

De Broglie wavelength of a macroscopic object

$$\left. \begin{array}{l} m = 5.17 \text{ kg} \\ v = 10.2 \text{ m/s} \end{array} \right\} p = mv$$

$$\lambda = \frac{h}{p} = \frac{h}{mv} = \frac{6.63 \cdot 10^{-34} \text{ Js}}{5.17 \text{ kg} \cdot 10.2 \text{ m/s}}$$

$$\lambda = 1.26 \cdot 10^{-35} \text{ m}$$

This is a very short wavelength.
The wave behavior of macroscopic objects is not very significant.

Classical, relativistic and ultra-relativistic electron

$\lambda = \frac{h}{p}$ for all of them, but p is calculated differently at different energies.

Classical: $KE = \frac{p^2}{2m} \Rightarrow p^2 = 2mKE$

$$\Rightarrow p = \sqrt{2mKE} \quad (\text{my } KE = 59.4 \text{ eV})$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mKE}} = \frac{hc}{\sqrt{2mc^2 \cdot KE}} = \frac{hc}{\sqrt{2E_0 \cdot KE}}$$

$$\lambda = \frac{1240 \text{ eVnm}}{\sqrt{2 \cdot 5.11 \cdot 10^5 \text{ eV} \cdot 59.4 \text{ eV}}} = 0.159 \text{ nm}$$

$$\lambda = 0.159 \text{ nm} = 1.59 \text{ \AA} = 159 \text{ pm}$$

Relativistic electron: my $KE = 1.44 \text{ MeV}$

$$E^2 = (pc)^2 + (m_0c^2)^2 = (pc)^2 + E_0^2 \Rightarrow$$

$$\Rightarrow E^2 - E_0^2 = (pc)^2 \Rightarrow \sqrt{E^2 - E_0^2} = pc$$

$$E = E_0 + KE \Rightarrow E^2 = E_0^2 + 2E_0 \cdot KE + KE^2$$

$$E^2 - E_0^2 = 2E_0 \cdot KE + KE^2$$

Relativistic electron continued:

$$pc = \sqrt{2E_0 \cdot KE + KE^2}$$

$$\lambda = \frac{h}{p} = \frac{hc}{pc} = \frac{hc}{\sqrt{2E_0 \cdot KE + KE^2}}$$

$$\lambda = \frac{1240 \text{ eV nm}}{\sqrt{(2 \cdot 0.511 \cdot 1.44 + 1.44^2) \cdot (10^6 \text{ eV})^2}}$$

$$\lambda = \frac{1240 \text{ eV nm}}{1.88 \cdot 10^6 \text{ eV}} = 658 \cdot 10^{-6} \text{ nm}$$

$$\lambda = 0.658 \text{ } \mu\text{m}$$

Ultrarelativistic electron:

$$KE \gg E_0 \quad \text{my } KE = 2.24 \text{ GeV}$$

$$\lambda = \frac{hc}{\sqrt{KE(2E_0 + KE)}} \approx \frac{hc}{\sqrt{KE^2}} = \frac{hc}{KE}$$

$$\lambda = \frac{1240 \text{ eV nm}}{2.24 \cdot 10^9 \text{ eV}} = 553 \cdot 10^{-9} \text{ nm}$$

$$\lambda = 0.553 \text{ fm}$$

Protons from the Tevatron

$E_0 = 938 \text{ MeV}$: rest energy of the proton

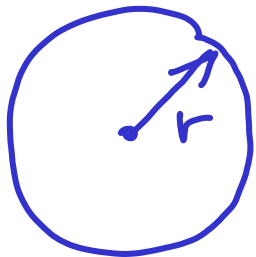
$KE = 554 \text{ GeV}$: kinetic energy of these protons. This is a very high energy, we need to use relativistic mechanics:

$$pc = \sqrt{KE^2 + 2KE \cdot E_0}$$

Since the kinetic energy is so huge ($554 \text{ GeV} \gg 0.938 \text{ GeV}$), we can use the $pc \approx KE$ approximation:

$$\lambda = \frac{h}{p} = \frac{hc}{pc} \approx \frac{hc}{KE} = \frac{1240 \text{ eV nm}}{554 \text{ GeV}}$$

$$\lambda = 2.24 \cdot 10^{-9} \text{ nm} = 2.24 \cdot 10^{-3} \text{ fm} = 2.24 \text{ am} \quad (\text{a} = \text{atto})$$



proton

$$r = 0.94 \text{ fm} = 940 \text{ am}$$

$$\frac{r}{\lambda} = \frac{940 \text{ am}}{2.24 \text{ am}} \approx 420$$

In theory we can probe $1/420$ of the proton radius with protons accelerated to this energy.

$$1/420 = 2.38 \cdot 10^{-3} \text{ or } 0.238\% \text{ of the } r.$$

Energy uncertainty of a particle

Lifetime: $\tau = 47.9 \text{ as} = 47.9 \cdot 10^{-18} \text{ s}$

Rest mass: $m_0 = 124.6 \text{ MeV}/c^2 \Rightarrow$

$\Rightarrow$ rest energy: $E_0 = 124.6 \text{ MeV}$.

Time uncertainty of this particle:

$$\Delta t \cong \tau$$

Heisenberg Uncertainty Principle:

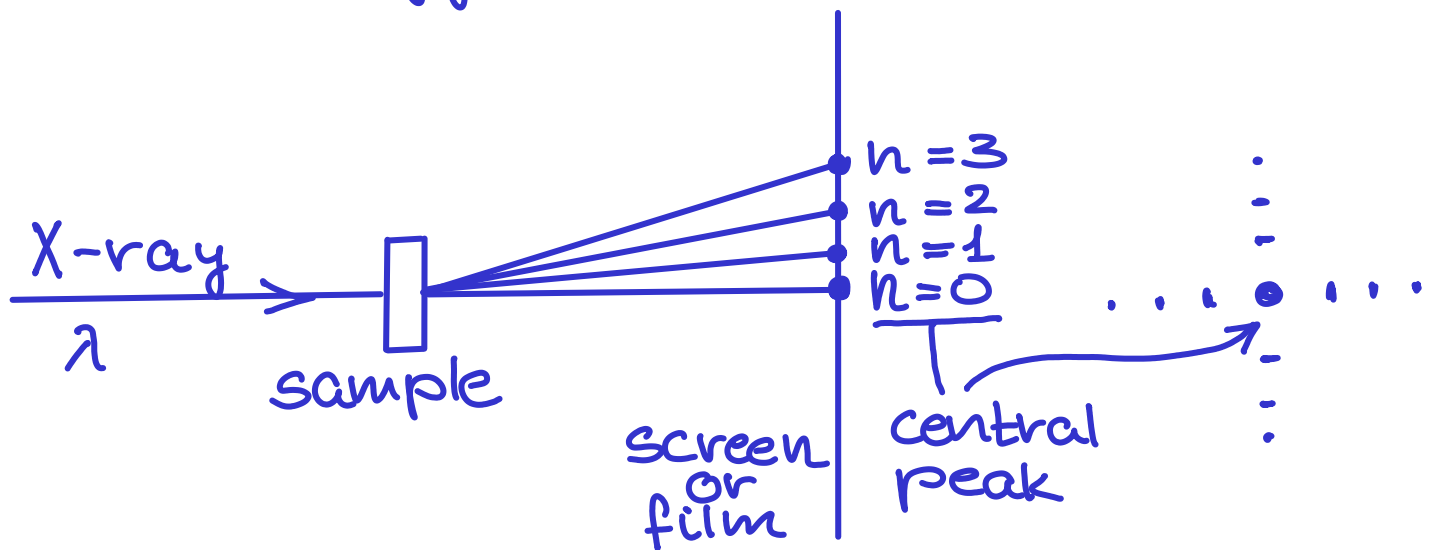
$$\Delta t \cdot \Delta E \geq \frac{\hbar}{2}$$

$$\Delta E \geq \frac{\hbar}{2\Delta t} \cong \frac{\hbar}{2\tau}$$

$$\hbar = 6.5821 \cdot 10^{-16} \text{ eVs}$$

$$\Delta E \geq 6.87 \text{ eV}$$

Bragg's law



Bragg's law:

$$2d \sin \theta = n\lambda \quad n=1,2,3,4,\dots$$

$$\left. \begin{aligned} 2d \sin \theta_1 &= 1 \cdot \lambda \\ 2d \sin \theta_2 &= 2 \cdot \lambda \\ 2d \sin \theta_3 &= 3 \cdot \lambda \end{aligned} \right\} \frac{\sin \theta_n}{n} = \frac{\lambda}{2d}$$

$$\frac{\sin \theta_1}{1} = \frac{\sin \theta_2}{2} = \frac{\sin \theta_3}{3} = \dots$$

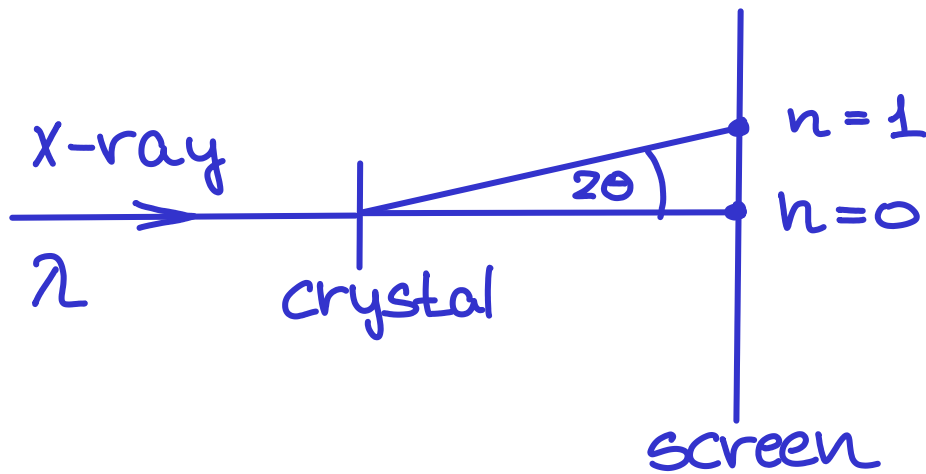
$$\sin \theta_2 = 2 \sin \theta_1 \Rightarrow \theta_2 = \arcsin(2 \sin \theta_1)$$

$$\sin \theta_3 = 3 \sin \theta_1 \Rightarrow \theta_3 = \arcsin(3 \sin \theta_1)$$

If $\theta_1 = 17.3^\circ$, then $\theta_2 = 36.5^\circ$

and $\theta_3 = 63.1^\circ$

Lattice constant of a crystal



X-ray wavelength: $\lambda = 0.890 \text{ nm}$
and $\theta = 17.8^\circ$

Bragg's law:

$$2d \cdot \sin \theta = n\lambda \quad n = 1, 2, 3, \dots$$

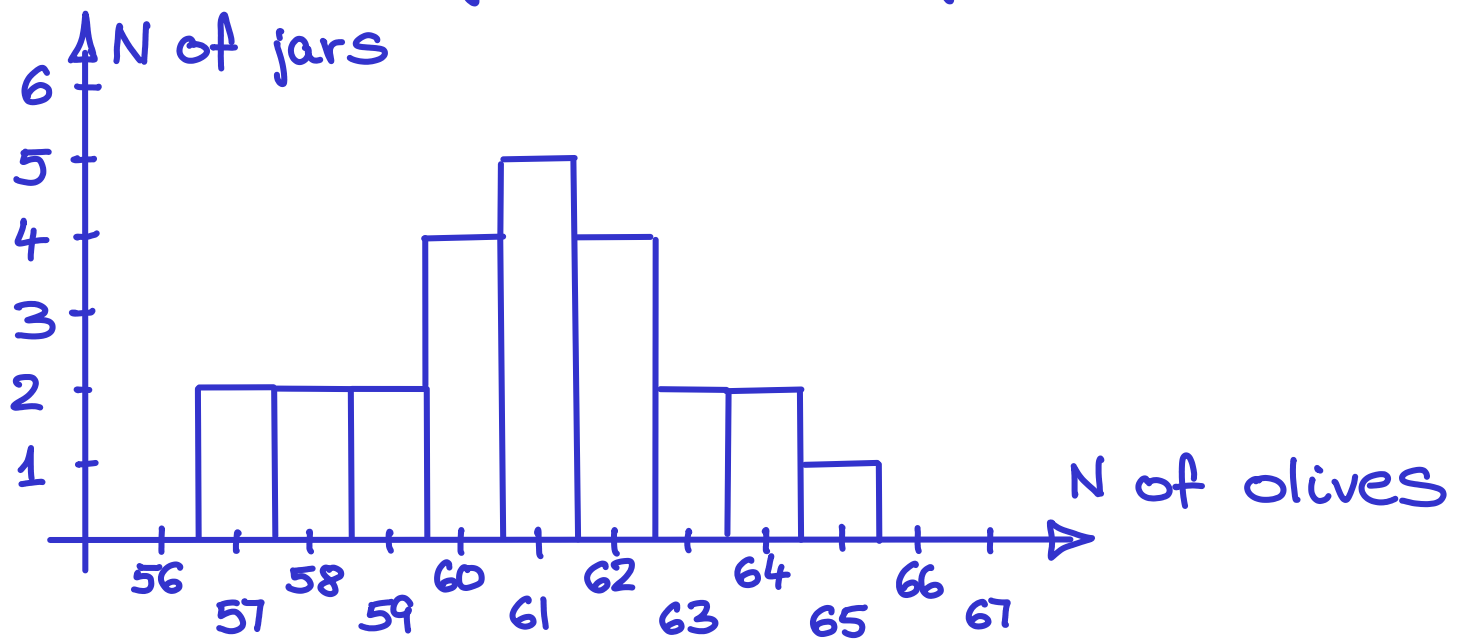
$$d = \frac{n\lambda}{2 \cdot \sin \theta}$$

$$d = \frac{1 \cdot 0.890 \text{ nm}}{2 \cdot \sin 17.8^\circ} = 1.46 \text{ nm}$$

For simple cubic lattice (SC):

$d = d_1 = D$ where D is the lattice constant. This $D = 1.46 \text{ nm}$ is larger than the lattice constant of simple metals (Ni: $0.215 \text{ nm} = 2.15 \text{ \AA}$). This is probably a molecular crystal.

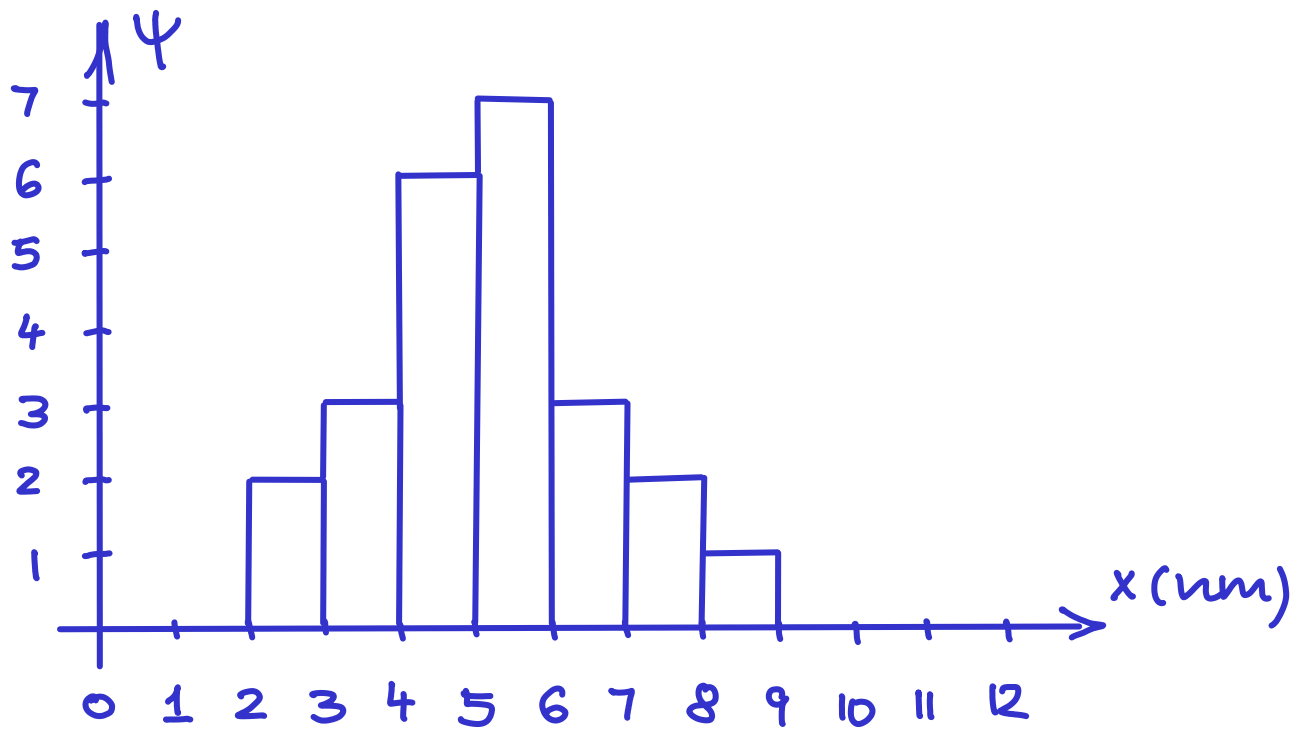
Quality control engineer



Sample size: $2+2+2+4+5+4+2+2+1=24$

$$P(N_{\text{olives}} < 59) = \frac{2+2}{24} = \frac{1}{6} = 0.167 (=16.7\%)$$

Wave function in one dim. (a)



$$\psi: 2, 3, 6, 7, 3, 2, 1$$

$$S: 4, 9, 36, 49, 9, 4, 1 \quad (S = \psi^* \psi = |\psi|^2)$$

$$\text{Total: } \Sigma = 112$$

$$P(4 \leq x \leq 8) = (36 + 49 + 9 + 4) / 112 = 98 / 112 = 0.875$$

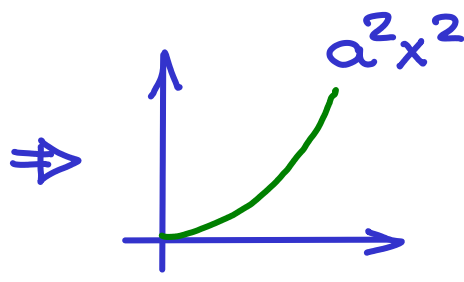
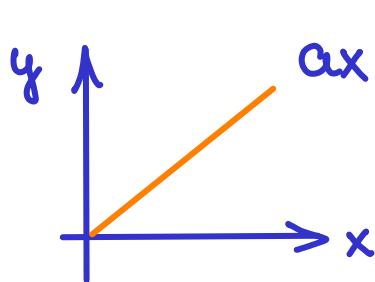
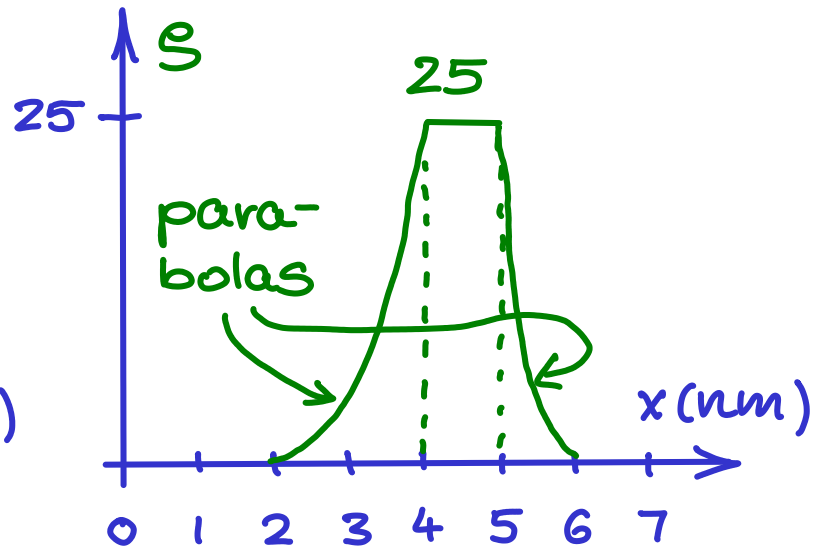
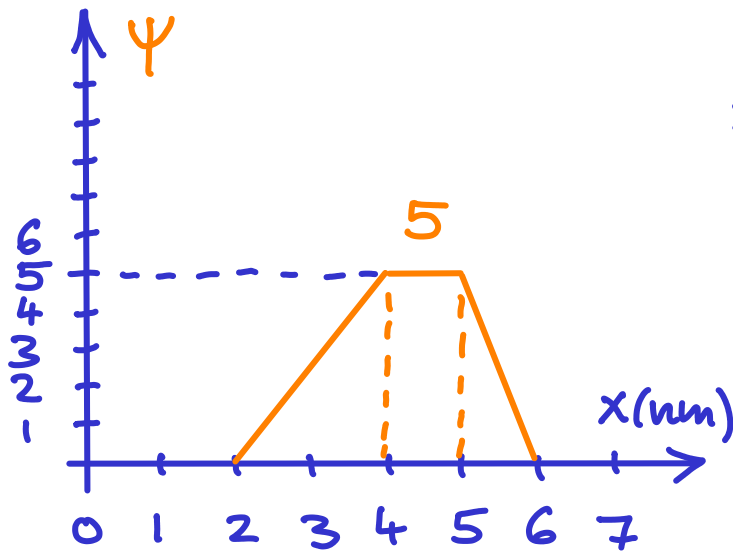
$$(\text{Normalization constant: } A = \frac{1}{\sqrt{112}})$$

Unit of the wavefunction in 1D:

$$1 = \int S(x) dx = \int |\psi|^2 dx$$

$$[S] = \frac{1}{m} \quad [\psi] = \frac{1}{\sqrt{m}}$$

Wave function in one dim. (b)



$$\int a^2 x^2 dx = a^2 \cdot \frac{x^3}{3}$$

Normalization: $1 = \int S(x) dx$

$$\Sigma_1 = \left(\frac{5}{2}\right)^2 \cdot \frac{2^3}{3} = \frac{50}{3} \approx 16.7$$

$$\Sigma_2 = 25 \cdot 1 = 25$$

$$\Sigma_3 = 5^2 \cdot \frac{1^3}{3} = \frac{25}{3} \approx 8.33$$

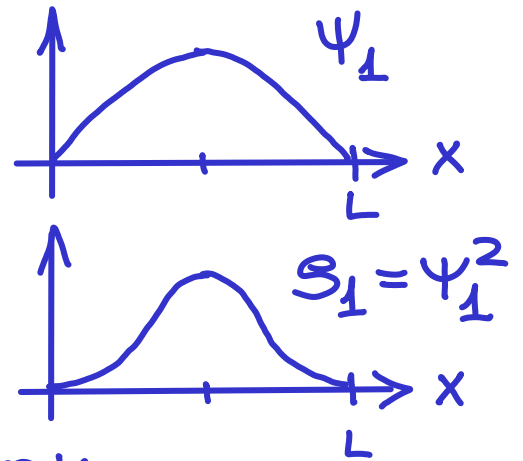
Total area:
 $\Sigma' = 50$

Normalization constant: $A = \frac{1}{\sqrt{50}}$

$$P(2 \leq x \leq 4) = \frac{\Sigma_1}{\Sigma'} = \frac{50/3}{50} = \frac{1}{3} = 0.333$$

Probabilities in an infinite square well

$$\psi_1 = \sqrt{\frac{2}{L}} \cdot \sin\left(\frac{\pi x}{L}\right)$$
$$\left(\psi_n = \sqrt{\frac{2}{L}} \cdot \sin\left(\frac{n\pi x}{L}\right) \right)$$



$$P(\text{left half}) = 0.5 = 50\%$$
$$P(\text{right half}) = 0.5 = 50\%$$

$$P(\text{1st third}) \neq 1/3$$
$$P(\text{2nd third}) \neq 1/3$$
$$P(\text{3rd third}) \neq 1/3$$

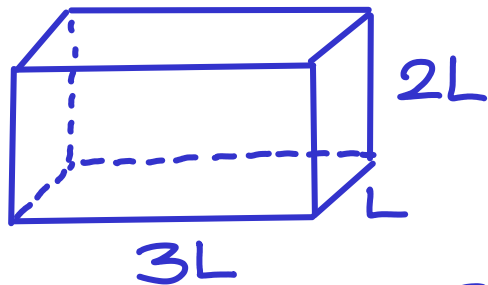
$$\text{Trig: } \sin^2(\alpha) = \frac{1 - \cos(2\alpha)}{2}$$

$$P(\text{1st third}) = \int_0^{L/3} S_1 dx = \frac{2}{L} \int_0^{L/3} \sin^2\left(\frac{\pi x}{L}\right) dx$$
$$= \frac{2}{L} \int_0^{\pi/3} \sin^2(x) dx = \frac{2}{L} \int_0^{\pi/3} \frac{1 - \cos(2x)}{2} dx =$$
$$= \frac{2}{L} \left[\frac{1}{2} x - \frac{1}{4} \sin(2x) \right] \Big|_0^{\pi/3} =$$
$$= \frac{2}{L} \left(\frac{\pi}{6} - \frac{1}{4} \cdot \frac{\sqrt{3}}{2} \right) = \underbrace{\frac{1}{3}}_{33.33\%} - \underbrace{\frac{\sqrt{3}}{4\pi}}_{13.78\%} = 0.1955$$

$$P(\text{3rd third}) = P(\text{1st third})$$

$$P(\text{2nd third}) = 1 - 2 \cdot P(\text{1st}) = 1 - 2 \cdot P(\text{3rd})$$

Box with sides $L, 2L, 3L$



$$E_{n_1, n_2, n_3} = \frac{h^2}{8m} \left(\frac{n_1^2}{L^2} + \frac{n_2^2}{(2L)^2} + \frac{n_3^2}{(3L)^2} \right)$$
$$= \frac{h^2}{8mL^2} \left(n_1^2 + \frac{n_2^2}{4} + \frac{n_3^2}{9} \right)$$

n_1	n_2	n_3		
1	1	1	gs	$1 + \frac{1}{4} + \frac{1}{9} = \frac{49}{36}$ #1
1	1	2		$1 + \frac{1}{4} + \frac{4}{9} = \frac{61}{36}$ #2
1	2	1		$1 + \frac{4}{4} + \frac{1}{9} = \frac{76}{36}$ #3
2	1	1		$4 + \frac{1}{4} + \frac{1}{9} = \frac{157}{36}$
1	1	3		$1 + \frac{1}{4} + \frac{9}{9} = \frac{81}{36}$ #4
1	3	1		$1 + \frac{9}{4} + \frac{1}{9} = \frac{121}{36}$
3	1	1		$9 + \frac{1}{4} + \frac{1}{9} = \frac{337}{36}$

Box with sides $L, 2L, 3L$ (cont'd)

$$1 \quad 2 \quad 2 \quad 1 + \frac{4}{4} + \frac{4}{9} = \frac{88}{36} \quad \#5$$

$$2 \quad 1 \quad 2 \quad 4 + \frac{1}{4} + \frac{4}{9} = \frac{169}{36}$$

$$2 \quad 2 \quad 1 \quad 4 + \frac{4}{4} + \frac{1}{9} = \frac{184}{36}$$

$$2 \quad 2 \quad 2 \quad 4 + \frac{4}{4} + \frac{4}{9} = \frac{196}{36}$$

Hydrogen molecule



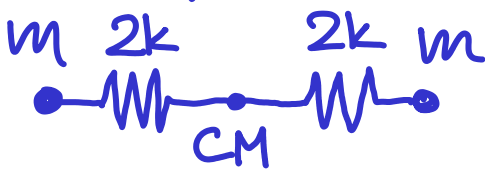
$$k = 1100 \text{ N/m}$$

$$m_p = 1.6726 \cdot 10^{-27} \text{ kg} : \text{proton}$$

$$(m_e = 0.0009 \cdot 10^{-27} \text{ kg} : \text{electron})$$



$$\omega = \sqrt{\frac{k}{m}}$$



$$\omega = \sqrt{\frac{2k}{m}}$$

Reduced mass:

$$\frac{1}{\mu} = \frac{1}{m} + \frac{1}{m} = \frac{2}{m} \Rightarrow \mu = \frac{m}{2}$$

$$\omega = \sqrt{\frac{k}{\mu}} = \sqrt{\frac{k}{\frac{m}{2}}} = \sqrt{\frac{2k}{m}}$$

$$E_n = (n + \frac{1}{2}) \hbar \omega ; E_0 = \frac{1}{2} \hbar \omega = \frac{1}{2} \hbar \sqrt{\frac{2k}{m}}$$

$$\Delta E = \hbar \omega = \hbar \sqrt{\frac{2k}{m}}$$

$$\lambda = \frac{c}{f} = \frac{c}{\frac{\Delta E}{h}} = \frac{hc}{\Delta E} = \frac{hc}{\hbar \sqrt{\frac{2k}{m}}} = 2\pi c \sqrt{\frac{m}{2k}}$$

$$\left(T = \frac{\lambda}{c} = 2\pi \sqrt{\frac{m}{2k}} = 2\pi \sqrt{\frac{\mu}{k}} \right)$$

Electron energies in 1D and 3D wells

Electron: $m_e = 511 \text{ keV}/c^2$

Width of the well: $L = 7.0 \text{ \AA} = 0.7 \text{ nm}$

$$\boxed{1D}: E_n = n^2 \frac{h^2}{8mL^2} = n^2 \frac{(hc)^2}{8m_e c^2 L^2} = n^2 E_1$$

$$E_1 = \frac{(1240 \text{ eV nm})^2}{8 \cdot 511,000 \cdot (0.7 \text{ nm})^2} = 0.767 \text{ eV}$$

$$E_{gs} = E_1 = 0.767 \text{ eV}$$

$$E_2 = 2^2 \cdot E_1 = 3.07 \text{ eV}$$

$$E_3 = 3^2 \cdot E_1 = 6.91 \text{ eV}$$

$$\boxed{3D}: E_{n_1, n_2, n_3} = \frac{h^2}{8m} \left(\frac{n_1^2}{L_1^2} + \frac{n_2^2}{L_2^2} + \frac{n_3^2}{L_3^2} \right)$$

$$\text{Cubic box: } E_{n_1, n_2, n_3} = \frac{h^2}{8mL^2} (n_1^2 + n_2^2 + n_3^2)$$

$$E_{gs, 3D} = 3 \cdot E_{gs, 1D} = 3 \cdot 0.767 \text{ eV} = 2.30 \text{ eV}$$

$$E_{1st, 3D} = 2 \cdot E_{gs, 3D} = 4.60 \text{ eV}$$

$$\begin{array}{r} \text{gs: } 111 : 3 \\ \hline 211 \} 6 \\ 121 \\ 112 \end{array}$$

$$\begin{array}{r} 221 \} 9 \\ 212 \\ 122 \\ \hline 311 \} 11 \\ 131 \\ 311 \end{array}$$

$$\begin{array}{r} 222 \} 14 \\ 312 \\ \hline 123 \} 14 \\ 132 \\ 213 \\ 231 \\ 312 \\ 321 \end{array}$$