this is not true of all lattice types. First Brillouin zone contains ALL unique $k$ points, and they are closer to $k = 0$ than any other. Just as $T$ is a vector that connects 2 lattice points in REAL space, so $G$ is a vector that connects 2 points in $k$-space or reciprocal space.
The Fermi surface:
Not all states are occupied with electrons. At $T=0$, the states fill sequentially from lowest to highest energy, consistent with the Pauli Principle. Highest occupied state defines the Fermi energy. Highest occupied states define a surface in $k$-space called Fermi surface. Fermi surface is still defined at $T \neq 0$. 
$$E(k_x, k_y) = \alpha + 2\beta \left[ \cos(k_x a) + \cos(k_y a) \right]$$

$$E(k_x, k_y) \approx \alpha + 2\beta \left[ 1 - \frac{1}{2}(k_x a)^2 + 1 - \frac{1}{2}(k_y a)^2 \right]$$

$$E_F = \alpha + 4\beta - \beta a^2 \left( k_{F,x}^2 + k_{F,y}^2 \right) = \alpha + 4\beta - \beta a^2 k_F^2$$

$$k_F = \sqrt{\frac{E_F - \alpha - 4\beta}{-\beta a^2}}$$

- Low filling, Small $E_F$,
  - $k_F \approx 0$

- Circle!

- $\alpha = 1$
- $\beta = -0.3$
- $a = 1$

Fermi surface
$\alpha = 1$
$\beta = -0.3$
$a = 1$
\[ E_F = \alpha = \alpha + 2\beta \left[ \cos(k_{F,x}a) + \cos(k_{F,y}a) \right] \]

\[ \cos(k_{F,x}a) + \cos(k_{F,y}a) = 0 \]

\[ k_{F,y} = \pm k_{F,x} \pm \pi / a \]

Half filling
\[ E_F = \alpha \]

Square!

\[ \alpha = 1 \]
\[ \beta = -0.3 \]
\[ a = 1 \]

Fermi surface
\[ E_F = \alpha = \alpha + 2\beta \left[ \cos(k_F,x,a) + \cos(k_F,y,a) \right] \]

Expand cosines about \( \pi/a \) - circles again, but "empty" circles, centered on \((\pm \pi/a, \pm \pi/a)\)

Almost full
\[ E_F \approx \alpha - 2\beta, \quad k_F \approx \pi/a - \delta \]
Fermi surfaces for different band fillings
Real Fermi surfaces can be measured by applying magnetic fields and measuring magnetoresistance at low $T$ in different directions (Schubnikov-de Haas oscillations). Other methods, too (PES).

http://www.phys.ufl.edu/fermisurface/
Position of the Fermi energy in the bands determines whether the material is a metal or an insulator.

Filled bands imply insulating or semiconducting behavior. (Depends on distance of Fermi energy from band edge compared to thermal energies).

Partially filled bands result in metallic behavior. Thermal energies do not determine number of carriers.