

Chapter 2 Introduction to Quantum Mechanics

→ some behavior of electrons, semiconductors, ... can't be explained by classical physics.

This led to the development of quantum mechanics, key to understanding the physics behind semiconductors.

2.1 Principles of Quantum Mechanics

2.1.1 Energy Quanta

photoelectric effect

→ light incident on a material can cause an electron to be emitted (photoelectron)

* Classical physics would say that the intensity of the incident light would be all that matters

* Reality, the frequency ν (Hz) of the incident light matters much more. ← lowercase Greek letter Nu

* As shown in Fig. 2.1, at a constant intensity, below frequency ν_0 no photoelectrons are emitted. Above ν_0 , the max. kinetic energy $T_{\max}$ of electron increases linearly w/ ν .

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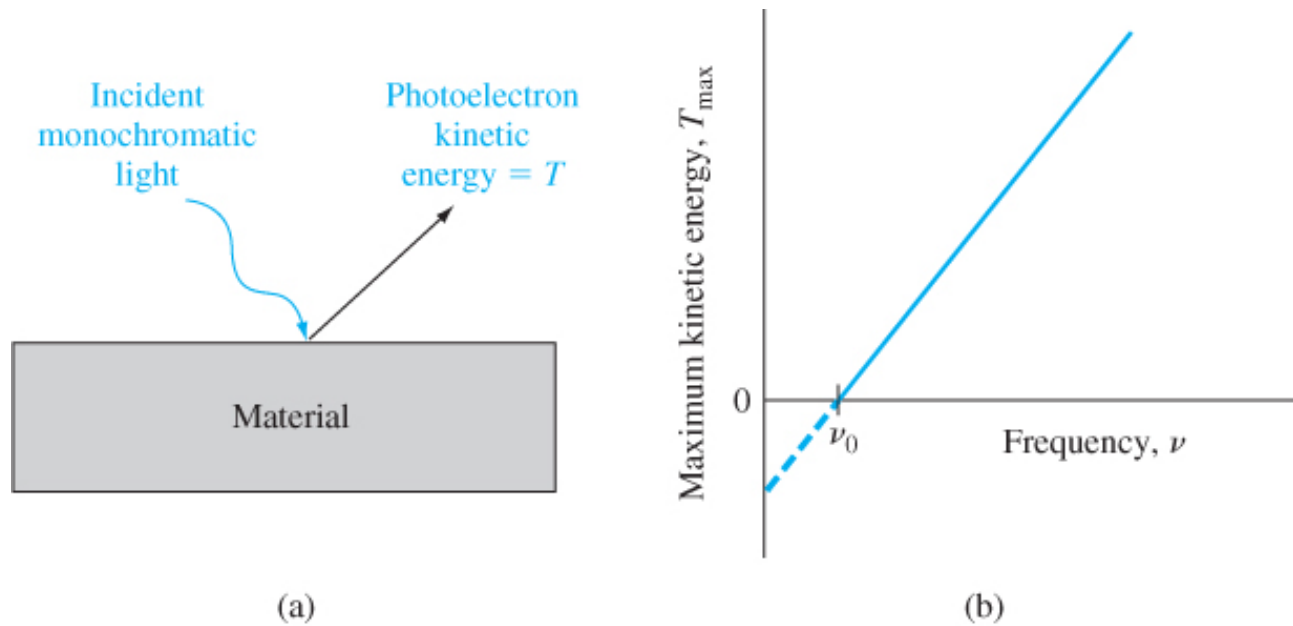


Figure 2.1 | (a) The photoelectric effect and (b) the maximum kinetic energy of the photoelectron as a function of incident frequency.

2.1.1 cont.

→ In 1900, Max Planck put forth the idea that energy from a heated surface, i.e., blackbody radiation, was emitted in discrete packets or quanta, i.e., $E = h\nu$, where

$\uparrow$ energy $\uparrow$ freq (Hz)

Planck's constant $\equiv h = 6.62607 \times 10^{-34} \text{ J}\cdot\text{s}$

→ Albert Einstein in 1905 made a splash (1921 Nobel in Physics) by theorizing that energy in light also came in discrete packets (i.e., like particles rather than waves) that he called photons. He developed this equation

$$T = \frac{1}{2}mv^2 = h\nu - \Phi \quad (2.1)$$

$\uparrow$ max. K.E. of photoelectron $\uparrow$ energy in photon $\uparrow$ work function to pry electron loose from surface

when RHS is less than zero $\rightarrow$ no photoelectrons

$\Phi = h\nu_0$ is the min. value required, all energy above goes to K.E. of photoelectron.

$$\underline{T = h(\nu - \nu_0) \quad \text{for } \nu \geq \nu_0}$$

2.1.1 cont.

ex. Find the energy associated w/ the photons of a 532 nm wavelength green laser.

$$E_g = h\nu = h\left(\frac{c}{\lambda}\right) = 6.62607 \times 10^{-34} \frac{2.9979 \times 10^8}{532 \times 10^{-9}}$$

$$= \underline{\underline{3.7339 \times 10^{-19} \text{ J}}}$$

For particle physics, the unit of electron-volts is often used. It's the energy gained by an electron going from rest through a 1V potential in vacuum. For SI units, $1\text{eV} = 1.602176634 \times 10^{-19} \text{ J}$.

$$E_g = 3.7339 \times 10^{-19} \left(\frac{1\text{eV}}{1.6022 \times 10^{-19} \text{ J}} \right) = \underline{\underline{2.3305 \text{ eV}}}$$

See Appendix D (p. 720) in text for a more detailed discussion of eV.

$$\text{EE 381} \quad V_{AB} = \frac{\text{Work}}{\text{charge}} = \frac{W}{Q}$$

$$\hookrightarrow W = QV_{AB}$$

$$\text{EE 362} \quad T = eV \quad \leftarrow \text{voltage}$$

$\uparrow$
 work/
 KE

$e = \text{mag. of charge of electron}$
 $= 1.6022 \times 10^{-19} \text{ C}$

2.1.2 Wave-Particle Duality

In 1924, Louis deBroglie (Fr. Phys) postulated that particles (e.g., electrons) can act like or w/ wave properties, the dual of waves acting like particles $\Rightarrow$ wave-particle duality

$\Downarrow$ led to

$$\text{momentum of a photon} \equiv p = \frac{h}{\lambda} \quad \leftarrow \text{Planck's constant} \quad (\text{kg m/s})$$

$$\text{deBroglie wavelength of a particle} \equiv \lambda = \frac{h}{p} \quad (\text{m}) \quad \leftarrow \text{momentum of particle}$$

This is evident or applies to very small particles, e.g., electrons and to protons + neutrons (harder). For macroscopic 'particles', the relevant equations converge w/ classical mechanics (Newtonian physics)

This will be used when examining how electrons behave in crystals.

2.1.3 The Uncertainty Principle

A German physicist Werner Heisenberg, another initial contributor to quantum mechanics, developed the uncertainty principle

part 1 $\Delta p \Delta x \geq \hbar = \frac{h}{2\pi} \equiv \text{reduced or modified Planck's constant}$

where Δp is uncertainty in momentum
while Δx " " " " location

→ can also apply to angular momentum
+ position

→ can't simultaneously know both p & x of
a particle

part 2 $\Delta E \Delta t \geq \hbar = 1.054572 \times 10^{-34} \text{ J.s}$

where ΔE is uncertainty of particle energy
while Δt is " " " " time @ which
particle has this energy

→ can't simultaneously know particle
energy & exact time @ which it has it

Since $\hbar$ is so small, this is typically
only an issue w/ subatomic particles
(e.g., electrons)

2.2 Schrodinger's Wave Equation

Erwin Schrodinger (Austrian) in 1926 proposed describing electron motion in crystals by wave theory (AKA wave mechanics)

2.2.1 The Wave Equation

→ 1D, nonrelativistic (Sorry Einstein) Schrodinger's Wave Equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x,t)}{\partial x^2} + V(x) \psi(x,t) = j\hbar \frac{\partial \psi(x,t)}{\partial t} \quad (2.6)$$

where $\psi(x,t) \equiv$ wave function,

$V(x) \equiv$ potential function, and

$m \equiv$ mass of particle

Next, assume the wave function is separable,

i.e., $\psi(x,t) = \psi(x)\phi(t)$. This leads to

$$-\frac{\hbar^2}{2m} \phi(t) \frac{\partial^2 \psi(x)}{\partial x^2} + V(x) \psi(x) \phi(t) = j\hbar \psi(x) \frac{\partial \phi(t)}{\partial t} \quad (2.8)$$

Dividing thru by $\psi(x)\phi(t)$, yields

$$\underbrace{-\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{\partial^2 \psi(x)}{\partial x^2} + V(x)}_{\text{all functions of } x} = j\hbar \underbrace{\frac{1}{\phi(t)} \frac{\partial \phi(t)}{\partial t}}_{\text{functions of } t} \quad (2.9)$$

2.2.1 cont.

From mathematics, the only way for the LHS and RHS to be equal for all positions 'x' and times 't' is for each to be equal to some constant which we'll call ' η ', the separation constant.

For the RHS, $j\hbar \frac{1}{\phi(t)} \frac{d\phi(t)}{dt} = \eta$

$$\frac{1}{\phi(t)} \frac{d\phi(t)}{dt} = \frac{\eta}{j\hbar}$$

$\times dt$ and integrate $\int \frac{d\phi(t)}{\phi(t)} = \int \frac{\eta}{j\hbar} dt$

$$\ln \phi(t) = \frac{\eta}{j\hbar} t$$

$$\phi(t) = e^{\frac{\eta}{j\hbar} t} = e^{-j(\frac{\eta}{\hbar})t}$$

letting $\omega = \eta/\hbar$, we get

$$\phi(t) = e^{-j\omega t} \leftarrow \text{complex exponential form of sinusoidal waves (negative time convention!)}$$

From earlier, $E = h\nu = h\left(\frac{\omega}{2\pi}\right) = \frac{h}{2\pi} \left(\frac{\eta}{\hbar}\right) = \eta!$
 $\uparrow$
 freq. $\Rightarrow \eta$ is total energy!

2.2.1 cont.

For the LHS, we can now write

$$-\frac{\hbar^2}{2m} \frac{1}{\psi(x)} \frac{d^2 \psi(x)}{dx^2} + V(x) = \eta = E.$$

This can be rearranged to

$$\frac{d^2 \psi(x)}{dx^2} + \frac{2m}{\hbar^2} \left\{ E - \overset{\substack{\text{pot. Energy}}}{V(x)} \right\} \psi(x) = 0 \quad (2.13)$$

called the time-independent Schrodinger's wave equation.

Appendix E shows how this can be explained or justified in terms of a voltage wave equation.

$$\frac{d^2 V(x)}{dx^2} + \left(\frac{\omega^2}{v_p^2} \right) V(x) = 0$$

If we replace $V(x)$ w/ $\psi(x)$ and use $v_p = \downarrow$ $\overset{\text{freq. (Hz)}}{v} \lambda$,

$$\text{we get } \frac{d^2 \psi(x)}{dx^2} + \left(\frac{2\pi}{\lambda} \right)^2 \psi(x) = 0$$

From earlier, $p = \hbar \lambda$ so $\frac{2\pi}{\lambda} = \frac{2\pi p}{\hbar} = \frac{p}{\hbar}$.

2.2.1 cont.

This allows us to say $\left(\frac{2\pi}{\lambda}\right)^2 = \left(\frac{p}{\hbar}\right)^2 = \frac{2m}{\hbar^2} \left(\frac{p^2}{2m}\right)$

where $\frac{p^2}{2m} = T = E - V$

$\uparrow$ Kinetic energy $\uparrow$ Total energy $\nwarrow$ potential energy

since $T = \frac{(mv)^2}{2m} = \frac{1}{2}mv^2$

Giving

$$\frac{\omega^2}{v_p^2} = \left(\frac{2\pi}{\lambda}\right)^2 = \frac{2m}{\hbar^2} (E - V).$$

This can be substituted into the wave equation

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

that looks like Schrodinger's 1D time-independent wave eq'n.

2.2.2 Physical Meaning of the Wave Function

Max Born (German physicist) postulated that

$|\Psi(x,t)|^2 dx$ is the probability of finding a particle between x and $x+dx$ around 1926,

Therefore, $|\Psi(x,t)|^2$ would be the probability density function for the particle.

Since, $\Psi(x,t) = \Psi(x)\phi(t) = \Psi(x)e^{-j\omega t}$ ← complex

$$|\Psi(x,t)|^2 = \Psi(x,t) \Psi(x,t)^*$$

$$= \Psi(x) e^{-j\omega t} \Psi^*(x) e^{+j\omega t}$$

$$(2.17) \quad \underline{|\Psi(x,t)|^2 = \Psi(x) \Psi^*(x) = |\Psi(x)|^2} \quad \leftarrow \text{NOT time dependent}$$

Classical physics - we can know precise location of an object

quantum mechanics - position of a particle is in terms of a probability density function

2.2.3 Boundary Conditions

Since a particle must be somewhere

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1 \quad (2.18)$$

Other boundary conditions, based on E and $V(x)$ being finite, are:

$\psi(x)$ must be finite, single-valued,
+ continuous

$$\frac{d\psi(x)}{dx} \quad \text{||}$$

Fig. 2.5 shows some consequences of these boundary conditions
(no solutions to $\psi(x)$ yet)

Finite well $\rightarrow$ Note that $\psi(x)$ is
continuous @ well edges

Infinite well $\rightarrow$ Note that $\psi(x)$ is continuous
@ well edges & $\psi(x) = 0$ when
 $V(x) \rightarrow \infty$ (particle can't
surmount infinite potential)

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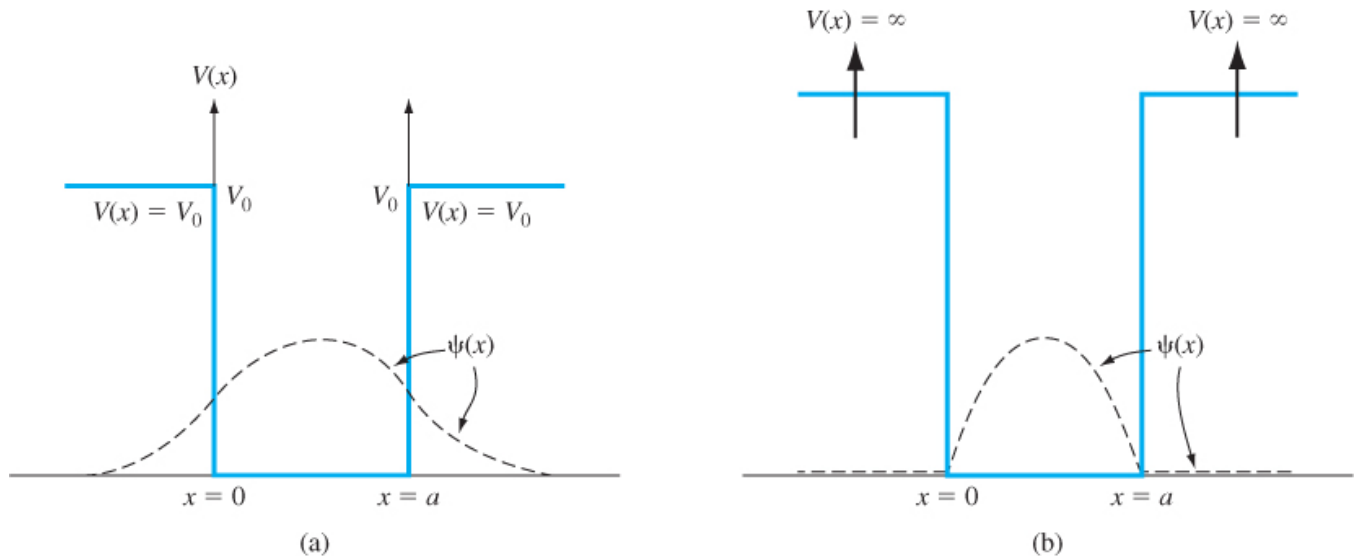


Figure 2.5 | Potential functions and corresponding wave function solutions for the case (a) when the potential function is finite everywhere and (b) when the potential function is infinite in some regions.

Handwaving arguments:

- For lefthand graph of $\psi(x)$ above, a particle is **less likely** to be in a region of higher potential than lower potential as it takes work/energy to move from lower potential to higher potential.
- For righthand graph of $\psi(x)$ above, a particle **cannot** be in a region of infinite potential as it would take infinite work/energy to reach such a region.

2.3 Applications of Schrodinger's Wave Equation

2.3.1 Electron in Free Space

Assume no applied force $\Rightarrow V(x) = \text{constant} \Rightarrow 0$

$$\Rightarrow E > V(x)$$

Here, $\frac{d^2 \psi(x)}{dx^2} + \frac{2mE}{\hbar^2} \psi(x) = 0$ 2nd-ord
ordinary
diff. Egn
(wave eqn)

has solution

$$\begin{aligned} \psi(x) &= A e^{j \sqrt{\frac{2mE}{\hbar^2}} x} + B e^{-j \sqrt{\frac{2mE}{\hbar^2}} x} \\ &= A e^{jKx} + B e^{-jKx} \end{aligned}$$

where wave number $\equiv K = \sqrt{\frac{2mE}{\hbar^2}}$.

The overall wave function is then

$$\begin{aligned} \Psi(x, t) &= \psi(x) \phi(t) \\ &= A e^{j(Kx - \omega t)} + B e^{-j(Kx + \omega t)} \quad (2.23) \\ &= A e^{-j(\omega t - Kx)} + B e^{-j(\omega t + Kx)} \end{aligned}$$

$\Rightarrow$ Traveling waves in the $\pm x$ -directions

$$K = \sqrt{\frac{2mE}{\hbar^2}} = \sqrt{\frac{p^2}{\hbar^2}} = p/\hbar \Rightarrow p = K\hbar$$

The deBroglie wavelength $\lambda = h/p = \frac{2\pi\hbar}{p}$

$$\hookrightarrow \lambda = \frac{2\pi\hbar}{K\hbar} = \frac{2\pi}{K} \Rightarrow K = \frac{2\pi}{\lambda}$$

2.3.1 cont.

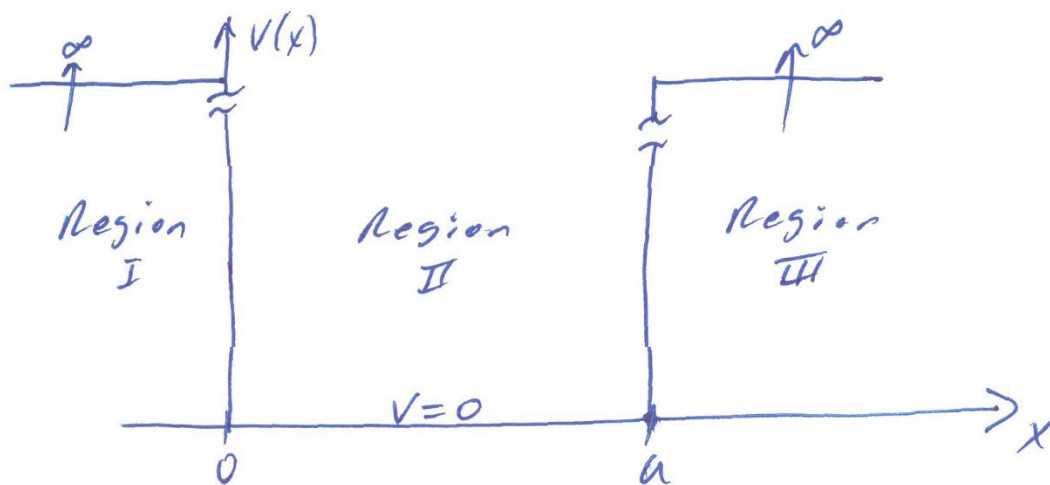
→ So, a free electron (particle) w/ well-defined energy E has a well-defined λ and momentum p . However, for the tx wave ($B=0$)

$$|\psi(x,t)|^2 = AA^* = \text{constant}$$

⇒ particle/electron equally likely to be anywhere! This agrees/supports Heisenberg uncertainty principle where if we know momentum p , then we can't also know position x .

2.3.2 The Infinite Potential Well

→ classic 'bound' particle problem



For a finite total energy E , $\psi(x) = 0$

for regions I & III as particle cannot reach them

2.3.2 cont.

In region II, $V(x)=0$. Therefore,

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

$$\text{becomes } \frac{d^2 \psi(x)}{dx^2} + \frac{2mE}{\hbar^2} \psi(x) = 0. \quad (2.28)$$

As we want a bounded sol'n, we'll choose a sol'n of the form

$$\psi(x) = A_1 \cos Kx + A_2 \sin Kx \quad (2.29)$$

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

Next, apply our boundary conditions that

$$\psi(x=0) = \psi(x=a) = 0.$$

$$\psi(0) = 0 = A_1 \overset{1}{\cos 0} + A_2 \overset{0}{\sin 0} \Rightarrow \underline{A_1 = 0}$$

$$\psi(a) = 0 = A_2 \sin(Ka)$$

For a non-trivial sol'n, $A_2 \neq 0$. Therefore,

$$\sin(Ka) = 0 \Rightarrow Ka = n\pi \text{ where } n=1,2,3,\dots$$

$$\hookrightarrow \underline{K = \frac{n\pi}{a} \text{ where } n=1,2,\dots}$$

2.3.2 cont.

How do we find A_2 ?

$\Rightarrow$ Recall that our particle must exist.

Therefore, $\int_{-\infty}^{\infty} \psi(x) \psi^*(x) dx = 1$ (2.18).

which reduces to

$$\int_{x=0}^a A_2 \sin Kx (A_2 \sin Kx) dx = 1$$

$$A_2^2 \int_{x=0}^a \sin^2 Kx dx = 1$$

$$A_2^2 \int_{x=0}^a \frac{1}{2} (1 - \cos 2Kx) dx = 1$$

$$\frac{A_2^2}{2} \left[x - \frac{1}{2} \sin 2Kx \right] \Big|_{x=0}^a = 1$$

$$\frac{A_2^2}{2} \left[(a - \frac{1}{2} \sin 2n\pi) - (0 - 0) \right] = 1$$

$$\hookrightarrow \underline{A_2 = \sqrt{2/a}}$$

Now, we have our particular sol'n

$$\psi(x) = \sqrt{2/a} \sin\left(\frac{n\pi}{a} x\right) \text{ where } n = 1, 2, \dots$$

$$0 \leq x \leq a$$

2.3.2 cont.

Further, note that $K = \sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{a}$

$$K^2 = \frac{2mE}{\hbar^2} = \frac{n^2 \pi^2}{a^2} = K_n^2 \quad \leftarrow \text{wave \# takes on discrete/quantized values!}$$

$$\hookrightarrow \underline{E = E_n = \frac{\hbar^2 n^2 \pi^2}{2ma^2} \quad n = 1, 2, \dots \quad (2.38)}$$

$\Rightarrow$ Energy of particle is quantized!

We can also write $\psi(x) = \sqrt{\frac{2}{a}} \sin(K_n x) \quad 0 \leq x \leq a$

The following MathCad example will illustrate the consequences for $n = 1, 2, 3, \dots$

Example- Let's examine the various quantities related to putting an electron in an infinite potential well that is 4 Angstroms wide.

Define some constants

$$h := 6.62607015 \cdot 10^{-34} \text{ J-s} \quad h_{\text{mod}} := \frac{h}{2 \cdot \pi} \quad h_{\text{mod}} = 1.05457 \times 10^{-34} \text{ J-s}$$

$$\underline{m} := 9.1093837015 \cdot 10^{-31} \text{ kg} \quad a := 4 \cdot 10^{-10} \text{ m}$$

Calculate some quantities and/or define equations

Per (2.33), the wave number (rad/m), in terms of quantum number n , is $k(n) := \frac{n \cdot \pi}{a}$

Per (2.35) $A2 := \sqrt{\frac{2}{a}} \quad \boxed{A2 = 7.071 \times 10^4} \text{ m}^{-0.5}$

Per (2.38), the quantized energy (J & eV), in terms of quantum number n , is

$$E(n) := \frac{h_{\text{mod}}^2 \cdot n^2 \cdot \pi^2}{2 \cdot m \cdot a^2} \quad E_{\text{eV}}(n) := \frac{E(n)}{1.602176634 \cdot 10^{-19}}$$

Per (2.39), the wave function ($\text{m}^{-0.5}$), in terms of quantum number n & position x , is

$$\psi(n, x) := A2 \cdot \sin(k(n) \cdot x)$$

Per (2.17), the probability density function (m^{-1}), in terms of quantum number n and position x , is

$$\Psi^2(n, x) := \psi(n, x) \cdot \overline{\psi(n, x)}$$

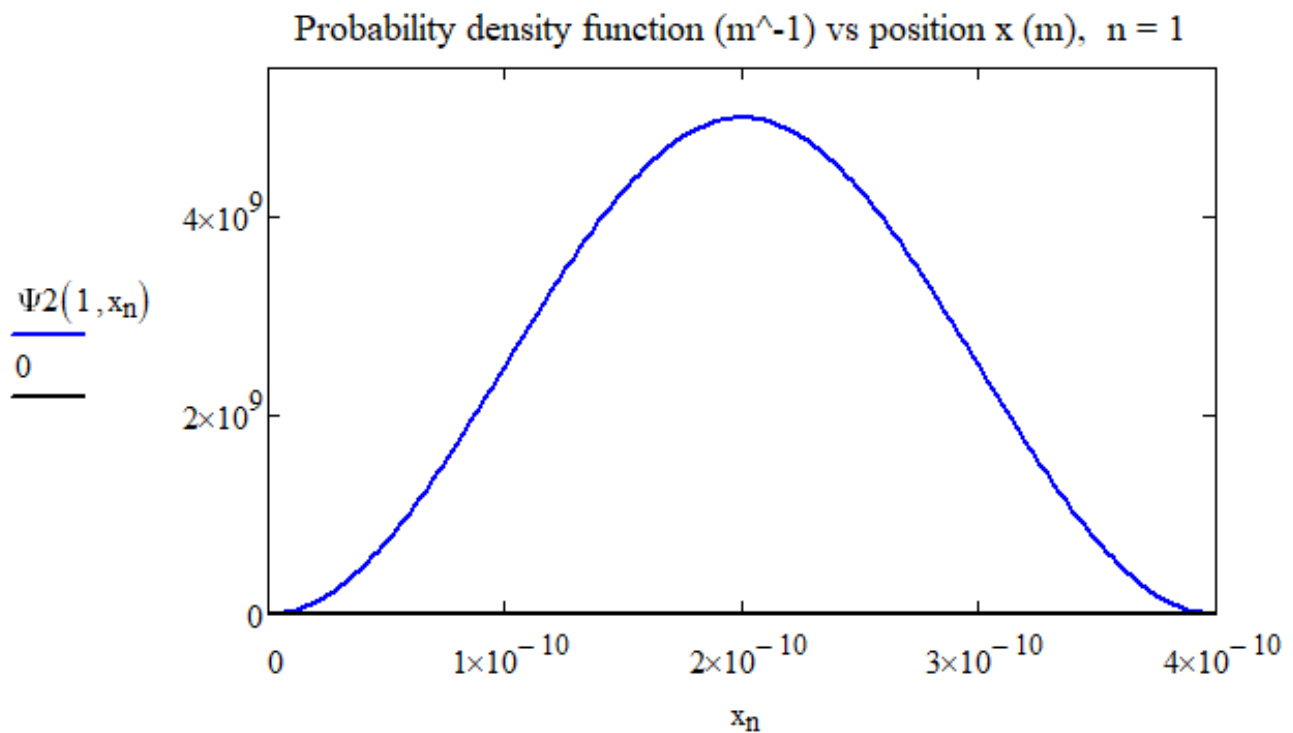
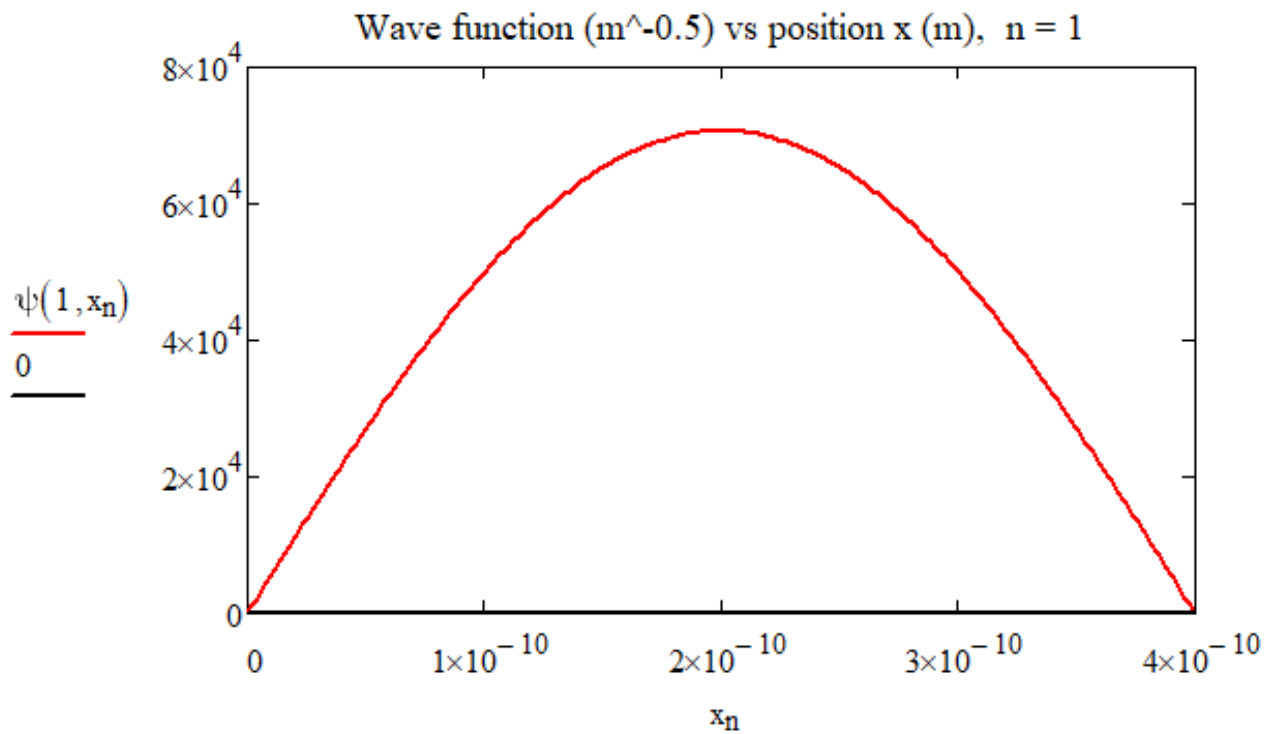
Define vector of positions x across the width of the potential well, i.e., $0 \leq x \leq a$.

$$N_{\text{max}} := 200 \quad n := 0 \dots N_{\text{max}} \quad x_n := \frac{n}{N_{\text{max}}} \cdot a$$

For the first quantum level, i.e., $n = 1$

$$k(1) = 7.854 \times 10^9 \quad (\text{rad/m})$$

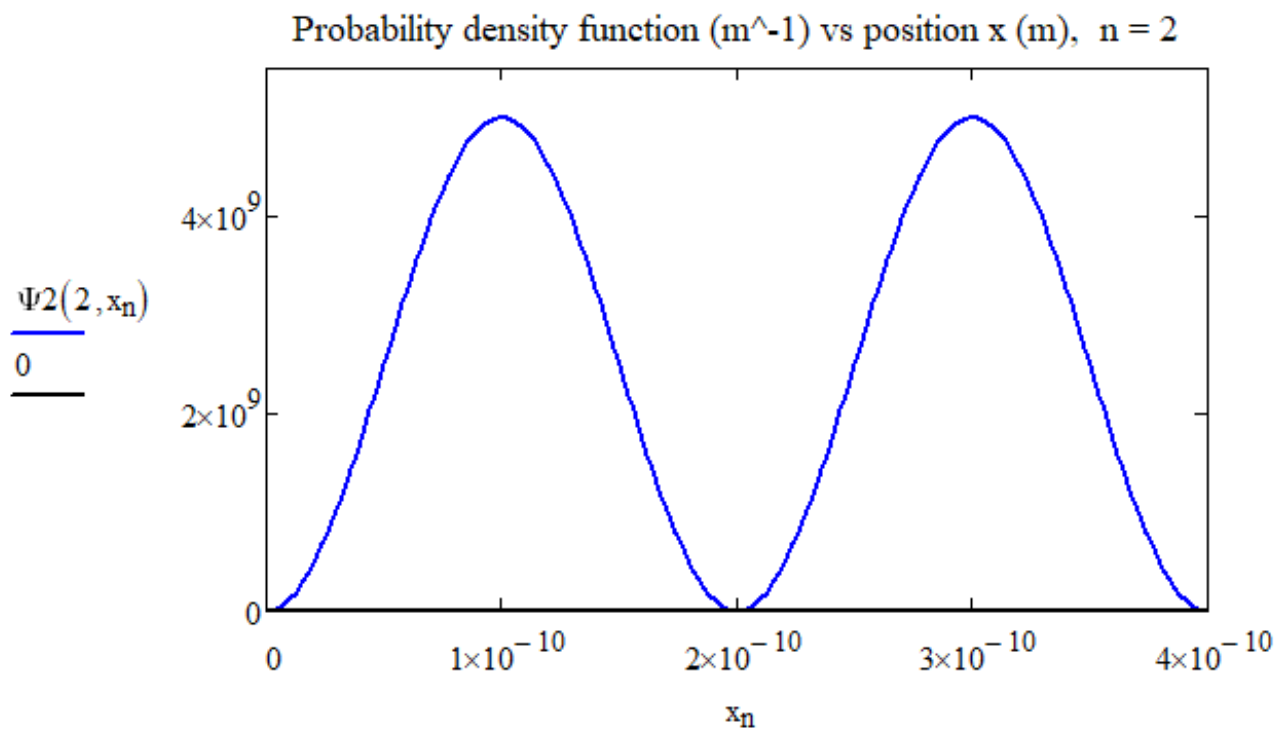
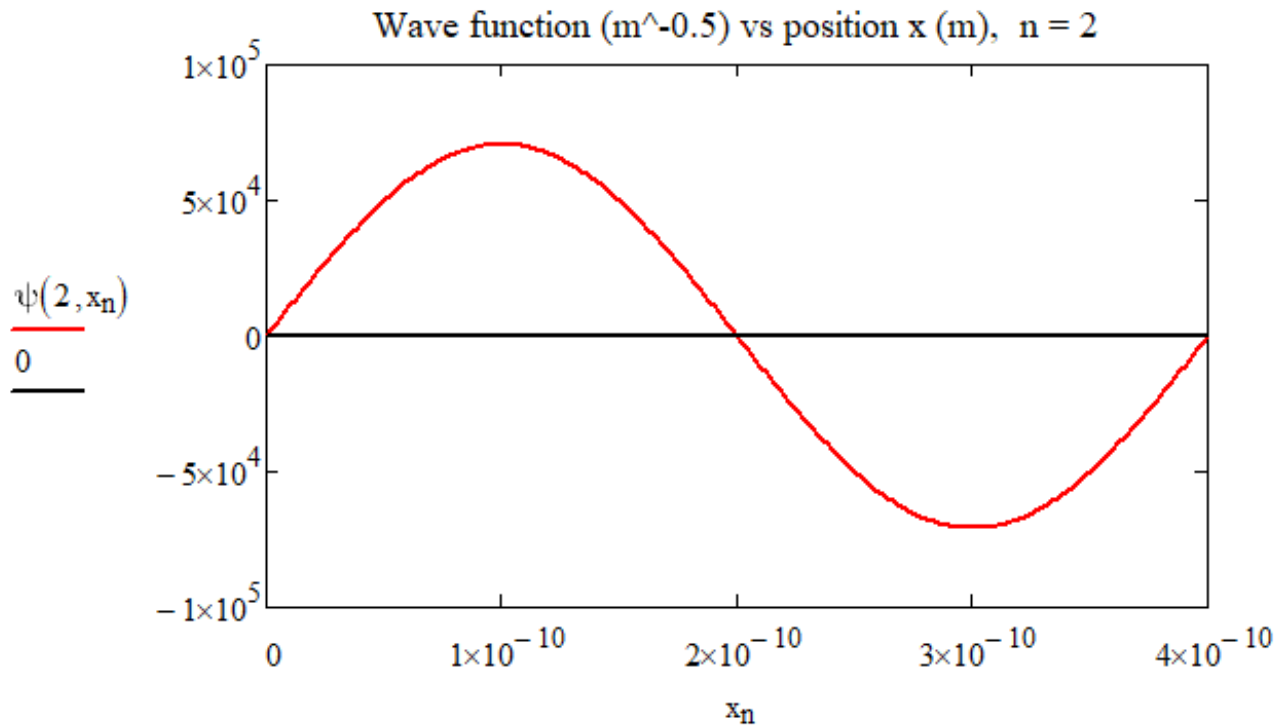
$$E(1) = 3.765 \times 10^{-19} \quad (\text{J}) \quad \text{or} \quad E_{\text{eV}}(1) = 2.3502 \quad (\text{eV})$$



For the second quantum level, i.e., $n = 2$

$$k(2) = 1.5708 \times 10^{10} \quad (\text{rad/m})$$

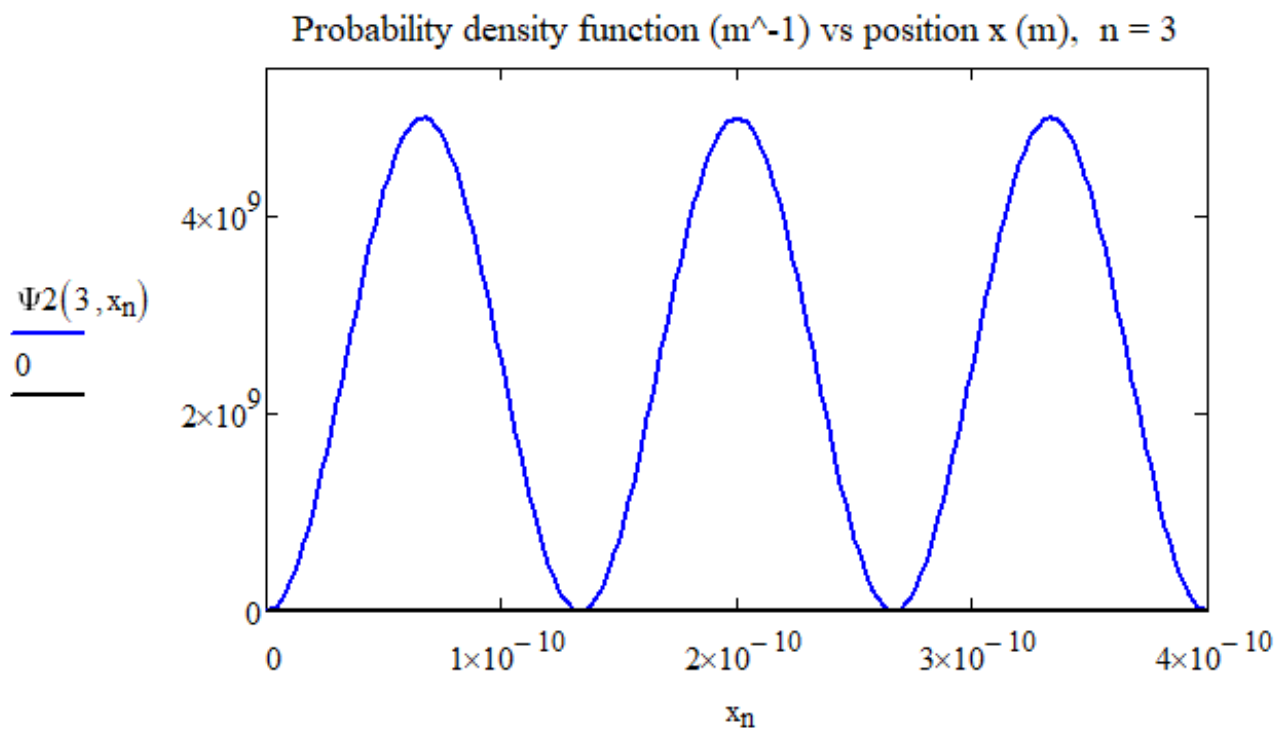
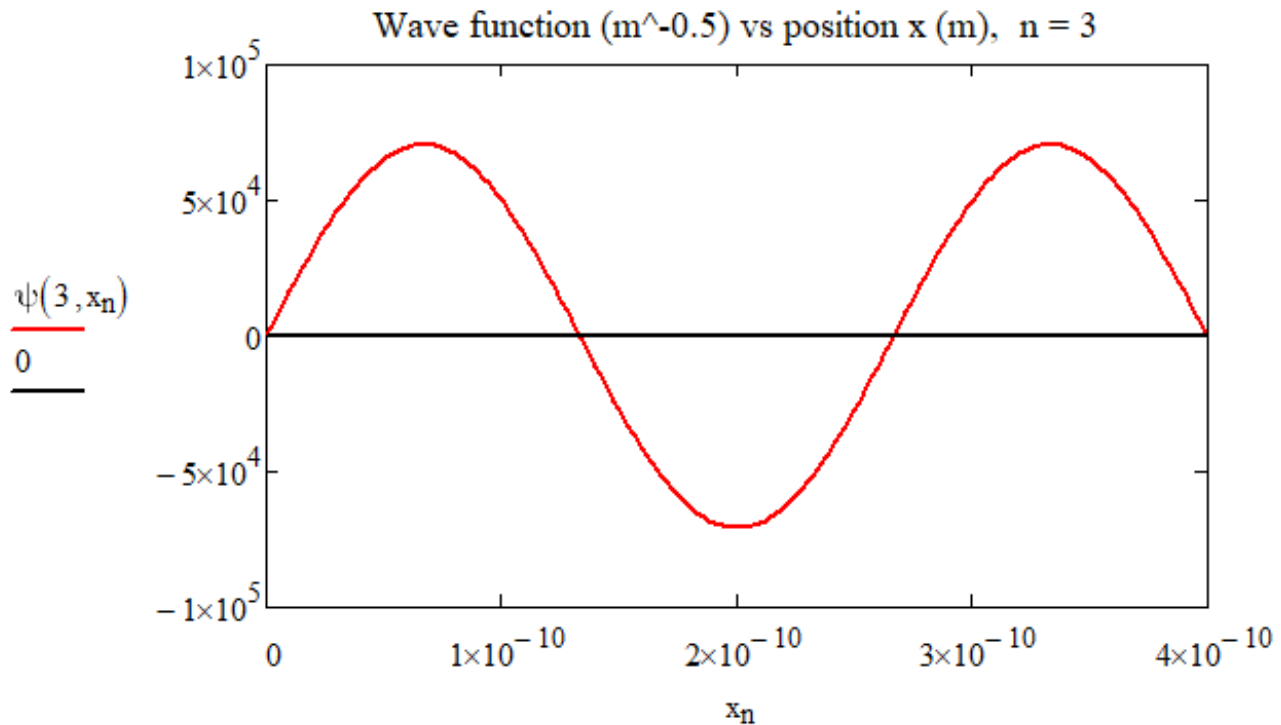
$$E(2) = 1.506 \times 10^{-18} \quad (\text{J}) \quad \text{or} \quad E_{\text{eV}}(2) = 9.4008 \quad (\text{eV}) \quad \frac{E_{\text{eV}}(2)}{E_{\text{eV}}(1)} = 4$$



For the third quantum level, i.e., $n = 3$

$$k(3) = 2.3562 \times 10^{10} \quad (\text{rad/m})$$

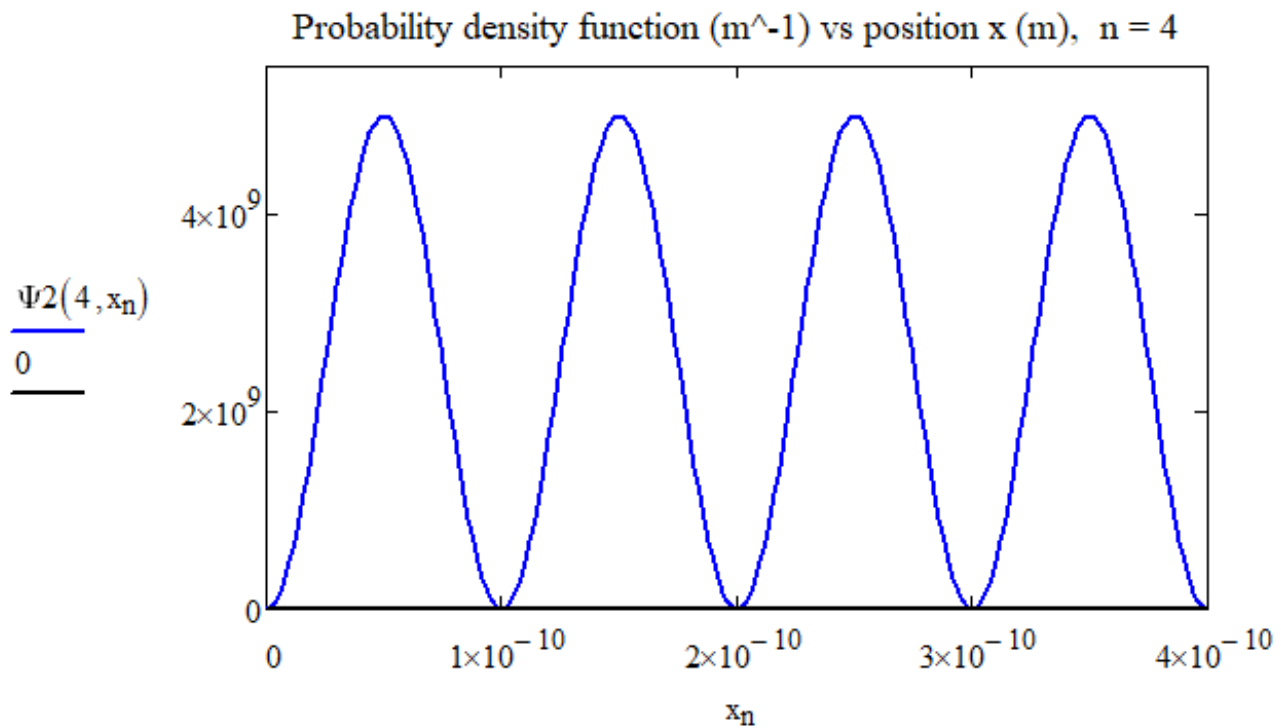
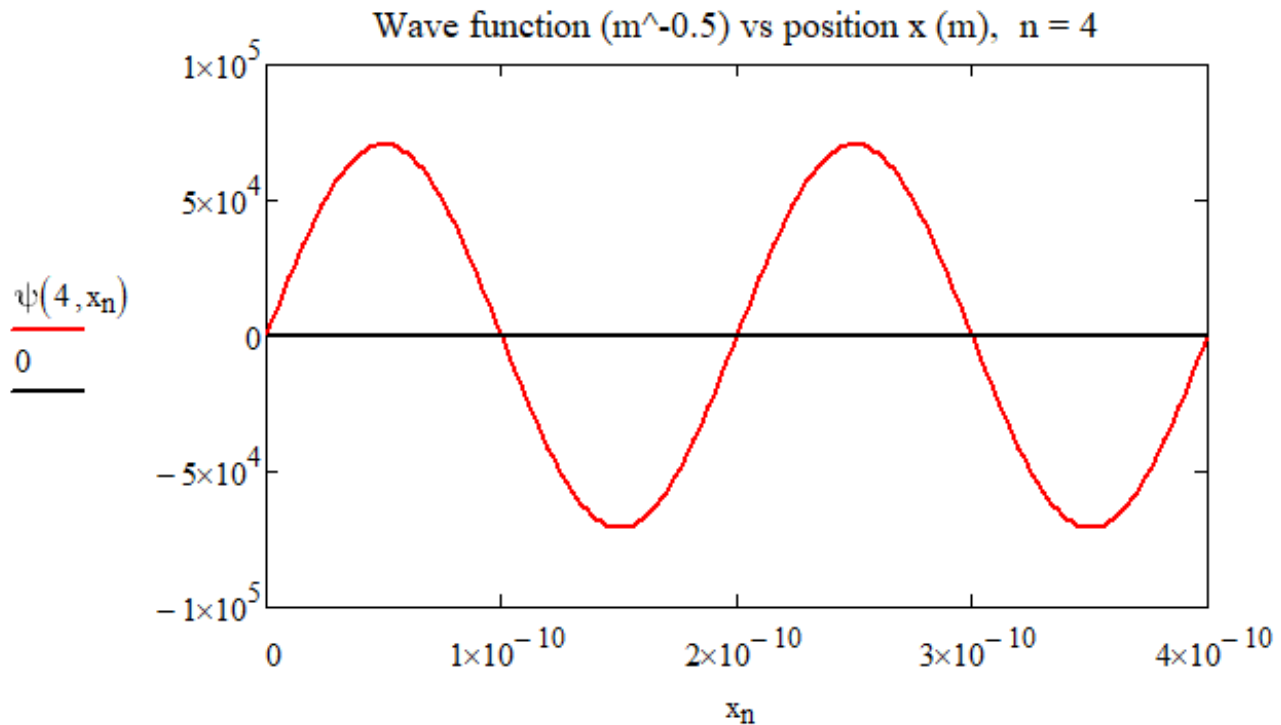
$$E(3) = 3.389 \times 10^{-18} \quad (\text{J}) \quad \text{or} \quad E_{\text{eV}}(3) = 21.517 \quad (\text{eV}) \quad \frac{E_{\text{eV}}(3)}{E_{\text{eV}}(1)} = 9$$



For the fourth quantum level, i.e., $n = 4$

$$k(4) = 3.1416 \times 10^{10} \text{ (rad/m)}$$

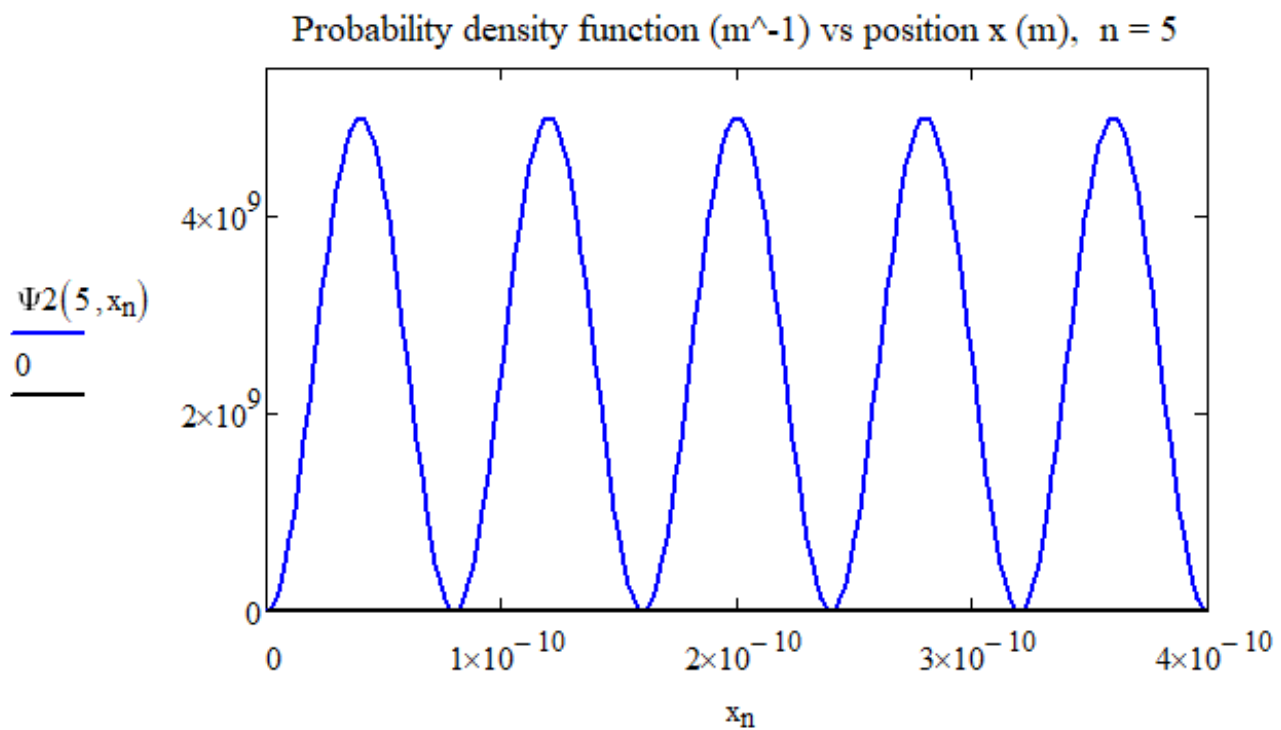
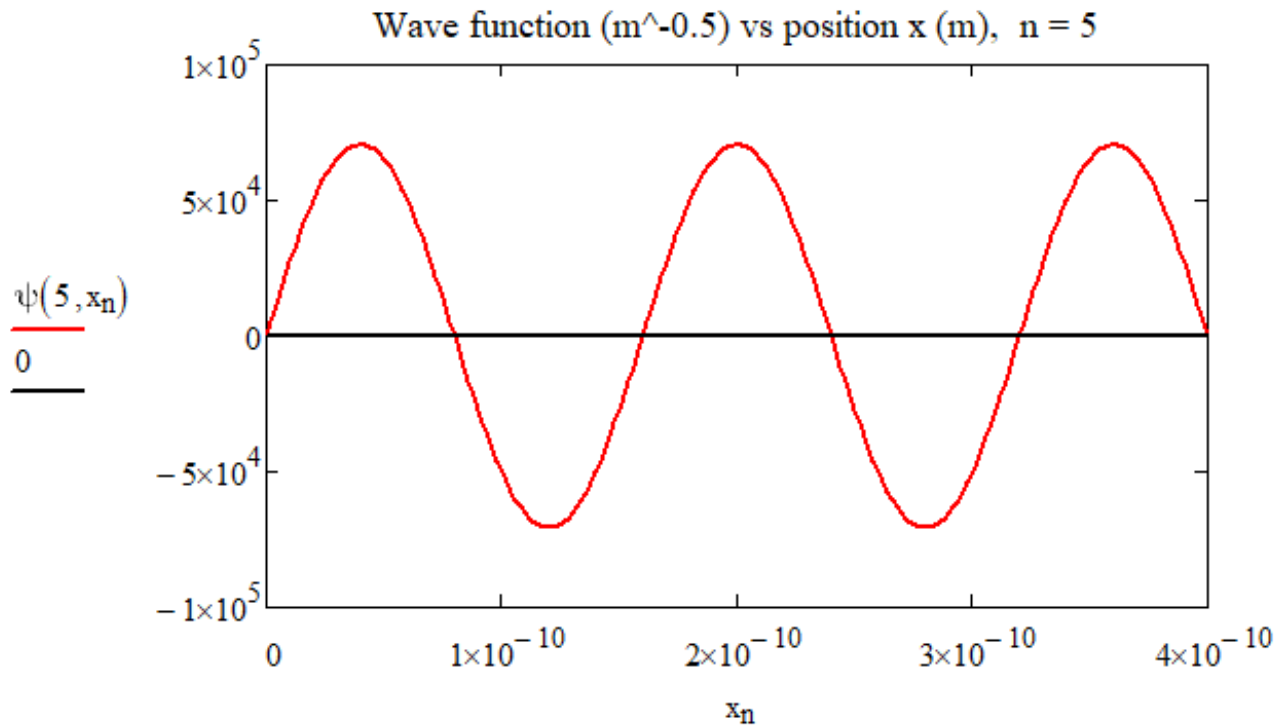
$$E(4) = 6.025 \times 10^{-18} \text{ (J)} \quad \text{or} \quad E_{\text{eV}}(4) = 37.603 \text{ (eV)} \quad \frac{E_{\text{eV}}(4)}{E_{\text{eV}}(1)} = 16$$



For the fifth quantum level, i.e., $n = 5$

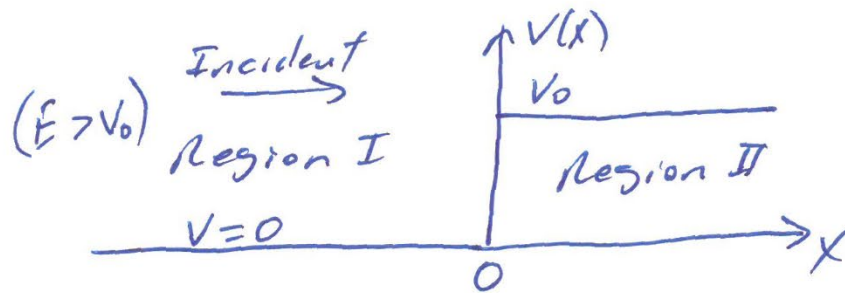
$$k(5) = 3.927 \times 10^{10} \quad (\text{rad/m})$$

$$E(5) = 9.414 \times 10^{-18} \quad (\text{J}) \quad \text{or} \quad E_{\text{eV}}(5) = 58.7547 \quad (\text{eV}) \quad \frac{E_{\text{eV}}(5)}{E_{\text{eV}}(1)} = 25$$



2.3.3 The Step Potential Function

What if we have traveling particles that encounter a potential barrier of finite 'height'?



In Region I, the time independent 1D Schrodinger Eqn is

$$\frac{d^2 \psi_1(x)}{dx^2} + \frac{2m}{\hbar^2} [E - V(x)] \psi_1(x) = 0 \quad \leftarrow \begin{array}{l} \text{2nd order} \\ \text{ODE} \\ \text{wave eqn} \end{array}$$

where $\psi_1(x)$ is the solution in Region I.

Since Region I is semi-infinite and contains traveling particles, we choose the soln form

$$\psi_1(x) = A_1 e^{jK_1 x} + B_1 e^{-jK_1 x} \quad (x \leq 0) \quad (2.41)$$

where $K_1 = \sqrt{\frac{2mE}{\hbar^2}}$ (rad/m). Like UPWs

and lossless TLs, the first term represents particles traveling in $+x$ -direction while the second term is for those going in the $-x$ -direction

2.3.3 cont.

From $|\psi(x,t)|^2 = \psi(x)\psi^*(x)$, we can note that

A, A^* = probability density of incident (+x-dir) particles

$$B, B^{\star} \equiv \quad " \qquad " \qquad " \text{ reflected } (-x\text{-dir})$$

If v_i & v_r are the velocities (magnitude) of the incident & reflected particles, we can define the flux of the incident & reflected particles as

$$v_i A, A_i^* \text{ \& } v_r B, B_i^* \left(\frac{\# \text{ particles}}{cm^2 s} \right)$$

In Region II, we will assume $V_0 > E$ and get the wave eq'n

$$\frac{d^2 \psi_2(x)}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \psi_2(x) = \frac{d^2 \psi_2(x)}{dx^2} - \frac{2m (V_0 - E)}{\hbar^2} \psi_2(x) = 0$$

w/ the "-" sign in the ODE, the sol'n is of form $y = e^{ax}$, no 'j'!!

$$\psi_2(x) = A_2 e^{-k_2 x} + B_2 e^{+k_2 x} \quad (x \geq 0) \quad (2.44)$$

where $k_2 = \pm \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$ (1/m)

2.3.3 cont.

Since $\psi_2(x)$ must be finite, set $B_2 = 0$ to prevent $e^{+k_2 x}$ term from approaching ∞ as $x \rightarrow \infty$.

$$\psi_2(x) = A_2 e^{-k_2 x} \quad (x \geq 0)$$

Next, since ψ must be continuous at $x=0$

$$\psi_1(x=0) = A_1 + B_1 = \psi_2(x=0) = A_2 \quad (1)$$

Need more information. Use $\frac{\partial \psi}{\partial x}$ must be continuous @ $x=0$

$$\left. \frac{\partial \psi_1}{\partial x} \right|_{x=0} = \left. \frac{\partial \psi_2}{\partial x} \right|_{x=0}$$

$$\left[jk_1 A_1 e^{jk_1 x} - jk_1 B_1 e^{-jk_1 x} \right] \Big|_{x=0} = -k_2 A_2 e^{-k_2 x} \Big|_{x=0}$$

$$jk_1 A_1 - jk_1 B_1 = -k_2 A_2 \quad (2)$$

2 eqns + 3 unknowns. Solving (1) + (2) for B_1 and A_2 in terms of A_1 , we get

$$B_1 = \frac{-(k_2^2 + 2jk_1 k_2 - k_1^2)}{k_2^2 + k_1^2} A_1 \quad (2.51a)$$

$$A_2 = \frac{2k_1 (k_1 - jk_2)}{k_2^2 + k_1^2} A_1 \quad (2.51b)$$

Why? $B_1/A_1 = \text{Part of incident } \psi_1 \text{ refl.}$ & $A_2/A_1 = \text{Part of incident } \psi_1 \text{ transmitted}$

2.3.3 cont.

Now, the reflected wave probability density function is

$$B, B_i^* = + \frac{(k_2^2 + j2k_1k_2 - k_1^2)(k_2^2 - j2k_1k_2 - k_1^2)}{(k_2^2 + k_1^2)^2} A, A_i^* \quad (2.52)$$

Also, we can define a reflection coeff. for the fluxes of incident + reflected particles

$$R = \frac{v_r B, B_i^*}{v_i A, A_i^*} \quad (2.53)$$

Now, in Region I, $V(x < 0) = 0 \Rightarrow E = T + V = T = \frac{1}{2}mv^2$

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}} = \sqrt{\frac{2m(\frac{1}{2}mv^2)}{\hbar^2}} = \frac{mv}{\hbar}$$

$$\hookrightarrow v = \frac{\hbar}{m} k_1$$

$\Rightarrow v_i = v_r$, since we have $\psi(x) = A, e^{j k_1 x} + B, e^{-j k_1 x}$

Therefore

$$R = \frac{\cancel{v_r} B, B_i^*}{\cancel{v_i} A, A_i^*} = \frac{B, B_i^*}{A, A_i^*}$$

2.59 has
Typo

$$= \frac{[(k_2^2 - k_1^2) + j2k_1k_2][(k_2^2 - k_1^2) - j2k_1k_2]}{(k_2^2 + k_1^2)^2} \frac{\cancel{A}, \cancel{A_i^*}}{\cancel{A}, \cancel{A_i^*}}$$

$$R = \frac{(k_2^2 - k_1^2)^2 + 4k_1^2 k_2^2}{(k_2^2 + k_1^2)^2} = \underline{\underline{1}} \quad ?!!$$

2.3.3 cont.

$R=1$ implies that particles incident @ $x=0$ w/ $E < V_0$ might go into Region II ($x > 0$), but will eventually be reflected. $A_2 \neq 0$ implies $|\Psi(x,t)|^2 \neq 0$ for $x > 0$, i.e., particle might penetrate potential barrier despite $E < V_0$! Different from classical mechanics.

ex. Consider an electron w/ a kinetic energy of 0.25 eV incident on a barrier of 2 eV . Find V_i , k_1 , k_2 and the 'skin depth' into region II, i.e., distance at which $\Psi_2(d) = e^{-1} \Psi_2(0)$.

$$T = \frac{1}{2} m v_i^2 = \frac{1}{2} (9.1093837 \times 10^{-31}) v_i^2 = 0.25 \text{ eV} (1.60218 \times 10^{-19} \frac{\text{J}}{\text{eV}})$$

$$\hookrightarrow v_i^2 = 8.79412 \times 10^{10} \Rightarrow \underline{\underline{v_i = 296,548.79 \text{ m/s}}}$$

$$(2.42) \quad k_1 = \sqrt{\frac{2mE}{\hbar^2}} = \sqrt{\frac{2(9.1094 \times 10^{-31}) 0.25 (1.60218 \times 10^{-19})}{(1.054572 \times 10^{-34})^2}}$$

$$= \underline{\underline{2.5616 \times 10^9 \text{ rad/m}}}$$

$$(2.46) \quad \Psi_2(x) = A_2 e^{-k_2 x} \quad + \quad (2.45) \quad k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

2.3.3 cont.

ex. cont.

$$K_2 = \sqrt{\frac{2(9.1094 \times 10^{-31})(2-0.25)1.60218 \times 10^{-19}}{(1.054572 \times 10^{-34})^2}}$$

$$= 6.77319 \times 10^9 \text{ NP/m}$$

$$\frac{\psi_2(d)}{\psi_2(0)} = \frac{A_2 e^{-K_2 d}}{A_2} = e^{-6.77319 \times 10^9 d} = e^{-1}$$

$$\Rightarrow d = \frac{1}{6.77319 \times 10^9} = 1.4755 \times 10^{-10} \text{ m}$$

$$= \underline{\underline{1.4755 \text{ \AA}}}$$

2.3.4 The Potential Barrier and Tunneling

Now, consider the situation where a particle(s) is incident from $-\infty$ on a potential barrier of finite 'height' and width.



Again, we assume incident particle(s) are moving in $+x$ -direction and have $T=E < V_0$. From the wave equation, we get general solutions of the form

$$\psi_1(x) = A_1 e^{jk_1 x} + B_1 e^{-jk_1 x} \quad x < 0 \quad (2.60a)$$

$$\psi_2(x) = A_2 e^{k_2 x} + B_2 e^{-k_2 x} \quad 0 < x < a \quad (2.60b)$$

$$\psi_3(x) = A_3 e^{jk_3 x} + B_3 e^{-jk_3 x} = A_3 e^{jk_1 x} + B_3 e^{-jk_1 x} \quad (x > a) \quad (2.60c)$$

$$\text{Where } k_1 = k_3 = \sqrt{\frac{2mE}{\hbar^2}} \quad (\text{rad/m}) \quad (2.61a)$$

$$\text{and } k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}} \quad (\text{Np/m}) \quad (2.61b)$$

2.3.4 cont.

We have 6 unknown constant coefficients ($A_1, B_1, A_2, B_2, A_3, \text{ and } B_3$) to find.

Given that there is nothing to cause a negative x traveling particle in Region III, assume/set $B_3 = 0$,

$\psi(x)$ is continuous B.C. gives:

$$\textcircled{1} \quad \psi_1(0) = A_1 + B_1 = \psi_2(0) = A_2 + B_2$$

$$\textcircled{2} \quad \psi_2(a) = A_2 e^{k_2 a} + B_2 e^{-k_2 a} = A_3 e^{j k_1 a} = \psi_3(a)$$

$\frac{d\psi(x)}{dx}$ is continuous B.C. gives:

$$\textcircled{3} \quad \left. \frac{d\psi_1(x)}{dx} \right|_{x=0} = j k_1 A_1 - j k_1 B_1 = k_2 A_2 - k_2 B_2 = \left. \frac{d\psi_2(x)}{dx} \right|_{x=0}$$

$$\textcircled{4} \quad \left. \frac{d\psi_2(x)}{dx} \right|_{x=a} = k_2 A_2 e^{k_2 a} - k_2 B_2 e^{-k_2 a} = j k_1 A_3 e^{j k_1 a} = \left. \frac{d\psi_3}{dx} \right|_{x=a}$$

We have 5 unknowns and 4 equations. We can solve for $B_1, A_2, B_2, \text{ and } A_3$ in terms of A_1 (long). If we do so, we get a sol'n that looks like Fig. 2.10.

From *Semiconductor Physics and Devices: Basic Principles* (4th Edition), Donald A. Neamen, McGraw Hill, 2012, ISBN 978-0-07-352958-5.

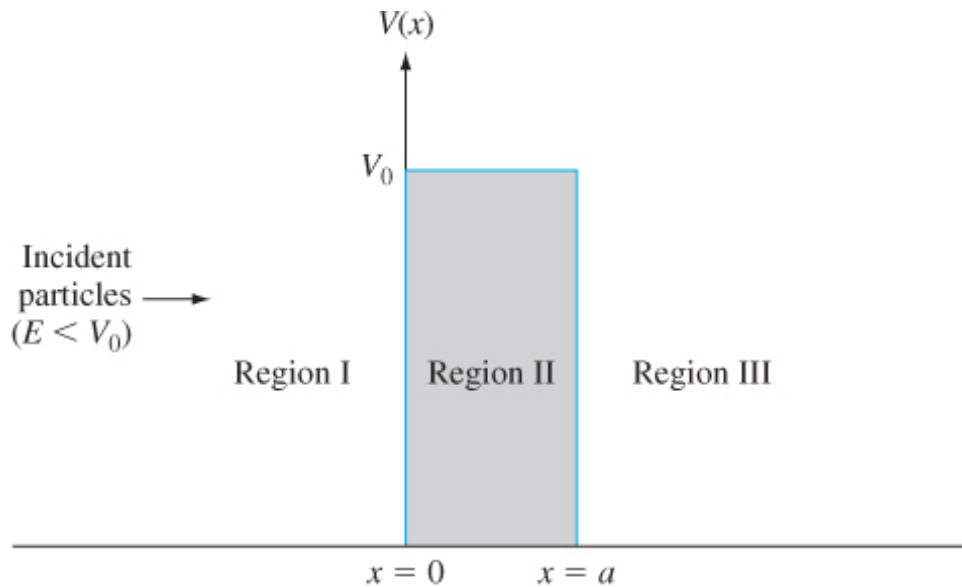


Figure 2.9 | The potential barrier function.

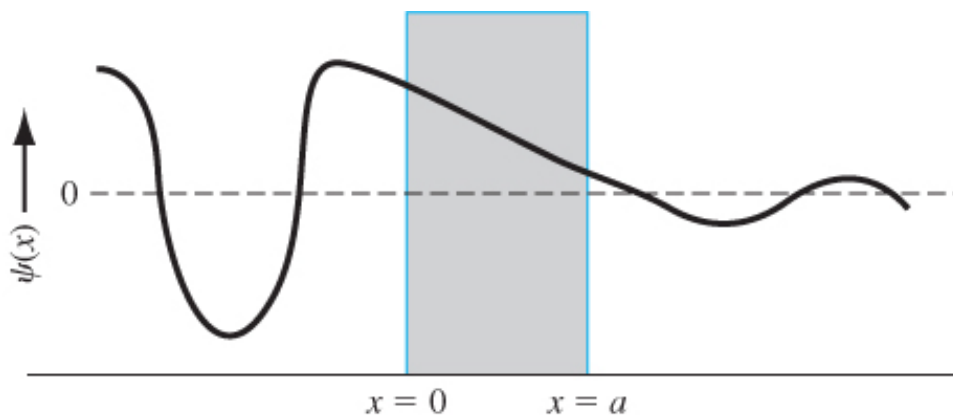


Figure 2.10 | The wave functions through the potential barrier.

- Unlike classical mechanics, there is a non-zero probability or finite probability that the particle will be in Regions II and III.
- The particle getting through the potential barrier is called *tunneling*.

2.3.4 cont.

A transmission coefficient T from Region I to Region III can be defined in terms of the fluxes of incident & transmitted particles.

$$T = \frac{v_t A_3 A_3^*}{v_i A_1 A_1^*} = \frac{A_3 A_3^*}{A_1 A_1^*}$$

where again $v_t = v_i$ since $V(x) = 0$ in Regions I & III.

With much effort, we can find

$$T = \frac{1}{1 + \frac{V_0^2 \sinh^2(k_2 a)}{4E(V_0 - E)}} \quad \text{where } \sinh(k_2 a) = \frac{e^{k_2 a} - e^{-k_2 a}}{2}$$

In the case that $E \ll V_0$, $k_2 a \gg 1$ and

$\sinh^2(k_2 a) \approx \frac{1}{4} e^{2k_2 a}$. Then,

$$T \approx \frac{1}{1 + \frac{V_0^2 \frac{1}{4} e^{2k_2 a}}{4E(V_0 - E)}} = \frac{16 \frac{E}{V_0} (1 - \frac{E}{V_0})}{\underbrace{16 \frac{E}{V_0} (1 - \frac{E}{V_0})}_{\substack{\uparrow \text{small} \quad \uparrow \text{small} \\ \text{ignore}}} + \underbrace{e^{2k_2 a}}_{\uparrow \text{big}}}$$

$$T \approx \frac{16 \frac{E}{V_0} (1 - \frac{E}{V_0})}{e^{2k_2 a}} \quad (2.63)$$

$\Rightarrow T$ is small but > 0 !!

Example- Let's examine various quantities when an electron with a kinetic energy of 1 eV in a region of zero potential is incident on a finite potential barrier at $x = 0$ of 12 eV that is 4 Angstroms wide followed by another zero potential region.

Define some constants

$$h := 6.62607015 \cdot 10^{-34} \text{ J-s} \quad h_{\text{mod}} := \frac{h}{2 \cdot \pi} \quad h_{\text{mod}} = 1.05457 \times 10^{-34} \text{ J-s}$$

$$m := 9.1093837015 \cdot 10^{-31} \text{ kg} \quad a := 4 \cdot 10^{-10} \text{ m}$$

Calculate some quantities and/or define equations

$$E_{\text{eV}} := 1 \text{ eV} \quad E := E_{\text{eV}} \cdot 1.602176634 \cdot 10^{-19} \quad \boxed{E = 1.60218 \times 10^{-19} \text{ J}}$$

$$V0_{\text{eV}} := 12 \text{ eV} \quad V0 := V0_{\text{eV}} \cdot 1.602176634 \cdot 10^{-19} \quad \boxed{V0 = 1.92261 \times 10^{-18} \text{ J}}$$

Per (2.61a), the wave number k_1 (rad/m) for **regions I & III** is

$$k_1 := \sqrt{\frac{2 \cdot m \cdot E}{h_{\text{mod}}^2}} \quad \boxed{k_1 = 5.12317 \times 10^9 \text{ rad/m}}$$

Per (2.61b), the wave number k_2 (Np/m) in **region II** is

$$k_2 := \sqrt{\frac{2 \cdot m \cdot (V0 - E)}{h_{\text{mod}}^2}} \quad \boxed{k_2 = 1.69916 \times 10^{10} \text{ Np/m}}$$

From notes, the exact transmission coefficient T is

$$T_{\text{exact}} := \frac{1}{1 + \frac{V0^2 \cdot \sinh(k_2 \cdot a) \cdot \sinh(k_2 \cdot a)}{4 \cdot E \cdot (V0 - E)}} \quad \boxed{T_{\text{exact}} = 1.52636 \times 10^{-6}}$$

Pretty small!

$$\text{For } k_2 \cdot a = 6.7966 \quad \sinh(k_2 \cdot a) \cdot \sinh(k_2 \cdot a) = 2.001859 \times 10^5$$

$$\text{which can be approximated as } 0.25 \cdot e^{2 \cdot k_2 \cdot a} = 2.001864 \times 10^5$$

Per (2.63), the approximate transmission coefficient T is

$$T_{\text{approx}} := 16 \cdot \frac{E}{V0} \cdot \left(1 - \frac{E}{V0}\right) \cdot e^{-2 \cdot k_2 \cdot a} \quad \boxed{T_{\text{approx}} = 1.52635 \times 10^{-6}}$$

Very good approximation!

2.4 Extensions of the Wave Theory to Atoms

→ We're going to do a reduced & simplified look as full coverage is lengthy (grad level).

2.4.1 The One-Electron Atom

Let's start w/ hydrogen where we have 1 proton ($m_p = 1.672622 \times 10^{-27} \text{ kg}$) and 1 electron ($m_e = 9.1093837 \times 10^{-31} \text{ kg}$). Obviously, the proton is much more massive than the electron.

The potential (energy) due to Coulomb force attraction between the two is

$$V(r) = \frac{-e^2}{4\pi\epsilon_0 r^2} \quad (2.64) \quad \hookrightarrow \underline{V(r \rightarrow 0) \rightarrow \infty}$$

where $e = 1.6021766 \times 10^{-19} \text{ C}$, $\epsilon_0 = 8.8541878 \times 10^{-12} \text{ F/m}$, and $r = \text{spherical distance (assume proton @ origin)}$.

⇒ Since e^- can be anywhere in three dimensions (r, θ, ϕ) for spherical coordinates, the time-independent Schrodinger's wave eqn becomes -

2.4.1 cont.

$$\nabla^2 \psi(r, \theta, \phi) + \frac{2m_0 \overset{\text{rest mass of electron}}{c^2}}{\hbar^2} [E - V(r)] \psi(r, \theta, \phi) = 0 \quad (2.65)$$

Where ∇^2 is the scalar Laplacian in spherical coordinates giving

$$\begin{aligned} \nabla^2 \psi = & \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) \\ & + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \end{aligned}$$

Again, we assume that $\psi(r, \theta, \phi)$ is a separable function $\psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi)$ (2.67).

Using this in the 3D Schrodinger wave equation yields (2.68) ← Text typo

$$\begin{aligned} \sin^2 \theta \frac{1}{R(r)} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R(r)}{\partial r} \right) + \frac{1}{\Phi(\phi)} \frac{\partial^2 \Phi(\phi)}{\partial \phi^2} \\ + \sin \theta \frac{1}{\Theta(\theta)} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Theta(\theta)}{\partial \theta} \right) + r^2 \sin^2 \theta \frac{2m_0}{\hbar^2} [E - V(r)] = 0 \end{aligned}$$

Note that The second and Third terms are only functions of a single variable.

2.4.1 cont.

For (2.68) to hold true for all r, θ, ϕ ,
we require/need

$$\frac{1}{\Phi(\phi)} \frac{d^2 \Phi(\phi)}{d\phi^2} = -m^2$$

where $m \equiv$ separation of variables constant
(NOT mass) which is why we used m_0 for
the electron rest mass,

The solution to (2.69) is $\Phi(\phi) = e^{jm\phi}$ (2.70)

where $m = 0, \pm 1, \pm 2, \dots$ since $\Psi(r, \theta, \phi)$
must be single-valued.

Similarly, we get two more separation
of variables constants from $R(r)$ (use n)
and $\Theta(\theta)$ (use l). We call $l, m, \& n$
the quantum numbers.

$n = 1, 2, 3, \dots \equiv$ principle quantum #

$l = n-1, n-2, \dots, 0 \equiv$ azimuthal or angular
quantum # (2.72)

$|m| = l, l-1, \dots, 0 \equiv$ magnetic quantum #

2.4.1 cont.

- Solutions to $R(r)$ & $\Theta(\theta)$ are 'complex'.
- Each set of n, l, m represents an electron quantum state.
- Finding solutions to $\Psi(r, \theta, \phi)$ is beyond the scope of this class. One surprising result is that even though $V(r)$ is spherically symmetric, $\Psi(r, \theta, \phi)$ may or may not be!
- As was the case for a particle in a infinite potential well, the energy for the electron is quantized.

$$E_n = \frac{-m_0 e^4}{(4\pi\epsilon_0)^2 2\hbar^2 n^2} \quad (2.73)$$

where $n=1, 2, 3, \dots$

For the quantum state $n=1, l=0, + m=0$,

$$\Psi_{100} = \frac{1}{\sqrt{\pi}} \left(\frac{1}{a_0}\right)^{3/2} e^{-r/a_0} \quad (2.74) \quad \text{~ spherically symmetric}$$

where

$$\text{Bohr radius} \equiv a_0 = \frac{4\pi\epsilon_0 \hbar^2}{m_0 e^2} = \underline{0.529177 \text{ \AA}}$$

Fig 2.11 shows the prob. density functions for $|\Psi_{100}|^2$ and $|\Psi_{200}|^2$ versus radius

From *Semiconductor Physics and Devices: Basic Principles* (4th Edition), Donald A. Neamen, McGraw Hill, 2012, ISBN 978-0-07-352958-5.

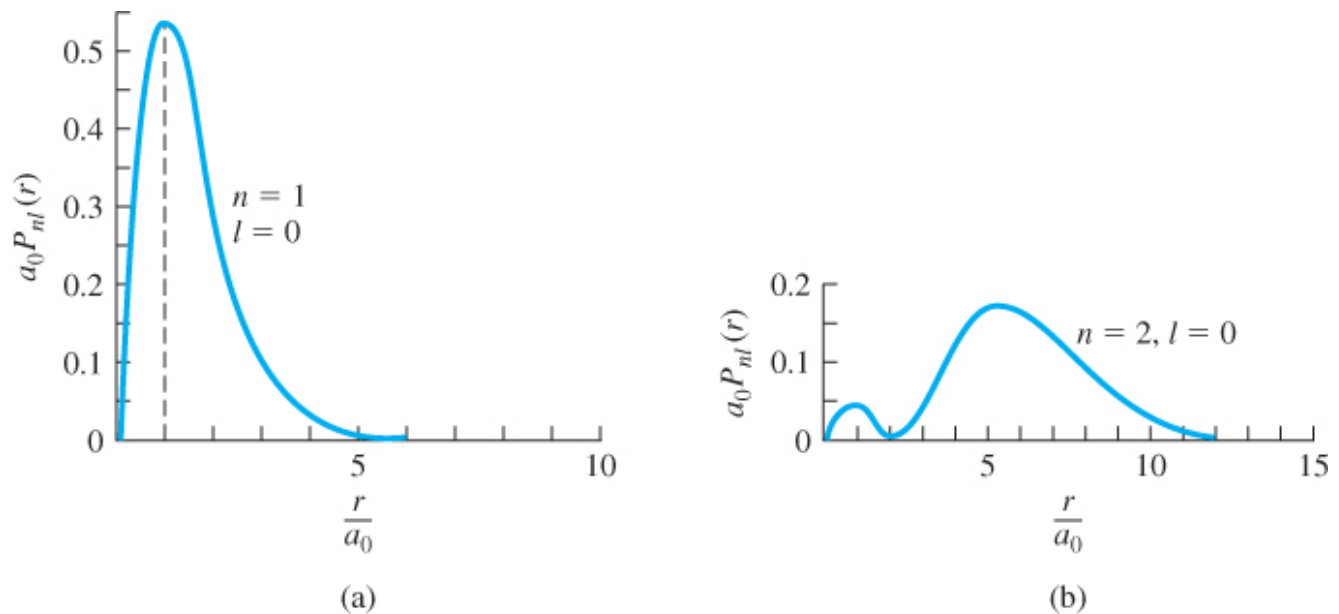


Figure 2.11 | The radial probability density function for the one-electron atom in the (a) lowest energy state and (b) next-higher energy state.
(From Eisberg and Resnick [5].)

- Per (2.72) $|m| = \ell, \ell - 1, \dots, 0$. Therefore, $m = 0$ when $\ell = 0$.
- When $\ell = m = 0$, the solutions for the probability density functions $|\Psi|^2$ are **spherically symmetric**, i.e., $|\Psi(r)|^2$.
- For $|\Psi_{100}(r)|^2$ (AKA: $1s$ shell/state), note that the electron is most likely to be found near $r/a_0 = 1$ or $r = a_0 = 0.529 \text{ \AA}$.
- For $|\Psi_{200}(r)|^2$ (AKA: $2s$ shell/state), note that the electron is most likely to be found farther from the proton/nucleus at $5 < r/a_0 < 6$.

2.4.1 cont.

How does this single H atom relate to semiconductors?

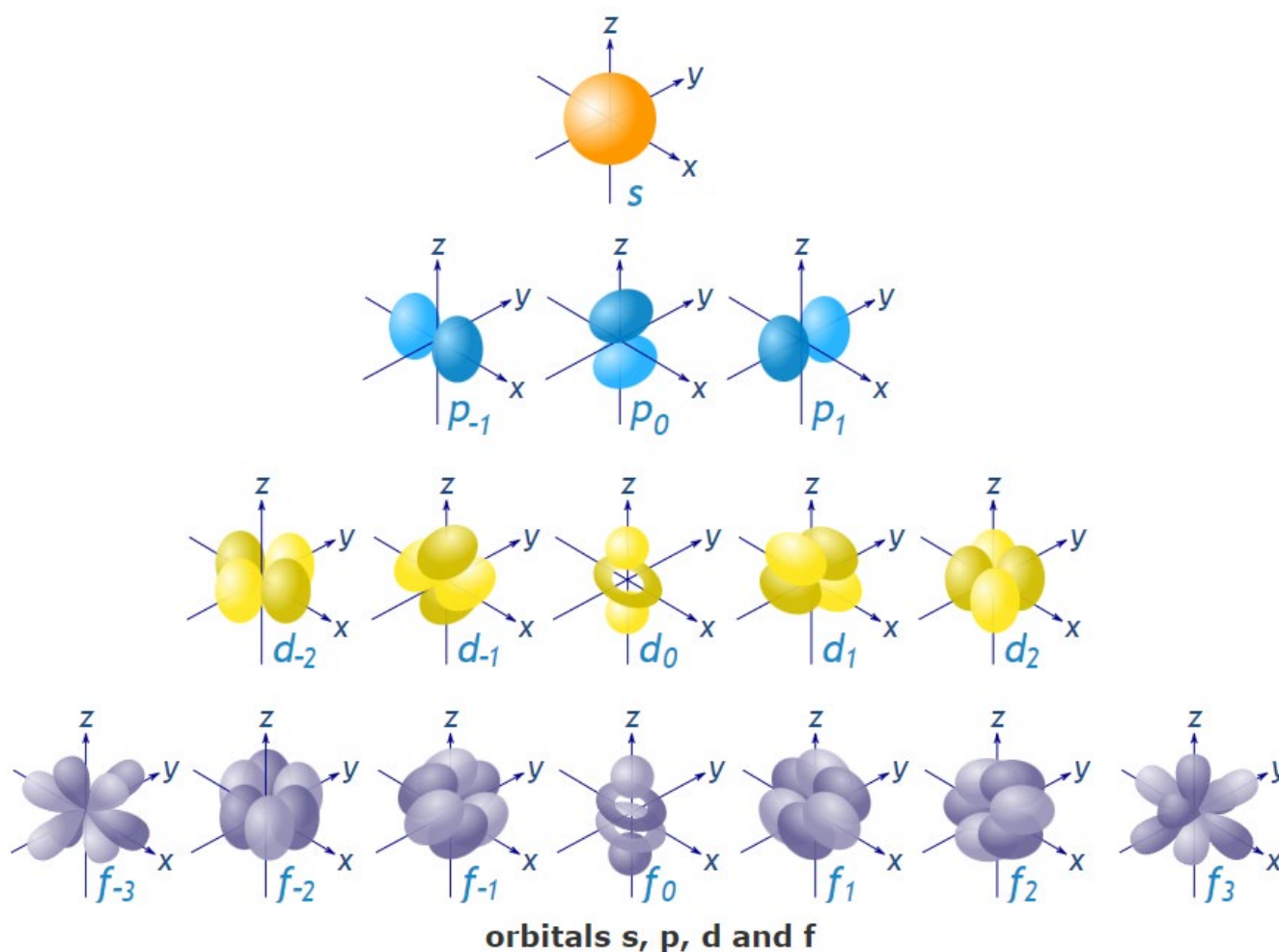
- 3D time-independent Schrodinger's wave eq'n.
- quantized energy levels/states for electrons
- quantum numbers & quantum states for electrons

When $l \neq 0$, we get $|\psi(r, \theta, \phi)|^2$ that are NOT rotationally symmetric (see pictures).

Shells go w/ $n=1, 2, \dots$, then we have subshells/orbitals

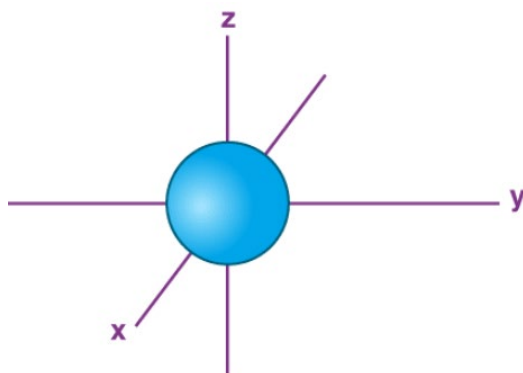
Subshells/orbitals	ℓ quantum #	Max # electrons per level
<i>s</i> (sharp)	0	2
<i>p</i> (principal)	1	6
<i>d</i> (diffuse)	2	10
<i>f</i> (fundamental)	3	14

From <https://www.mathsisfun.com/physics/atom-orbitals.html>

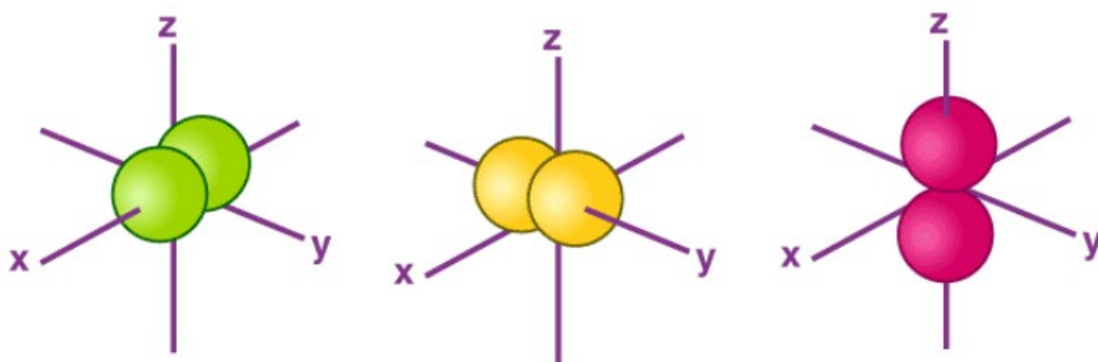


- As a caution, these are plots of where the probability density function $|\Psi|^2$ **peaks**; the orbitals are actually more diffuse than can be shown by the pictures.

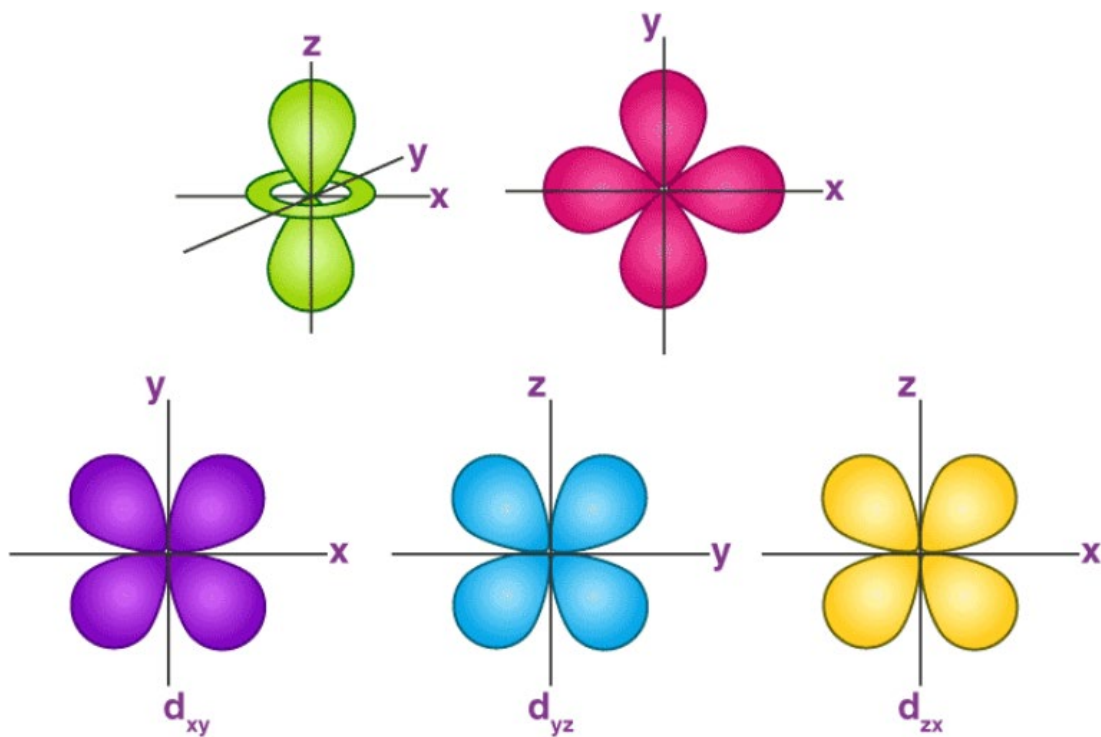
From <https://byjus.com/chemistry/shapes-of-orbitals/>



s orbitals



p orbitals



d orbitals

2.4.2 The Periodic Table

For more complex atoms, we need two more items

1) the 'spin' quantum # denoted 's'.

[Now, we have $n, l, m, \& s.$]

This is related to electron spin / angular momentum, $s = +\frac{1}{2}$ or $-\frac{1}{2}$



2) Pauli exclusion principle -

In a system (i.e., atom, molecule, ...), no two electrons can occupy the same quantum state, i.e., they must have different quantum numbers