VE320 Intro to Semiconductor Devices

Chapter 2 & 3

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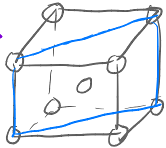
PS：中文都是后加的，
这个版本的PPT上有一些小错误，RC前传的无note版已经修改了，
大差不差

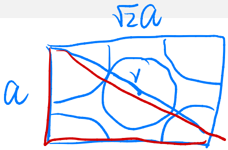
看不懂欢迎来找我捏

老师进来搞得我很紧张
脑子和嘴都瓦特了 TT sorry

Lattice Types

这个面的原子密度最大





$4r = \sqrt{3}a$

$r = \frac{\sqrt{3}a}{4}$

在FCC中，6个面原子密度相同且最大，因此

$4r = \sqrt{2}a$

$r = \frac{\sqrt{2}}{4}a$

- Simple cubic: $\#\text{atom} = \frac{1}{8} \times 8 = 1$, $r(\text{atom}) = \frac{a}{2}$
- Body-centered cubic: $\#\text{atom} = \frac{1}{8} \times 8 + 1 = 2$, $r(\text{atom}) = \frac{\sqrt{3}a}{4}$
- Face-centered cubic: $\#\text{atom} = \frac{1}{8} \times 8 + \frac{1}{2} \times 6 = 4$, $r(\text{atom}) = \frac{\sqrt{2}a}{4}$
- Volume Density $= \frac{\#\text{atoms per unit cell}}{\text{volume of unit cell}}$
- Surface Density $= \frac{\#\text{atoms per lattice plane}}{\text{area of lattice plane}}$

* What is the radius of atom?

Ans: Half the equilibrium distance between two adjacent atoms in a cell along the direction of maximum atomic density.

Miller Index

- Steps:
  - Find the intersection (∞ if parallel to the axis)
  - Write the reciprocal
  - Times the lowest common denominator
- All parallel planes are equivalent.
- $[hkl]$: Crystal direction
  (hkl): Crystal plane direction
  $[hkl]$ direction is perpendicular to the (hkl) plane in the simple cubic lattice.

Basic: Wave-particle Duality

- For matters: $p = mv$, $E = \frac{1}{2}mv^2$
- For photons: $p = \frac{h\nu}{c}$, $E = h\nu$, $\nu = \frac{\lambda}{c}$
- For both: $k = \frac{2\pi}{\lambda}$, $p = \frac{h}{\lambda}$, $\hbar = \frac{h}{2\pi}$

* $E=mc^2$ for photons.

Basic Concepts

$\Psi(x,t) = \psi(x)\cdot\phi(t)$

一维非相对论的薛定谔方程

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x,t)}{\partial x^2} + V(x)\psi(x,t) = i\hbar\frac{\partial\psi(x,t)}{\partial t}$$

- Wave function: $\Psi(x)$
- Probability density function: $|\Psi(x)|^2 = \Psi(x) \times \Psi^*(x)$.
  Note: In quantum mechanics, we cannot determine the exact coordinates of a particle, only the probability that it is at a certain coordinate position.

① 将ψ(x,t)代入
② 左右同除ψ(x,t)

$$-\frac{\hbar^2}{2m}\cdot\frac{1}{\psi(x)}\frac{\partial^2\psi(x)}{\partial x^2} + V(x) = i\hbar\frac{1}{\phi(t)}\frac{\partial\phi(t)}{\partial t} = \eta$$

- Schrodinger Equation:

经典正弦波 → $\phi(t) = e^{\frac{\eta}{i\hbar}t}$

$$\frac{\partial^2\Psi(x)}{\partial x^2} + \frac{2m}{\hbar}(E - V(x))\Psi(x) = 0$$

$\begin{cases} \omega = \eta/\hbar \\ E = h\nu = h\frac{\omega}{2\pi} \end{cases} \Rightarrow \eta = \boxed{E}$

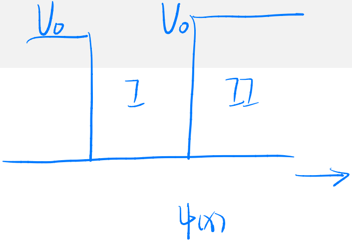
where m: mass of the particle, V(x): potential function, E: total energy of the particle.

* what if $V(x) \to \infty$?

- Boundary condition:
  - $\int_{-\infty}^{\infty} |\Psi(x)|^2 dx = 1$
  - $\Psi(x)$ must be finite and continuous
  - $\partial\Psi(x)/\partial x$ must be finite and continuous

$|\psi(x)| < \infty$

Solution of 2nd Order DE



- $\frac{\partial^2 y}{\partial x^2} = k^2 y$

$$y = Ae^{kx} + Be^{-kx}$$

- $\frac{\partial^2 y}{\partial x^2} = -k^2 y$

$$\begin{aligned} y &= Ae^{ikx} + Be^{-ikx} \\ &= C\sin(kx) + D\cos(kx) \end{aligned}$$

Electrons in Free Space

- Suppose $V(x) = 0$

$$\frac{\partial^2 \Psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\Psi(x) = 0$$

- General solution:

$$\Psi(x) = Ae^{ikx} + Be^{-ikx}$$

  where the wave number $k = \sqrt{\frac{2mE}{\hbar}}$.

- Particles in free space behave as traveling waves, and we have $k = \sqrt{\frac{2mE}{\hbar}} = \frac{p}{\hbar}, \lambda = \frac{h}{p} = \frac{2\pi}{k}$.

Electrons in Infinite Quantum Well

- $\frac{\partial^2\Psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\Psi(x) = 0, \begin{cases} V(x) = +\infty, & x \le 0 \text{ or } x \ge a \\ V(x) = 0, & 0 < x < a \end{cases}$
- General solution:

$Ae^{jkx} + Be^{jkx}$

$$\Psi(x) = A_1 \cos kx + A_2 \sin kx$$

- Boundary condition:

$$\begin{cases} \Psi(x=0) = \Psi(x=a) = 0 \\ \int_0^a \Psi(x)\Psi^*(x) = 1 \end{cases}$$

$\frac{\partial \psi(x)}{\partial x}$

- Conclusion:

$$A_1 = 0, A_2 = \sqrt{\frac{2}{a}}, k_n = \frac{n\pi}{a}, n = 1, 2, 3, \cdots$$

$$\Psi(x) = \sqrt{\frac{2}{a}} \sin k_n x, \quad E = E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2}$$

Electrons in Finite Quantum Well

- $\frac{\partial^2 \Psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}(E - V(x))\Psi(x) = 0, \begin{cases} \underline{V(x) = V_0}, & x \leq 0 \text{ or } x \geq a \\ V(x) = 0, & 0 < x < a \end{cases}$
- General solution:

$$\Psi(x) = \begin{cases} Ae^{-ik_1 x} + Be^{ik_1 x}, & k_1 = \sqrt{\frac{2m(E-V_0)}{\hbar^2}}, x \underline{\leq 0 \text{ or } x} \geq a \\ Ce^{-ik_2 x} + De^{ik_2 x}, & k_2 = \sqrt{\frac{2mE}{\hbar^2}}, 0 < x < a \end{cases}$$

① $E > V_0$ sinusoid

② $E < V_0$ k_1 complex

$\psi(x) = \exp(\quad)$

- Boundary condition:

0, a

$$\Psi(x)|_{\cancel{x=0}} \text{ continuous}$$

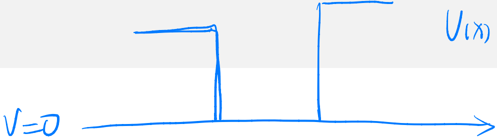
$\psi'(x)|_{x=0,a}$ continuous

$$\Psi(x)|_{x=a} \text{ continuous}$$

$$\int_{-\infty}^{\infty} \Psi(x)\Psi^*(x) = 1$$

- Conclusion: Depending on the relationship between E and V_0, $\Psi(x)$ is different.

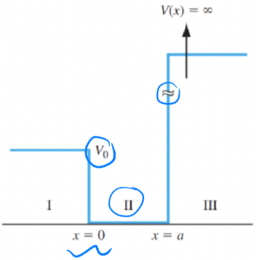
Exercise



Homework 1 Exercise 1.7

Exercise 1.7

Consider the one-dimensional potential function shown in Figure 1. Assume the total energy of an electron is $E < V_0$. (a) Write the wave solutions that apply in each region. (b) Write the set of equations that result from applying the boundary conditions. (c) Show explicitly why, or why not, the energy levels of the electron are quantized.



Exercise

a> Region I. $V(x)=V_0$ $\quad \frac{\partial^2 \psi_1(x)}{\partial x^2} - \frac{2m}{\hbar}(V_0-E)\psi_1(x)=0$

Region II. $V(x)=0$ $\quad \frac{\partial^2 \psi_2(x)}{\partial x^2} + \frac{2m}{\hbar^2} V_0 \psi_2(x)=0$

Region III. $V(x)=\infty$ $\quad \psi_3(x)=0$

I: $\psi_1(x) = B_1 e^{k_1 x}$ $\quad k_1=\sqrt{\frac{2m(V_0-E)}{\hbar^2}}$ $\quad (|\psi(x)|<\infty)$

II. $\psi_2(x) = A_2 \sin(k_2 x) + B_2 \cos(k_2 x)$ $\quad k_2=\sqrt{\frac{2mE}{\hbar^2}}$

III. $\psi_3(x)=0$

b> when $x=0$ $\quad \psi_1(x)=\psi_2(x) \Rightarrow \underline{B_1=B_2}$

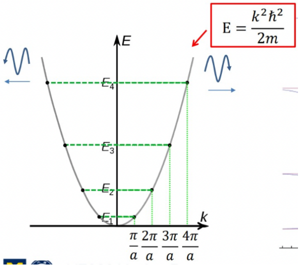
$\frac{\partial \psi_1(x)}{\partial x} = \frac{\partial \psi_2(x)}{\partial x} \Rightarrow k_1 B_1 = k_2 A_2$

when $x=a$ $\quad \psi_2(x)=\psi_3(x) \Rightarrow A_2\sin(k_2 a)+B_2\cos(k_2 a)=0 \Rightarrow B_2 = \underline{-A_2\tan(k_2 a)}$

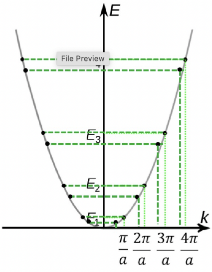
c> $k_1 B_1 = k_2 A_2$

$\cancel{A_2} = \frac{k_1}{k_2} B_1 = \frac{k_1}{k_2} B_2 = -\frac{k_1}{k_2}\cancel{A_2}\tan(k_2 a) \Rightarrow \sqrt{\frac{E}{V_0-E}} = -\tan\left[\sqrt{\frac{2mE}{\hbar^2}}\cdot a\right]$

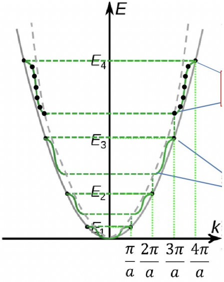
Energy Bands



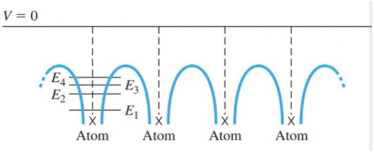
(a) Isolated atom



(b) 2 atoms



(c) N atoms



(d) Potential function of 1-D crystal

Figure: Energy bands

1-D Kronig-Penny Model

* Bloch theorem: In periodic potential field, for a single electron,

① $\psi(x) = u(x)e^{jkx}$ $u(x)$: periodic function with period $(a+b)$, k: parameter

- Idealized model of one dimensional single crystal

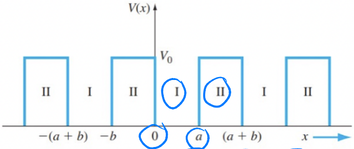
Plug ① into Schr Eq.

$\psi_1(x) = A_1 e^{u} + A_2 e^{u}$

$\psi_2(x) = B_1 e^{u} + B_2 e^{u}$

$Ax = b$

$\det(A) = 0$



* what is α?

$\alpha^2 = \frac{2mE}{\hbar^2}$

$\beta^2 = \frac{2m}{\hbar^2}(E - V_0) = \alpha^2 - \frac{2mV_0}{\hbar^2}$

Figure: Potential function of 1-D crystal in KP model

- Conclusion:

$$\boxed{P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a = \cos ka}$$

where $P' = \frac{mV_0 ba}{\hbar^2}$. This equation gives the condition that the Schrodinger wave equation has a solution.

用boundary condition解两个ψ，有4个未知系数，得到4个线性齐次方程，表示为 $Ax=b$ 有解条件是 $\det A = 0$，得到该式

Energy Bands in K Space

$\alpha^2 = \frac{2mE}{\hbar^2}$

- Consider the E-k relation of particles in the lattice.
- Let $f(\alpha a) = P' \frac{\sin \alpha a}{\alpha a} + \cos \alpha a$ $= \cos ka$ $[-1, 1]$

αa

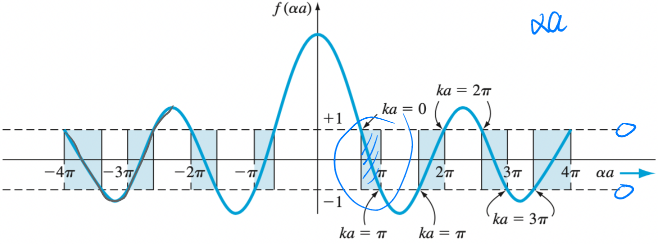


Figure: The entire $f(\alpha a)$ function

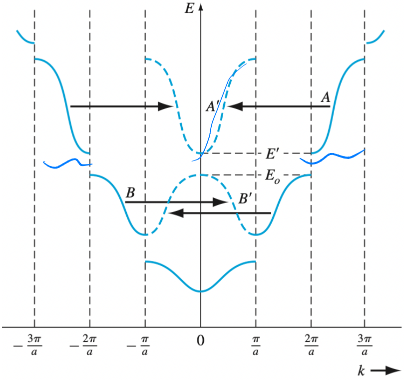
where the shared areas show the allowed values of αa corresponding to real values of k.

E can't take all values $\Longrightarrow$ Forbidden bands!

The E versus k diagram

$\cos ka = \cos(ka+2\pi)$
$= \cos(ka-2\pi)$

since $\alpha^2 = \frac{2mE}{\hbar^2}$, get the E-k diagram



$p = \hbar k = \frac{h}{\lambda}$

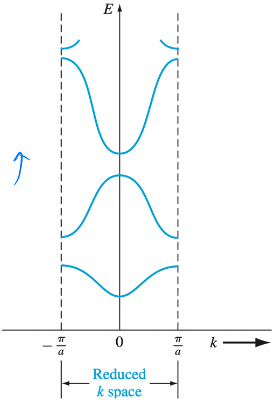
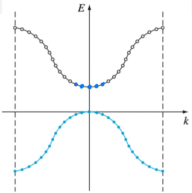


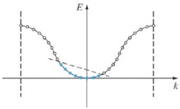
Figure: E vs. k diagram

Energy bands

* What if T>0K ?
* What's the difference between semiconductor and insulator ?
* What if external $\vec{E}$ applied ?

- Metal:
- Insulator:
- Semiconductor:





$dE = F\,dx$
$= F v\,dt$

$J = -e\sum v_i$

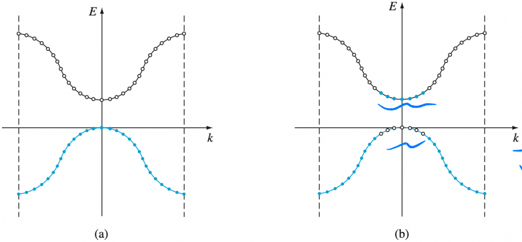


Figure: E-k diagram of semiconductor. (a)T=0K; (b)T>0K

- Drift current density: $J = qNv_d = q\sum_{i=1}^{N} v_i$.

$q>0$.

Effective Mass

- Background: for the electrons in the lattice,

$$F_{\text{total}} = F_{\text{ext}} + F_{\text{int}} = ma$$

内力难以一一考虑.

where m is the static mass of the electron. Consider only the external force,

$$F_{\text{ext}} = m^* a$$

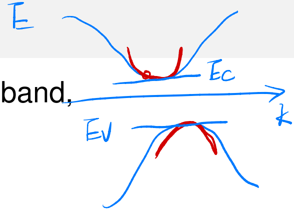
where m^* is the effective mass of the electron.

- For electron in free space, we have $E = \frac{\hbar^2 k^2}{2m}$, i.e.,

$$\frac{1}{\hbar}\frac{dE}{dk} = v$$

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m}$$

Effective Mass



- For electrons at the bottom of the conduction band, $E - E_c = C_1(k)^2$, i.e.,

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{2C_1}{\hbar^2} = \frac{1}{m^*}$$

- For electrons at the top of the valance band, $E - E_v = -C_2(k)^2$, i.e.,

$$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{-2C_2}{\hbar^2} = \frac{1}{m^*}$$

which is equivalent to holes with positive mass and positive charge.

-

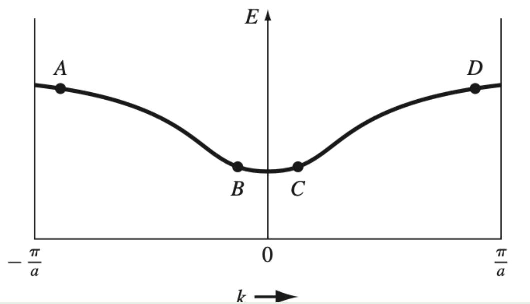
$$\begin{cases} E = E(k) = E_c + \dfrac{\hbar^2}{2m_n^*}(k - k_1)^2 \\ E = E(k) = E_v - \dfrac{\hbar^2}{2m_p^*}(k - k_2)^2 \end{cases}$$

where m_n^* and m_p^* are effective mass of electrons and holes.

Exercise

Effective mass

The E versus k diagram for a particular allowed energy band is shown in Figure below. Determine (a) the sign of the effective mass and (b) the direction of velocity for a particle at each of the four positions shown.



Exercise

$$\begin{cases} \frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{1}{m^*} \\ \frac{1}{\hbar}\frac{dE}{dk} = v \end{cases}$$

① A. $\frac{dE}{dk} < 0$ $\quad \frac{d^2E}{dk^2} < 0$

② B. $\frac{dE}{dk} < 0$ $\quad \frac{d^2E}{dk^2} > 0$

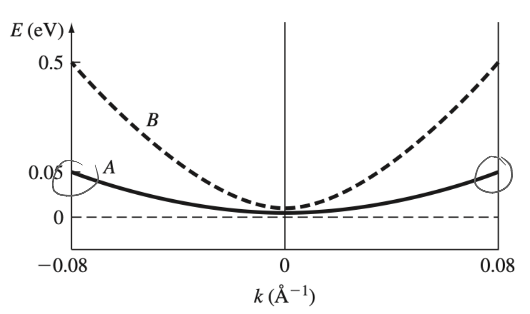
③ C $\quad > 0$ $\quad > 0$

④ D $\quad > 0$ $\quad < 0$

Exercise

Effective mass

Figure below shows the parabolic E versus k relationship in the conduction band for an electron in two particular semiconductor materials. Determine the effective mass (in units of the free electron mass) of the two electrons.



Exercise

For A. $E - E_c = C_1 k^2$

at $k = 0.08 \times 10^{10}\ m^{-1}$

$E = 0.05\ eV = 0.05 \times 1.6 \times 10^{-19} = 8 \times 10^{-21}\ J$

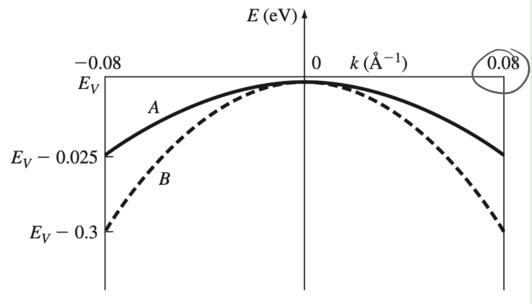
$\Rightarrow C_1 = 1.25 \times 10^{-38}$

$\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{2C_1}{\hbar^2} = \frac{1}{m_1^*} \Rightarrow m_1^* = \frac{\hbar^2}{2C_1}$

Exercise

Effective mass

Figure below shows the parabolic E versus k relationship in the valence band for a hole in two particular semiconductor materials. Determine the effective mass (in units of the free electron mass) of the two holes.



Exercise

$$E_V - E = C_2 k^2$$

① C_2

② $\frac{1}{\hbar^2}\frac{d^2E}{dk^2} = \frac{-2C_2}{\hbar^2} = \frac{1}{m^*}$

Exercise

$\psi(x) = \underbrace{Ae^{-ikx}} - \underbrace{Ae^{ikx}}$

$\psi(x) = -Ae^{ikx}$

b)

c) $E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 k_0^2}{9m_n^*}$

$k = \frac{\sqrt{2}}{3}k_0$

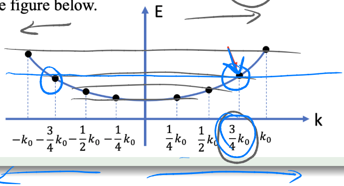
Problem Example 1

1. In a quantum system, the wavenumber k and energy E is quantized as shown in Figure 1. Please answer the following questions:

a) Write the static wavefunction of the dot ($k = \frac{3}{4}k_0$) that the red arrow is pointing to. Find the wavelength of this wavefunction.

b) If all the states are filled with electrons, how many electrons can be filled in the figure below? The electron spin is not considered.

c) If the effective mass of this quantum system is m_n^*, can this system allow an electron to have a quantized energy of $\frac{\hbar^2 k_0^2}{9m_n^*}$? If yes, mark the state of this electron in the figure below. How about a quantized energy of $\frac{\hbar^2 k_0^2}{8m_n^*}$? If yes, mark the state of this electron in the figure below.



Exercise

如果搞不懂下一面的推导也问题不大，会用下面的公式做题就行 (bushi

Density of States Function Derivation

Consider an electron bounded in a 3D infinite quantum well (crystal)

$V(x,y,z)=0 \quad 0<x<a$

$\quad\quad\quad\quad\quad\quad 0<y<a$

$\quad\quad\quad\quad\quad\quad 0<z<a$

$V(x,y,z)=\infty \quad$ o.w.

Apply Schrodinger Eq. $\quad k=\frac{n\pi}{a}$

$$\frac{2mE}{\hbar^2}=k^2=k_x^2+k_y^2+k_z^2$$
$$=(n_x^2+n_y^2+n_z^2)\frac{\pi^2}{a^2}$$

Positive / Negative k_x, k_y, k_z represents the same energy level

Consider 1/8 sphere in k-space is enough

Volume of one quantum state: $\left(\frac{\pi}{a}\right)^3$

Volume element in k space: $4\pi k^2 dk$

$$g_T(k)dk=\underbrace{2\cdot\frac{1}{8}}\frac{4\pi k^2 dk}{\left(\frac{\pi}{a}\right)^3}$$
$$=\frac{\pi k^2 dk}{\pi^3}\cdot a^3$$

2: 量子有两种自旋状态

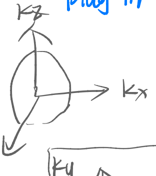
$\frac{1}{8}$: 考虑的是 k_x, k_y, k_z 全正

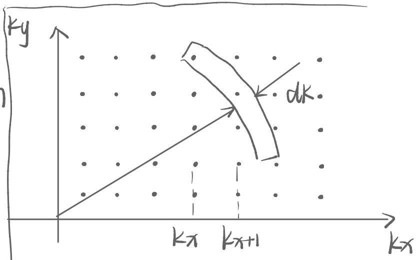
For free particle, we have

$$k^2=\frac{2mE}{\hbar^2} \Rightarrow \begin{cases} k=\frac{\sqrt{2mE}}{\hbar} \\ dk=\frac{1}{\hbar}\sqrt{\frac{m}{2E}}\cdot dE \\ (\hbar=h/2\pi) \end{cases}$$

plug in ①

$$g_T(k)=\frac{4\pi(2m)^{3/2}}{h^3}\sqrt{E}$$



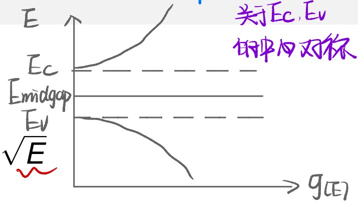


$$k_{x+1}-k_x=\frac{\pi}{a}$$

Density of States Function

* What if $m_n^* = m_p^*$?

关于Ec,Ev的中心对称



- For electrons in the lattice, $E = \frac{\hbar^2 k^2}{2m}$,

$$g(E) = \frac{4\pi(2m)^{3/2}}{h^3}\sqrt{E}$$

- For electrons at the bottom of the conduction band, $E - E_c = \frac{\hbar^2 k^2}{2m_n^*}$,

$$g_c(E) = \frac{4\pi(2m_n^*)^{3/2}}{h^3}\sqrt{E - E_c}, \quad E \geq E_c$$

- For holes at the top of the valance band, $E_v - E = \frac{\hbar^2 k^2}{2m_p^*}$,

$$g_v(E) = \frac{4\pi(2m_p^*)^{3/2}}{h^3}\sqrt{E_v - E}, \quad E \leq E_v$$

- There is no energy states in the forbidden band, $g(E) = 0$, when $E_v < E < E_c$.

Fermi-Dirac Probability Function

- Fermi level E_F: hypothetical levels with a 50% probability of electron occupancy in thermodynamic equilibrium.
- $f_F(E)$ represents the possibility that a quantum state of energy E is occupied by an electron

$$f_F(E) = \underbrace{\frac{1}{1+\exp(\frac{E-E_F}{kT})}}$$

* $P(E>E_F$ occupied)
$P(E<E_F$ empty)

都随T↑而↑

* $f_F(E)$ and $1-f_F(E)$?

对E_F对称

T = 0K:

① $E<E_F$ $\frac{E-E_F}{kT} \to -\infty$
$\exp(\ ) \to 0$
$f_F(E) = 1$

② $E>E_F$ $\frac{E-E_F}{kT} \to \infty$
$\exp(\ ) \to \infty$
$f_F(E) = 0$

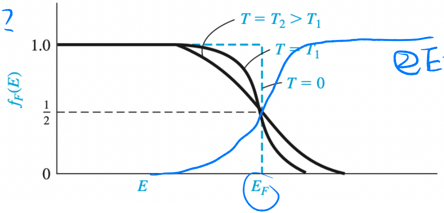


Figure: The Fermi probability function versus energy for different temperatures.

Exercise

Different distributions

Assume that the Fermi energy level for a particular material is 6.25 eV and that the electrons in this material follow the Fermi–Dirac distribution function. Calculate the temperature at which there is a 1 percent probability that a state 0.30 eV below the Fermi energy level will not contain an electron.

$$1 - f_F(E) = 1 - \frac{1}{1+\exp\left(\frac{E-E_F}{kT}\right)}$$

$$E - E_F = -0.3$$

$$0.01 = 1 - \frac{1}{1+\exp\left(\frac{-0.3}{kT}\right)}$$

$$\Rightarrow kT = 0.06529\,\text{eV}$$

$$T = 756\,\text{K}$$

Boltzmann Distribution

3kT

- When $\exp(\frac{E-E_F}{kT} \gg 1)$ $(E - E_F > \cancel{2}kT)$,

$$f_F(E) \cancel{=} \approx \underbrace{\exp(-\frac{E-E_F}{kT})}$$

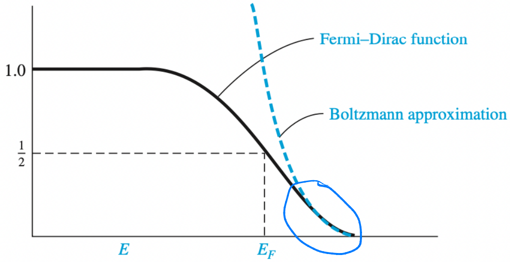


Figure: The Fermi–Dirac probability function and the Maxwell–Boltzmann approximation.

Exercise

$$\frac{\exp\left(-\frac{E-E_F}{kT}\right) - \frac{1}{1+\exp(\ )}}{\frac{1}{1+\exp(\ )}} = 0.05$$

$1+\exp(\ )$

Different distributions

Calculate the energy, in terms of kT and E_F, at which the difference between the Boltzmann approximation and the Fermi–Dirac function is 5 percent of the Fermi function.

$$E - E_F = kT \cdot \ln\left(\frac{1}{0.05}\right) \approx 3kT$$