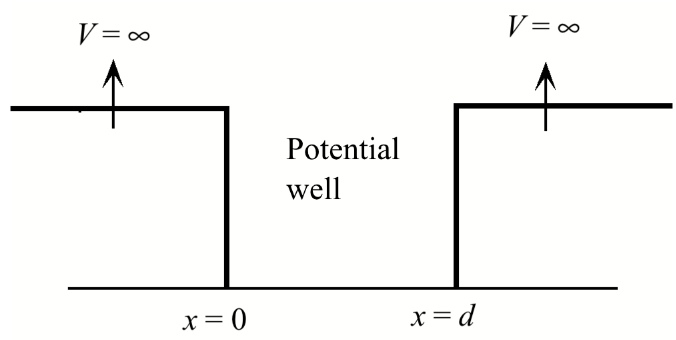
The Electron in a Box

The problem of an electron in an infinite potential well is a classic example of a bound particle. This situation is depicted in the figure below



Here, the potential field is constant (zero) potential for $0 < x < d$, but infinite for $x > d$ and $x < d$. Since no particle can have infinite energy, the electron is confined to the range $0 \le x \le d$.

To see what affect this has on the electron's possible energy states, we note that the electron wave function Ψ must satisfy Schrodinger's equation in the range $0 \le x \le d$, where the potential field $V(x)$ is zero in this range:

$$\frac{-\hbar^2}{2m}\frac{1}{\Psi}\frac{\partial^2 \Psi}{\partial x^2} = E$$

which has a general solution of:

$$\Psi(x) = A\sin(kx) + B\cos(kx)$$

where

$$k = \frac{1}{\hbar}\sqrt{2mE}$$

and A and B are yet to be determined constants. We can find these constants and the allowed values of k (and therefore E) by noting the following conditions:

a)The electron cannot exist outside the range $0 \le x \le d$, $|\Psi|^2 = 0$ for all $x > d$ and $x < d$. Since Ψ must be a continuous function, we must have $\Psi(0) = \Psi(d) = 0$

b)The probability of finding the electron somewhere within the potential well is unity, so we must have: $\int_0^d |\Psi(x)|^2 dx = 1$

Requiring the first condition, we find:

$$\Psi(0) = A\sin(0) + B\cos(0) = 0$$

and

$$\Psi(d) = A\sin(kd) + B\cos(kd) = 0$$

The first equation requires: B=0. The second requires

$$\sin(kd) = 0$$

which means that the product kd must be restricted to values:

$kd = n\pi$, n=0,1, 2 ….

Since $k = \frac{1}{\hbar}\sqrt{2mE}$, this means that E can only have values

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2md^2}$$

Finally, since the probability of finding the electron within the potential well is unity, we must have

$$\int_0^d \left|\Psi(x)\right|^2 dx = \int_0^d A^2 \sin^2\left(\frac{n\pi}{d}x\right)dx = 1$$

Which yields $A = \sqrt{\frac{2}{d}}$ and a wave function

$$\Psi(x) = \sqrt{\frac{2}{d}}\sin\left(\frac{n\pi}{d}x\right)$$

This wave function represents a standing wave, consisting of a series of peaks and nulls, corresponding to positions where the particle is most likely to be found, and least likely.