A particle in a 3 dimensional box

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$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Phi+V(\vec{x})\Phi=E\Phi$$

$$V(\vec{x})=\begin{cases}0 & \text{inside the box: } x\in[0,a],\quad y\in[0,b],\quad z\in[0,c]\\ \infty & \text{outside the box}\end{cases}$$

Search energies **E** for which functions $\Phi(\vec{x})$ with

$\Phi(\vec{x})=0$ at the surface of the box and inside: $-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\Phi=E\Phi$

Custumary first try: $\Phi(\vec{x})=f(x)g(y)h(z)$

$$-\frac{\hbar^2}{2m}fgh[\underbrace{\frac{1}{f}\frac{\partial^2}{\partial x^2}f(x)}_{F(x)}+\underbrace{\frac{1}{g}\frac{\partial^2}{\partial y^2}g(y)}_{G(y)}+\underbrace{\frac{1}{h}\frac{\partial^2}{\partial z^2}h(z)}_{H(z)}]=E\,fgh$$

$F(x)+G(y)+H(z)=-\frac{2m}{\hbar^2}E=const. \quad\rightarrow\quad F(x),G(y),H(z)$ **are constant.**

$$F(x)=-k_x^2,\quad G(y)=-k_y^2,\quad H(z)=-k_z^2,\quad k_x^2+k_y^2+k_z^2=\frac{2m}{\hbar^2}E$$

$$\frac{\partial^2}{\partial x^2}f(x)=-k_x^2 f(x),\quad f(0)=f(a)=0$$

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Products of one dimensional wave functions

$$\frac{\partial^2}{\partial x^2} f(x) = -k_x^2 f(x), \quad f(0) = f(a) = 0$$ **A one dimensional wave function**

$$\rightarrow f(x) \propto \sin(k_x x) \text{ and } k_x = n_x \frac{\pi}{a} \text{ for integers } n_x$$

$$\rightarrow g(y) \propto \sin(k_y y) \text{ and } k_y = n_y \frac{\pi}{b} \text{ for integers } n_y$$

$$\rightarrow h(z) \propto \sin(k_z z) \text{ and } k_z = n_z \frac{\pi}{c} \text{ for integers } n_z$$

$$E = \frac{\hbar^2 \pi^2}{2m} \left(\frac{n_x^2}{a^2} + \frac{n_y^2}{b^2} + \frac{n_z^2}{c^2} \right)$$

$$\Phi(\vec{x}) \propto \sin(k_x x) \sin(k_y y) \sin(k_z z)$$

If Φ_1 and Φ_2 are solutions of for the same energy **E**,

then also $\Phi = \Phi_1 + \Phi_2$ is a solution.

Any linear combination of states for the energy E is also a state for the energy E.

Degeneracy: There two or more stationary wave functions which do not only differ by a phase factor.

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Normalization

$$\Phi(\vec{x}) = C\sin(n_x \tfrac{\pi}{a} x)\sin(n_y \tfrac{\pi}{b} y)\sin(n_z \tfrac{\pi}{c} z)$$

What does **C** have to be to normailize the wave function, i.e. $\int_0^c\int_0^b\int_0^a |\Phi|^2 dxdydz = 1$

$$\int_0^a \sin^2(n_x \tfrac{\pi}{a} x)\, d\,x = \tfrac{a}{\pi}\int_0^\pi \sin^2(n_x \tfrac{\pi}{a} x)\, d(\tfrac{\pi}{a} x) = \tfrac{a}{\pi}\int_0^\pi \sin^2(n_x\xi)\, d\xi = \tfrac{a}{2}$$

$$\boxed{\Phi_{n_x n_y n_z}(\vec{x}) = \sqrt{\tfrac{2}{a}}\sin(n_x \tfrac{\pi}{a} x)\sqrt{\tfrac{2}{b}}\sin(n_y \tfrac{\pi}{b} y)\sqrt{\tfrac{2}{c}}\sin(n_z \tfrac{\pi}{c} z)}$$

Φ is a **product of stationary states of a one dimensional wave functions.**

These are orthogonal for different quantum numbers.

$$\int_0^a f_{n_x}^*(x)\, f_{m_x}(x)\, dx = \delta_{n_x m_x}$$

Two three dimensional wave functions Φ are therefore orthogonal when one of their three quantum numbers differ.

$$\int_0^c\int_0^b\int_0^a \Phi_{n_x n_y n_z}(\vec{x})\Phi_{m_x m_y m_z}(\vec{x})\, dxdydz = \delta_{n_x m_x}\delta_{n_y m_y}\delta_{n_z m_z}$$

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Spherically symmetric potentials and wave functions

3D Schrödinger equation: $-\frac{\hbar^2}{2m}(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2})\Phi+V(\vec{x})\Phi=E\Phi$

$$d\vec{x}\cdot\vec{\nabla}\Phi=(dr\vec{e}_r+rd\vartheta\vec{e}_\vartheta+r\sin\vartheta\, d\varphi\vec{e}_\varphi)\cdot\vec{\nabla}\Phi=dr\frac{\partial}{\partial r}\Phi+d\vartheta\frac{\partial}{\partial\vartheta}\Phi+d\varphi\frac{\partial}{\partial\varphi}\Phi$$

$$\frac{\partial}{\partial k}\vec{e}_k\perp\vec{e}_k\ ,\ \frac{\partial}{\partial\vartheta}\vec{e}_r=\vec{e}_\vartheta\ ,\ \frac{\partial}{\partial\vartheta}\vec{e}_\vartheta=-\vec{e}_r\ ,\ \frac{\partial}{\partial\varphi}\vec{e}_r=\sin\vartheta\,\vec{e}_\varphi\ ,\ \frac{\partial}{\partial\varphi}\vec{e}_\vartheta=\cos\vartheta\,\vec{e}_\varphi$$

$$\vec{\nabla}\Phi=\vec{e}_r\frac{\partial}{\partial r}\Phi+\vec{e}_\vartheta\frac{1}{r}\frac{\partial}{\partial\vartheta}\Phi+\vec{e}_\varphi\frac{1}{r\sin\vartheta}\frac{\partial}{\partial\varphi}\Phi$$

all other $\frac{\partial}{\partial k}\vec{e}_j=0$

$$\vec{\nabla}^2\Phi(r,\vartheta,\varphi)=\frac{1}{r}\frac{\partial^2}{\partial r^2}(r\Phi)+\frac{1}{r^2\sin\vartheta}\frac{\partial}{\partial\vartheta}(\sin\vartheta\frac{\partial}{\partial\vartheta}\Phi)+\frac{1}{\sin^2\vartheta\, r^2}\frac{\partial^2}{\partial\varphi^2}\Phi$$

Search for only those wave functions for a spherically symmetric potential that are spherically symmetric. The other wave functions will be found later.

$$-\frac{\hbar^2}{2m}\frac{1}{r}\frac{\partial^2}{\partial r^2}[r\Phi(r)]+V(r)\Phi(r)=E\Phi(r)$$

$$u(r)=r\Phi(r)$$

↓

$$\frac{\partial^2}{\partial r^2}u(r)=\frac{2m}{\hbar^2}[V(r)-E]u(r)$$

↔ Like a 1D Schrödinger equation

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