A Brief Introduction to

Quantum Mechanics and Electronic Band Theory

Lecture Notes for INEL 6055

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Abstract

Quantum mechanics is not part of the traditional curriculum in electrical engineering because classic concepts suffice to explain the main aspects of the device's operation. However, due to the small size of the devices used in modern integrated circuits, which approach atomic dimensions, an understanding of quantum concepts is increasingly important for device engineers. Furthermore, many new technologies make used of quantum effects to produce novel devices that might find place in commercial circuits in the future. This document offers a brief introduction to the basic ideas of quantum theory as they apply to solid state devices.

1 The Need for a Quantum Theory

In the early 1900's, experimental disagreement between predictions of classical mechanics and some experimental observations drove some well known scientists to formulate alternative theories. Some of the most important examples in which quantum concepts were used are:

- Blackbody radiation: solids emit light when they are heated. The emission spectra was in disagreement with classical predictions (Rayleigh-Jeans law). In 1901 Max Planck explained the measured spectra by assuming that atoms could only absorb or emit light in discrete packets.
- Sharp spectral lines emitted by heated Hydrogen gas: In 1910 Bohr explained the results based on a model that assumed angular momentum quantization
- Photoelectric effect: electro-magnetic waves exhibit particle-like properties. In the mid 1920, De Broglie suggested that particles should also exhibit wave-like behavior, and hypothesized that the wavelength can be found from momentum using the relationship

$$p = h/\lambda$$

2 Basic Postulates

- There exist a complex quantity called the *wavefunction* $\Psi = \Psi(x, y, z, t)$ from which the all desirable variables of a system can be obtained.
- For a given system constrains, Ψ is determined by solving the time dependent Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar}{2m}\nabla^2\Psi + U(x, y, z)\Psi$$

where U represents the potential energy of the system and $i = \sqrt{-1}$.

- Ψ and $\nabla\Psi$ must be finite, continuous and single-valued.
- The probability of finding the particle in the spacial volume dV is $\Psi^*\Psi dV$, where Ψ^* is the complex conjugate of Ψ.

  This implies that

  $$\int_V \Psi^*\Psi dV = 1$$
- There is a mathematical operator α_{op} associated to each dynamic system's variable α, such as energy and momentum. The expectation value of the quantity can be found from

  $$< \alpha >= \int_V \Psi^* \alpha_{op} \Psi dV$$
- The momentum operator is $\frac{\hbar}{i}\frac{\partial}{\partial r}$, where r can be x, y or z. Thus once the wavefunction has been found, the expectation value of the momentum in the x direction can be determined from

  $$< p_x >= \int_V \Psi^* \frac{\hbar}{i}\frac{\partial \Psi}{\partial x} dV$$
- The energy operator is $-\frac{\hbar}{i}\frac{\partial}{\partial t}$

2.1 Time-independent Formulation

If the total energy E is constant, the problem can be simplified as follows. The energy expectation value is

$$< E >= \int_V \Psi^* \left(-\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} \right) dV$$

For this integral to equal E, one must have that

$$-\frac{\hbar}{i}\frac{\partial \Psi}{\partial t} = E\Psi$$

This requires a general solution of the form:

$$\Psi(x,y,z,t) = \psi(x,y,z)e^{-iEt/\hbar}$$

The Schrödinger equation can then be expressed in its simpler, time-independent form:

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

3 Examples

3.1 Free Particle

Consider a particle of mass m that finds itself alone in the universe and that has total energy equal to E. Such particle experiences no forces ($\mathbf{F} = \nabla U = 0$) so the potential energy is constant and can be chosen to be zero. For simplicity, let the particle's universe be one-dimensional,

To characterize the particle from the point of view of quantum mechanics, one must solve the time-independent Schrödinger equation

$$\frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2}\psi = 0$$

Using the trial solution

$$\psi = Ae^{ikx} + Be^{-ikx}$$

one obtains

$$\begin{aligned}\frac{\partial \psi}{\partial x} &= ikAe^{ikx} - ikBe^{-ikx} \\ \frac{\partial^2 \psi}{\partial x^2} &= -k^2\left(Ae^{ikx} + Be^{-ikx}\right) \\ &= -k^2\psi\end{aligned}$$

which demonstrates that ψ is a solution provided that

$$k = \frac{\sqrt{2mE}}{\hbar}$$

Thus for this problem

$$\Psi(x,t) = Ae^{i\left(kx - \frac{E}{\hbar}t\right)} + Be^{-i\left(kx + \frac{E}{\hbar}t\right)}$$

The right hand side terms have the form of results from classical wave analysis dealing with electromagnetism, sound, etc,

$$e^{i(kx-\omega t)}$$

and

$$e^{-i(kx+\omega t)}$$

These expressions correspond to waves traveling in the $+x$ and $-x$ directions, respectively, where $k = \frac{2\pi}{\lambda}$ is the wavenumber and ω is the angular momentum of the traveling wave. By analogy:

- The free particle wavefunction is interpreted as a traveling wave.
- If the particle moves in the x direction, $B = 0$. If it moves in the $-x$ direction, $A = 0$.
- Since, for a particle moving in the $+x$ direction,

  $$\psi^*\psi = A^*A = constant$$

  for all values of x, one has equal probability of finding the particle anywhere.
- The particle's momentum is

  $$\begin{aligned}< p_x > &= \int_{-\infty}^{\infty} \psi^* \frac{\hbar}{i}\frac{d\psi}{dx} dx \\ &= \hbar k \int_{-\infty}^{\infty} \psi^*\psi dx \\ &= \hbar k = \frac{h}{\lambda} = \sqrt{2mE}\end{aligned}$$

  in agreement with classical mechanics.
- We know the particle's momentum with complete precision but know nothing about the particle's position. This is in agreement with the *Heisenberg's Uncertainty Principle*, which postulates that

  $$\Delta p \times \Delta x \approx \hbar$$

  where Δ expresses uncertainty. Thus complete certainty of the particles momentum requires complete uncertainty of the position.
- The particle can be localized in some region of space by forming adding several different versions of ψ, each with different values of k, A, and B. Such superposition of sinusoids form what is known as a *wavepacket*, and resembles the formation of a waveform of arbitrary shape with a Fourier series. By doing so we have to use different values of momentum; thus we reduce the uncertainty in position by increasing that of momentum, in agreement with the above uncertainty principle.

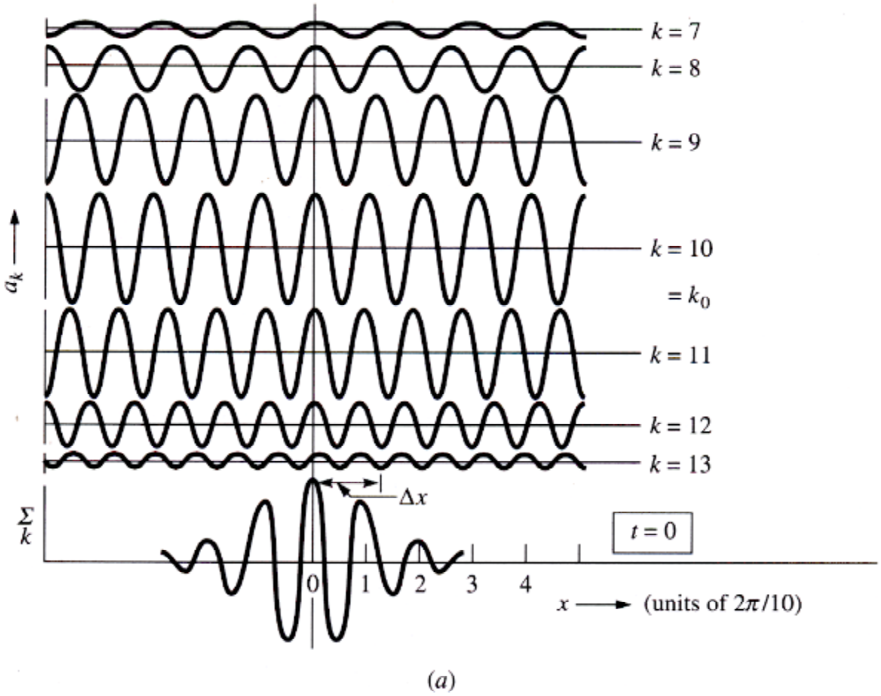

Figure 1: Example illustrating wafefunction superposition. (Taken from Craig Casey, 1999).

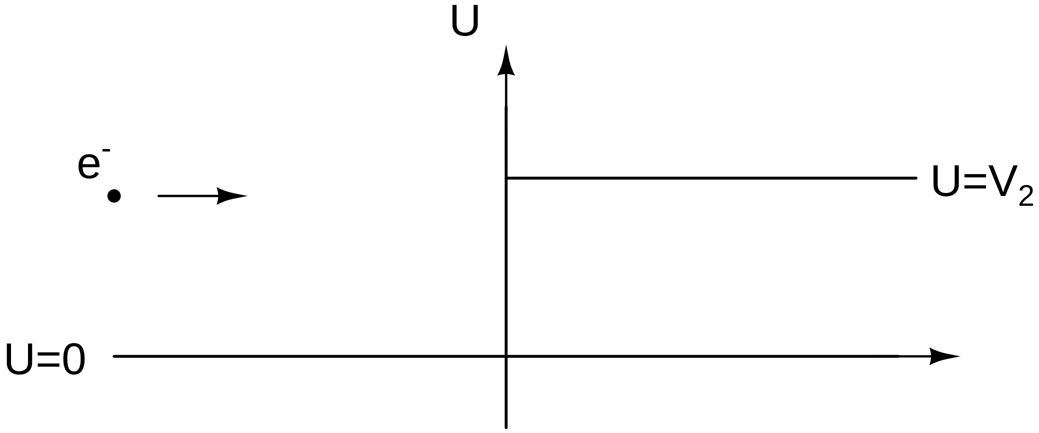

Figure 2: An electron approaching a potential barrier.

3.2 Electron Meeting a Potential Barrier

Consider a potential with the shape shown in figure 2. For simplicity lets consider again a one-dimensional universe.

We must now solve two equations. For $x \leq 0$ the electron is free ($U = 0$), and the solution is the one found in the previous example:

$$\psi = Ae^{ikx} + Be^{-ikx}$$

For $x > 0$, $U = V_2$ and the Schrdinger Equation becomes

$$\frac{\partial^2 \psi}{\partial x^2} + \frac{2m}{\hbar^2}\left(E - V_2\right)\psi = 0$$

which is similar to the one obtained for the free electron. Thus we should obtain solutions of the form

$$\psi = Ce^{ik_2 x} + De^{-ik_2 x}$$

where

$$k_2 = \frac{2m(E - V_2)}{\hbar}$$

Since at $x = 0$ the wavefunction must be continuous $\psi(0-) = \psi(0+)$ and $A + B = C + D$ Now consider a particle incident from the left. For this case, we can set $D = 0$ and get that

$$A + B = C$$

Because $\frac{\partial \psi}{\partial x}$ is also required to be continuous,

$$ikA - ikB = ik_2 C$$

or $k(A - B) = k_2 C$, which can be expressed as $C = \frac{k}{k_2}(A - B)$. Substituting in the previous expression yields

$$\begin{aligned} A + B &= \frac{k}{k_2}(A - B) \\ A\left(1 - \frac{k}{k_2}\right) &= -B\left(1 + \frac{k}{k_2}\right) \\ A\frac{k - k_2}{k_2} &= B\frac{k + k_2}{k_2} \\ \frac{B}{A} &= \frac{k - k_2}{k + k_2} \end{aligned}$$

and

$$\frac{C}{A} = \frac{2k}{k + k_2}$$

We can make the following observations about these results:

- If $E > V_2$,
  - both k and k_2 are real;
  - solutions are oscillatory;
  - $\frac{B}{A} = \frac{k - k_2}{k + k_2}$ is finite! Thus, there is a finite probability that the barrier will reflect back the electron, causing it to turn back to the left.
- If $E < V_2$,
  - $k_2 = \frac{2m(E - V_2)}{\hbar}$ is imaginary;
  - the wavefunction declines exponentially for $x > 0$.
  - $\frac{C}{A} = \frac{2k}{k + k_2} > 0$ so there is a non-zero probability for the electron to penetrate the barrier!

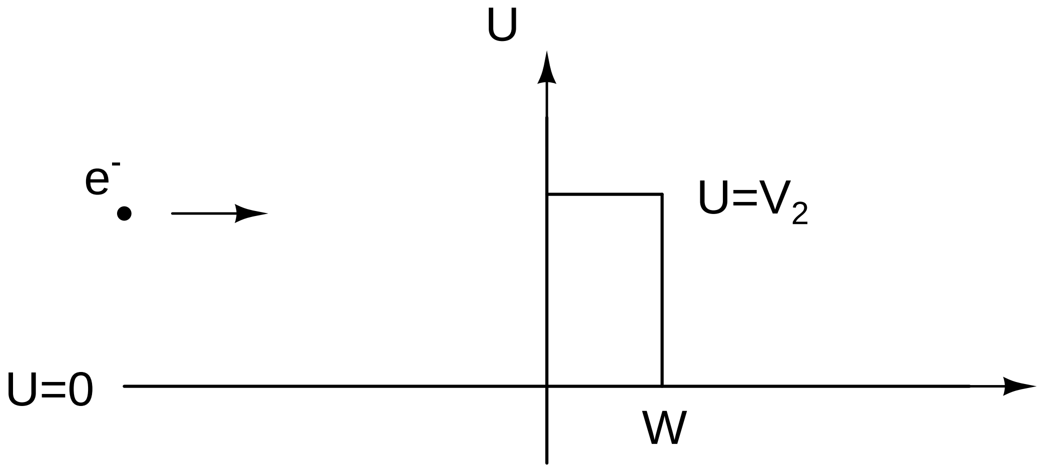

Figure 3: An electron approaching a finite-width potential barrier.

3.3 Tunneling

Consider an electron approaching the potential barrier of finite width shown in figure 3 The wavefunction will be the same as the one we found for a free electron for $x < 0$ and for $x > W$. For $0 \leq x \leq W$, the wavefunction will be similar to ψ_2 in the previous example. Thus,

$$\psi(x) = \begin{cases} A_+e^{ikx} + A_-e^{-ikx} & \forall x < 0 \\ B_+e^{ik_2x} + B_-e^{-ik_2x} & \forall 0 \leq x \leq W \\ C_+e^{ikx} + C_-e^{-ikx} & \forall x > W \end{cases}$$

where $\hbar k = \sqrt{2mE}$ and $\hbar k_2 = \sqrt{2m(E - V_2)}$.

Again, we can limit ourselves to the case of an electron approaching the barrier from the left, so that $C_- = 0$. Rather than proceeding to match the wave-functions and its derivative at $x = 0$ and $x = W$ to determine the relation between coefficients explicitly , we shall be happy by expressing the result in terms of the transmission coefficient, defined as

$$T = \left|\frac{C_+}{A_+}\right|^2$$

For $E > V_2$,

$$T = \frac{1}{1 + \frac{V_2^2}{4E(E-V_2)}S^2} \tag{1}$$

where $S = sin(k_2W)$. Notice that this equals unity for any barrier width for which $k_2W = n\pi$, where n is any integer. For the case in which $E < V_2$,

$$T = \frac{1}{1 + \frac{V_2^2}{4E(V_2-E)}S_h^2} \tag{2}$$

where $S = sinh(ik_2W)$. Wave-functions for both cases are shown in figure 4. It can be observed that an electron with a an energy lower than V_2 have a finite probability of penetrating the barrier.

3.4 The Quantum Well

Another problem of practical interest is the *quantum well*, shown in figure 5 for the one dimensional case. It is convenient in this case to express the imaginary exponentials in terms of sinusoids and chose wave-functions of the form

$$\psi(x) = \begin{cases} A_1e^{\alpha x} + B_1e^{-\alpha x} & \forall x < 0 \\ A_0sin(kx) + B_0cos(kx) & \forall 0 \leq x \leq W \\ A_2e^{\alpha x} + B_2e^{-\alpha x} & \forall x > W \end{cases}$$

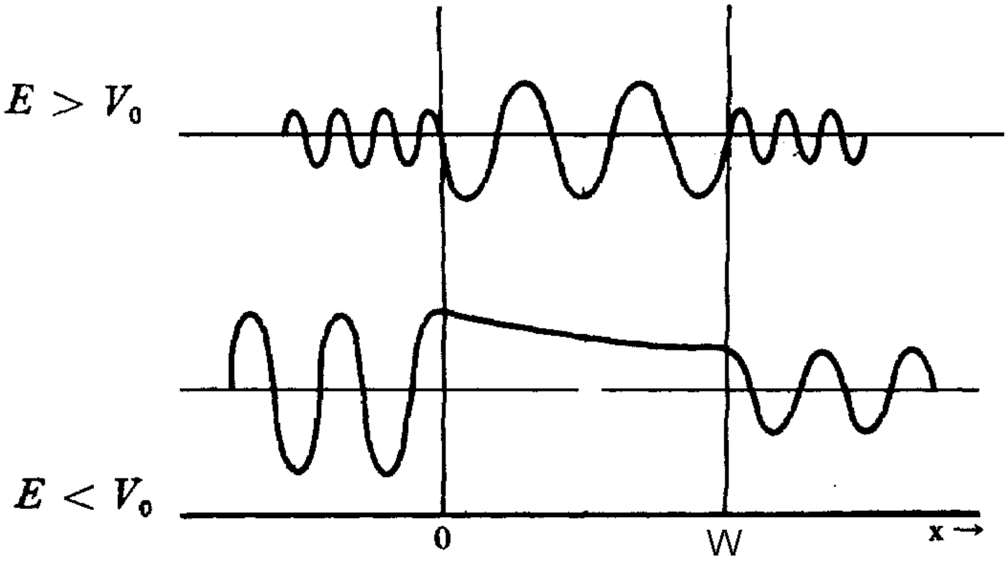

Figure 4: Wavefunction shape for the tunneling example.

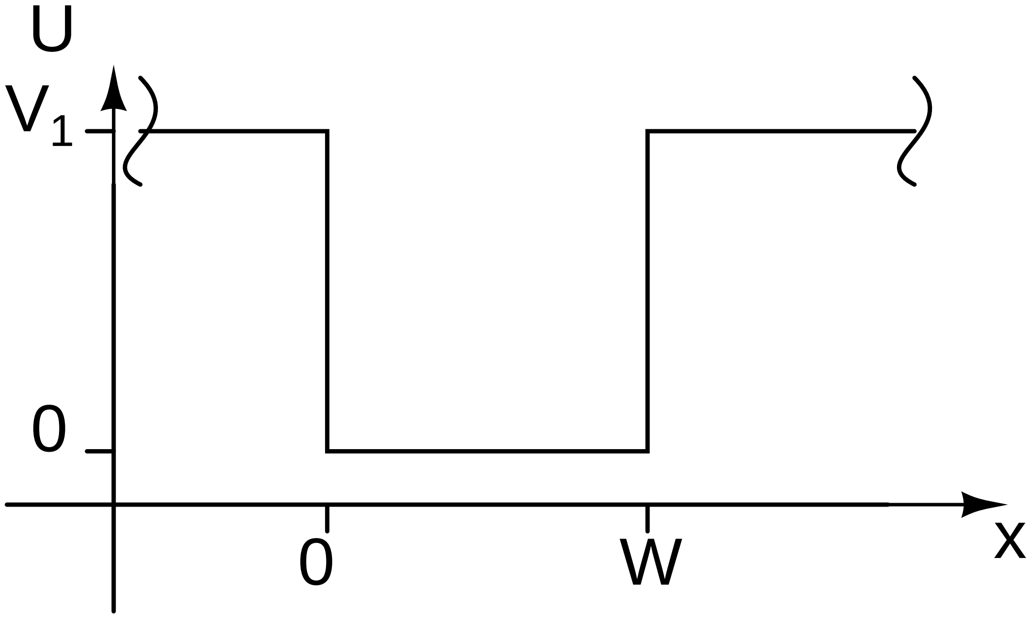

Figure 5: A one-dimensional quantum well.

where

$$\alpha = \frac{\sqrt{2m(V_1 - E)}}{\hbar}$$

and

$$k = \frac{\sqrt{2mE}}{\hbar}$$

Notice that if $E > V_1$ then alpha is imaginary and the corresponding exponential terms in the wavefunction display oscillations that extend to infinity. In the other hand, if $E < V_1$ we expect the wavefunction to decay as it penetrates the barrier, an to vanish far from it. This behavior requires that $B_1 = A_2 = 0$.

The resulting wavefunction,

$$\psi(x) = \begin{cases} A_1 e^{\alpha x} & \forall x < 0 \\ A_0 sin(kx) + B_0 cos(kx) & \forall 0 \leq x \leq W \\ B_2 e^{-\alpha x} & \forall x > W \end{cases}$$

must satisfy the continuity boundary conditions at $x = 0$ and $x = W$: $\psi(0-) = \psi(0+)$, $\psi(W-) = \psi(W+)$, $\frac{d\psi}{dx}(0-) = \frac{d\psi}{dx}(0+)$, and $\frac{d\psi}{dx}(W-) = \frac{d\psi}{dx}(W+)$. Evaluation of these conditions into the wavefunction yield

$$A_1 = B_0 \tag{3}$$

$$B_0 = \frac{k}{\alpha} A_0 \tag{4}$$

$$A_0 sin(kW) + B_0 cos(kW) = B_2 e^{-\alpha W} \tag{5}$$

$$k\left(A_0 cos(kW) - B_0 sin(kW)\right) = -\alpha B_2 e^{-\alpha W} \tag{6}$$

Solving equation 5 for B_2, substituting into eq. 6 and rearranging yields

$$A_0\left(k cos(kW) + \alpha sin(kW)\right) - B_0\left(k sin(kW) - \alpha cos(kW)\right) = 0$$

which, after eliminating A_0 and B_0 by using eqs. 3 and 4 can be expressed as

$$tan(kW) = \frac{2k\alpha}{k^2 - \alpha^2} \tag{7}$$

Since V_1 and W are constants, this is a single-variable equation in E. It is, however, convenient to re-write it in terms of a normalized energy $\xi = E/V_1$. Notice that

$$kW = \frac{\sqrt{2mE}}{\hbar} = \frac{W\sqrt{2mV_1}}{\hbar}\sqrt{\frac{E}{V_1}} = Wa\sqrt{\xi}$$

where $a = \frac{\sqrt{2mV_1}}{\hbar}$, and that

$$\frac{2k\alpha}{k^2 - \alpha^2} = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1}$$

Equation 7 thus becomes

$$tan(Wa\sqrt{\xi}) = \frac{2\sqrt{\xi(1-\xi)}}{2\xi - 1}$$

The following observations can be made about this result:

- The tangent of an angle θ increases from 0 at $\theta = 0$ to $+\infty$ at $\theta = \pi/2$; it then jumps discontinuously to $-\infty$ and increases again to 0 at $\theta = \pi$. This behavior repeats with a period π.
- The function in the right-hand side of the above expression is compared to the tangent on the left-hand side on figure 6 for the case in which $Wa = 4\pi$. It can be observed that the two sides of the above expression intercept at four different points. Thus there are four energy levels for which the particle is confined to the well ($0 < E < V_1$).

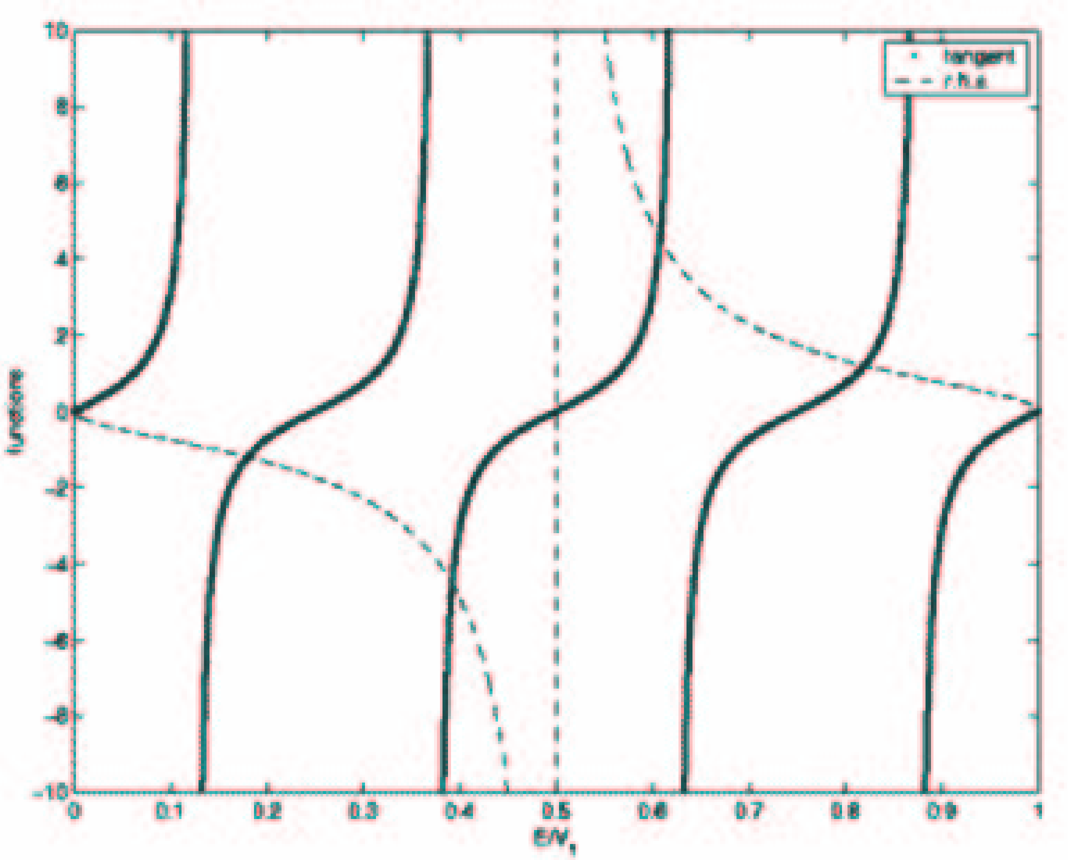

Figure 6: Comparison of the two functions in the result obtained for the quantum well example.

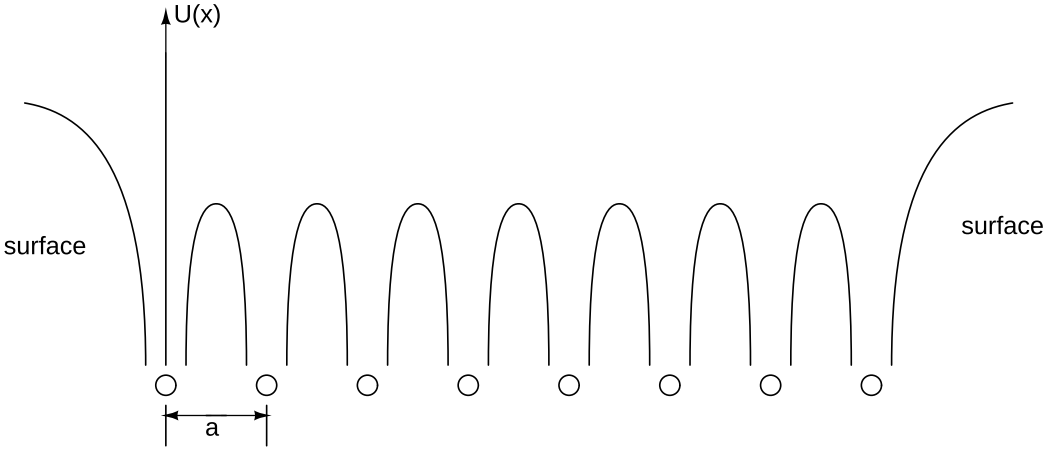

Figure 7: Potential due to a one-dimensional Crystal lattice. The distance between ion cores is a .

4 Energy Bands

When a particle is subject to a periodic potential, quantum mechanics predicts that the particle's energy is not arbitrary, but must be within one of several continuous ranges of allowable energies. In a crystal, these ranges are called *allowable energy bands* and are separated by *energy gaps*. They give place to the *electronic structure* of the crystal and determine its chemical and electrical properties.

The determination of the electronic structure of a three-dimensional solid is a complex exercise that is beyond the scope of our discussion here. The book by Harrison [1] provides a relatively friendly introduction to the subject. Our discussion will be limited to a simplified one-dimensional model in which electrons are subject to the potential produced by fixed ions. These ions are arranged in a periodic lattice like the one shown in figure 7, and consist of the atomic nuclei and tightly-bound electrons.

Some of the simplifying assumptions that we will make are:

- The effects of lattice defects and atomic-core vibrations are considered as second-order corrections to our analysis.
- Electron-electron interaction is neglected.
- Atomic cores extend from $x = 0$ to $x = (N-1)a$ where N is the number of atoms in the crystal.
- To avoid the complexity of considering the potential at the solid's surfaces, we shall assume a *ring* of atoms, with the last atom being followed by the first one.

4.1 Bloch Theorem

The quantum mechanical analysis of systems that involve periodic potentials is greatly simplified by the use of the *Bloch Theorem*:

Theorem 1 *For a periodic potential $U(x)$ such that $U(x+a) = U(x)$, the solutions to Schrdinger's Equation consist of wave-functions that obey*

$$\psi(x+a) = e^{ika}\psi(x)$$

This is equivalent to

$$\psi(x) = e^{ikx}u(x)$$

where $u(x)$ is also periodic with period a, i.e. $u(x+a) = u(x)$.

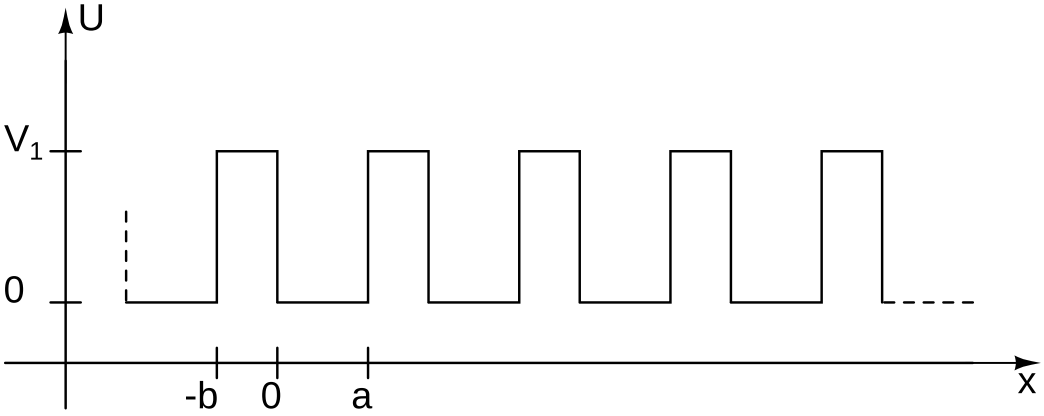

Figure 8: Potential used in the Kronig-Penney Model.

The last statement can be seen to result from the first by direct substitution,

$$\begin{aligned} \psi(x+a) &= e^{ik(x+a)}u(x+a) \\ &= e^{ikx}e^{ika}u(x) \\ &= e^{ika}\psi(x) \end{aligned}$$

Notice that our assumption of a ring-shaped lattice imposes restrictions in the values that k can assume. To see this, consider that for the N-atom lattice with inter-atomic distance a,

$$\psi(x) = \psi(x + N \times a) = e^{ikNa}\psi(x)$$

Thus

$$e^{ikNa} = 1$$

and

$$k = \frac{2\pi n}{Na}$$

where n assumes the integer values $0, \pm 1, \pm 2, ... \pm N/2$.

4.2 Kronig-Penney Model

The complexity of the potential shown in 7 prevent us from obtaining an algebraic solution to Schrdinger's Equation. An algebraic solution can be obtained if this lattice potential is replaced by the one shown in figure 8. Albeit highly unrealistic, the use of this potential is standard practice in introductory solid state courses and provides us with valuable insight into the nature of the real problem. It is known as the *Kronig-Penney Model*.

For this potential, for the segments in which $U = 0$, the time-independent Schrdinger Equation can be written as

$$\frac{d^2\psi}{dx^2} + \alpha^2\psi = 0$$

where $\alpha = \sqrt{2mE}/\hbar$. If $U = V_1$, the equation becomes

$$\frac{d^2\psi}{dx^2} + \beta^2\psi = 0$$

where $\beta = \sqrt{2m(E - V_1)}/\hbar$. Notice that β is imaginary if $E < V_1$.

If we assume wave-functions of the form

$$\psi(x) = \begin{cases} A_0 sin(\alpha x) + B_0 cos(\alpha x) & \forall 0 < x < a \\ A_1 sin(\beta x) + B_1 cos(\beta x) & \forall -b < x < 0 \end{cases}$$

which repeats itself around each lattice point[1].

The requirements imposed on these equations can be expressed as

- ψ and $d\psi/dx$ must be continuous, and
- the Bloch Theorem must be satisfied.

Applying these requirements to the previously shown ψ yields:

- For $\psi(0-) = \psi(0+)$:
$$B_1 = B_0$$
for $\frac{d\psi}{dx}(0-) = \frac{d\psi}{dx}(0+)$:
$$\beta A_1 = \alpha A_0$$
or
$$A_1 = \frac{\alpha}{\beta} A_0$$
- For $\psi(a-) = e^{ik(a+b)}\psi(-b+)$:
$$\begin{aligned} \psi(a-) &= A_0 sin(\alpha a) + B_0 cos(\alpha a) \\ &= e^{ik(a+b)}\psi(-b+) \\ &= e^{ik(a+b)}(A_1 sin(\beta \times -b) \\ &\quad +B_1 cos(\beta \times -b)) \\ &= e^{ik(a+b)}(-A_1 sin(\beta b) + B_1 cos(\beta b)) \end{aligned}$$
- for $\frac{d\psi}{dx}(a-) = e^{ik(a+b)}\frac{d\psi}{dx}(-b+)$:
$$\begin{aligned} \frac{d\psi}{dx}(a-) &= \alpha(A_0 cos(\alpha a) - B_0 sin(\alpha a)) \\ &= e^{ik(a+b)}\beta(A_1 cos(\beta b) + B_1 sin(\beta b) \end{aligned}$$

Rearranging and substituting the first two results into the last two, we obtain the following equations

$$\begin{aligned} &A_0\left(sin(\alpha a) + \frac{\alpha}{\beta} sin(\beta b)\right) \\ &\quad +B_0\left(cos(\alpha a) - e^{ik(a+b)}cos(\beta b)\right) = 0 \end{aligned}$$

$$\begin{aligned} &A_0\left(\alpha cos(\alpha a) - \alpha e^{ik(a+b)}cos(\beta b)\right) \\ &\quad +B_0\left(-\alpha sin(\alpha a) - \beta e^{ik(a+b)}sin(\beta b)\right) = 0 \end{aligned}$$

The requirement for a non-trivial solution is that the determinant of the quantities inside parenthesis vanish, or that

$$\begin{aligned} &\left(sin(\alpha a) + \frac{\alpha}{\beta} sin(\beta b)\right) \\ &\quad \times\left(-\alpha sin(\alpha a) - \beta e^{ik(a+b)}sin(\beta b)\right) \\ &\quad = \left(cos(\alpha a) - e^{ik(a+b)}cos(\beta b)\right) \\ &\quad \times\left(\alpha cos(\alpha a) - \alpha e^{ik(a+b)}cos(\beta b)\right) \end{aligned}$$

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[1] Notice that because β is imaginary if $E < V_1$, and

$$\begin{aligned} cos\theta &= \frac{e^{i\theta} + e^{-i\theta}}{2} \\ sin\theta &= \frac{e^{i\theta} - e^{-i\theta}}{2i} \end{aligned}$$

in that case the trigonometric functions will become hyperbolic in the last equation.

This can be rearranged to get

$$-\frac{\beta^2+\alpha^2}{\beta}e^{ik(a+b)}sin(\alpha a)sin(\beta b)$$
$$+2\alpha e^{ik(a+b)}cos(\alpha a)cos(\beta b)=\alpha\left(1+e^{i2k(a+b)}\right)$$

which, after multiplying by $\frac{1}{2\alpha}e^{-ik(a+b)}$ and using the identity $cos\theta=\frac{e^{i\theta}+e^{-i\theta}}{2}$ yields

$$cos(\alpha a)cos(\beta b)-\frac{\beta^2+\alpha^2}{2\alpha\beta}sin(\alpha a)sin(\beta b)=cos\left(k(a+b)\right) \tag{8}$$

4.3 Discussion

Equation 8 can be considered the result of the analysis using the Kronig-Penney model. To understand its implications it is convenient to express it in terms of a normalized energy $\xi=E/V_1$. Defining $\alpha_0=\frac{\sqrt{2mV_1}}{\hbar}$ such that

$$\alpha=\frac{\sqrt{2mE}}{\hbar}=\alpha_0\sqrt{\xi}$$
$$\beta=\frac{\sqrt{2m(E-V_1)}}{\hbar}=\frac{\sqrt{2mV_1(E/V_1-1)}}{\hbar}=\alpha_0\sqrt{\xi-1}$$

we can express equation 8 as

$$cos\left(k(a+b)\right)=cos(\alpha_0 a\sqrt{\xi})cos(\alpha_0 b\sqrt{\xi-1})$$
$$-\frac{1-2\xi}{2\sqrt{\xi(\xi-1)}}sin(\alpha_0 a\sqrt{\xi})sin(\alpha_0 b\sqrt{\xi-1})$$

Recall that, because we are considering a ring of atoms with period $a+b$, $k=\frac{2\pi n}{N(a+b)}$ where n is an integer between $\pm N/2$. Since this is a real quantity

$$0\le cos(k(a+b))\le 1$$

for all the allowed values of k. Thus, the energy levels for which the right-hand side of the above equation is in this range satisfy Schrdinger Equation and are therefore allowed. These energies form the *energy bands* of the solid. The range of energies that do not satisfy this criterion form the *forbidden gaps* between the bands. These bands are shown as boxes in figure 9 for the specific case in which $a=b=\frac{\pi}{\alpha_0}$.

4.4 Carrier Effective Mass

In our discussion of the free electron wavefunction, it was said that to limit the existence of a particle to some region in space a *wavepacket* had to be constructed by superimposing wavefunctions with different energies. Wave theory describes the motion of a packet of electromagnetic waves in terms of a *dispersion relation* that defines the *group velocity* of the packet,

$$v_g=\frac{d\omega}{dk}$$

To apply the same concept to wavepackets, the angular frequency ω must be replaced by its quantum mechanical equivalent, $E/\hbar$ to obtain that

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

If an external force is applied to the packet such that work is done,

$$dE=Fdx=Fv_gdt=F\frac{1}{\hbar}\frac{dE}{dk}dt=\frac{F}{\hbar\frac{dk}{dt}}dE$$

which implies that

$$F=\hbar\frac{dk}{dt}$$

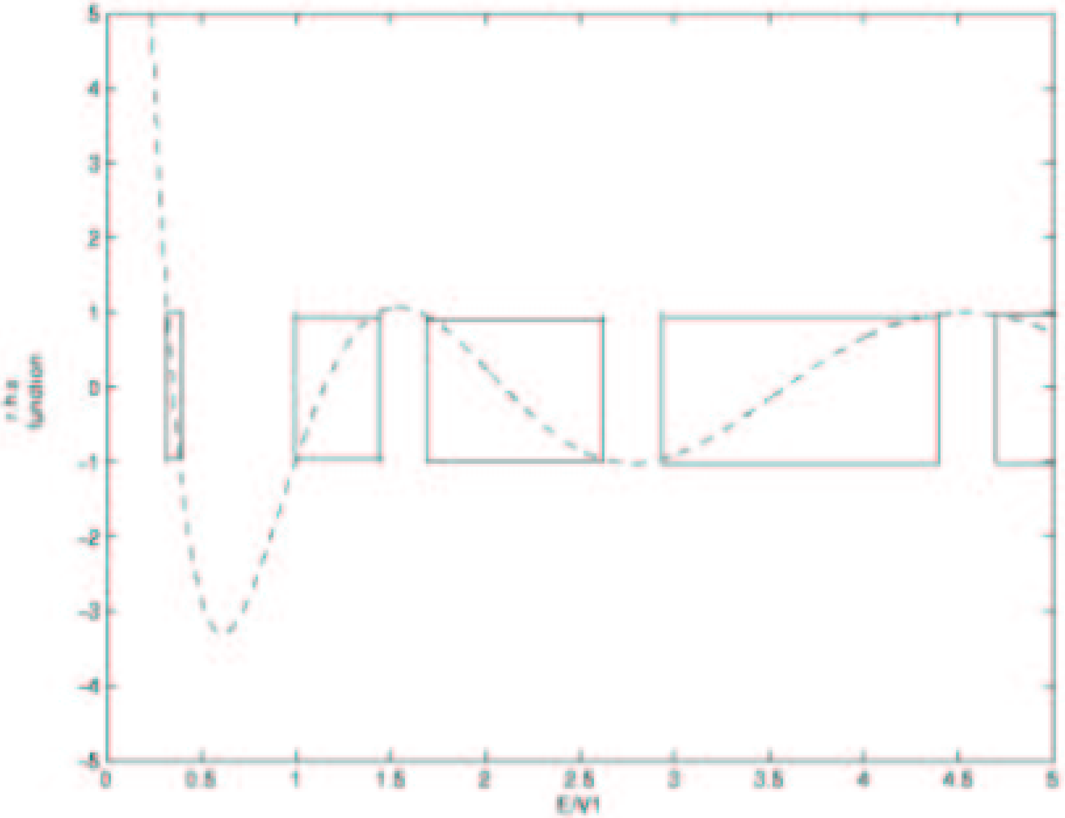

Figure 9: Result from the analysis of a periodic potential represented by the Kronig-Penney model for $a = b = \frac{\pi}{\alpha_0}$.

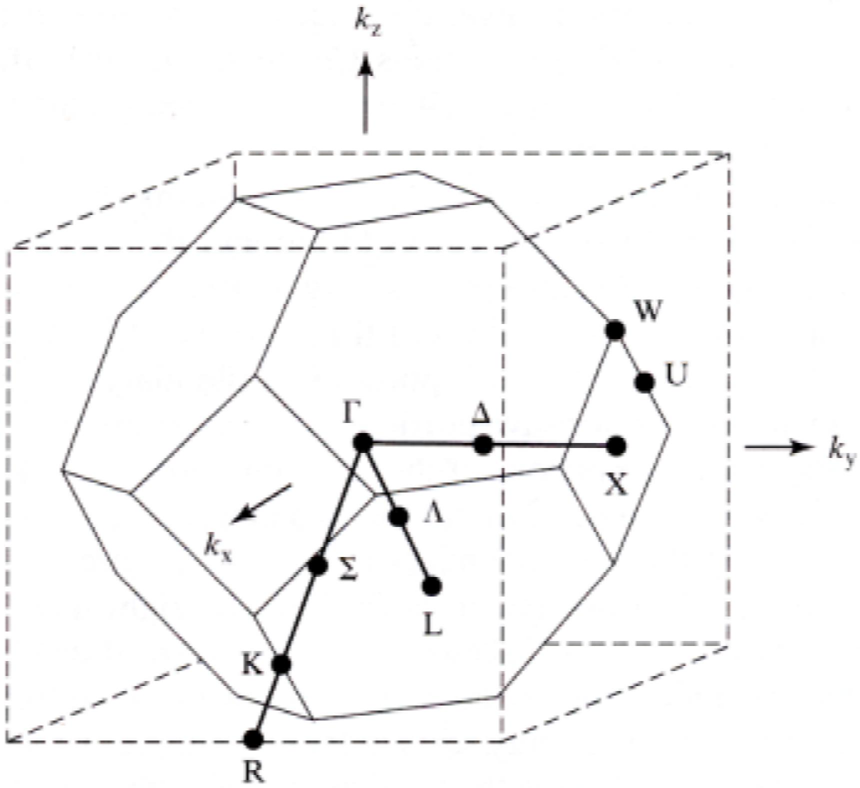

Figure 10: First Brillouin zone for materials crystalilizing in the diamond and zincblende lattices.

In the other hand,

$$\frac{dv_g}{dt} = \frac{1}{\hbar}\frac{d}{dt}\left(\frac{dE}{dk}\right) = \frac{1}{\hbar}\frac{d^2E}{dk^2}\frac{dk}{dt}$$

is the acceleration of the wavepacket. Solving for $\frac{dk}{dt}$, substituting into our previous expression for F, we get

$$F = \frac{1}{\frac{1}{\hbar^2}\frac{d^2E}{dk^2}}\frac{dv_g}{dt}$$

Recalling that force equals mass times acceleration and taking the group velocitys rate of change as the acceleration, we identify the particles *effective mass* as

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

- Brillouin zone: ranges of k associated with a given energy band.
- In three dimensions, the Block wavenumber becomes a vector and the Brillouin zones become volumes.
- Γ: identifies the zone center ($k = 0$)
- X: denotes the zone end along a $< 100 >$ direction
- L: denotes the zone end along a $< 111 >$ direction

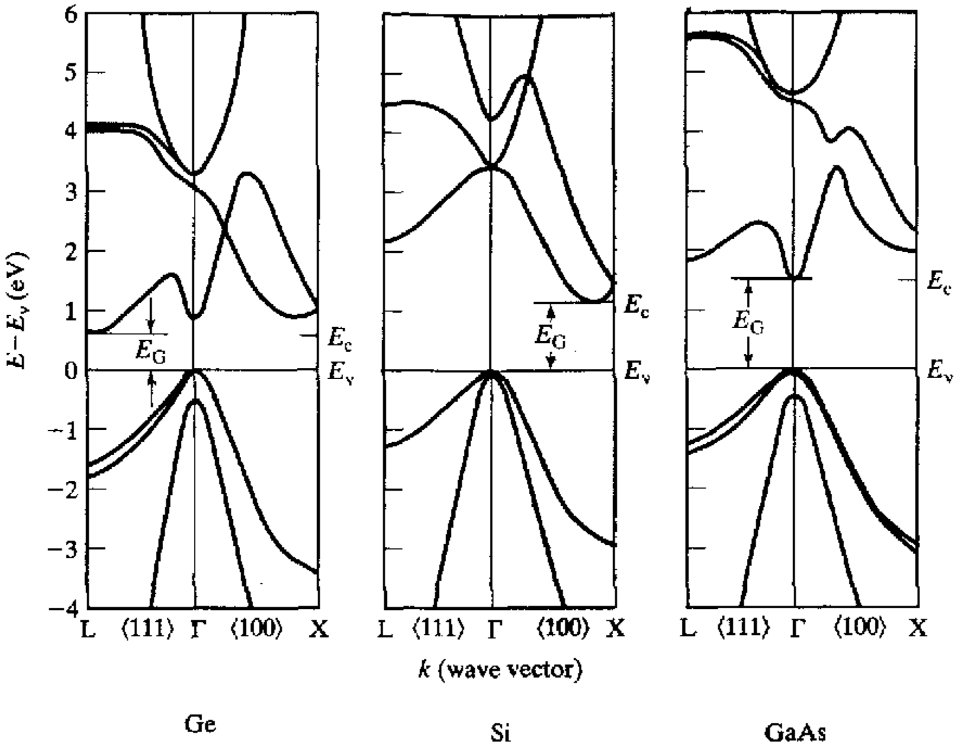

Figure 11: Electronic structure of Si, Ge and GaAs.

Effective Mass	Ge	Si	GaAs
m_l^*/m_0	1.588	0.9163	-
m_t^*/m_0	0.08152	0.1905	-
m_e^*/m_0	-	-	0.067
m_{hh}^*/m_0	0.347	0.537	0.51
m_{lh}^*/m_0	0.0429	0.153	0.082
m_{so}^*/m_0	0.077	0.234	0.154

Table 1: Electron and hole effective masses. The meaning of the subscripts is: l=longitudinal, t=transversal, e=?, hh=heavy-hole, lh=light-hole, and so=split-off. Numbers are in reference to m_0, the electron rest mass.

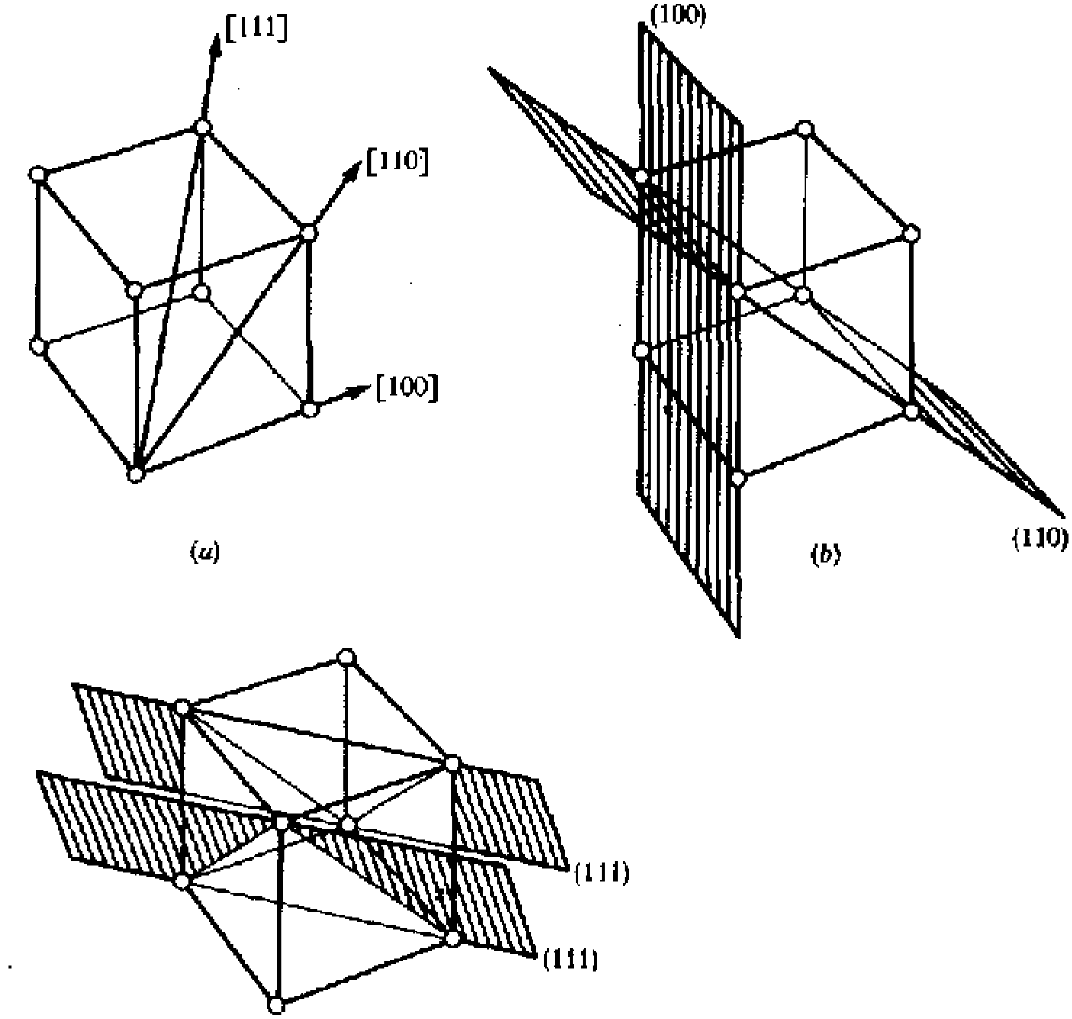

Figure 12: Description of the Miller indeces for the simple cubic structure: (a) directions, (b) (100) an (110) planes, and (c) two parallel (111) planes.

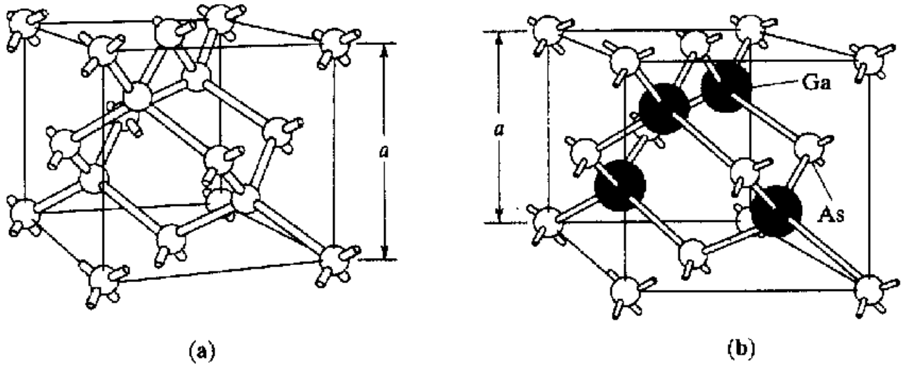

Figure 1.5 (a) Diamond lattice unit cell. (b) Zincblende lattice unit cell (GaAs used for illustration).

Figure 13: Diamond and Zincblende unit cells. While the diamond lattice is found in Silicon and Germanium crystals, GaAs adopts the Zincblende structure.

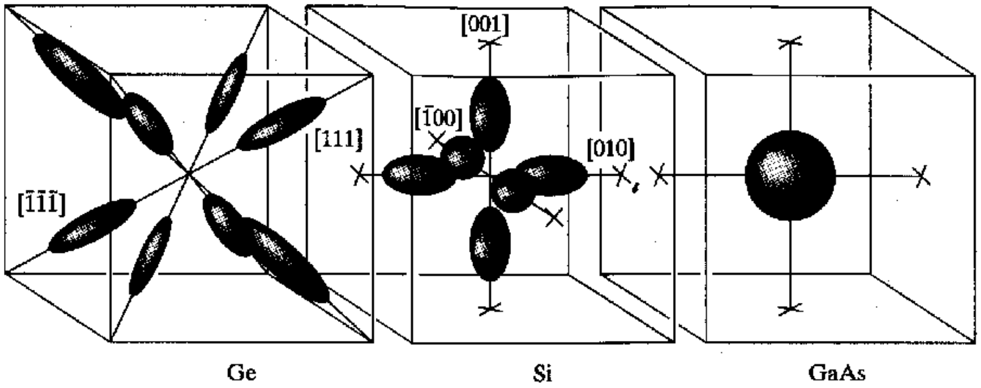

Figure 14: Representation of the constant energy surfaces near the bottom of the conduction band.

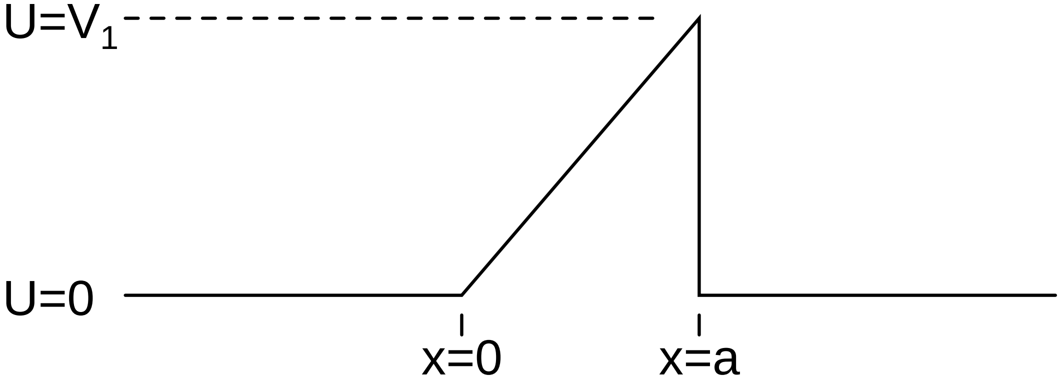

Figure 15: Triangular barrier discussed in problem 2.

5 Homework

1. Derive equations 1 and 2 from the wavefunction given in the text.
2. For the triangular potential barrier shown in figure 15
    (a) Assuming that the wavefunction will have different forms for $0 \leq x \leq a$ and for $x < 0$ or $x > a$, write down Schrdingers equation for the specified problem. Let $k = \frac{\sqrt{2mE}}{\hbar}$.
    (b) Show that the specified wavefunctions are indeed a solution to Schrdingers equation.
    (c) Indicate the boundary conditions that must be employed to solve the problem.
    (d) Derive the set of simultaneous equations that must be solved.
    (e) (optional) Find an expression for the energy states that correspond to $E < V_1$.

6 Further Reading

1. I extensively used the following two books to prepare this document:

    Advanced Semiconductor Fundamentals, by Robert F. Pierret, Second Edition, *Modular Series on Solid State Devices*, vol. VI, Prentice Hall, 2003.

    Solid State and Semiconductor Physics, John P. McKelvey, Robert E. Krieger Publishing Company, Malabar, Florida, 1966.

2. It you are interested in applications of quantum theory to electronic devices, you can consult:

    Quantum Phenomena, by Supriyo Datta First Edition, *Modular Series on Solid State Devices*, vol. VIII, Prentice Hall, 1989.

3. There are many books that offer a more complete introduction to Quantum Mechanics. One of them is:

    Modern Physics and Quantum Mechanics, by Elmer E. Anderson, W. B. Saunders Co., Phil., PA, 1971.

4. Figure 1 was taken from the book *Devices for Integrated Circuits*, by H. Craig Casey, jr., John Wiley and Sons, 1999.

5. The following book offers an introduction to electronic band calculations using pseudo-potentials, written by a leading researcher in the field.

    Electronic Structure and the properties of Solids: The Physics of the Chemical Bond, by Walter A. Harrison, Dover Publications, 1989.

6. The following Internet link gives you access to what appear to be a draft for a whole book on semiconductor devices. It includes chapters about Quantum Mechanics and energy bands.

   http://ece-www.colorado.edu/ bart/book/

7. Check this one out for an interactive applet demonstrating the Kronig-Penney model predictions:

   http://www.benfold.com/sse/kp.html