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) ← Nu of the incident light matters much more.

  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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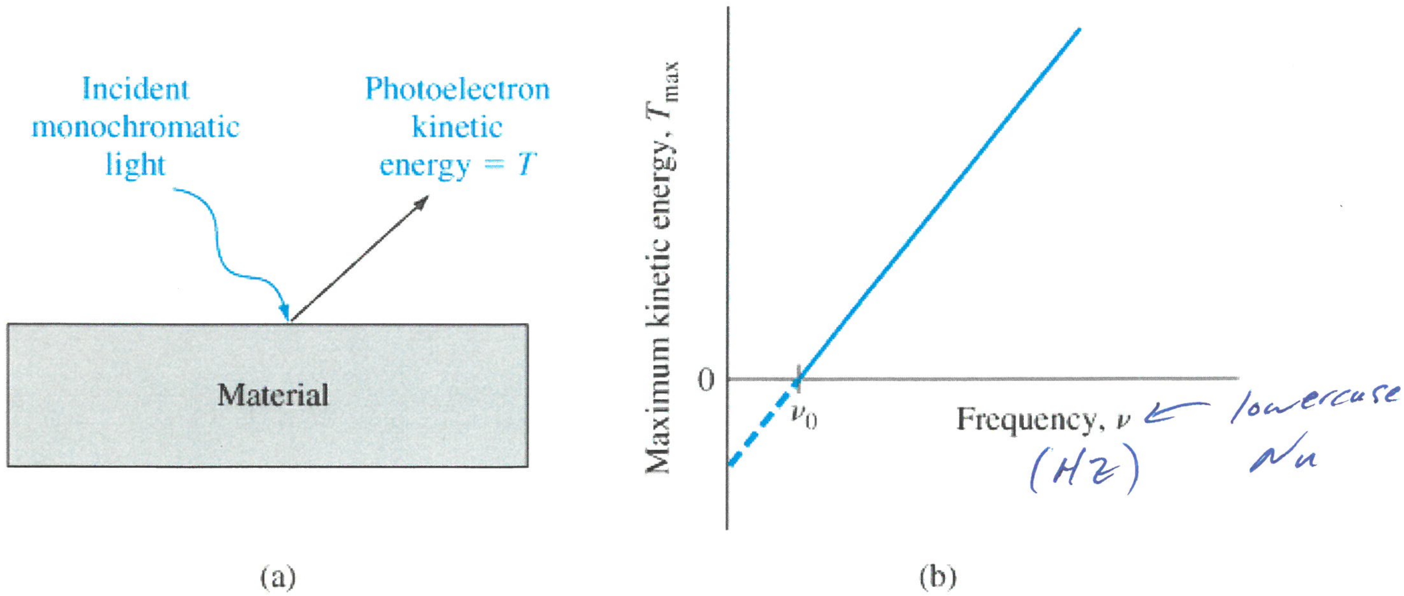

Figure 2.1 | (a) The photoelectric effect and (b) the maximum kinetic energy of the photoelectron as a function of incident frequency.

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

energy   freq (Hz)

Planck's constant $\equiv h = 6.62607 \times 10^{-34}$ J·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 <u>photons</u>. He developed this equation

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

max. K.E. of photoelectron

energy in photon

work function to pry electron loose from surface

when the RHS is less than zero, no photoelectron

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

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

2.1.1 cont.

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

$$E_g = h\nu = h\,c/\lambda = 6.62607\times10^{-34}\ \frac{2.9979\times10^{8}}{532\times10^{-9}}$$

$$= \underline{\underline{3.7339\times10^{-19}\ \text{J}}}$$

For particle physics, the unit of electron-volts is often used. It's the energy gained by an electron going from rest through 1V in vacuum. For SI units, $1\text{eV} = 1.602176634\times10^{-19}\ \text{J}$.

$$E_g = 3.7339\times10^{-19}\ \frac{1\text{eV}}{1.6022\times10^{-19}\ \text{J}} = \underline{\underline{2.3305\ \text{eV}}}$$

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

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

$\hookrightarrow W = V_{AB}\,Q$

EE 362 $\quad T = eV \qquad e = $ mag. of charge of electron $= 1.6022\times10^{-19}\ \text{C}$

work/ KE

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

momentum of a photon $\equiv p = \dfrac{h}{\lambda}$ ← Planck's constant (kg m/s)

deBroglie wavelength of a particle $\equiv \lambda = \dfrac{h}{p}$ (m) ← 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 $\Delta p \Delta x \geq \hbar = \frac{h}{2\pi} \equiv$ 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 $\Delta E \Delta t \geq \hbar = 1.054572 \times 10^{-34}$ 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

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

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 LHS

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

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

x dt and integrate

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

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

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

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

$$\phi(t) = e^{-j\omega t}$$ ← complex exponential form of sinusoidal waves

From earlier, $E = h\nu = h\left(\frac{\omega}{2\pi}\right) = \frac{h}{2\pi}\left(\frac{\eta}{\hbar}\right) = \eta$!

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

pot. Energy

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m}{\hbar^2}\left[E - V(x)\right]\psi(x) = 0 \qquad (2.13)$$

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.

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

freq. (Hz)

If we replace $V(x)$ w/ $\psi(x)$ and use $v_p = \nu\lambda$,

we get

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

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

2.2.1 cont.

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

where $\frac{p^2}{2m} = T = E - V$ since $\frac{(mv)^2}{2m} = \frac{1}{2}mv^2 = T$

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

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

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

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) $$\underline{|\Psi(x,t)|^2 = \psi(x)\psi^*(x) = |\psi(x)|^2}$$ ← 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 someplace

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

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

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

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

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

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

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

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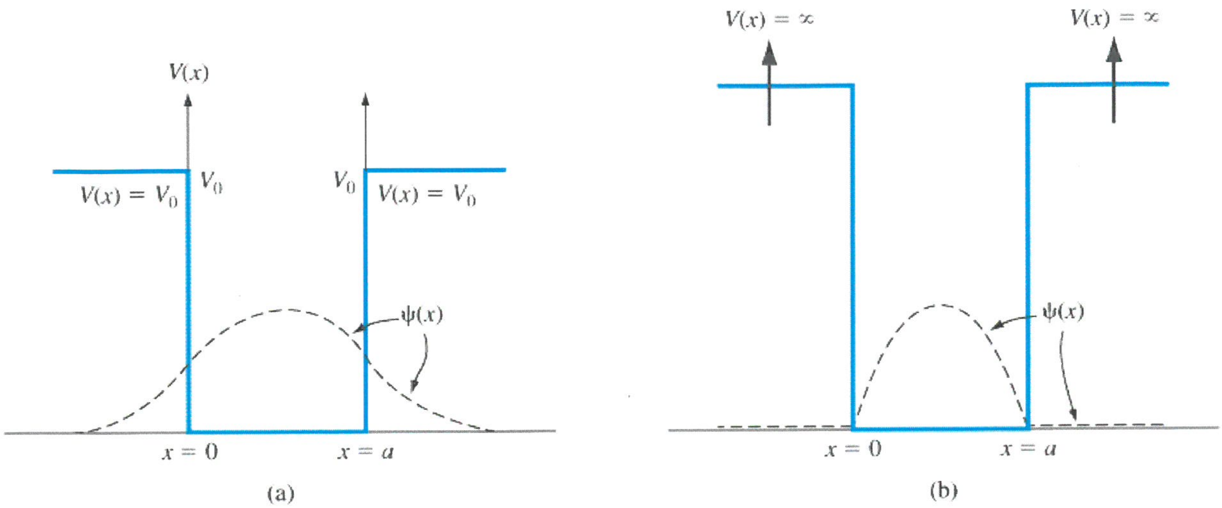


Figure 2.5 | Potential functions and corresponding wave function solutions for the case (a) when the potential function is finite everywhere and (b) when the potential function is infinite in some regions.

Handwaving arguments:

- 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.
- By conservation of energy, a particle can **not** 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 $\dfrac{d^2\psi(x)}{dx^2} + \dfrac{2mE}{\hbar^2}\psi(x) = 0$ ← 2nd-ord ordinary diff. Eq'n (wave eq'n)

has solution

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

$$= A e^{jKx} + B e^{-jKx}$$

where wave number $\equiv K = \sqrt{\dfrac{2mE}{\hbar^2}}$. The overall wave function is then

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

$$= A e^{j(Kx - \omega t)} + B e^{-j(Kx + \omega t)} \qquad (2.23)$$

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

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

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

↳ $\lambda = \dfrac{2\pi\hbar}{K\hbar} = 2\pi/K \quad \Rightarrow K = 2\pi/\lambda$

2.3.1 cont.

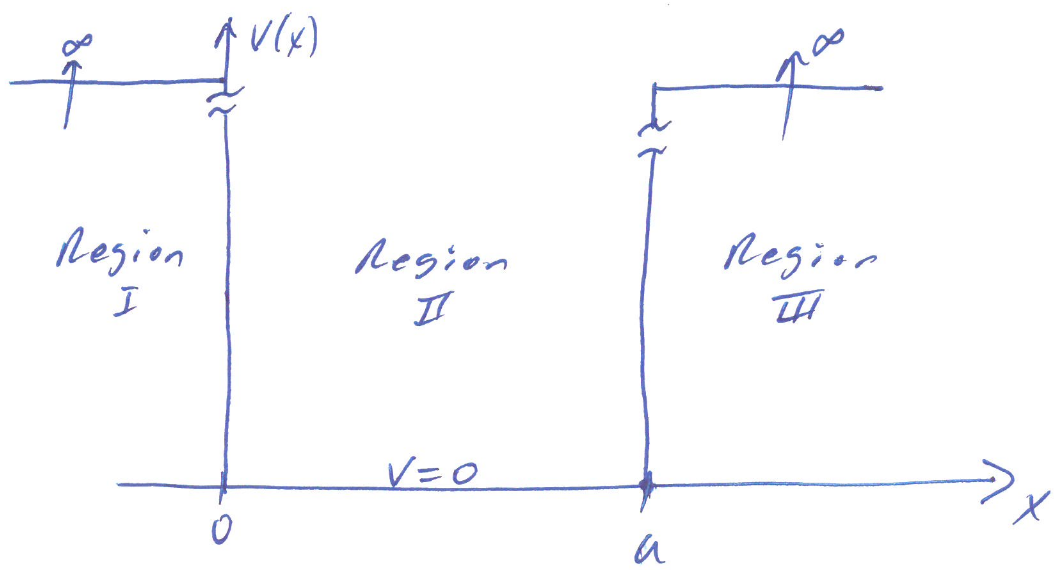
⇒ So, a free electron (particle) w/ well-defined energy E has a well-defined λ and momentum p. However, for the $+x$ wave ($B=0$)

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

⇒ particle/electron equally lilkely to be <u>anywhere</u>! 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 can <u>NOT</u> reach them.

2.3.2 cont.

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

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m}{\hbar^2}\left[E - \cancel{V(x)}^{\,0}\right]\psi(x) = 0$$

becomes

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2mE}{\hbar^2}\psi(x) = 0. \qquad (2.28)$$

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

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

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

Next, apply our boundary conditions that $\psi(x=0) = \psi(x=a) = 0$.

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

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

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

$\sin Ka = 0 \Rightarrow Ka = n\pi$ where $n = 1, 2, 3, \ldots$

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

2.3.2 cont.

How do we find A_2?

⇒ Recall that our particle must exist.

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

which reduces to

$$\int_{x=0}^{a} A_2 \sin kx \; A_2 \sin kx \, dx = 1$$

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

$$A_2^2 \int_{x=0}^{a} \tfrac{1}{2}(1 - \cos 2kx)\, dx = 1$$

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

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

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

Now, we have our particular sol'n

$$\boxed{\psi(x) = \sqrt{2/a}\, \sin\left(\frac{n\pi}{a}x\right) \quad \text{where } n = 1, 2, \ldots \quad 0 \le x \le a}$$

Further, note that

$$k = \sqrt{\frac{2mE}{\hbar^2}} = \frac{n\pi}{a}$$

2.3.2 cont.

$$k^2 = \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{a^2} = k_n^2$$ ← wave # takes on discrete/quantized values!

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

⇒ Energy of particle is quantized!

We can also write $\underline{\psi(x) = \sqrt{2/a}\,\sin(k_n x) \quad 0 \le x \le a}$

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

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

$h := 6.62607015 \cdot 10^{-34}$ J-s $\qquad hmod := \dfrac{h}{2 \cdot \pi}$ $\qquad hmod = 1.05457 \times 10^{-34}$ J-s

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

Calculate some quantities and/or define equations

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

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

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

$$E(n) := \frac{hmod^2 \cdot n^2 \cdot \pi^2}{2 \cdot m \cdot a^2} \qquad EeV(n) := \frac{E(n)}{1.602176634 \cdot 10^{-19}}$$

Per (2.39), the wave function ($m^{-0.5}$), in terms of quantum number *n* and 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

$$\Psi2(n,x) := \psi(n,x) \cdot \overline{\psi(n,x)}$$

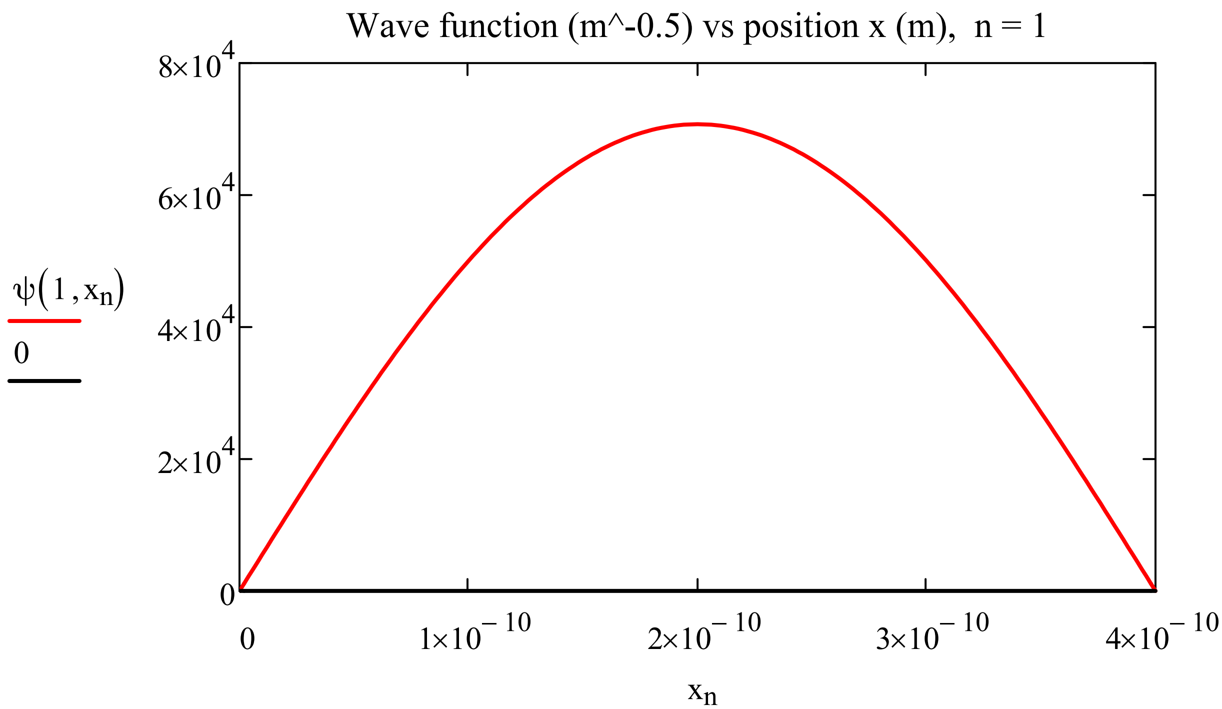
Define a vector of positions *x* across the width of the potential well, i.e., 0 <= *x* <= *a*.

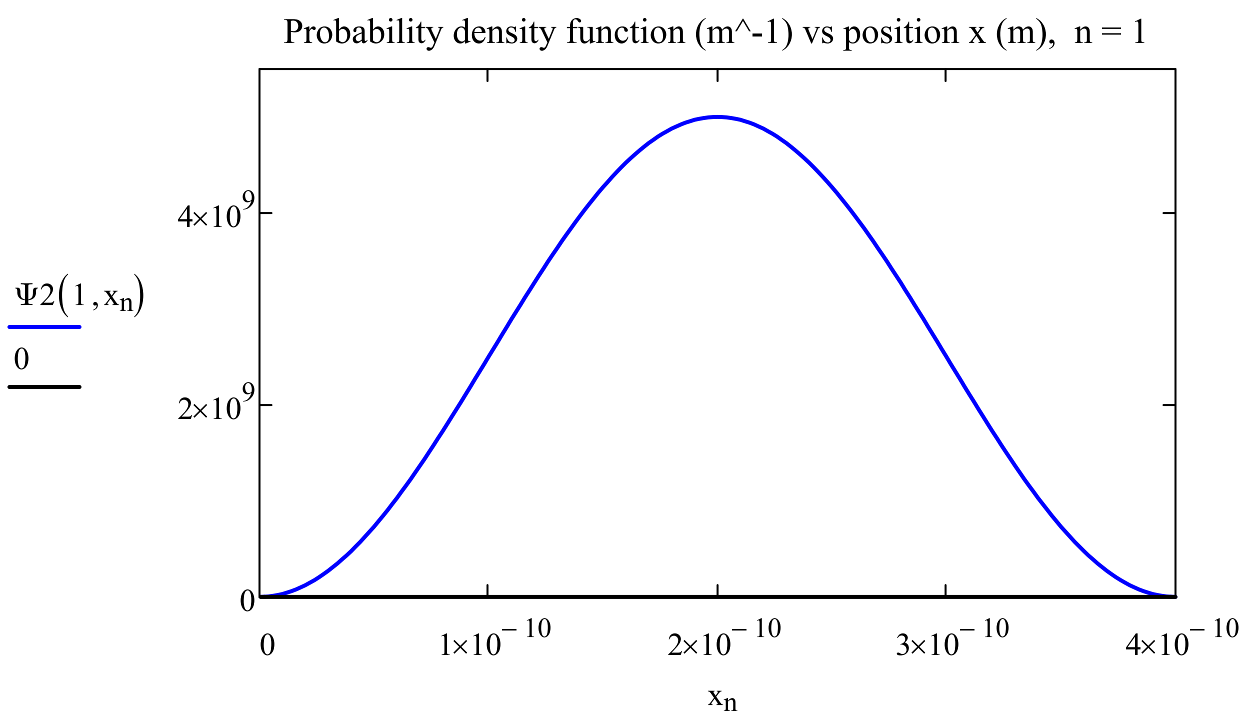
$$Nmax := 200 \qquad n := 0 .. Nmax \qquad x_n := \frac{n}{Nmax} \cdot a$$

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

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

$\boxed{E(1) = 3.765 \times 10^{-19}}$ (J) or $\boxed{EeV(1) = 2.3502}$ (eV)

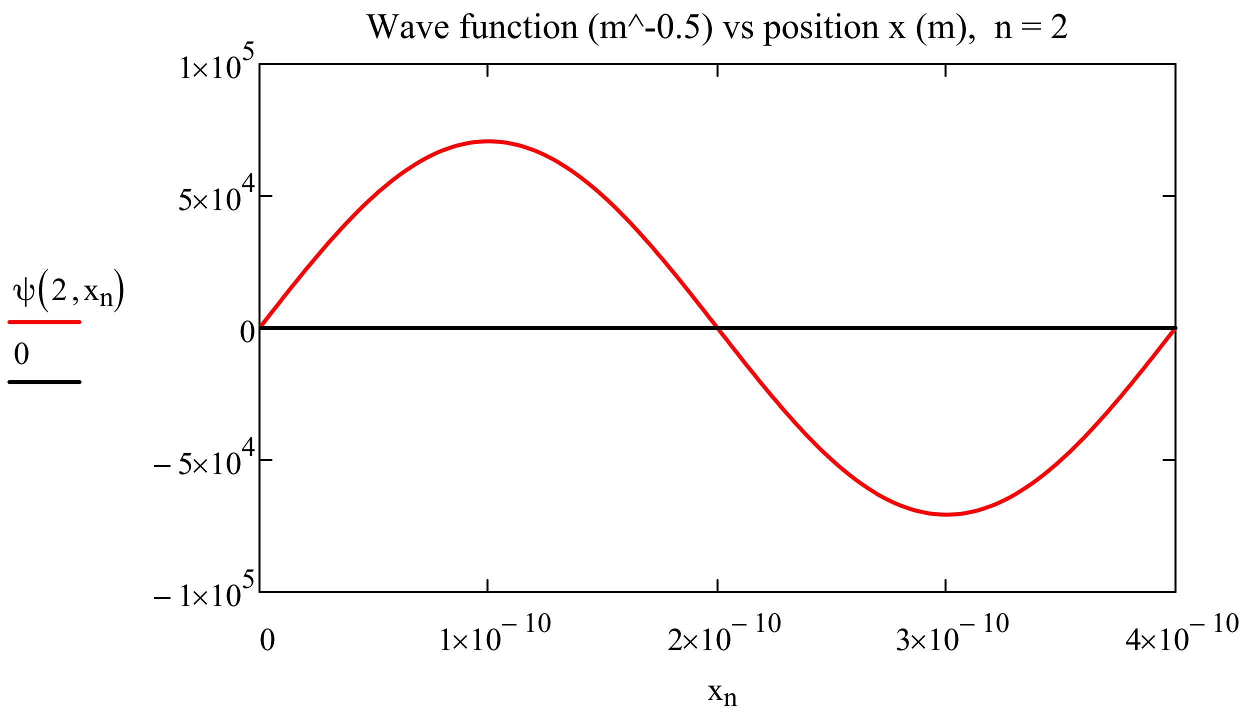


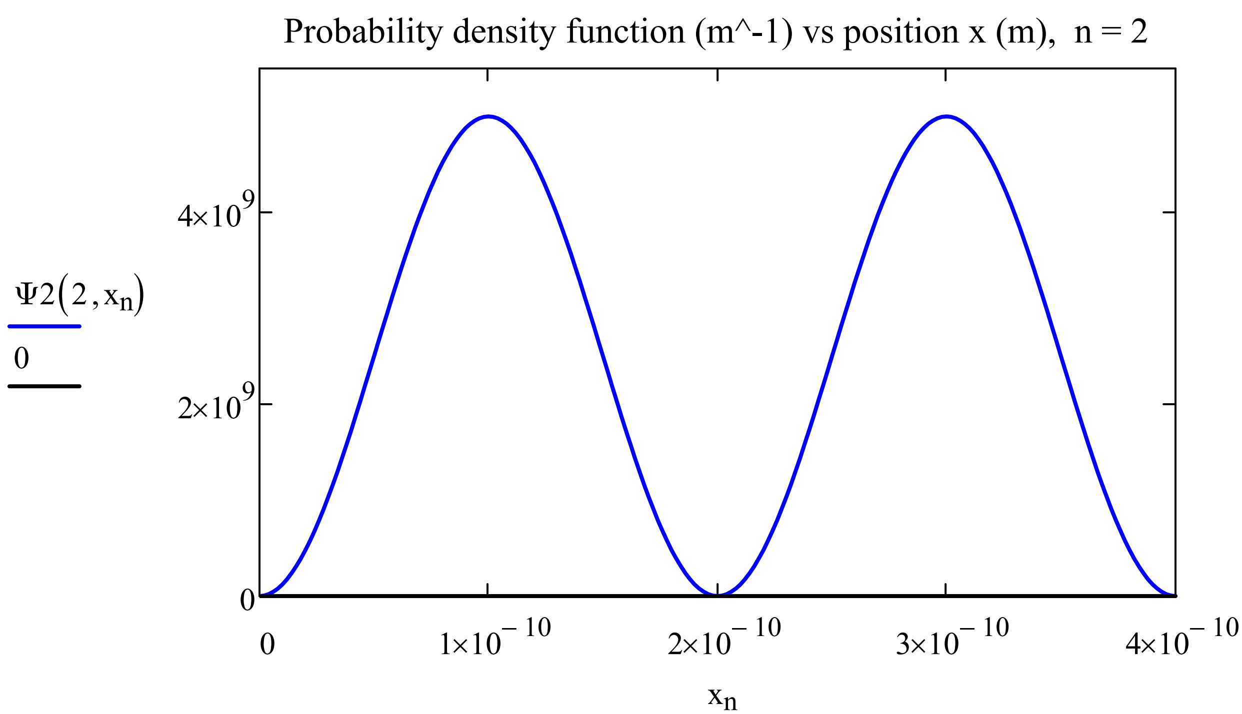


For the second quantum level, i.e., *n* = 2

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

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

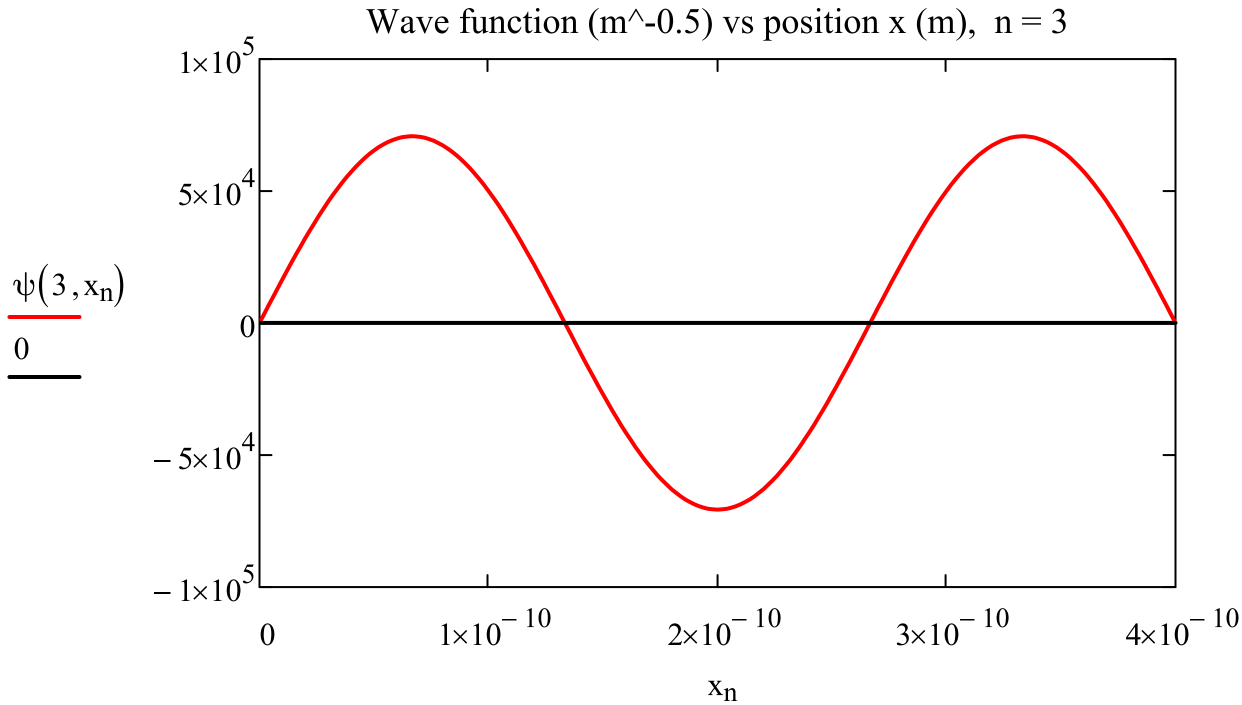


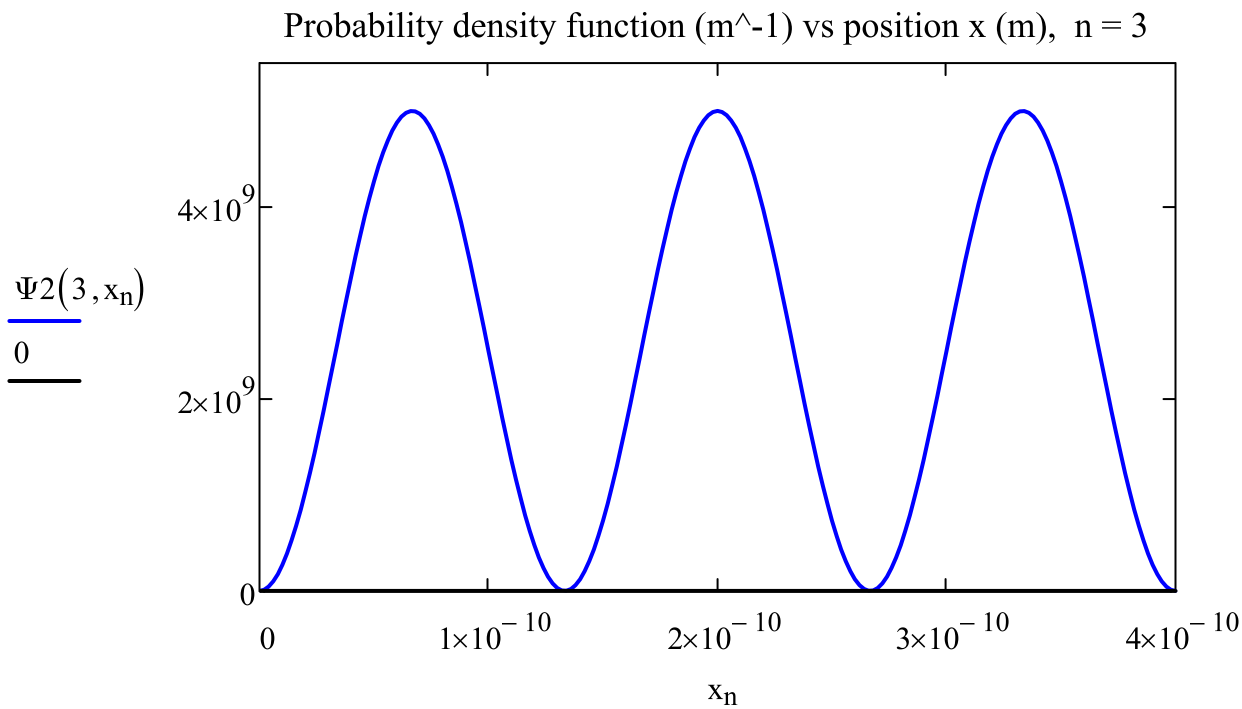


For the third quantum level, i.e., *n* = 3

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

$\boxed{E(3) = 3.389 \times 10^{-18}}$ (J) or $\boxed{EeV(3) = 21.1517}$ (eV) $\frac{EeV(3)}{EeV(1)} = 9$

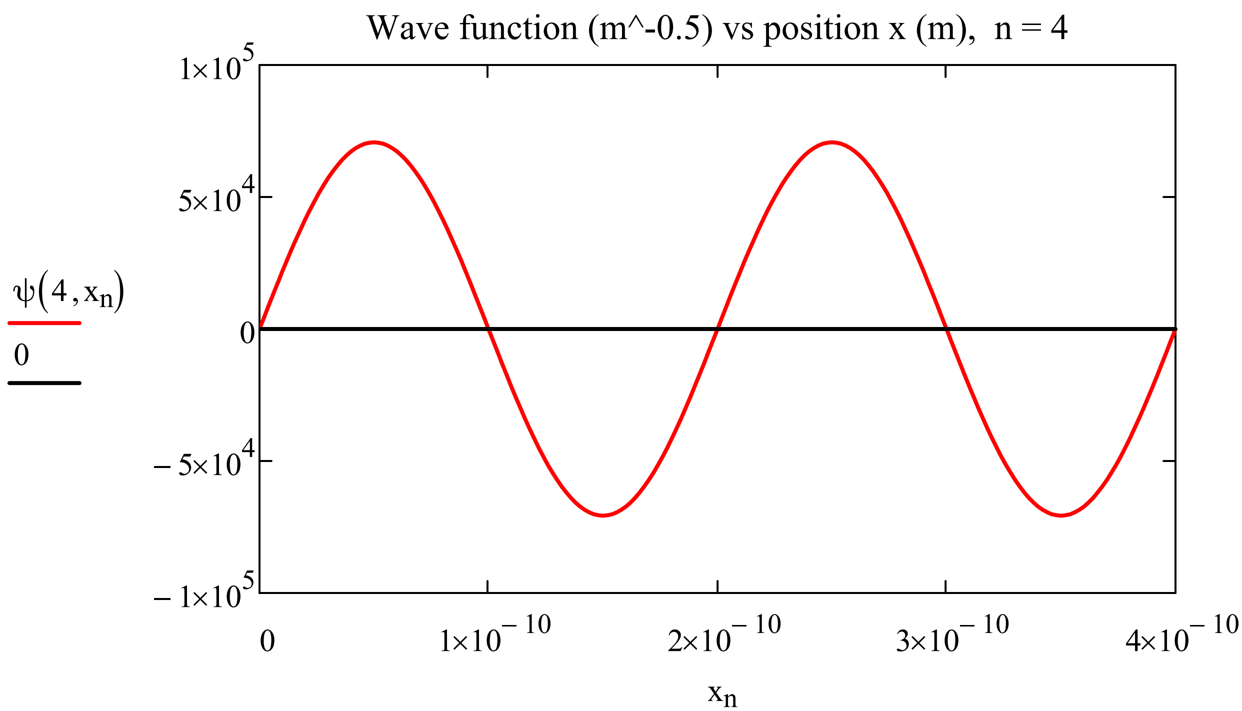


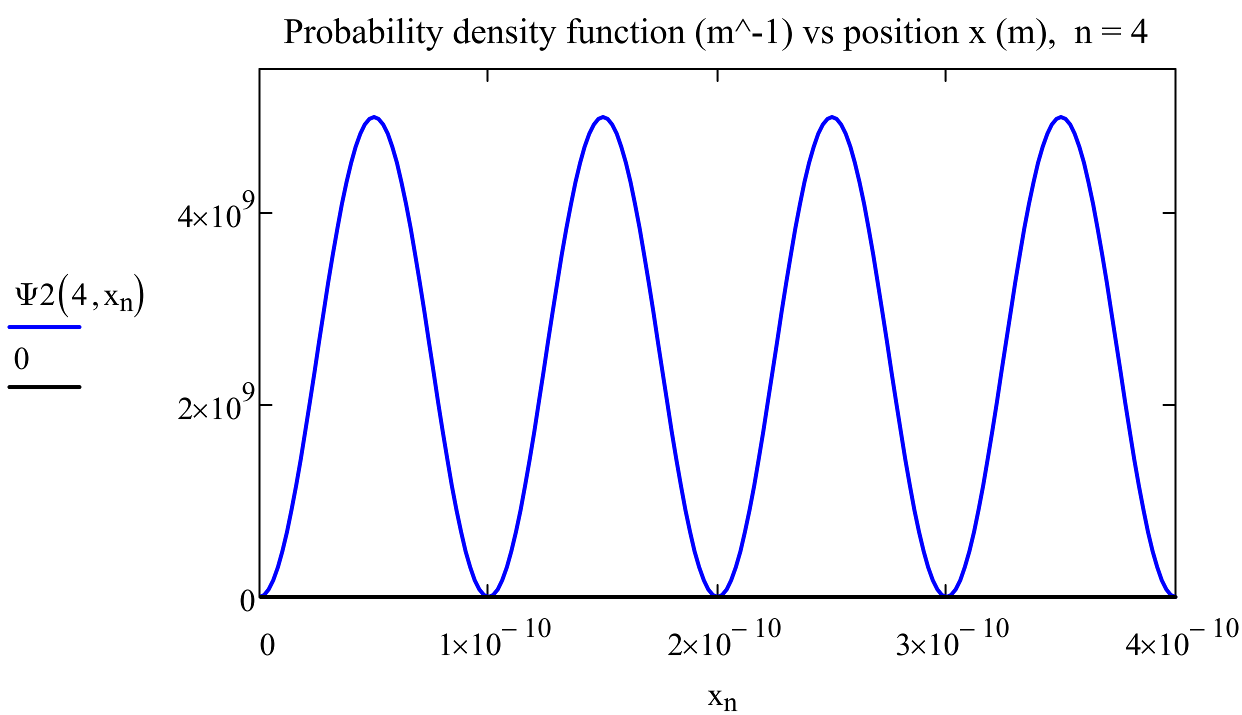


<u>For the fourth quantum level, i.e., *n* = 4</u>

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

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

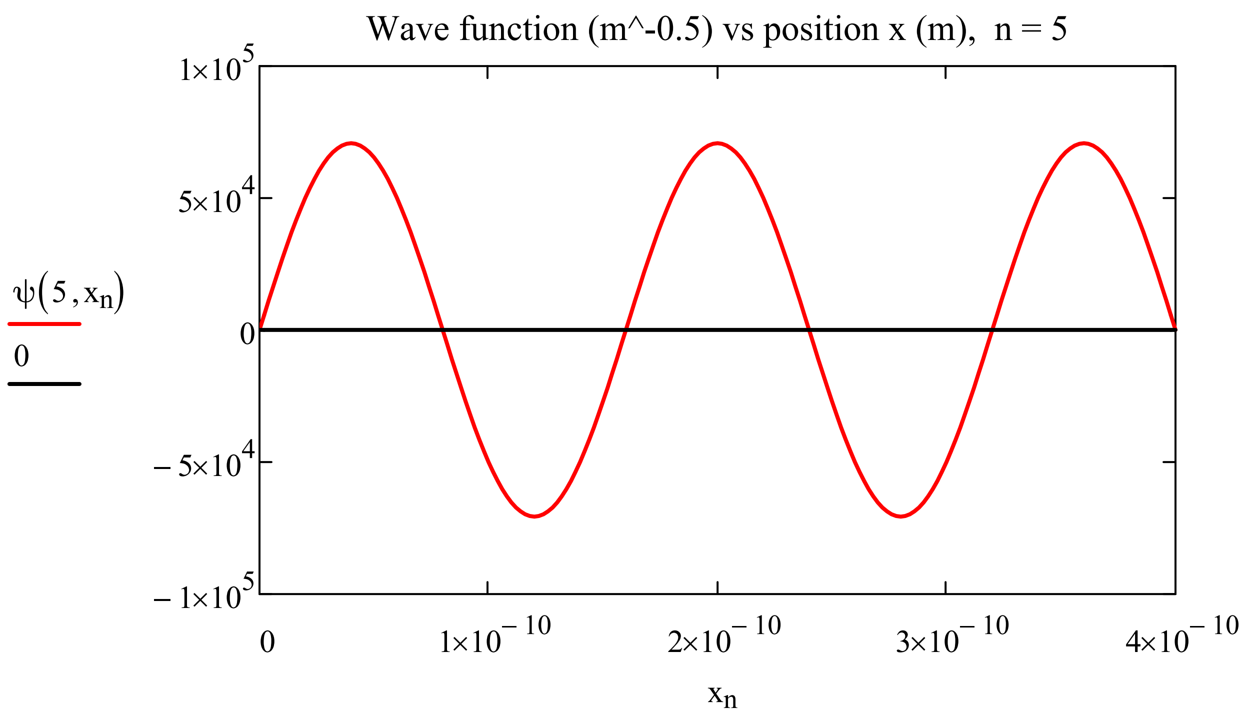


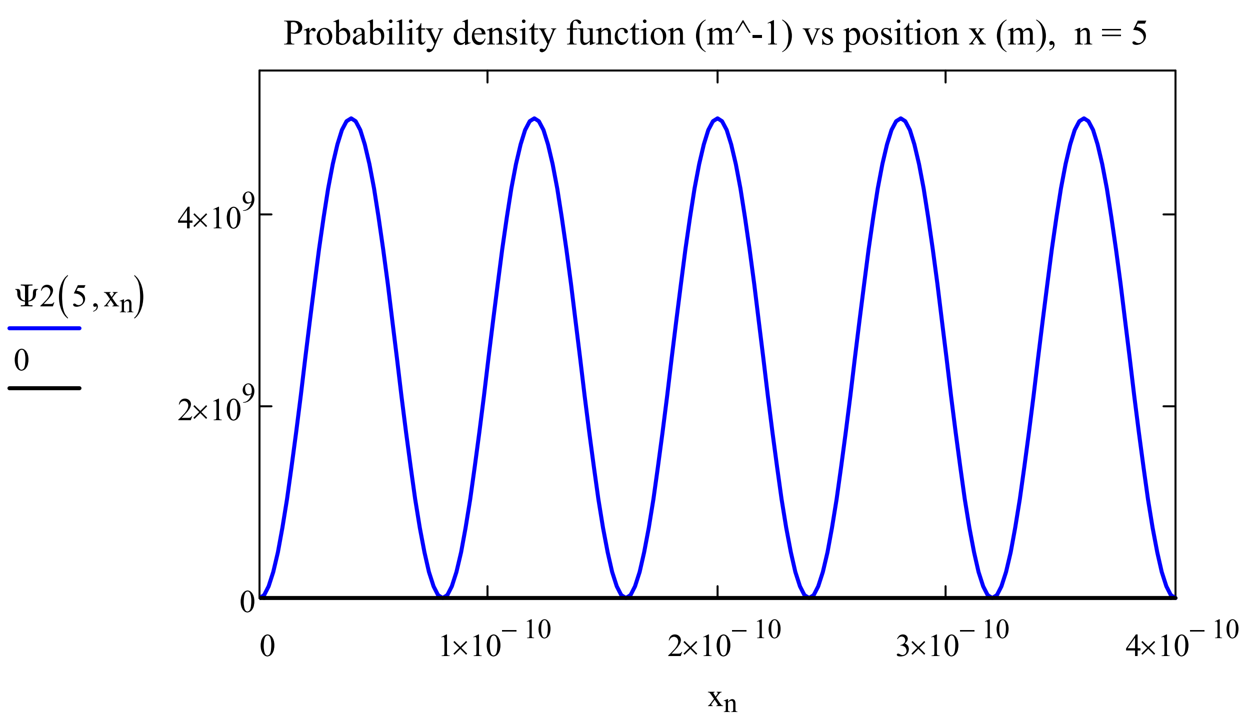


For the fifth quantum level, i.e., *n* = 5

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

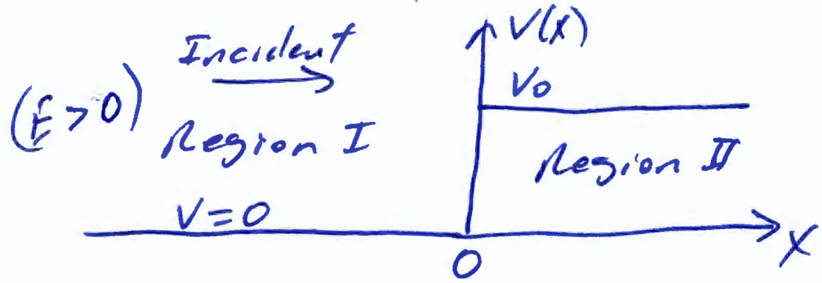
$\boxed{E(5) = 9.414 \times 10^{-18}}$ (J) or $\boxed{EeV(5) = 58.7547}$ (eV) $\frac{EeV(5)}{EeV(1)} = 25$





2.3.3 The Step Potential Function

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



<u>In Region I</u>, the time independent 1D Schrodinger Eq'n is

$$\frac{d^2\psi_1(x)}{dx^2} + \frac{2m}{\hbar^2}\left[E - \cancelto{0}{V(x)}\right]\psi_1(x) = 0$$

← 2nd order ODE wave eq'n

where $\psi_1(x)$ is the solution in Region I. Since Region I is semi-infinite and contains traveling particles, we choose the sol'n form

$$\psi_1(x) = A_1 e^{jK_1x} + B_1 e^{-jK_1x} \qquad (x \le 0) \qquad (2.41)$$

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 $|\Psi(x,t)|^2 = \psi_1(x)\psi_1^*(x)$, we can note that

$A_1 A_1^* \equiv$ probability density of incident (+x-dir) particles

$B_1 B_1^* \equiv$ " " " reflected (-x-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

$$v_i A_1 A_1^* \quad \& \quad v_r B_1 B_1^* \quad \left(\frac{\#\text{particles}}{\text{cm}^2\,\text{s}}\right)$$

or m^2

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

neg. pos.

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

w/ the "-" sign in the ODE, the sol'n is of form

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

2.3.3 cont.

Since $\psi_2(x)$ must be finite, set $B_2 = 0$ to prevent $e^{+\kappa_2 x}$ term from approaching ∞ as $x \to \infty$.

$$\psi_2(x) = A_2 e^{-\kappa_2 x} \qquad (x \geq 0)$$

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

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

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

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

$$\left[jk_1 A_1 e^{jk_1 x} - jk_1 B_1 e^{-jk_1 x} \right]\Big|_{x=0} = -\kappa_2 A_2 e^{-\kappa_2 x}\Big|_{x=0}$$

② $$jk_1 A_1 - jk_1 B_1 = -\kappa_2 A_2$$

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

$$B_1 = \frac{-(\kappa_2^2 + 2jk_1\kappa_2 - k_1^2)}{\kappa_2^2 + k_1^2} A_1 \quad (2.51a)$$

$$A_2 = \frac{2k_1(k_1 - j\kappa_2)}{\kappa_2^2 + k_1^2} A_1 \quad (2.51b)$$

Why? B_1/A_1 = Part of incident ψ_1 refl. + A_2/A_1 = Part of incident ψ_1 transmitted

2.3.3 cont.

Now, the reflected wave probability density function is

$$B_1 B_1^* = \frac{+(K_2^2 + j2K_1K_2 - K_1^2)(K_2^2 - j2K_1K_2 - K_1^2)}{(K_2^2+K_1^2)^2} A_1 A_1^* \quad (2.52)$$

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

$$R = \frac{v_r B_1 B_1^*}{v_i A_1 A_1^*} \quad (2.53)$$

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

$$K_1 = \sqrt{\frac{2mE}{\hbar^2}} = \sqrt{\frac{2m(\frac{1}{2}mv^2)}{\hbar^2}} = \frac{mv}{\hbar}$$

$\hookrightarrow v = \frac{\hbar}{m} K_1$

$\Rightarrow v_i = v_r$, since we have $\psi_1(x) = A_1 e^{jK_1x} + B_1 e^{-jK_1x}$

Therefore

2.59 has Typo

$$R = \frac{\cancel{v_r} B_1 B_1^*}{\cancel{v_i} A_1 A_1^*} = \frac{B_1 B_1^*}{A_1 A_1^*}$$

$$= \frac{\{(K_2^2-K_1^2) + j2K_1K_2\}[(K_2^2-K_1^2) - j2K_1K_2]}{(K_2^2+K_1^2)^2} \frac{\cancel{A_1 A_1^*}}{\cancel{A_1 A_1^*}}$$

$$R = \frac{(K_2^2-K_1^2)^2 + 4K_1^2K_2^2}{(K_2^2+K_1^2)^2} = \underline{\underline{1}} \quad ?!!$$

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 $\psi_2(d) = e^{-1}\psi_2(0)$.

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

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

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

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

$$(2.48) \quad \psi_2(x) = A_2 e^{-k_2 x} \quad \& \quad (2.45) \quad k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

2.3.3 cont.

ex. cont.

$$K_2 = \sqrt{\frac{2(9.1094\times10^{-31})(2-0.25)1.60218\times10^{-19}}{(1.054572\times10^{-34})^2}}$$

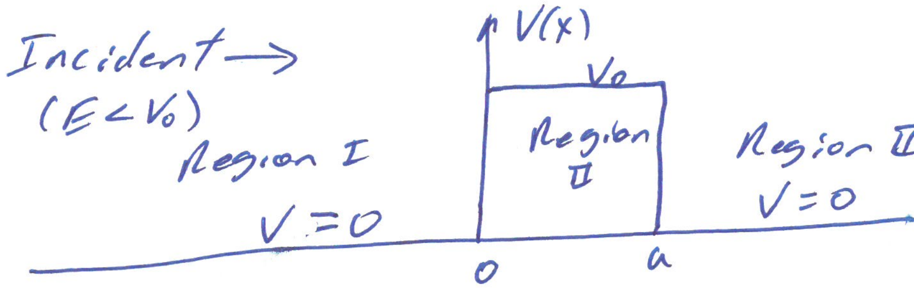
$$= 6.77319\times10^{9}\ \text{Np/m}$$

$$\frac{\psi_2(d)}{\psi_2(0)} = \frac{A_2 e^{-K_2 d}}{A_2} = e^{-6.77319\times10^{9} d} = e^{-1}$$

$$\Rightarrow\ d = \frac{1}{6.77319\times10^{9}} = 1.4755\times10^{-10}\ \text{m} = \underline{\underline{1.4755\ \text{Å}}}$$

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

$$\psi_1(x) = A_1 e^{jK_1 x} + B_1 e^{-jK_1 x} \qquad x < 0 \qquad (2.60a)$$

$$\psi_2(x) = A_2 e^{K_2 x} + B_2 e^{-K_2 x} \qquad 0 < x < a \qquad (2.60b)$$

$$\psi_3(x) = A_3 e^{jK_3 x} + B_3 e^{-jK_3 x} = A_3 e^{jK_1 x} + B_3 e^{-jK_1 x} \qquad (2.60c)$$

$(x > a)$

where $K_1 = K_3 = \sqrt{\dfrac{2mE}{\hbar^2}}$ (rad/m) (2.61a)

and $K_2 = \sqrt{\dfrac{2m(V_0 - E)}{\hbar^2}}$ (Np/m) (2.61b)

2.3.4 cont.

We have 6 unknown constant coefficients (A_1, B_1, A_2, B_2, A_3, & 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:

① $\psi_1(0) = A_1 + B_1 = \psi_2(0) = A_2 + B_2$

② $\psi_2(a) = A_2 e^{K_2 a} + B_2 e^{-K_2 a} = A_3 e^{jK_1 a} = \psi_3(a)$

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

③ $\left.\frac{\partial \psi_1(x)}{\partial x}\right|_{x=0} = jK_1 A_1 - jK_1 B_1 = K_2 A_2 - K_2 B_2 = \left.\frac{\partial \psi_2(x)}{\partial x}\right|_{x=0}$

④ $\left.\frac{\partial \psi_2(x)}{\partial x}\right|_{x=a} = K_2 A_2 e^{K_2 a} - K_2 B_2 e^{-K_2 a} = jK_1 A_3 e^{jK_1 a} = \left.\frac{\partial \psi_3}{\partial x}\right|_{x=a}$

We have 5 unknowns and 4 equations.

We can solve for B_1, A_2, B_2, + 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.

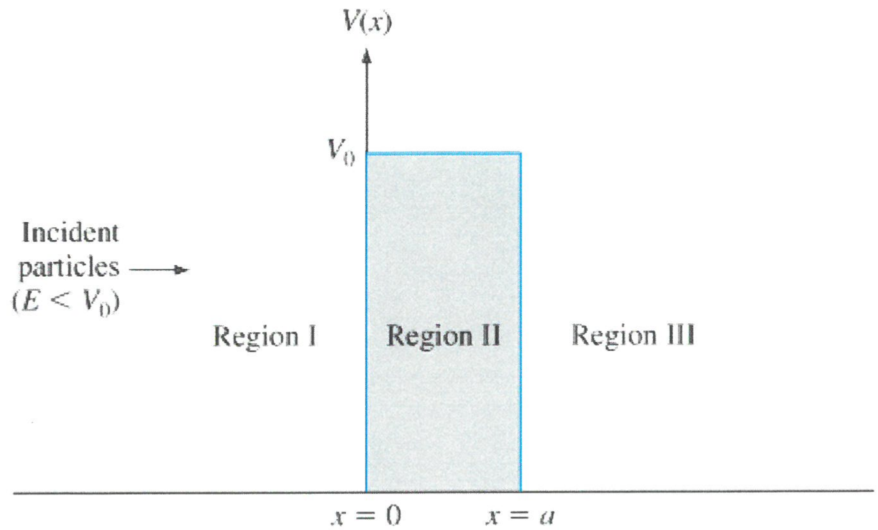


Figure 2.9 | The potential barrier function.

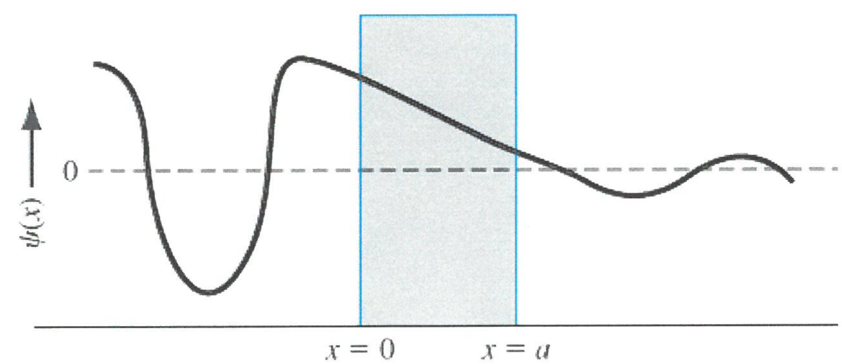


Figure 2.10 | The wave functions through the potential barrier.

- 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

$$T = \frac{1}{1 + \frac{V_0^2 \sinh^2(K_2 a)}{4E(V_0 - E)}}$$ 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 $\sinh^2(K_2 a) \simeq \frac{1}{4} e^{2K_2 a}$. Then,

$$T \simeq \frac{1}{1 + \frac{V_0^2 \frac{1}{4} e^{2K_2 a}}{4E(V_0 - E)}} = \frac{16 \frac{E}{V_0}\left(1 - \frac{E}{V_0}\right)}{\underbrace{\underset{\uparrow \text{small}}{16 \frac{E}{V_0}}\underset{\uparrow \text{small}}{\left(1 - \frac{E}{V_0}\right)}}_{\text{ignore}} + \underset{\uparrow \text{big}}{e^{2K_2 a}}}$$

$$\underline{T \simeq 16 \frac{E}{V_0}\left(1 - \frac{E}{V_0}\right) e^{-2K_2 a}} \quad (2.63)$$

$\Rightarrow T$ is small <u>but</u> > 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

$h := 6.62607015 \cdot 10^{-34}$ J-s $\quad hmod := \dfrac{h}{2 \cdot \pi}$ $\quad hmod = 1.05457 \times 10^{-34}$ J-s

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

Calculate some quantities and/or define equations

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

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

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

$$k1 := \sqrt{\frac{2 \cdot m \cdot E}{hmod^2}} \qquad \boxed{k1 = 5.12317 \times 10^{9}} \text{ rad/m}$$

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

$$k2 := \sqrt{\frac{2 \cdot m \cdot (V0 - E)}{hmod^2}} \qquad \boxed{k2 = 1.69916 \times 10^{10}} \text{ Np/m}$$

From notes, the exact transmission coefficient T is

$$Texact := \frac{1}{1 + \dfrac{V0^2 \cdot \sinh(k2 \cdot a) \cdot \sinh(k2 \cdot a)}{4 \cdot E \cdot (V0 - E)}} \qquad \boxed{Texact = 1.52636 \times 10^{-6}}$$

Pretty small!

For $\quad k2 \cdot a = 6.7966 \qquad \sinh(k2 \cdot a) \cdot \sinh(k2 \cdot a) = 2.001859 \times 10^{5}$

which can be approximated as $\quad 0.25 \cdot e^{2 \cdot k2 \cdot a} = 2.001864 \times 10^{5}$

Per (2.63), the approximate transmission coefficient T is

$$Tapprox := 16 \cdot \frac{E}{V0} \cdot \left(1 - \frac{E}{V0}\right) \cdot e^{-2 \cdot k2 \cdot a} \qquad \boxed{Tapprox = 1.52635 \times 10^{-6}}$$

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 ($m_p = 1.672622 \times 10^{-27}$ kg) and 1 electron ($m_e = 9.1093837 \times 10^{-34}$ kg). Obviously, the proton is much more massive than the electron.

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

$$V(r) = \frac{-e^2}{4\pi\epsilon_0 r^2} \qquad (2.64) \quad \leftarrow V(r \to 0) \to \infty$$

where $e = 1.6021766 \times 10^{-19}$ C, $\epsilon_0 = 8.8541878 \times 10^{-12}$ F/m, and r = 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 eq'n becomes –

2.4.1 cont.

rest mass of electron

$$\nabla^2 \psi(r,\theta,\phi) + \frac{2m_0}{\hbar^2}\left[E - V(r)\right]\psi(r,\theta,\phi) = 0 \quad (2.65)$$

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

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

Again, we assume that $\psi(r,\theta,\phi)$ is a separable function

$$\psi(r,\theta,\phi) = R(r)\,\Theta(\theta)\,\Phi(\phi) \quad (2.67).$$

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

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

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 $r, \theta, \& \phi$, we require/need

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

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 $m = 0, \pm 1, \pm 2, \ldots$ 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 $\ell, m, \& n$ the quantum numbers.

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

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

$|m| = \ell, \ell-1, \ldots 0 \equiv$ magnetic quantum #

2.4.1 cont.

→ Solutions to $R(r)$ & $\Theta(\theta)$ are 'complex'.

→ Each set of n, l, and 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.

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

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

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

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

where

$$\text{Bohr radius} \equiv a_o = \frac{4\pi\epsilon_o \hbar^2}{m_o e^2} = \underline{0.529177\,\text{Å}}$$

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.

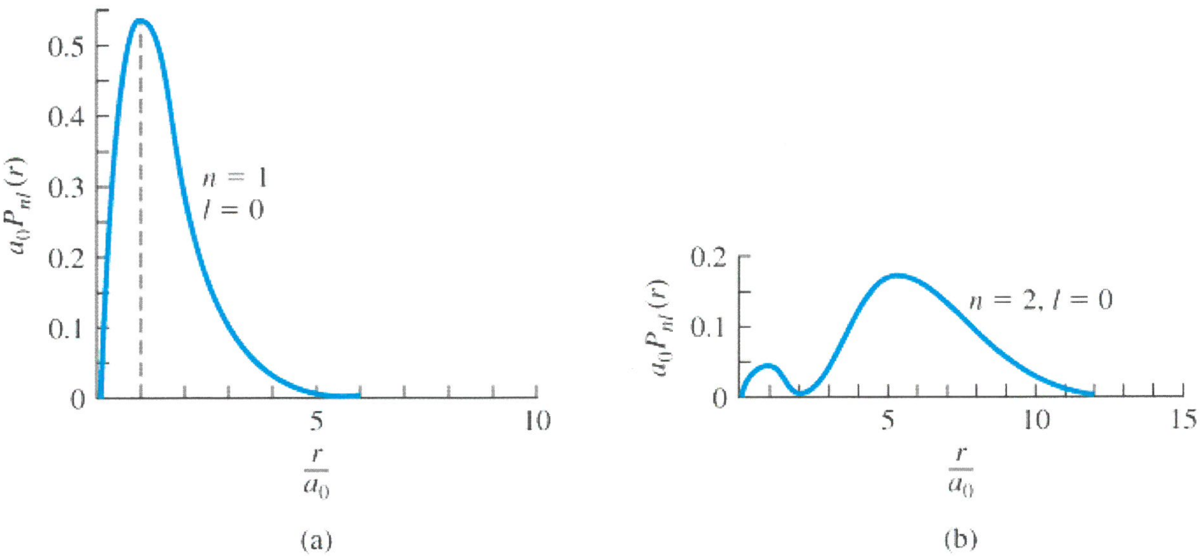


Figure 2.11 | The radial probability density function for the one-electron atom in the (a) lowest energy state and (b) next-higher energy state.
(From Eisberg and Resnick [5].)

- Per (2.72) $|m| = \ell, \ell\text{-}1, \ldots, 0$. 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, 1*s* shell/state), note that the electron is most likely to be found near $r/a_0 = 1$ or $r = a_0 = 0.529$ Å.
- For $|\Psi_{200}(r)|^2$ (AKA, 2*s* 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?

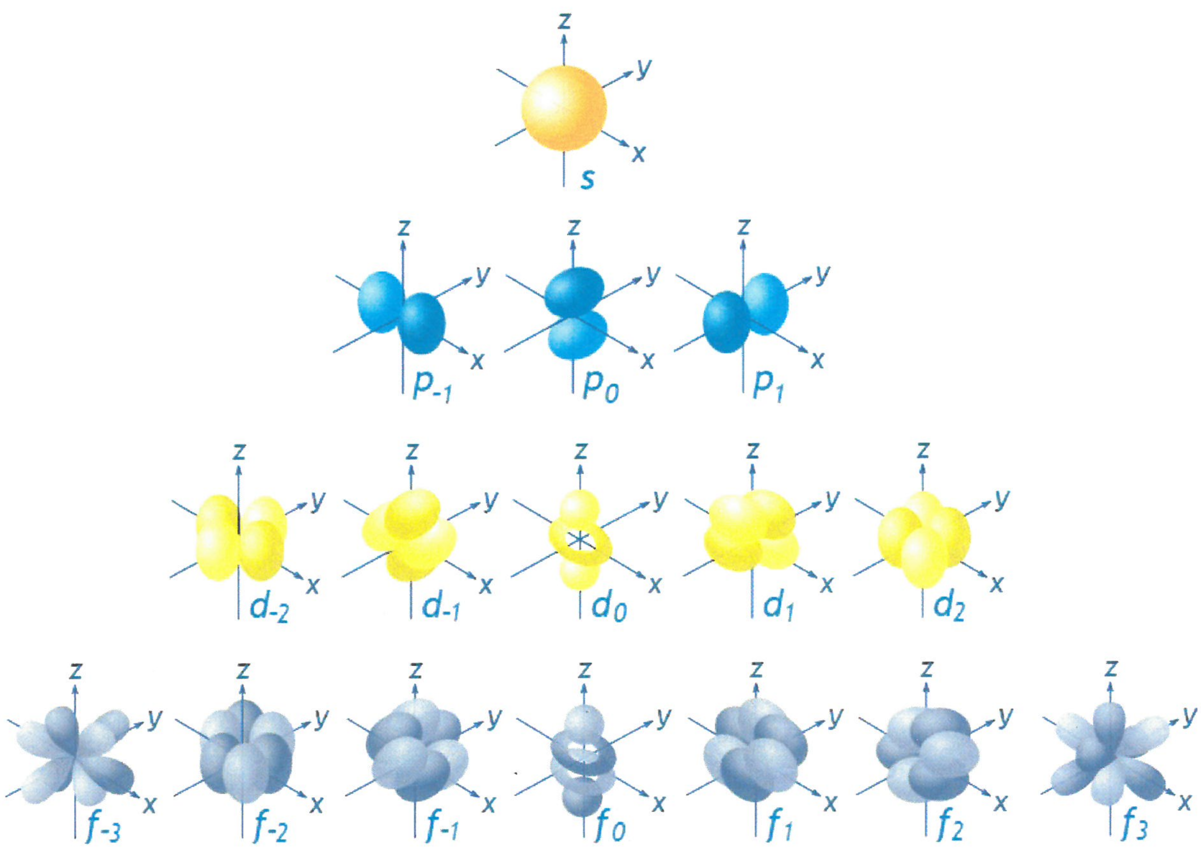
- → 3D time-independent Schrodinger's wave eq'n.
- → quantized energy levels/states for electrons
- → quantum numbers & quantum states for electrons

When $l \neq 0$, , we get $|\psi(r,\theta,\phi)|^2$ that are NOT rotationally symmetric (see pictures). Shells go w/ $n = 1, 2, \ldots$, then we have subshells/orbitals

subshells/orbitals	max # e^-
s (sharp)	
p (principal)	
d (diffuse)	
f (fundamental)	

Subshells/orbitals	ℓ quantum #	Max # electrons per level
s (**s**harp)	0	2
p (**p**rincipal)	1	6
d (**d**iffuse)	2	10
f (**f**undamental)	3	14

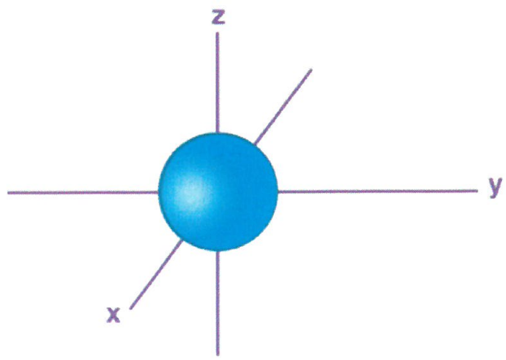
From https://www.mathsisfun.com/physics/atom-orbitals.html



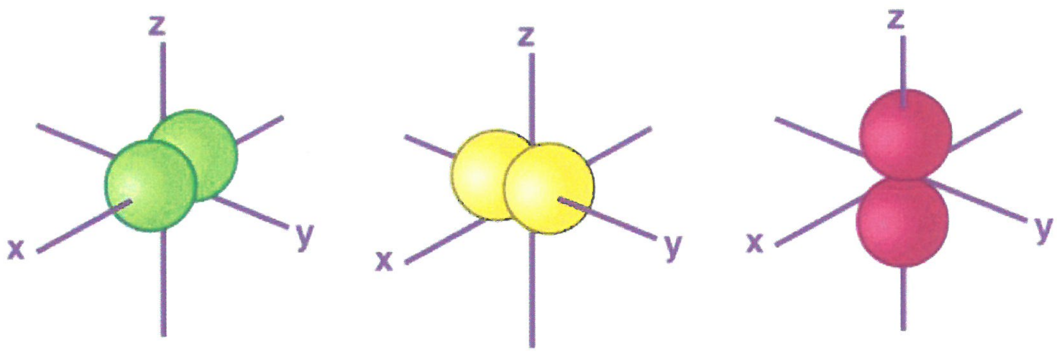
orbitals s, p, d and f

- 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.

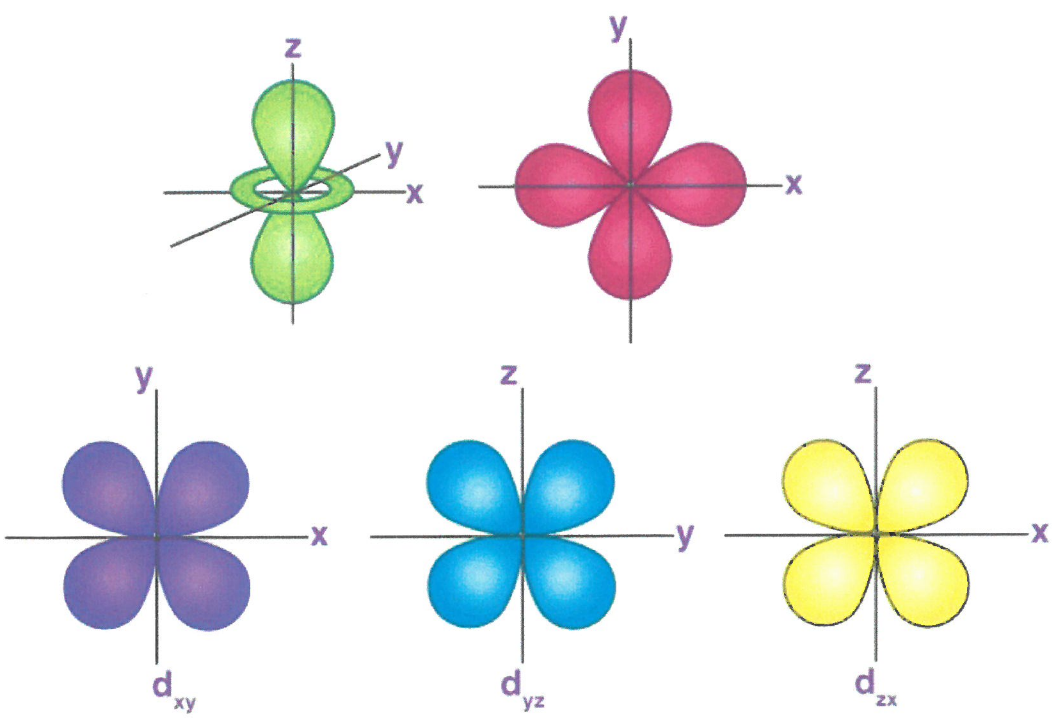
From https://byjus.com/chemistry/shapes-of-orbitals/



s orbitals



p orbitals

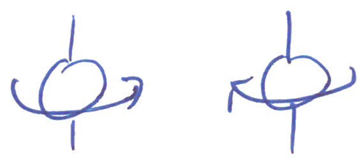


d orbitals

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) <u>Pauli exclusion principle</u> - In a system (i.e., atom, molecule, ...), no two electrons can occupy the same quantum state, i.e., they must have different quantum numbers