재료의 전자기적 성질

Electronic Properties of Materials

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Grading

30-min Quiz #1	10%
Midterm Exam	25%
30-min Quiz #2	10%
Final Exam	35%
Homework	20%

(# absence more than 4 lectures = F)

Evaluation: Relative

A:	20%
B:	30%
C:	30%
D–F:	20%

Overall Contents

Part Ⅰ Fundamentals

Electron Theory : Matter Waves

Chap. 1 Introduction

Chap. 2 The Wave-Particle Duality (Review)

Chap. 3 The Schördinger Equation (Review)

Chap. 4 Solution of the Schördinger Equation for Four Specific Problems

Chap. 5 Energy Bands in Crystals

Chap. 6 Electrons in a Crystal

1. Introduction

3 approaches for the undersdtanding of the electronic properties of materials

- In 19C, a phenomenological description of the experimental observation

:Continuum theory

Only macroscopic quantities and interrealted experimental data
The empirical laws: Ohm's law, the Maxwell equations, Newton's law, Hagen-Rubens equation

- At the turn to 20C, introcuction of atomistic principles into the description of matter

: Classical electron theory

Postulated that free electrons in materials drift as a response to an external force and interac with certain lattice atoms
Drude equations

- At the beginning of 20C, explanation of experimental observations

: Quantum theory

Quantum theory lacks vivid visualization of the phenomena which it descibes. Thus, a considerable effort needs to be undertaken to comprehend its basic concepts; but mastering its principles leads to a much deeper understanding of the electronic properties of materials.

2. The Wave-Particle Duality

- **Light : electromagnetic wave**

  light quantum (called a photon)

Energy $E = h\nu = \hbar\omega$

Planck constant $\hbar = \dfrac{h}{2\pi}$

In 1924 yr, de Broglie $\lambda p = h$

"wave nature of electrons" "matter wave"

For a general wave $\upsilon = \nu\lambda$

"wave number"

$$k = \frac{2\pi}{\lambda} \longrightarrow \upsilon = \frac{\omega}{k}$$

2. The Wave-Particle Duality

➤ Description of electron wave

- The simplest waveform: harmonic wave
- A wave function (time- and space-dependent)

$$\Psi = \sin(kx - \omega t)$$

Electron wave: a combination of several wave trains

Assuming two waves,

$$\Psi_1 = \sin[kx - \omega t]$$

$$\Psi_2 = \sin[(k + \Delta k)x - (\omega + \Delta\omega)t]$$

Mathematical description of traveling waves

Consider a string stretched along the x axis whose vibrations are in the y direction.

Assuming simple harmonic motion,

At $t = 0$, $y = A\sin 2\pi \nu t$

where A is the amplitude of the vibrations

If t is replaced by $\frac{x}{\upsilon} - t$, then $y = A\sin 2\pi \nu(\frac{x}{\upsilon} - t)$: **Wave Formula**

where υ is the wave speed

Since the wave speed is given by $\upsilon = \nu\lambda$,

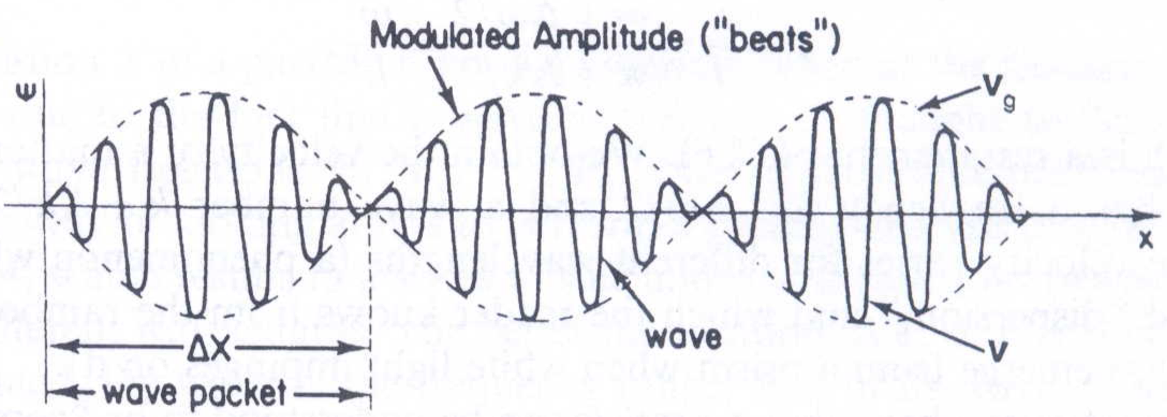
we have $y = A\sin 2\pi(\frac{x}{\lambda} - \nu t) = A\sin(kx - \omega t)$

➢ Description of electron wave

Supposition of two waves:

$$\Psi_1 + \Psi_2 = \Psi = \underbrace{2\cos\left(\frac{\Delta\omega}{2}t - \frac{\Delta k}{2}x\right)}_{\text{modulated amplitude}} \cdot \underbrace{\sin\left[\left(k + \frac{\Delta k}{2}\right)x - \left(\omega + \frac{\Delta\omega}{2}\right)t\right]}_{\text{sine wave}}$$

modulated amplitude **sine wave**



"Wave Packet"

Figure 2.1. Combination of two waves of slightly different frequencies. ΔX is the distance over which the particle can be found.

The extreme conditions

(a) No variation in angular frequency and wave number : monochromatic wave

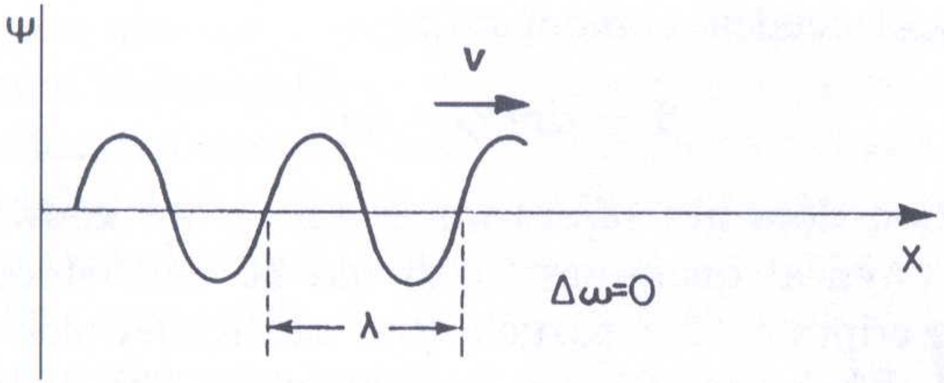


Figure 2.2. Monochromatic matter wave ($\Delta\omega$ and $\Delta k = 0$). The wave has constant amplitude. The matter wave travels with the phase velocity, v.

The extreme conditions

(b) Very large variation in angular frequency and wave number

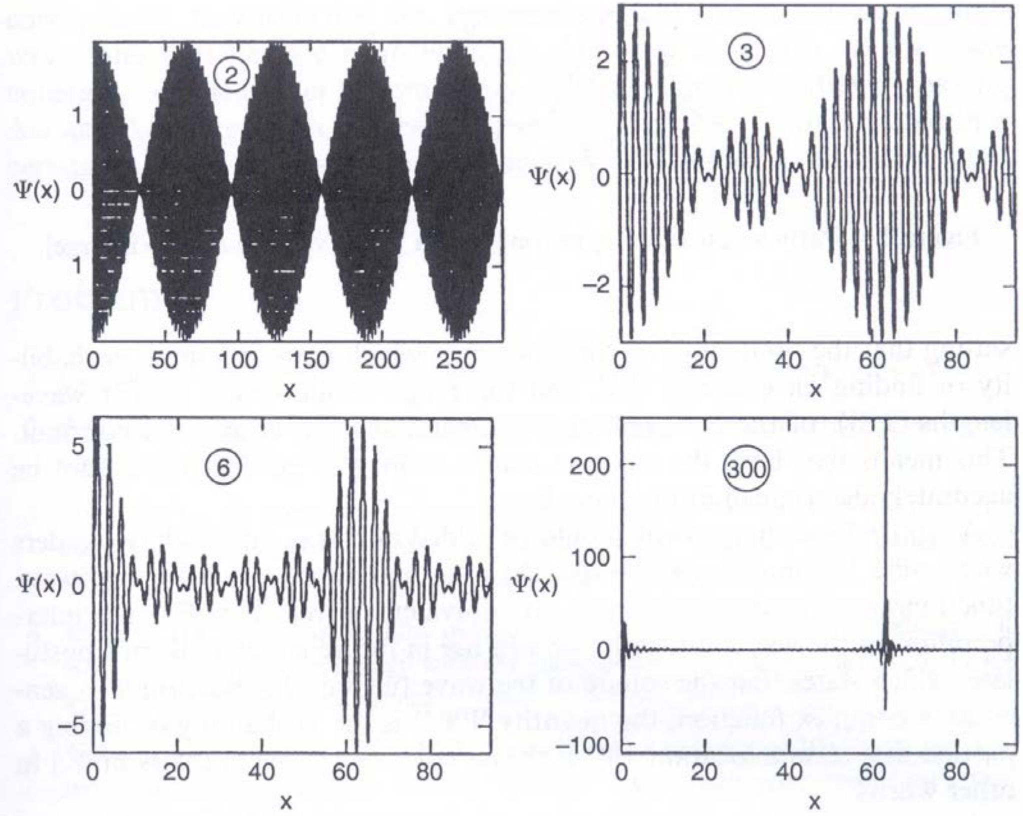


Figure 2.3. Superposition of Ψ-waves. The number of Ψ-waves is given in the graphs. (See also Fig. 2.1 and Problem 2.8.)

Phase velocity:

velocity of a matter wave

$$\upsilon = \frac{x}{t} = \frac{\omega + \Delta\omega / 2}{k + \Delta k / 2} = \frac{\omega'}{k'}$$

Group velocity:

velocity of a pulse wave

(i.e., a moving particle)

$$\upsilon_g = \frac{x}{t} = \frac{\Delta\omega}{\Delta k} = \frac{d\omega}{dk}$$

The extreme conditions

(b) Very large variation in angular frequency and wave number (continued)

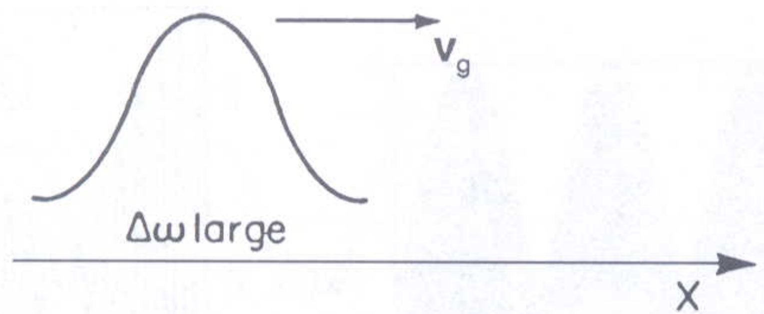


Figure 2.4. Particle (pulse wave) moving with a group velocity v_g ($\Delta\omega$ is large).

Heisenberg's Uncertainty principle $\Delta p \cdot \Delta X \geq h$

Probability of finding a particle at a certain location

$$\Psi\Psi^* dxdydz = \Psi\Psi^* d\tau$$

3.1 The Time-Independent Schrödinger Equation

- Time-independent Schrödinger equation: *a vibration equation*

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E - V)\psi = 0$$

$$\nabla^2\psi = \frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}$$

where, m = the (rest) mass of the electron,

E = the total energy of the system,

E_{kin} = kinetic energy,

V = the potential energy (or potential barrier)

$$E = E_{kin} + V$$

- Applicable to the calculation of the properties of atomic systems in *stationary* **conditions**

3.2 The Time-Dependent Schrödinger Equation

Time-dependent Schrödinger equation: *a wave equation*

$$\nabla^2\Psi - \frac{2mV}{\hbar^2}\Psi - \frac{2mi}{\hbar}\frac{\partial\Psi}{\partial t} = 0$$

Since $\Psi(x,y,z,t) = \psi(x,y,z)\cdot e^{i\omega t}$

$$\frac{\partial\Psi}{\partial t} = \psi i\omega e^{i\omega t} = \Psi i\omega \longrightarrow \omega = -\frac{i}{\Psi}\cdot\frac{\partial\Psi}{\partial t}$$

and $E = \nu h = \omega\hbar \longrightarrow E = -\frac{\hbar i}{\Psi}\cdot\frac{\partial\Psi}{\partial t}$

Then $\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0 \longrightarrow \nabla^2\Psi - \frac{2mV}{\hbar^2}\Psi - \frac{2mi}{\hbar}\frac{\partial\Psi}{\partial t} = 0$

Applying differential operators to the wave function $\mathrm{E} = -\hbar i\frac{\partial}{\partial t}$ $\mathbf{p} = -\hbar i\nabla$

(Hamiltonian operators)

$$E_{total} = E_{kin} + E_{pot} = \frac{p^2}{2m} + V \longrightarrow -\hbar i\frac{\partial\Psi}{\partial t} = \frac{\hbar^2 i^2}{2m}\nabla^2\Psi + V\Psi$$