## Introductory Nanotechnology <br> ~Basic Condensed Matter Physics ~



## Atsufumi Hirohata

Department of Electronics
The University offork

y
Quick Review over the Last Lecture
Wave / particle duality of an electron:

|  | Particle nature | Wave nature |
| :---: | :--- | :--- |
| Kinetic energy |  |  |
| Momentum |  |  |

Brillouin zone (1st \& 2nd) :


Fermi-Dirac distribution (T-dependence) :


## Contents of Introductory Nanotechnology

```
First half of the course
Basic condensed matter physics
1. Why solids are solid?
2. What is the most common atom on the earth ?
```

3. How does an electron travel in a material ?
4. How does lattices vibrate thermally ?
5. What is a semi-conductor ?
6. How does an electron tunnel through a barrier?
7. Why does a magnet attract / retract ?
8. What happens at interfaces ?

Second half of the course
Introduction to nanotechnology (nano-fabrication / application)

## How Does an Electron Travel

 in a Material ?- Group / phase velocity
- Effective mass
- Hall effect
- Harmonic oscillator
- Longitudinal / transverse waves
- Acoustic / optical modes
- Photon / phonon

Electron wave under a uniform E:


Group velocity :

$$
\boldsymbol{v}_{\mathrm{g}}=\frac{d \omega}{d \boldsymbol{k}}
$$

Wave packet

Here, energy of an electron wave is

$$
E=h v=\hbar \omega
$$

Accordingly,

$$
\boldsymbol{v}_{\mathrm{g}}=\frac{1}{\hbar} \frac{d E}{d \boldsymbol{k}}
$$

Therefore, electron wave velocity depends on gradient of energy curve $E(\mathbf{k})$.

## Equation of Motion for an Electron with $\boldsymbol{k}$

For an electron wave travelling along $\mathbf{E}$ :

$$
\frac{d \boldsymbol{v}_{\mathrm{g}}}{d t}=\frac{1}{\hbar} \frac{d}{d t}\left(\frac{d E}{d \boldsymbol{k}}\right)=\frac{1}{\hbar} \frac{d}{d \boldsymbol{k}}\left(\frac{d E}{d \boldsymbol{k}}\right) \frac{d \boldsymbol{k}}{d t}=\frac{1}{\hbar} \frac{d^{2} E}{d \boldsymbol{k}^{2}} \frac{d \boldsymbol{k}}{d t}
$$

Under $\mathbf{E}$, an electron is accelerated by a force of $-q \mathbf{E}$.
In $\Delta t$, an electron travels $\mathbf{v}_{\mathrm{g}} \Delta t$, and hence $\mathbf{E}$ applies work of $(-q \mathbf{E})\left(\mathbf{v}_{\mathrm{g}} \Delta t\right)$.
Therefore, energy increase $\Delta \mathrm{E}$ is written by

$$
\Delta E=-q \boldsymbol{E} \boldsymbol{v}_{\mathrm{g}} \Delta t=-q \boldsymbol{E} \frac{1}{\hbar} \frac{d E}{d \boldsymbol{k}} \Delta t
$$

At the same time $\Delta \mathbf{E}$ is defined to be

$$
\Delta E=\frac{d E}{d \boldsymbol{k}} \Delta \boldsymbol{k}
$$

From these equations,
$\Delta \boldsymbol{k}=-\frac{1}{\hbar} q \boldsymbol{E} \Delta t \quad \therefore \frac{d \boldsymbol{k}}{d t}=-\frac{1}{\hbar} q \boldsymbol{E} \quad \therefore \hbar \frac{d \boldsymbol{k}}{d t}=-q \boldsymbol{E}$
$\rightarrow$ Equation of motion for an electron with $\mathbf{k}$

By substituting $\hbar \frac{d \boldsymbol{k}}{d t}=-q \boldsymbol{E}$ into $\frac{d \boldsymbol{v}_{\mathrm{g}}}{d t}=\frac{1}{\hbar} \frac{d^{2} E}{d \boldsymbol{k}^{2}} \frac{d \boldsymbol{k}}{d t}$

$$
\frac{d \boldsymbol{v}_{\mathrm{g}}}{d t}=-\frac{1}{\hbar^{2}} \frac{d^{2} E}{d \boldsymbol{k}^{2}} q \boldsymbol{E}
$$

By comparing with acceleration for a free electron :

$$
\begin{aligned}
& \frac{d \boldsymbol{v}}{d t}=-\frac{1}{m} q \boldsymbol{E} \\
& m^{*}=\hbar^{2} /\left(\frac{d^{2} E}{d \boldsymbol{k}^{2}}\right)
\end{aligned}
$$

$\rightarrow$ Effective mass

## Hall Effect

Under an applications of both a electrical current $\mathbf{i}$ an magnetic field $\mathbf{B}$ :


Lattice vibration in a crystal :

spring constant: $k$


Hooke's law :

$$
M \frac{d^{2} u}{d t^{2}}=-k x
$$

Here, we define
$\omega=\sqrt{\frac{k}{M}} \quad \therefore \frac{d^{2} u}{d t^{2}}=-\omega^{2} u$
$\therefore u(t)=A \sin (\omega t+\alpha)$
$\rightarrow$ 1D harmonic oscillation

Displacement per unit length :

$$
\delta=\frac{(\partial u / \partial x) d x}{d x}=\frac{\partial u}{\partial x}
$$

Young's law (stress $=$ Young's modulus $\times$ strain) :

$$
\frac{\boldsymbol{F}}{S}=\boldsymbol{E}_{\mathrm{Y}} \frac{\partial u}{\partial x} \quad S: \text { area }
$$

Here,

$$
+\boldsymbol{F}(x+d x)=\boldsymbol{F}(x)+(\partial \boldsymbol{F} / \partial x) d x+\cdots
$$

For density of $\rho$,

$\rho S d x \frac{\partial^{2} u}{\partial t^{2}}=\frac{\partial \boldsymbol{F}}{\partial \boldsymbol{x}} d x$
$\therefore \frac{\partial^{2} u}{\partial t^{2}}=\frac{\boldsymbol{E}_{\mathrm{Y}}}{\rho} \frac{\partial^{2} u}{\partial x^{2}} \equiv v_{\ell} \frac{\partial^{2} u}{\partial x^{2}}$
$\rightarrow$ Wave eqution in an elastomer
Therefore, velocity of a strain wave (acoustic velocity) :

$$
v_{\ell} \equiv \sqrt{\frac{\boldsymbol{E}_{\mathrm{Y}}}{\rho}}
$$

Longitudinal wave : vibrations along or parallel to their direction of travel


Transverse wave : vibrations perpendicular to their direction of travel




http://www12.plala.or.jp/ksp/wave/waves/

## Acoustic / Optical Modes

For a crystal consisting of 2 elements ( $k$ : spring constant between atoms) :

By assuming,

$$
\begin{aligned}
& \left\{\begin{array}{l}
u_{n}(n a, t)=A \exp \{i(\omega t-q n a)\} \\
v_{n}(n a, t)=B \exp \{i(\omega t-q n a)\}
\end{array}\right. \\
& \left\{\begin{array}{c}
-M \omega^{2} A=k B\{1+\exp (i q a)\}-2 k A \\
-m \omega^{2} B=k A\{\exp (-i q a)+1\}-2 k B
\end{array}\right. \\
& \therefore\left\{\begin{array}{cc}
\left(2 k-M \omega^{2}\right) A-k\{1+\exp (i q a)\} B=0 \\
-k\{\exp (-i q a)+1\} A+\left(2 k-m \omega^{2}\right) B=0
\end{array}\right. \\
& \therefore\left|\begin{array}{cc}
2 k-M \omega^{2} & -k\{1+\exp (i q a)\} \\
-k\{\exp (-i q a)+1\} & 2 k-m \omega^{2}
\end{array}\right|=0
\end{aligned}
$$

Therefore, $\omega^{2}=k\left(\frac{1}{M}+\frac{1}{m}\right) \pm k \sqrt{\left(\frac{1}{M}+\frac{1}{m}\right)^{2}-\frac{4}{M m} \sin ^{2} \frac{q a}{2}}$
For $q a=0$,

$$
\left\{\begin{array}{l}
\omega_{+}=\sqrt{2 k\left(\frac{1}{M}+\frac{1}{m}\right)} \\
\omega_{-}=0
\end{array}\right.
$$

For $q a \sim 0$,

$$
\left\{\begin{array}{l}
\omega_{+} \approx \sqrt{2 k\left(\frac{1}{M}+\frac{1}{m}\right)} \\
\omega_{-} \approx \sqrt{\frac{k / 2}{M+m}} q a
\end{array}\right.
$$

For $q a=\pi$,

$$
\left\{\begin{array}{l}
\omega_{+}=\sqrt{\frac{2 k}{m}} \\
\omega_{-}=\sqrt{\frac{2 k}{M}}
\end{array}\right.
$$

## Figure 22.10

Dispersion relation for the diatomic linear chain. The lower branch is the acoustic branch and has the same structure as the single branch present in the monatomic case (Figure 22.8). In addition, there is now an optical branch (upper branch.)


* N. W. Ashcroft and N. D. Mermin, Solid State Physics (Thomson Learning, London, 1976).


## Why Acoustic / Optical Modes ?

Oscillation amplitude ratio between $M$ and $m(A / B)$ :
Optical mode : $\frac{m}{M}$
Neighbouring atoms changes their position in opposite directions, of which amplitude is larger for $m$ and smaller for $M$, however, the cetre of gravity stays in the same position.

Acoustic mode : 1
All the atoms move in parallel.

|  | $k=0$ | small $k$ |  | large $k$ |
| :---: | :---: | :---: | :---: | :---: |
| Optical | $\frac{\circ \circ 0}{\circ} \frac{\circ}{\circ}$ |  |  |  |
| Acoustic | 0.00000 |  |  |  |

Quantum hypothesis by M. Planck (black-body radiation) :

$$
E=\frac{1}{2} h v+n h v \quad(n=0,1,2, \ldots)
$$

Here, $h v$ : energy quantum (photon)
mass: 0, spin : 1
Similarly, for an elastic wave, quasi-particle (phonon) has been introduced by P. J. W. Debye.
$E=\frac{1}{2} \hbar \omega+n \hbar \omega \quad(n=0,1,2, \ldots)$
Oscillation amplitude : larger $\rightarrow$ number of phonons: larger

## What is a conductor?

Number of electron states (including spins) in the 1st Brillouin zone :

$$
\int_{-\pi / a}^{\pi / a} 2 \frac{L}{2 \pi} d k=\frac{2 L}{a}=2 N \quad\left(N=\frac{L}{a}\right)
$$

Here, $N$ : Number of atoms for a monovalent metal As there are $N$ electrons, they fill half of the states. By applying an electrical field $\mathbf{E}$, the occupied states become asymmetric.

- E increases asymmetry.
- Elastic scattering with phonon / non-elastic scattering decreases asymmetry.
$\rightarrow$ Stable asymmetry
$\rightarrow$ Constant current flow
$\rightarrow$ Conductor:
Only bottom of the band is filled by electrons



Forbidden

Allowed with unoccupied upper band.

