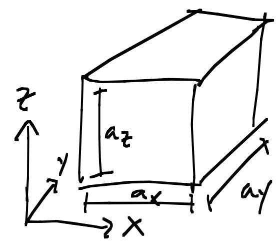
QM in higher dimensions: 3D infinite cubical well

$$V(x,y,z) = \begin{cases} 0 & \left\{ \begin{array}{l} 0<x<a_x \\ 0<y<a_y \\ 0<z<a_z \end{array} \right. \\ \infty & \text{otherwise} \end{cases}$$



Schrödinger Equation: $$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi(x,y,z) + V(x,y,z)\,\psi(x,y,z) = E\,\psi(x,y,z)$$

solution by separation of variables: $\psi(x,y,z) = \psi_x(x)\,\psi_{yz}(y,z)$

$$\frac{-\frac{\hbar^2}{2m}\left[\left(\frac{\partial^2}{\partial x^2}\psi_x\right)\psi_{yz} + \psi_x\left(\left(\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi_{yz}\right)\right]}{\psi_x\psi_{yz}} = \frac{E\,\psi_x\psi_{yz}}{\psi_x\psi_{yz}}$$

$$-\frac{\hbar^2}{2m}\frac{\frac{\partial^2}{\partial x^2}\psi_x}{\psi_x} - E = \frac{\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi_{yz}}{\psi_{yz}} = -E_{yz}$$

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$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_x = (E-E_{yz})\psi_x = E_x\psi_x}$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)\psi_{yz} = E_{yz}\psi_{yz}$$

Separation of Variables (Again!)

$$\varphi_{yz}(y,z) = \varphi_y(y)\,\varphi_z(z)$$

$$\frac{-\frac{\hbar^2}{2m}\left[\varphi_z \frac{\partial^2}{\partial y^2}\varphi_y + \varphi_y \frac{\partial^2}{\partial z^2}\varphi_z\right]}{\varphi_y\varphi_z} = \frac{E_{yz}\varphi_y\varphi_z}{\varphi_y\varphi_z}$$

$$\frac{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2}\varphi_y}{\varphi_y} - E_{yz} = \frac{\frac{\hbar^2}{2m}\frac{\partial^2}{\partial z^2}\varphi_z}{\varphi_z} = -E_z$$

2 $$\boxed{-\frac{\hbar^2}{2m}\frac{d^2}{dy^2}\varphi_y = (E_{yz}-E_z)\varphi_y = E_y\varphi_y}$$

3 $$\boxed{-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\varphi_z = E_z\varphi_z}$$

Note: $E_x + E_y + E_z = (E - E_{yz}) + (E_{yz} - E_z) + E_z = E$!

Full Solution

Solve each equation independently, then sum eigenvalues.

Apply B.C.'s

$$\varphi(0,y,z) = \varphi(a_x,y,z) = 0 \rightarrow \varphi_x(0) = \varphi(a_x) = 0$$

$$\varphi(x,0,z) = \varphi(x,a_y,z) = 0 \rightarrow \varphi_y(0) = \varphi(a_y) = 0$$

$$\varphi(x,y,0) = \varphi(x,y,a_z) = 0 \rightarrow \varphi_z(0) = \varphi(a_z) = 0$$

This yields familiar solutions $\sqrt{\frac{2}{a_x}}\sin k_x x$, $\sqrt{\frac{2}{a_y}}\sin k_y y$ and $\sqrt{\frac{2}{a_z}}\sin k_z z$ with eigenvalues:

$$E_x = \frac{\hbar^2}{2m}k_x^2 = \frac{\hbar^2\pi^2 n_x^2}{2m\,a_x^2} \qquad n_x = 1,2,3,\ldots$$

$$E_y = \frac{\hbar^2}{2m}k_y^2 = \frac{\hbar^2\pi^2 n_y^2}{2m\,a_y^2} \qquad n_y = 1,2,3\ldots$$

so $E = E_x + E_y + E_z = \frac{\hbar^2}{2m}\left(\frac{n_x^2}{a_x^2} + \frac{n_y^2}{a_y^2} + \frac{n_z^2}{a_z^2}\right)$

$$E_z = \frac{\hbar^2}{2m}k_z^2 = \frac{\hbar^2\pi^2 n_z^2}{2m\,a_z^2} \qquad n_z = 1,2,3\ldots$$

Full eigenfunction given by $\Psi(x,y,z,t) = \varphi_{n_x}(x)\,\varphi_{n_y}(y)\,\varphi_{n_z}(z)\,e^{-i\frac{E}{\hbar}t}$

Total Energies (for $a_x = a_y = a_z = a$)

n_x	n_y	n_z	$E\left(\frac{\hbar^2}{2ma^2}\right)$	degeneracy
1	1	1	3	1
1 1 2	1 2 1	2 1 1	6	3
1 2 2	2 1 2	2 2 1	9	3
3 1 1	1 3 1	1 1 3	11	3
2	2	2	12	1
1 1 2 2 3 3	2 3 1 3 1 2	3 2 3 1 2 1	14	6

These degenencies are caused by symmetry (equivalence of x, y, and z dimensions for $a_x = a_y = a_z$.

If, instead, $a_x \neq a_y \neq a_z$, the degenencies will be broken, except for "accidental" degenencies when

$$\frac{n_x^2}{a_x^2} + \frac{n_y^2}{a_y^2} + \frac{n_z^2}{a_z^2} = \frac{n_x'^2}{a_x^2} + \frac{n_y'^2}{a_y^2} + \frac{n_z'^2}{a_z^2}$$