

# Physical Electronics

## Schrodinger Equation

### Time-dependent (one-dimensional)

The Schrodinger equation is

$$\frac{-\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi = i\hbar \frac{\partial \Psi}{\partial t}$$

where  $\Psi = \Psi(x, t)$   
 $V = V(x)$  (potential energy)

Solve the differential equation by separation of variables. Assume that

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

$$\frac{-\hbar^2}{2m} \phi(t) \frac{d^2 \psi}{dx^2} + V(x)\psi(x)\phi(t) = i\hbar \psi(x) \frac{d\phi}{dt}$$

Divide by  $\psi(x)\phi(t)$ .

$$\frac{-\hbar^2}{2m} \left( \frac{1}{\psi} \frac{d^2 \psi}{dx^2} \right) + V(x) = i\hbar \frac{1}{\phi} \frac{d\phi}{dt} = G \text{ (constant)}$$

Solving for  $\phi$  gives

$$\phi(t) = e^{-\frac{i}{\hbar} Gt}$$

which should be  $e^{-i\omega t}$  for a matter wave by analogy with an E.M wave with

$$\omega = \frac{E}{\hbar} \Rightarrow G = E$$

$\therefore \Psi(x, t) = \psi(x)e^{-\frac{i}{\hbar} Et}$  is the solution to the time-dependent Schrodinger equation.

### Time-independent

The Schrodinger equation is

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

This can easily be extended to three dimensions as

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

### Born interpretation of wave functions

The intensity (energy/m<sup>2</sup>/sec) of an E.M wave is proportional to the square of the  $\vec{E}$  or  $\vec{B}$  field. It may be better to consider energy density in an electric field ( $\frac{1}{2}\epsilon_0 E^2$ ). The energy should be proportional to the probability of finding a photon there. By analogy with this, Born suggested that the probability density of observing a particle is given by

$$|\Psi(x,t)|^2 = \Psi^*(x,t) \Psi(x,t) \quad \text{Complex conjugate}$$

This leads to a so-called normalization for the wave function since the probability density integrated over all space should be 1 for a given particle. In one dimension this becomes

$$\int_{-\infty}^{\infty} \psi^* \psi dx = 1$$

From probability theory, the expectation value of a given quantity is

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} x P(x) dx}{\int_{-\infty}^{\infty} P(x) dx} \quad \text{where } P(x) \text{ is the probability density.}$$

For particles this becomes (with normalized wave functions)

$$\langle x \rangle = \frac{\int_{-\infty}^{\infty} \psi^* x \psi dx}{\int_{-\infty}^{\infty} \psi^* \psi dx} = \int_{-\infty}^{\infty} \psi^* x \psi dx$$

Recall that for E.M. waves of the form  $e^{i(kx - \omega t)}$  then

$$\begin{aligned} -i\hbar \frac{\partial}{\partial x} [e^{i(kx - \omega t)}] &= \hbar k e^{i(kx - \omega t)} \\ &= p_x e^{i(kx - \omega t)} \end{aligned}$$

Therefore we associate the operator  $-i\hbar \frac{\partial}{\partial x}$  with momentum  $p_x$ . With normalized wave functions

$$\langle p_x \rangle = \frac{\int_{-\infty}^{\infty} \psi^* (-i\hbar \frac{\partial}{\partial x}) \psi dx}{\int_{-\infty}^{\infty} \psi^* \psi dx} = \int_{-\infty}^{\infty} \psi^* (-i\hbar \frac{\partial}{\partial x}) \psi dx$$

(notice the importance of operator position)

Now consider the following requirements on wave functions:

<u><math>\psi(x)</math></u>	<u><math>\frac{d\psi}{dx}</math></u>
1. finite	1. finite
2. single-valued	2. single-valued
3. continuous	3. continuous

Conditions 1 and 2 arise from the fact that measurements (expectation values) of position ( $x$ ) and momentum ( $p_x$ ) should be unique and finite. If  $\frac{d\psi}{dx}$  is finite, then  $\psi(x)$  is continuous; and since

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V - E)\psi(x)$$

$\frac{d^2\psi}{dx^2}$  is finite which implies that  $\frac{d\psi}{dx}$  is continuous.

**Example I: Free particle ( $V(x) = 0$ ) with energy  $E$**

The time-independent Schrodinger equation becomes

$$\frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} - E\psi = 0$$

The solutions are

$$\psi = Ae^{\frac{i}{\hbar}\sqrt{2mE}x} + Be^{-\frac{i}{\hbar}\sqrt{2mE}x}$$

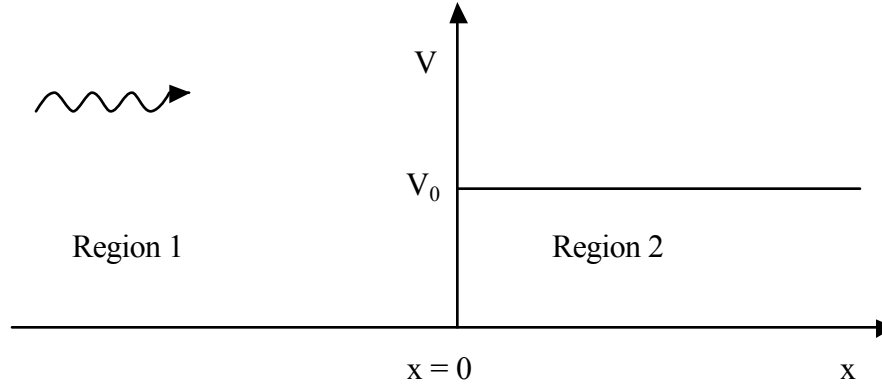
The time-dependent wave function is

$$\begin{aligned} \Psi(x,t) &= \psi(x)e^{-\frac{i}{\hbar}Et} \\ &= Ae^{\frac{i}{\hbar}(\sqrt{2mE}x - Et)} + Be^{-\frac{i}{\hbar}(\sqrt{2mE}x + Et)} \end{aligned}$$

For a wave traveling in the +x-direction,  $B = 0$ , thus

$$\begin{aligned} \langle p_x \rangle &= \frac{\int_{-\infty}^{\infty} \psi^* \left( -i\hbar \frac{\partial}{\partial x} \right) \psi dx}{\int_{-\infty}^{\infty} \psi^* \psi dx} \\ &= \frac{\sqrt{2mE} \int_{-\infty}^{\infty} \psi^* \psi dx}{\int_{-\infty}^{\infty} \psi^* \psi dx} = \sqrt{2mE} \end{aligned}$$

**Example II: Particle of energy  $E$  incident from the left on a potential barrier of height  $V_0$  ( $E > V_0$ )**



Solve the Schrodinger equation in regions 1 and 2; then demand continuity of  $\psi(x)$  and  $\frac{d\psi}{dx}$  at

$x = 0$  to match the solutions. In region 1

$$\frac{-\hbar^2}{2m} \frac{d^2\psi_1}{dx^2} = E\psi_1 \Rightarrow \psi_1(x) = Ae^{ik_1x} + Be^{-ik_1x} \text{ for } x < 0$$

$$\text{where } k_1 = \frac{\sqrt{2mE}}{\hbar}$$

In region 2

$$\frac{-\hbar^2}{2m} \frac{d^2\psi_2}{dx^2} + V\psi_2 = E\psi_2 \Rightarrow \psi_2(x) = Ce^{ik_2x} + De^{-ik_2x} \text{ for } x > 0$$

$$\text{where } k_2 = \frac{\sqrt{2m(E - V)}}{\hbar}$$

Now try to find the constants by applying the continuity conditions at the boundary. Also note that  $D = 0$  since the wave in region 2 only propagates to the right.

$$\psi_1|_{x=0} = \psi_2|_{x=0} \Rightarrow A + B = C$$

$$\left. \frac{d\psi_1}{dx} \right|_{x=0} = \left. \frac{d\psi_2}{dx} \right|_{x=0} \Rightarrow ik_1(A - B) = ik_2C$$

Find B and C in terms of A

$$A + B = C \Rightarrow 2A = \left(1 + \frac{k_2}{k_1}\right)C \Rightarrow C = \frac{2k_1}{k_1 + k_2} A$$

$$A - B = \frac{k_2}{k_1}C \Rightarrow \left(1 - \frac{k_1}{k_2}\right)A + \left(1 + \frac{k_1}{k_2}\right)B = 0 \Rightarrow B = \frac{k_1 - k_2}{k_1 + k_2} A$$

In principle, A should be determined by applying the normalization condition on  $\psi$ , but for unbounded traveling wave solutions it's a bit tricky. Instead find the probability of the particle being transmitted and being reflected. The reflected wave is given by  $Be^{-ik_1x}$  in region 1. Let us look at the ratio of the reflected wave amplitude divided by the incoming wave amplitude.

$$\frac{B}{A} = \frac{k_1 - k_2}{k_1 + k_2}$$

Remembering that the particle probabilities are related to the  $\psi^* \psi$ , we need to look at  $\left(\frac{B}{A}\right)^2$  to get the probability of reflection.

$$R \equiv \left(\frac{B}{A}\right)^2 = \frac{(k_1 - k_2)^2}{(k_1 + k_2)^2}$$

More care needs to be taken in the case of the transmission coefficient. We really need to know the flux of the particles incident on the barrier. Current density is the flux of the charge density ( $\vec{J} = \rho \vec{v}$ ), so likewise we need to multiply the probability density by the velocity of the particle (given by  $\frac{p}{m} = \frac{\hbar k}{m}$ ). Therefore we need only to multiply the probability density by k in a given region. Thus

$$T \equiv \frac{k_2 |C|^2}{k_1 |A|^2} = \frac{k_2}{k_1} \frac{(2k_1)^2}{(k_1 + k_2)^2}$$

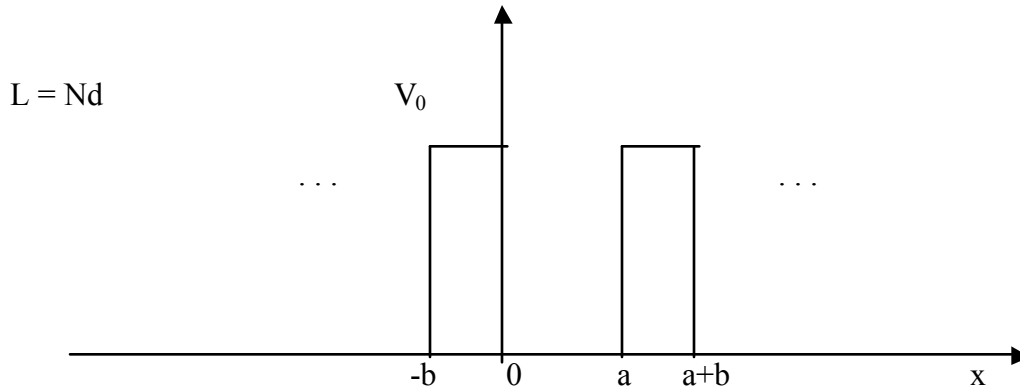
You may verify that  $R + T = 1$ .

### **Kronig-Penney Model**

Given a one-dimensional lattice of length L and  $E < V_0$

V

$$d = a+b$$



$$1) \frac{-\hbar^2}{2m} \frac{d^2\psi_1}{dx^2} - E\psi_1 = 0 \quad \text{for } 0 < x < a$$

$$2) \frac{-\hbar^2}{2m} \frac{d^2\psi_2}{dx^2} - (V_0 - E)\psi_2 = 0 \quad \text{for } -b < x < 0$$

Felix Bloch showed that the solutions to the Schrodinger equation for a periodic potential are of the form  $\psi(x) = e^{ikx}u(x)$  where  $u(x) = u(x + d)$ .

Transforming Eqs. 1) and 2) into differential equations involving  $u(x)$ :

$$\frac{d\psi}{dx} = e^{ikx}u' + ike^{ikx}u$$

$$\frac{d^2\psi}{dx^2} = e^{ikx}u'' + 2ike^{ikx}u' - k^2e^{ikx}u$$

Define  $\alpha^2 \equiv \frac{2mE}{\hbar^2}$ ,  $\beta^2 \equiv \frac{2m(V_0 - E)}{\hbar^2}$ . Then 1 and 2 become

$$1') \quad u_1'' + 2iku_1' + (\alpha^2 - k^2)u_1 = 0 \quad \text{for } 0 < x < a$$

$$2') \quad u_2'' + 2iku_2' - (\beta^2 + k^2)u_2 = 0 \quad \text{for } -b < x < 0$$

and the solutions are

$$u_1(x) = Ae^{-ikx + i\alpha x} + Be^{-ikx - i\alpha x} \quad \text{for } 0 < x < a$$

$$u_2(x) = Ce^{-ikx + \beta x} + De^{-ikx - \beta x} \quad \text{for } -b < x < 0$$

The boundary conditions are

$$u_1(0) = u_2(0)$$

$$u_1(a) = u_2(-b) = u_2(a)$$

$$\left. \frac{du_1}{dx} \right|_0 = \left. \frac{du_2}{dx} \right|_0$$

$$\left. \frac{du_1}{dx} \right|_a = \left. \frac{du_2}{dx} \right|_{-b} = \left. \frac{du_2}{dx} \right|_a$$

Substituting  $u_1$  and  $u_2$  into the boundary conditions gives:

$$3) \quad A + B = C + D$$

$$4) \quad (-ik + i\alpha)A + (-ik - i\alpha)B = (-ik + \beta)C + (-ik - \beta)D$$

$$5) Ae^{-ika+i\alpha a} + Be^{-ika-i\alpha a} = Ce^{ikb-\beta b} + De^{ikb+\beta b}$$

$$6) (-ik + i\alpha)Ae^{-ika+i\alpha a} + (-ik - i\alpha)Be^{-ika-i\alpha a} = (-ik + \beta)Ce^{ikb-\beta b} + (-ik - \beta)De^{ikb+\beta b}$$

Set the determinant of the coefficients equal to zero so that a non-trivial solution exists (by Kramer's Rule) gives:

$$7) \frac{\beta^2 - \alpha^2}{2\alpha\beta} \sinh(\beta b) \sin(\alpha a) + \cosh(\beta b) \cos(\alpha a) = \cos(k(b+a))$$

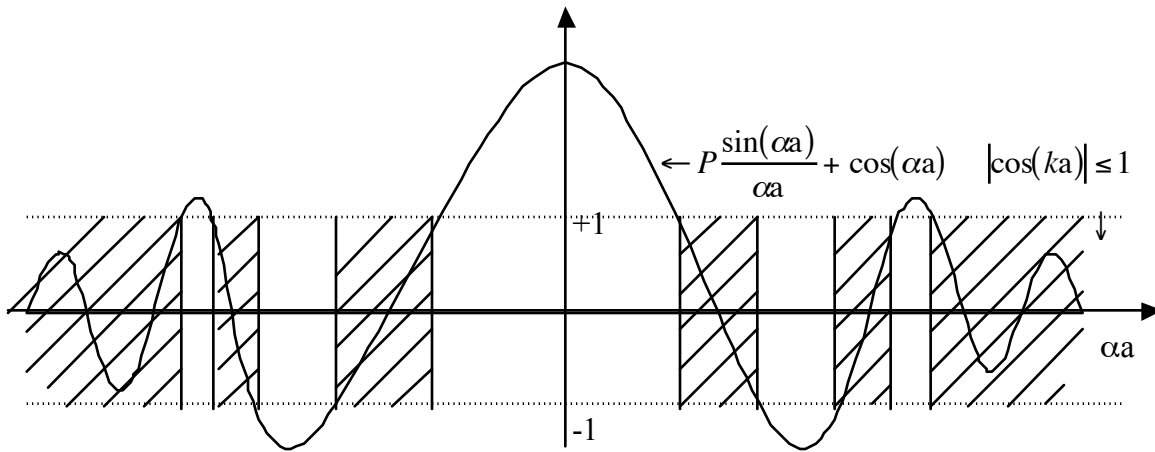
Let  $b \rightarrow 0$  and  $V_0 \rightarrow \infty$  such that  $bV_0 = \text{constant} \Rightarrow \beta b \rightarrow 0$ . Remember that  $\beta = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$ .

Take the limit of 9 as  $\beta b \rightarrow 0$ . In the limit, 9 becomes

$$8) \frac{\beta^2 b}{2\alpha} \sin(\alpha a) + \cos(\alpha a) = \cos(ka)$$

or  $P \frac{\sin(\alpha a)}{\alpha a} + \cos(\alpha a) = \cos(ka)$  where  $P \equiv \frac{a\beta^2 b}{2}$

The graphical solution is



Solutions are found for values of  $\alpha a$  in the cross-hatched areas. Conclusion: Energy bands exist in periodic structures.

### Particle in a box

Assume infinite potential barriers at  $x = y = z = 0$  and  $x = y = z = L$  (box has side  $L$  and volume  $L^3$ ). Inside the box, the Schrodinger equation becomes

$$\frac{-\hbar^2}{2m} \left( \frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right) - E\psi = 0$$

Assume that

$$\begin{aligned} \psi(x, y, z) &= f(x)g(y)h(z) \\ \therefore \frac{-\hbar^2}{2m} \left( \frac{f''}{f} + \frac{g''}{g} + \frac{h''}{h} \right) - E &= 0 \end{aligned}$$

Since this is true for all values of x, y, and z in the box, then

$$\begin{aligned} \frac{f''}{f} &= -k_x^2 \\ \therefore f(x) &= A \sin(k_x x) + B \cos(k_x x) \\ f(0) = f(L) = 0 &\Rightarrow B = 0 \\ A \sin(k_x L) = 0 &\Rightarrow k_x L = n_x \pi \Rightarrow k_x = \frac{n_x \pi}{L} \end{aligned}$$

Similarly for g(y) and h(z)

$$\begin{aligned} k_y &= \frac{n_y \pi}{L} \text{ and } k_z = \frac{n_z \pi}{L} \\ \therefore \psi(x, y, z) &= B_0 \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right) \end{aligned}$$

Find  $B_0$  by normalization

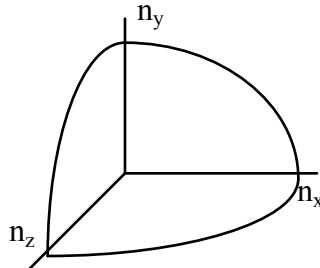
$$\begin{aligned} 1 &= \int_0^L \int_0^L \int_0^L \psi^* \psi dx dy dz = B_0^2 \left(\frac{L}{2}\right) \left(\frac{L}{2}\right) \left(\frac{L}{2}\right) = \frac{B_0^2 L^3}{8} \\ \therefore B_0 &= \left(\frac{2}{L}\right)^{\frac{3}{2}} \end{aligned}$$

Substituting  $\psi$  into the Schrodinger equation we get

$$E = \frac{\pi^2 \hbar^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2) \text{ where } n_x, n_y, \text{ and } n_z \text{ are all positive integers}$$

Define  $n^2 = n_x^2 + n_y^2 + n_z^2$  so that n is like the radius of a sphere in n-space.

$$\therefore E = \frac{\pi^2 \hbar^2}{2mL^2} n^2$$





Now the number of energy states between E and E + dE is equal to dN where

$$dN = \frac{4\pi n^2}{8} dn$$

(volume of a spherical shell of thickness dn in the first quadrant).

$$2ndn = \frac{2mL^2}{\pi^2\hbar^2} dE \quad \text{where } n = \left( \frac{2mL^2}{\pi^2\hbar^2} E \right)^{\frac{1}{2}}$$

$$\therefore dn = \frac{1}{2} \left( \frac{2mL^2}{\pi^2\hbar^2} \right)^{\frac{1}{2}} E^{-\frac{1}{2}} dE$$

$$\therefore dN = \frac{\pi}{2} n^2 dn = \frac{\pi}{4} \left[ \frac{2mL^2}{\pi^2\hbar^2} \right]^{\frac{3}{2}} E^{\frac{1}{2}} dE$$

It will be useful to define a density of states per unit energy given by

$$\frac{dN}{dE} = \frac{1}{4\pi^2} \left[ \frac{2mL^2}{\hbar^2} \right]^{\frac{3}{2}} E^{\frac{1}{2}}$$

Because electrons can have either spin of  $+\frac{1}{2}$  or  $-\frac{1}{2}$ , each state denoted by a value of n can contain 2 electronic states. Multiplying by 2 gives the density of states per energy for electrons as

$$9) \quad \frac{dN}{dE} = \frac{1}{2\pi^2} \left[ \frac{2mL^2}{\hbar^2} \right]^{\frac{3}{2}} E^{\frac{1}{2}}$$

Now consider the density of states/unit energy/unit volume (in a cube of volume  $L^3$ ) given by

$$\frac{1}{L^3} \frac{dN}{dE} = \frac{1}{2\pi^2} \left[ \frac{2m}{\hbar^2} \right]^{\frac{3}{2}} E^{\frac{1}{2}}$$

(Note that L drops out so the shape of the box is unimportant)

It is now possible to calculate the concentration of the electrons (number/unit volume) by integrating over all the possible energies and including the probability that a given energy state will be occupied. This probability is the Fermi-Dirac distribution.

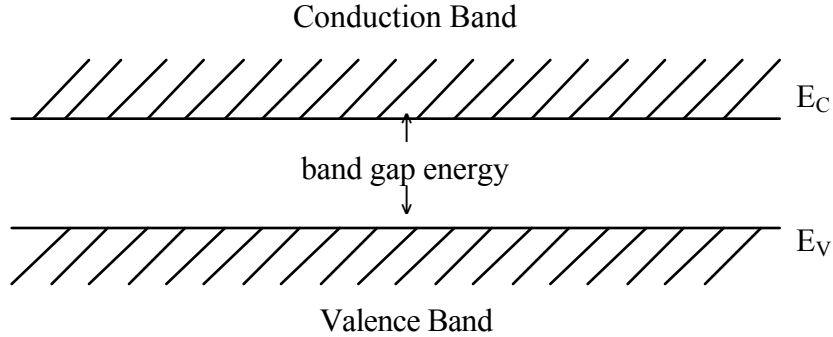
$$\therefore e^- \text{ concentration} = n = \int_0^{E_{\max}} \left( \frac{1}{L^3} \frac{dN}{dE} \right) E f_D dE$$

(note the different n,  $f_D$  = Fermi-Dirac distribution)

$$10) \quad n = \int_0^{E_{\max}} \frac{1}{2\pi^2} \left[ \frac{2m}{\hbar^2} \right]^{\frac{3}{2}} \frac{E^{\frac{1}{2}}}{1 + e^{\frac{(E-E_F)}{kT}}} dE$$

## Semiconductors

Now let us apply this formalism to semiconductors. At low temperatures a semiconductor acts like an insulator because the Fermi energy lies in the band gap, implying that the valence band is filled and the conduction band is empty.



Conduction takes place when an electron is free to move to a new energy state. Since the valence band is filled (at low temperatures), no conduction is possible. As the temperature increases, the thermal excitation can excite some electrons into the conduction band, leaving behind vacant states, or holes, in the valence band. Now conduction can readily take place since states are available for electrons to move into. This explains the increasing conductivity of semiconductors with increasing temperatures.

Let's assume that densities of states similar to equation 11 (pg. 9) exist at the conduction and valence band edges, but referenced with respect to  $E_C$  and  $E_V$  respectively.

$$\therefore \left. \frac{dN}{dE} \right|_{E_C} = \frac{1}{2\pi^2} \left( \frac{2m_e}{\hbar^2} \right)^{\frac{3}{2}} (E - E_C)^{\frac{1}{2}} \text{ for } E_C \leq E < \infty \text{ and}$$

$$\left. \frac{dN}{dE} \right|_{E_V} = \frac{1}{2\pi^2} \left( \frac{2m_h}{\hbar^2} \right)^{\frac{3}{2}} (E_V - E)^{\frac{1}{2}} \text{ for } -\infty < E \leq E_V$$

The rationale for assuming a similar density of states in the conduction band is that the electrons are essentially free there (ie. no potentials), just as they were in the box. This allows us to use a similar state density. Clearly this isn't the correct density to use for energies approaching infinity, but since the Fermi-Dirac distribution approaches zero there, errors should be small. It

is not quite so easy to argue that this is OK to do at the valence band edge. It depends on a so-called ‘negative mass’ behavior of the electrons at the top of an energy band.

To calculate the electron concentration in the conduction band (from equation 12)

$$11) n = \int_{E_C}^{\infty} \frac{1}{2\pi^2} \left[ \frac{2m_e}{\hbar^2} \right]^{\frac{3}{2}} \frac{(E - E_C)^{\frac{1}{2}}}{1 + e^{\frac{(E-E_F)}{kT}}} dE$$

define  $E' = E - E_C$  and  $dE' = dE \quad \therefore 0 \leq E' < \infty$  so equation 13 becomes

$$12) n = \int_0^{\infty} \frac{1}{2\pi^2} \left[ \frac{2m_e}{\hbar^2} \right]^{\frac{3}{2}} \frac{E'^{\frac{1}{2}}}{1 + e^{\frac{(E'+E_C-E_F)}{kT}}} dE'$$

At room temperature  $kT \approx 0.026\text{eV}$ . For lightly doped Si,  $(E_C - E_F) \approx 0.5\text{eV}$  which says that the Fermi-Dirac distribution can be approximated as follows

$$\frac{1}{1 + e^{\frac{(E'+E_C-E_F)}{kT}}} \approx \frac{1}{e^{\frac{(E'+E_C-E_F)}{kT}}} = e^{-\frac{(E'+E_C-E_F)}{kT}}$$

Now equation 14 can be written as

$$13) n = \frac{1}{2\pi^2} \left[ \frac{2m_e}{\hbar^2} \right]^{\frac{3}{2}} e^{-\frac{(E_C-E_F)}{kT}} \int_0^{\infty} E'^{\frac{1}{2}} e^{-\frac{E'}{kT}} dE'$$

From the CRC tables

$$\therefore \int_0^{\infty} E'^{\frac{1}{2}} e^{-\frac{E'}{kT}} dE' = (kT)^{\frac{3}{2}} \frac{\sqrt{\pi}}{2}$$

Then equation 15 becomes

$$14) n = \frac{1}{4} \left[ \frac{2m_e kT}{\pi \hbar^2} \right]^{\frac{3}{2}} e^{-\frac{(E_C-E_F)}{kT}} \quad \text{or} \quad n = N_C e^{-\frac{(E_C-E_F)}{kT}} \quad \text{where} \quad N_C \equiv \frac{1}{4} \left[ \frac{2m_e kT}{\pi \hbar^2} \right]^{\frac{3}{2}}$$

$N_C$  is called the effective density of states at the conduction band edge.

The hole concentration in the valence band (denoted by  $p$ ) can be found by remembering that the probability of finding a hole is  $[1 - (\text{the probability of finding an electron})]$ . Thus the Fermi function is modified for holes

$$p = \int_{-\infty}^{E_V} \frac{dN}{dE} \Big|_{E_V} (1 - f_D E) dE$$

$$\Rightarrow p = \frac{1}{2\pi^2} \left[ \frac{2m_h}{\hbar^2} \right]^{\frac{3}{2}} \int_{-\infty}^{E_V} (E_V - E)^{\frac{1}{2}} \frac{e^{\frac{(E-E_F)}{kT}}}{1 + e^{\frac{(E-E_F)}{kT}}} dE \quad \text{for } E < E_F$$

Then it follows that

$$15) p = \frac{1}{4} \left[ \frac{2m_h kT}{\pi \hbar^2} \right]^{\frac{3}{2}} e^{-\frac{(E_F - E_V)}{kT}} \text{ or } p = N_V e^{-\frac{(E_F - E_V)}{kT}} \text{ where } N_V \equiv \frac{1}{4} \left[ \frac{2m_h kT}{\pi \hbar^2} \right]^{\frac{3}{2}}$$

An intrinsic semiconductor has no doping impurities, therefore  $n = p = n_i$ , where  $n_i$  is the intrinsic electron or hole concentration. This must be the case since each electron in the conduction band leaves a hole behind in the valence band. An extrinsic semiconductor has been doped so that extra holes or electrons are present. Thus  $n \neq p$ . From equations 16 and 17 it is clear that

$$16) n_i^2 = N_C N_V e^{-\frac{(E_C - E_V)}{kT}}$$

Notice that the right side of this equation is a constant at a given temperature so that even for extrinsic semiconductors

$$17) np = n_i^2$$

## Special Homework Problems

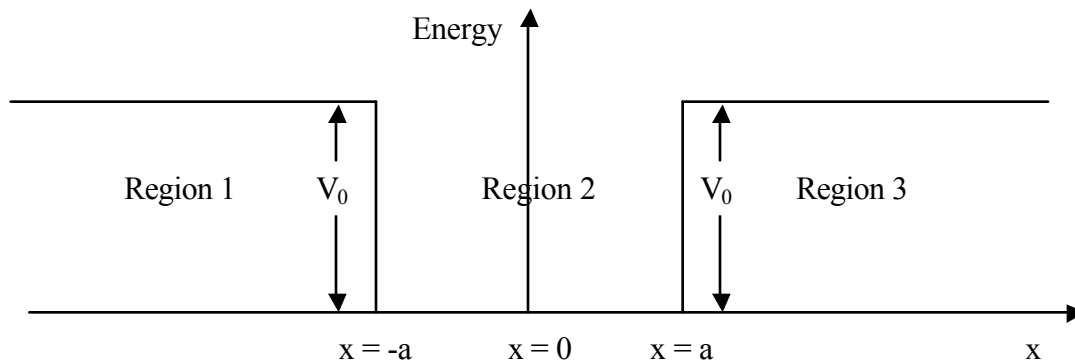
1. A wave function is given by

$$\psi(x) = A \cos\left(\frac{\pi x}{2a}\right) \text{ for } a \leq x \leq 3a$$

$$\psi(x) = 0 \text{ for } x < a \text{ and } x > 3a$$

Find the constant A so that  $\psi$  is normalized.

2. Use the wave function from problem 1 to find  $\langle x \rangle$ , the expectation value of position, and  $\langle p_x \rangle$ , the expectation value of momentum. Do your results make physical sense? Explain.
3. A particle is in a one-dimensional box with finite barrier heights (see figure). The total energy, E, of the particle is less than the barrier height,  $V_0$ .



Find the probability that the particle is outside the box for the lowest energy state (i.e. the particle lies outside  $-a \leq x \leq a$ ). You will find it useful to make the following definitions:

$$\hbar k_1 \equiv \sqrt{2m(V_0 - E)}$$

$$\hbar k_2 \equiv \sqrt{2mE}$$

In region 2, the general form of  $\psi$  is  $Ce^{ik_2x} + De^{-ik_2x}$ . Show that

$$\left. \frac{C}{D} \right|_{-a} \cdot \left. \frac{C}{D} \right|_a = 1 = \frac{C^2}{D^2} \Rightarrow C = \pm D \text{ etc.}$$

4. Graphically solve equation 10 (pg. 7) to find the allowed energy ranges when the product  $bV_0 = 10\text{eV}\cdot\text{\AA} = 1.6 \times 10^{-28} \text{J}\cdot\text{m}$  and  $a = 4\text{\AA}$ . Express your answers in eV. Assume that the particles involved are electrons.

5. Plot the Fermi-Dirac distribution function with  $E_F = 0.5\text{eV}$  at temperatures of 0, 50, and 300K. Plot  $f_D(E)$  vs.  $E$ .
6. Use your results from problem 5 to evaluate equation 12 (pg. 9). Then, assuming that the concentration of conduction electrons in Cu is  $1\text{ e}^-/\text{atom}$ , find the value of the Fermi energy at 0 Kelvins. Do you expect this value to change much at 300K? Explain. (You only need to evaluate the integral in equation 12 for a temperature of 0 K; this simplifies things greatly!)