PartInBoxPrep & Lambert-Beers

Sine, Cosine & the Exponential

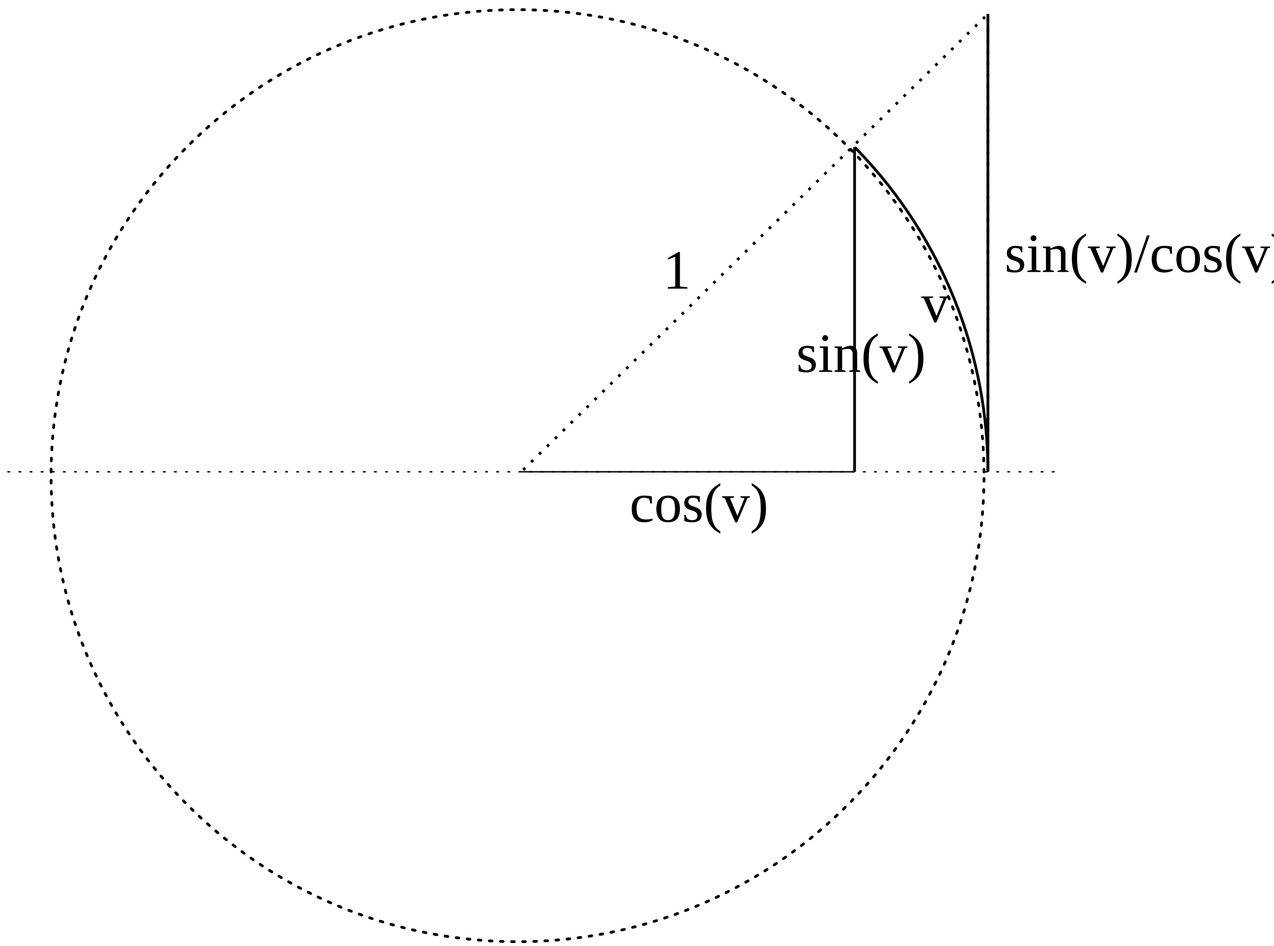
prep for understanding the partInBox model & Lambert-Beers law

startup

Learn why

- $-1 \le \sin(v) \le 1$, $-1 \le \cos(v) \le 1$ for all v
- $\cos(v) = \cos(-v)$ and $\sin(v) = -\sin(-v)$ for all v
- $\cos(v)^2 + \sin(v)^2 = 1$ for all v
- $\sin(v) \approx v$ for “small” v
- more precisely, $\cos(v) \le \frac{\sin(v)}{v} \le 1$ for all v,
- where $\cos(v) \approx 1$ for “small” v
- more precisely, $1 - \frac{1}{2}v^2 \le \cos(v) \le 1$.

why?



why?

Can you now see why $\sin(v) \leq v$ and why $v \leq \frac{\sin(v)}{\cos(v)}$, and why this implies that

$$\cos(v) \leq \frac{\sin(v)}{v} \leq 1,$$

for all v.

why?

Further, from the formula

$$\cos(\beta - \alpha) = \cos(\beta)\cos(\alpha) + \sin(\beta)\sin(\alpha)$$

from AMB&S ch 7, with $\beta = h/2$ and $\alpha = -h/2$, we have

$$\cos(h) = \cos(\frac{h}{2})^2 - \sin(\frac{h}{2})^2 = 1 - 2\sin(\frac{h}{2})^2,$$

so that indeed

$$\cos(h) \geq 1 - \frac{1}{2}h^2.$$

derivatives

Recalling

$$\cos(\beta - \alpha) = \cos(\beta)\cos(\alpha) + \sin(\beta)\sin(\alpha)$$

now with $\beta = x$ and $\alpha = -h$ we find

$$\cos(x+h) = \cos(x)\underbrace{\cos(-h)}_{=\cos(h)} + \sin(x)\underbrace{\sin(-h)}_{=-\sin(h)},$$

that is

$$\cos(x+h) = \cos(x) + (-\sin(x))\,h + E,$$

where

$$E = \cos(x)\,(\cos(h) - 1) + \sin(x)\,(h - \sin(h)).$$

derivatives

We note that E is of size $\approx h^2$ for h small. This is because

$$0 \leq 1 - \cos(h) \leq \frac{1}{2}h^2,$$

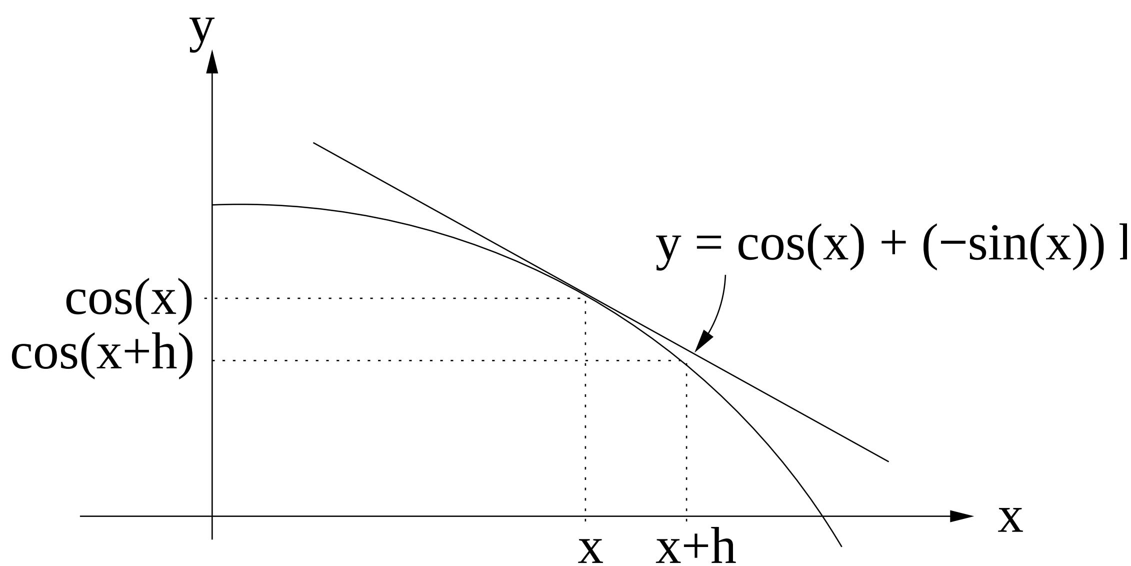
$$h - \sin(h) = h(1 - \frac{\sin(h)}{h})$$

and

$$0 \leq 1 - \frac{\sin(h)}{h} \leq 1 - \cos(h).$$

Thus ..

generalizations



We conclude that

$$D\cos(x) = -\sin(x)$$

generalizations

Similarly

$$\sin(\beta - \alpha) = \cos(\beta)\sin(\alpha) - \sin(\beta)\cos(\alpha),$$

leads to

$$D\sin(x) = \cos(x).$$

Replacing x and $x + h$ by kx and $k(x + h)$, respectively, we find that

$$D\cos(kx) = -k\sin(kx)$$

and

$$D\sin(kx) = k\cos(kx)$$

for any constant k.

In particular

In particular, we note that

$$D^2 \cos(kx) = D(\underbrace{D\cos(kx)}_{-k\sin(kx)}) = -k\,\underbrace{D\sin(kx)}_{k\cos(kx)} = -k^2\cos(kx),$$

and

$$D^2 \sin(kx) = D(k\cos(kx)) = k\,\underbrace{D\cos(kx)}_{-k\sin(kx)} = -k^2\sin(kx),$$

that is, both $\cos(kx)$ and $\sin(kx)$ have the property that their second derivative is $-k^2$ as large as the function itself, that is, they solve the equation

$$-D^2\psi = k^2\psi$$

Schrödinger

E. Schrödinger claimed that the likelihood of finding a particle in a (one-dimensional) box of length L, say in the interval $[0, L]$ along an x-axis, is given by $|c\psi|^2$, where c is a normalization constant and ψ is a solution of

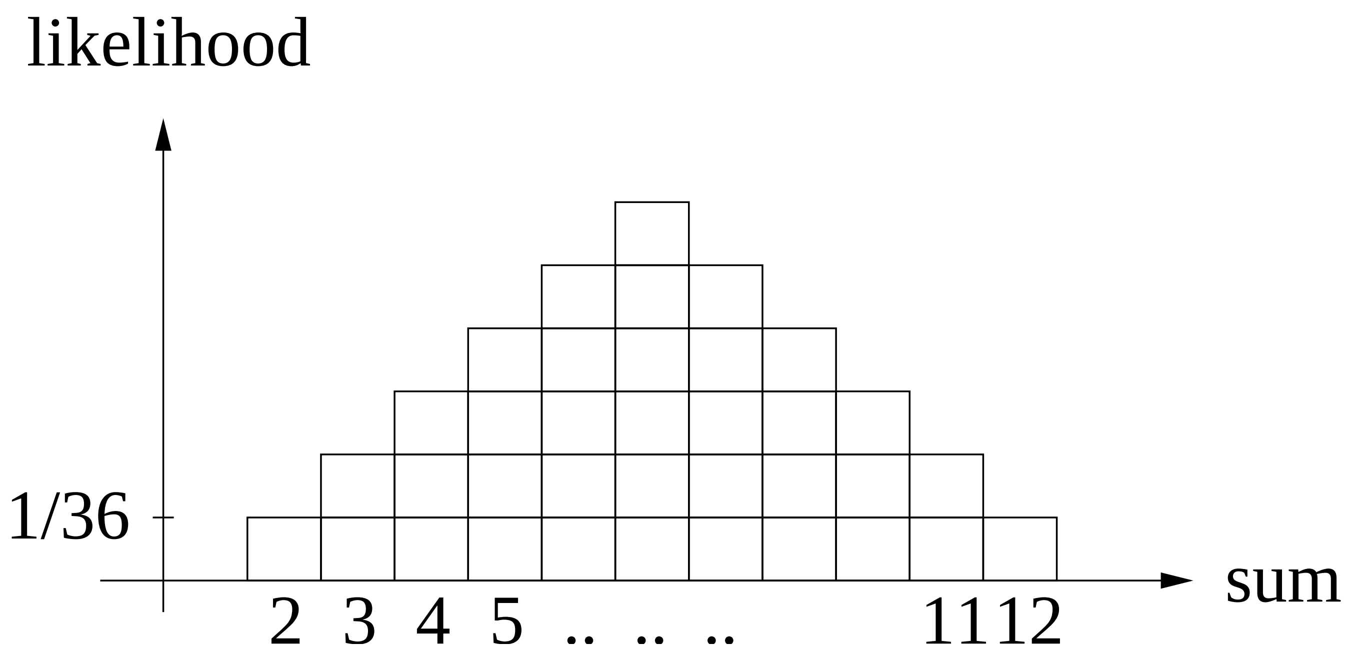
$$-D^2\psi = \lambda\psi$$

where λ is related to the energy of the particle, and ψ satisfies $\psi(0) = 0$ and $\psi(L) = 0$, corresponding to the likelihood of finding the particle right at the walls of the box is zero.

Above we have found that $\cos(kx)$ and $\sin(kx)$ possibly can fit into this equation and boundary conditions. For what values of λ can you find such a solution?

Normalization

For $|c\psi|^2$ to be a likelihood distribution the constant c must be chosen such that the integral $\int_0^L |c\psi(x)|^2 dx$, representing the total likelihood of the particle being found somewhere, equals one. Compare the likelihood for getting the sum 2, 3, .. or 12 out of throwing two dice as follows:

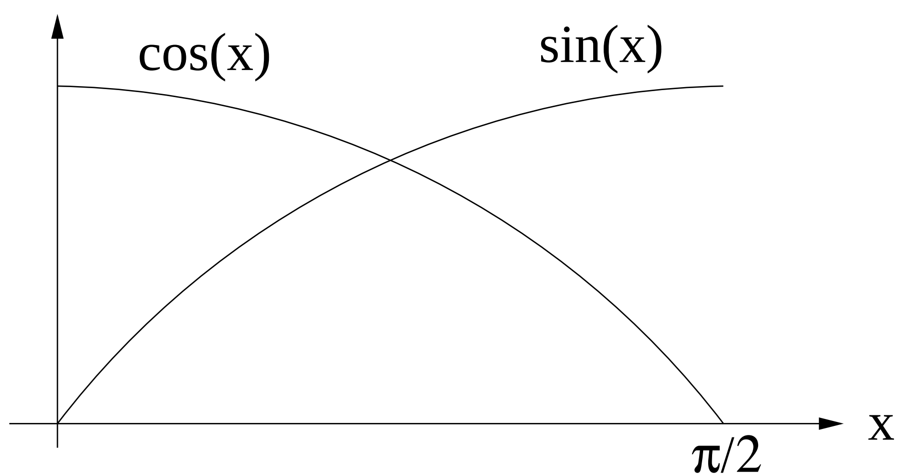


Normalization

We note that for $\psi(x) = \sin(kx)$ we would want to have

$$1 = \int_0^L |c\psi|^2 = c^2 \int_0^L \sin^2(kx)dx$$

To compute $\int \sin^2(kx)dx$ we can use a counterpart for $\sin(kx)$ of the observation that by symmetri $\int_0^{\pi/2} \sin^2 = \int_0^{\pi/2} \cos^2$, see



Normalization

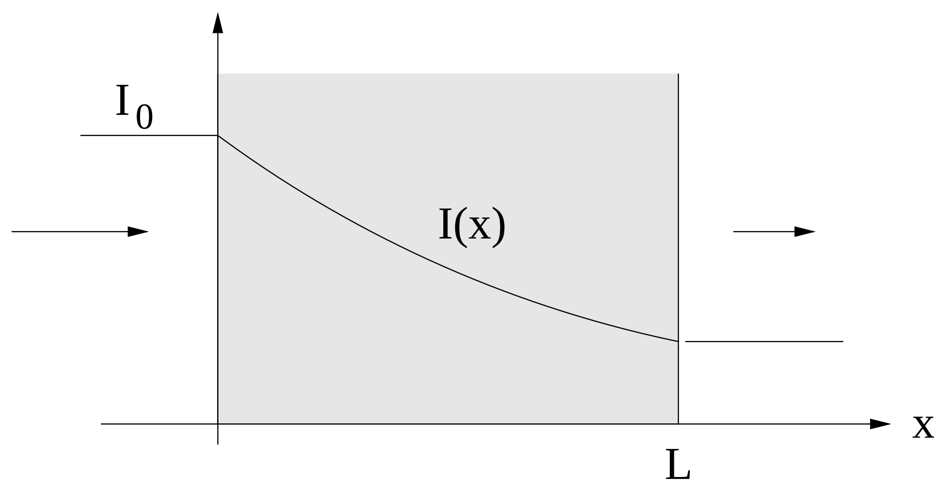
by which

$$\int_0^{\pi/2} \sin^2 = \frac{1}{2}\int_0^{\pi/2} \underbrace{\sin^2 + \cos^2}_{=1} = \pi/4.$$

The conclusion is that the integral of $\sin(kx)$ over an interval over which $\sin(kx)$ changes from zero to one equals the length of the interval divided by two.

Lambert-Beers law

Consider light of intensity $I = I(x)$ passing through a liquid where it is partially absorbed depending on the concentration c of the absorbing substance in the liquid, with the intensity varying as in the figure:



Lambert-Beers law

But exactly how does the intensity $I(x)$ decay in the liquid?

It is reasonable to believe (why?) that the decay dI over an interval of length dx in the liquid is given by $dI = -\,\epsilon\, c\, I\, dx$, where ϵ is a proportionality constant characteristic of the absorbing substance (and type of light). This leads to the differential equation

$$\frac{dI}{dx} = -\,\epsilon\, c\, I,$$

for $I = I(x)$ with the side condition $I(0) = I_0$. We recall that the solution of this type of equation is the exponential

$$I(x) = I_0\, \exp(-\,\epsilon\, c\, x) = e^{-\,\epsilon\, c\, x}$$

where $e \approx 2.71$.

Lambert-Beers law

One question that can be asked about a relation of the form

$$I(x) = I_0 \, \exp(-\,\epsilon c\, x) = I_0 \, e^{-\,\epsilon c\, x}$$

involving exponential decay is for which x the intensity has decreased to half of the original intensity I_0. The answer, of course, is given by $e^{-k\,x} = \frac{1}{2}$, where $k = \epsilon c$, with solution $x = \text{log}(1/2)/(-k) = \text{log}(2)/k$.

Lambert-Beers law

The properties of the exponential follow from the fact that

$$I(x + dx) = I(x) - \epsilon\, c\, I(x)\, dx = I(x)\, (1 - \epsilon\, c\, dx)$$

Adding up all these infinitesimal changes in I we arrive at

$$I(x) = I_0(1 - \epsilon\, c\, dx)^{x/dx},$$

corresponding to the original intensity I_0 multiplied by a (very!) large number of factors “somewhat” smaller than one. Exactly what this means will be considered in more detail later in the math course!

Lambert-Beers law

We also recall that we may rewrite $I(x) = I_0\, e^{-\epsilon\, c\, x}$ as

$$I_0/I(x) = e^{\epsilon\, c\, x},$$

which after taking logarithms takes the form

$$\log(I_0/I(x)) = \epsilon\, c\, x,$$

which by a logarithm rule may also be written as

$$\log(I_0) - \log(I(x)) = \epsilon\, c\, x.$$

Lambert-Beers law

By measuring I_0 and $I(L)$, corresponding to the intensity of the light leaving the liquid, and knowing c, we can calculate ϵ.