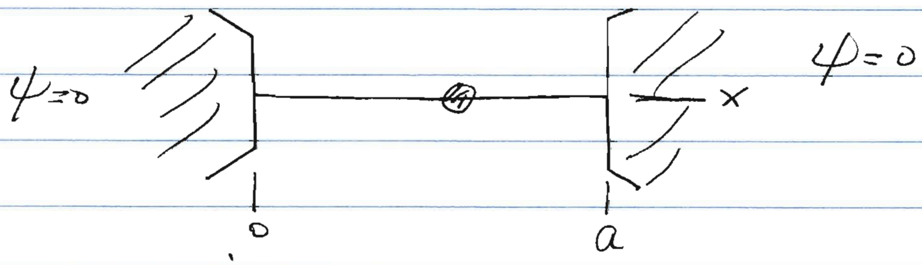
Particle on a line



Consider a particle of mass M confined to move on a line between $x=0$ & $x=a$. In the region $0 \le x \le a$ the potential energy is zero so the Schrödinger equation is

$$-\frac{\hbar^2}{2M}\frac{d^2}{dx^2}\psi = E\psi$$

or

$$\frac{d^2\psi}{dx^2} = -\left(\frac{2ME}{\hbar^2}\right)\psi = -\omega^2\psi$$

The general solution is

$$\psi(x) = A\cos\omega x + B\sin\omega x$$

Since the wavefunction is zero for $x<0$ & $x>a$ we will require that its zero at $x=0$ & $x=a$.

$$\psi(0) = A = 0$$

So $\quad \psi(x) = B \sin \omega x$

& then $\quad \psi(a) = 0 = B \sin \omega a$

$\Rightarrow \quad \omega a = N\pi \quad ; \quad N = 1, 2, \ldots$

So the wavefunction is

$$\psi(x) = B \sin\left(\frac{N\pi x}{a}\right)$$

Fix B by normalization

$$\int_0^a \psi^2(x)\,dx = 1 = B^2 \int_0^a \sin^2\left(\frac{N\pi x}{a}\right) dx$$

Let $z = \frac{N\pi x}{a}$

$$\int_0^a \sin^2\left(\frac{N\pi x}{a}\right) dx = \frac{a}{N\pi} \int_0^{N\pi} \sin^2 z \, dz$$

$$= \frac{a}{N\pi}\left(\frac{z}{2} - \frac{\sin 2z}{4}\right)\Bigg|_0^{N\pi} = \frac{a}{2}$$

So $\quad B = \sqrt{\frac{2}{a}} \quad$ &

$$\psi_N(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{N\pi x}{a}\right)$$

The energy is given by

$$E = \frac{\hbar^2 \omega^2}{2M} = \frac{\hbar^2}{2m}\left(\frac{N\pi}{a}\right)^2,$$

for an electron in a box of a (Å), the energy in eV is

$$E_N(eV) = \frac{37.61}{a^2(\text{Å})} N^2 \, (eV)$$