The Infinite Well

Today we are learning a little more complicated system that solves:

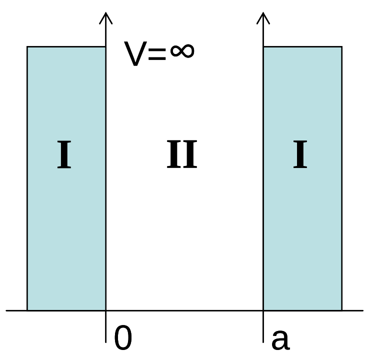
$$\hat{\mathbf{H}}\psi(\vec{r}) = E\psi(\vec{r})$$

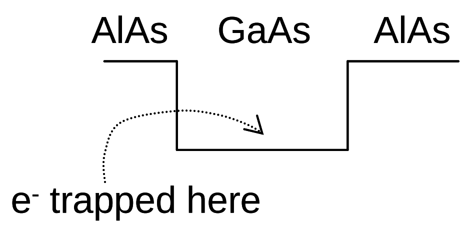
Here, the Hamiltonian includes a potential:

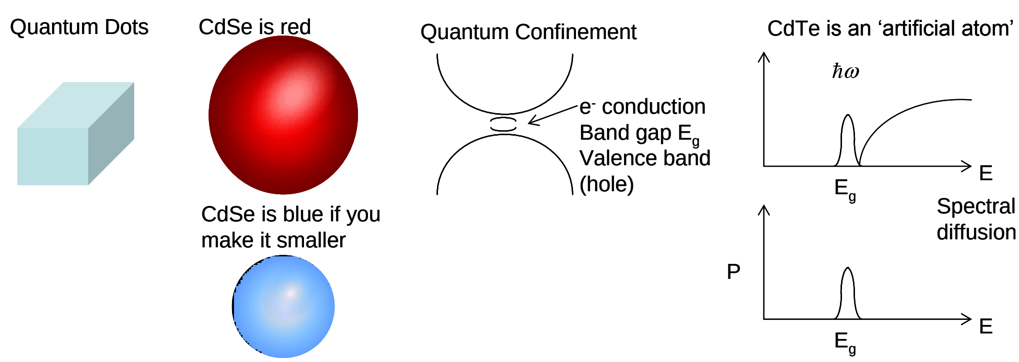
$V=\infty \qquad x \geq a,\ x \leq 0$

$V = 0 \qquad 0 < x < a$

This system is very simple, but also very useful for solid state as a model of a quantum well. An example is GaAs and AℓAs two materials with a band gap that traps an electron.







back to the infinite well problem…Solving for energy levels:

$$\hat{\mathbf{H}}_{\mathrm{I}} = \infty$$

$$\hat{\mathbf{H}}_{\mathrm{II}} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}$$

$$\hat{\mathbf{H}}_{\mathrm{I}}\psi_{\mathrm{I}}(x) = E\psi_{\mathrm{I}}(x)$$

$\psi_{\mathrm{I}}(x) = 0$ same as classical

$$\hat{\mathbf{H}}_{\mathrm{II}}\psi_{\mathrm{II}}(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi_{\mathrm{II}}(x) = E\psi_{\mathrm{II}}(x)$$

$$\frac{\partial^2}{\partial x^2}\psi_{\mathrm{II,n}}(x) + k_n^2\psi_{\mathrm{II,n}}(x) = 0$$

$$k_n^2 = \frac{2mE_n}{\hbar^2}$$

Two ways to express the result:

$$\psi_{\mathrm{II,n}}(x) = Ae^{-k_n x} + Be^{+k_n x}$$

$$\psi_{\mathrm{II,n}}(x) = A\sin k_n x + B\cos k_n x$$

Boundary conditions:

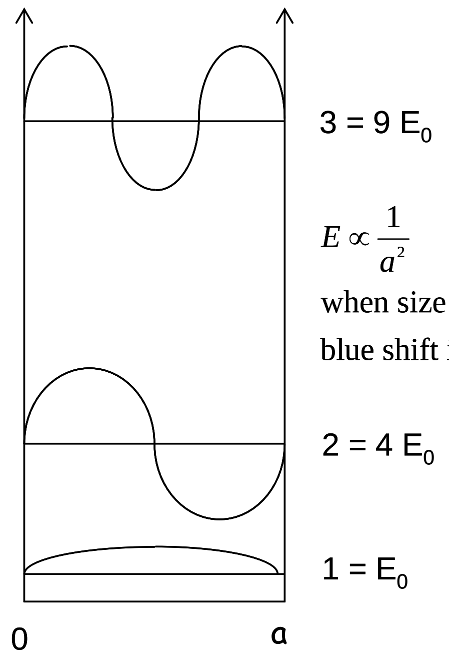
$$\psi_{\mathrm{II,n}}(0) = \psi_{\mathrm{II,n}}(a) = 0$$

$$\therefore B = 0$$

$$\psi_{\mathrm{II,n}}(x) = A\sin k_n x$$

$$\sin(k_n a) = 0$$

$$\therefore k_n a = n\pi \qquad \text{n=0,1,2,3,…}$$



$E \propto \frac{1}{a^2}$

when size is smaller
blue shift is larger

$|\psi|^2 =$ Probability, but n=0 gives all probability zero - so the state is not allowed.

$$\left(\frac{n\pi}{a}\right)^2 = \frac{2mE_n}{\hbar^2}$$

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

$\psi_n = A\sin\left(\frac{n\pi}{a}x\right)$ $\quad A$ is a complex coefficient

normalize

$$\int \psi_n{*}(x)\psi_n(x)dx = 1 \Rightarrow |A|^2\int_0^a \sin^2\left(\frac{n\pi}{a}x\right)dx = 1 \Rightarrow |A|^2 = \frac{2}{a}$$

$A = \sqrt{\frac{2}{a}}e^{i\alpha}$ where $e^{i\alpha}$ is a phase term - final result:

$$\psi_n(x) = \sqrt{\frac{2}{a}}e^{i\alpha}\sin\left(\frac{n\pi}{a}x\right)$$

☼ **Homework: 3.11 and 4.1**

Dirac Notation

$\varphi(x)$ $\psi(x)$

$|\varphi\rangle$ $|\psi\rangle$

$$\langle \varphi | \psi \rangle = \int_{-\infty}^{\infty} \varphi * \psi \, dx$$

$\langle \varphi |$ bra $|\psi\rangle$ ket

$\underbrace{\langle \varphi |}_{bra} \underbrace{|\psi\rangle}_{ket}$ $\underbrace{|\varphi\rangle}_{bra} \underbrace{\langle \psi |}_{ket}$

$$\langle \varphi | a\psi \rangle = a \langle \varphi | \psi \rangle$$

$$\langle a\varphi | \psi \rangle = a * \langle \varphi | \psi \rangle$$

$$\langle a\varphi + b\psi | = a * \langle \varphi | + b * \langle \psi |$$

$$| a\varphi + b\psi \rangle = a | \varphi \rangle + b | \psi \rangle$$

Hilbert Space

We have real space, 3-basis vector: $\vec{r} = r_x \hat{e}_x + r_y \hat{e}_y + r_z \hat{e}_z$. Generalize this concept to 'more large' – any kind of state can write:

$$\varphi(x) = \sum_n a_n \varphi_n(x)$$

$$\varphi_n(x) \leftarrow eigenfunction$$

$$\vec{r} = \sum_{i=1}^{3} r_i \vec{e}_i$$

$\Rightarrow$ state function (gradually use Dirac notation)

$$|\varphi(x)\rangle = \sum_{\text{n}} a_n \underbrace{|\varphi(x)\rangle}_{\text{unit vectors } \vec{e}_i \cdot \vec{e}_i = 1}$$

$$\langle \varphi_n | \varphi_n \rangle = 1$$

$$\vec{e}_i \cdot \vec{e}_j = \delta_{ij} \qquad \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

$\langle \varphi_m | \varphi_n \rangle \overset{m \neq n}{=} 0$ a property of the eigenfunctions

$$\langle \varphi_m | \varphi_n \rangle = \delta_{nm} \qquad \delta_{nm} = \begin{cases} 1 & n = m \\ 0 & n \neq m \end{cases}$$

$$\varphi_n = \sqrt{\frac{2}{a}} \sin\left(\frac{nx}{a}\right) \qquad \varphi_k = \frac{1}{\sqrt{2\pi}} e^{ikx}$$

$|\psi(x)\rangle = \int_{-\infty}^{\infty} f_k \varphi_k \, dk$ continuous Fourier tranform is special treatment