# Intro. to Electro-physics <br> The basics of a band theory 

## Previous

Crystal waves (i.e. phonons) in periodic 1D crystal


This lecture
Electrons (i.e. electron waves) in periodic 1D crystal

Jaesang Lee<br>Dept. of Electrical and Computer Engineering<br>Seoul National University<br>(email: jsanglee@snu.ac.kr)

## Electrons in 1D crystal

- Orbitals in a 1D crystal = A linear chain of atomic orbitals
- A single orbital on the $n^{\text {th }}$ atom $:|n\rangle$
- Periodic boundary conditions: $(N+1)^{\text {th }}$ atom $=1$ st atom
- All of the orbitals are orthonormal to each other : $\langle m \mid n\rangle=\delta_{m n}$

Orbitals in a 1D crystal constructed by a Linear Combination of Atomic Orbitals (LCAO) $\triangleq|\psi\rangle=\sum_{n} \phi_{n}|n\rangle$
<Tight-binding chain>
One orbital per atom;
electrons can hop from one atom
to the neighboring atom

<Periodic boundary condition>

## Schrödinger's equation (1/3)

- Schrödinger's equation for a 1D crystal

$$
H|\psi\rangle=E|\psi\rangle
$$

- Wave function: $|\psi\rangle=\sum \phi_{n}|n\rangle \quad$ (Linear Combination of Atomic Orbitals)
$-H|\psi\rangle=E|\psi\rangle \longrightarrow \sum_{m}\langle n| H|m\rangle \phi_{m}=E \phi_{n} \quad(n=1,2,3, \cdots, N) \quad$ (A set of $N$ eigenvalue equations)
- The matrix element of the Hamiltonian : $\langle n| H|m\rangle \triangleq H_{n m} \quad(N \times N$ matrix $)$
- The Hamiltonian (i.e., the energy operator)

$$
H=K+\sum_{j} V_{j}, \text { where }\left\{\begin{array}{l}
K=\frac{p^{2}}{2 m}: \text { Kinetic energy } \\
V_{j}=V\left(\boldsymbol{r}-\boldsymbol{R}_{j}\right): \text { Coulombic potential of the electron due to } j^{\text {th }} \text { nucleus }
\end{array}\right.
$$

where $\boldsymbol{r}$ : The position of the electron, $\boldsymbol{R}_{j}$ : The position of the $j$-th nucleus

## Schrödinger's equation (2/3)

- The matrix element of the Hamiltonian

The matrix element $H_{n m}=\langle n| H|m\rangle$ The Hamiltonian

- $H|m\rangle=\left(K+V_{m}\right)|m\rangle+\sum_{j \neq m} V_{j}|m\rangle$,
- $K+V_{m}$ : The Hamiltonian if there were only an isolated $m^{\text {th }}$ atom
where $\left(K+V_{m}\right)|m\rangle=\varepsilon_{\text {atomic }}|m\rangle$
- $\varepsilon_{\text {atomic }}$ : Eigen-energy of an electron on the isolated $m^{\text {th }}$ atom

$$
H_{n m}=\langle n| H|m\rangle=\varepsilon_{\text {atomic }} \delta_{n m}+\sum_{j \neq m}\langle n| V_{j}|m\rangle
$$

- Meaning of $\langle n| V_{j}|m\rangle$
- An electron on $m^{\text {th }}$ atom can hop onto $n^{\text {th }}$ atom via the interaction with the $j^{\text {th }}$ atom
- Simplifying assumption: Such a hopping occurs only if $n$ and $m$ are the nearest neighbor

$$
\sum_{j \neq m}\langle n| V_{j}|m\rangle=\left\{\begin{array}{ll}
V_{0}, & n=m \longrightarrow \text { Coulomb potential due to all the nuclei except the } m^{\text {th }} \text { one } \\
-t, & n=m \pm 1 \\
0, & \text { otherwise }
\end{array} \longrightarrow\right. \text { Hopping term }
$$

## Schrödinger's equation (3/3)

$$
\sum_{j \neq m}\langle n| V_{j}|m\rangle= \begin{cases}V_{0}, & n=m \\ -t, & n=m \pm 1 \\ 0, & \text { otherwise }\end{cases}
$$

- The Hamiltonian matrix element (contd.)

$$
H_{n m}=\langle n| H|m\rangle=\varepsilon_{\text {atomic }} \delta_{n m}+\sum_{j \neq m}\langle n| V_{j}|m\rangle=\left(\varepsilon_{\text {atomic }}+V_{0}\right)-t\left(\delta_{n+1, m}+\delta_{n-1, m}\right)
$$

$$
H_{n m}=\left(\begin{array}{ccccc}
\varepsilon_{0} & -t & 0 & \cdots & 0 \\
-t & \varepsilon_{0} & -t & \cdots & 0 \\
0 & -t & \varepsilon_{0} & \cdots & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & 0 & -t & \varepsilon_{0}
\end{array}\right)
$$

- Let $\varepsilon_{0} \triangleq \varepsilon_{\text {atomic }}+V_{0}$ : Kinetic energy + Coulomb potential due to all the nuclei
- $t$ : the hopping energy that allows for an electron to move from one site to another site
- Magnitude of $t$ depends on how close together the adjacent orbitals are


## Solution to Schrödinger's equation

- Results of tight-binding model in 1D
- Proposed coefficient : $\phi_{n}=\frac{e^{-j k n a}}{\sqrt{N}}$ (for time-independent S.E $\rightarrow$ no $\omega$ term!)
- The substitution into the Schrödinger's equation :

$$
\sum_{m} H_{n m} \phi_{m}=E \phi_{n} \longrightarrow\left\{\begin{array}{l}
\text { (l.h.s.) } \frac{1}{\sqrt{N}}\left[\varepsilon_{0} e^{-j k n a}-t\left(e^{-j k(n+1) a}+e^{-j k(n-1) a}\right)\right] \\
\text { (r.h.s) } \frac{1}{\sqrt{N}} E e^{-j k n a}
\end{array}\right.
$$

- Dispersion relation : $E=\varepsilon_{0}-2 t \cos (k a)$
- Periodic in $k \rightarrow k+2 \pi / a$
- Periodic boundary conditions with $N$ unit cells $\rightarrow \Delta k=2 \pi / L$
(* $N$ unit cells $\rightarrow N$ allowed $k$-values)


## Dispersion relation for a 1D crystal



- Important characteristics

- Allowed $k$ value : quantized in units of $\Delta k=2 \pi / L$ (c.f., continuous for free electrons)
- Energy band : The "finite" energy range where the electrons can be populated
- Bandwidth (4t) determined by the magnitude of hopping (or the interatomic distance)


## Characteristics of band structure $(1 / 2)$

- Energy band
- Hopping $(t)$ splits the $N$ electronic states into some higher energy states and some lower energy states with respect to $\varepsilon_{0}$
- Splitting becomes intense as interatomic spacing decreases

- Total energy of all of the electrons
- Average energy of all $N$ states : $\varepsilon_{0}$
- If the band is completely filled : $E=N \varepsilon_{0}$
- If the band is not filled : $E<N \varepsilon_{0}$
( $\because$ Some of the higher energy states not filled)
- $E-N \varepsilon_{0} \triangleq \Delta E$ : Binding energy of the crystal



## Characteristics of band structure (2/2)

- Dispersion relation near the bottom of the band

$$
E(k)=\varepsilon_{0}-2 t \cos (k a) \rightarrow E(k) \approx t a^{2} k^{2}+C
$$

( $\because$ Expanded for small $k \sim 0$ )

- Effective mass

$$
E(k)=t a^{2} k^{2}+C=\frac{\hbar^{2} k^{2}}{2 m^{*}}+C
$$

- The dispersion near the bottom of the band =

The dispersion of free particles with effective mass $m^{*}$

Taylor series

## Electrons filling a band

- Monovalent atomic crystal
- Each atom donates "one" electron into the band
- The crystal consists of $N$ atoms (or unit cells)
$\rightarrow N$ possible $k$-values
- Half-filled band : Due to "two" possible spin states for electrons, only $N / 2 k$-values can be occupied
- Only a small amount of energy (e.g. $\boldsymbol{E}$-field) needed to shift the

Fermi surface and move electrons $\rightarrow$ An electric current induced!

- Such a monovalent atomic crystals are mostly metallic!


## - Divalent atomic crystal

- Completely filled band: no response of the electrons upon the application of an $\boldsymbol{E}$-field $\rightarrow$ No electric current!
- Such a divalent atomic crystals are mostly insulators!





## Metal-to-insulator transition

## Previous tight-binding model

One atom per unit cell
One orbital per atom


Realistically
One atom per unit cell
Several orbitals per atom (e.g., s, p, d, f, $\cdots$ )

## Monatomic, Divalent

One atom per unit cell
$\approx$
Two orbitals per atom

Diatomic, monovalent
Two different atoms per unit cell
One orbital per atom


## Energy gap (From diatomic crystal vibrations)



Reduced zone scheme

"Extended" zone scheme

- Above is when $\kappa_{1} \neq \kappa_{2}$ and $\kappa_{1}<\kappa_{2}$
- The case of $\kappa_{1}=\kappa_{2}$
- A simple monatomic chain with a lattice constant $a / 2$
- The 1st Brillouin zone : $\left[-\frac{2 \pi}{a}, \frac{2 \pi}{a}\right]$
- When the two atoms are only slightly different
- A small perturbation applied to a situation where all atoms are identical
- Due to the perturbation, a small energy gap opens up at the zone boundary, but the rest of the dispersion mostly looks alike that of the monatomic chain!


## Energy gap (From electronic band)

- Two different atoms per unit cell
- Two bands exist (two possible energy eigenstates per each $k$ )
- Energy gap
- A gap between two bands where no eigenstates exist
- A gap opens up at the Brillouin zone boundary (i.e., where the Fermi surface is)



Divalent atom
Insulator


Monovalent atom Insulator


Monovalent atom
Semiconductor

