1-D Infinite Potential Box

Recall that for the 1D box, we write the Hamiltonian this way:

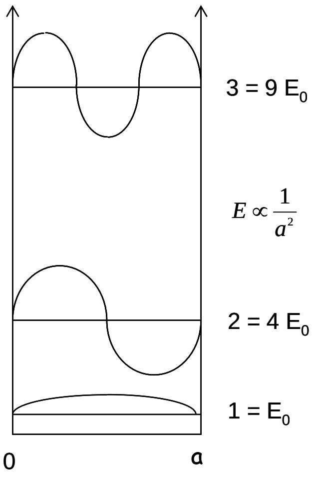
$$\hat{H}_{\mathrm{I}} = \tfrac{p_x^2}{2m} + V(x) \qquad V(x)\begin{cases} = \infty & \text{for } x \le 0 \text{ and } x \ge a \\ = 0 & \text{for } 0 < x < a \end{cases}$$

We solved the Schrödinger equation to find wavefunction and E_n:

$$\hat{H}\psi_n = E_n \psi_n$$

eigenfunction: $\psi_n\left(x\right) = \sqrt{\tfrac{2}{a}}\sin\left(\tfrac{n\pi x}{a}\right) \quad n = 1, 2, 3, \ldots$

eigenvalue: $E_n = \tfrac{\hbar^2\pi^2}{2ma^2} n^2$



2-D Infinite Potential Box

For the 2D box, we write the Hamiltonian this way (Section 8.5, page 317):

$$\hat{H}_{\mathrm{2D}} = \tfrac{p_x^2}{2m} + V(x) + \tfrac{p_y^2}{2m} + V(y) \qquad V(x)\begin{cases} = \infty & \text{for } x \le 0 \text{ and } x \ge a \\ = 0 & \text{for } 0 < x < a \end{cases}$$

$$V(y)\begin{cases} = \infty & \text{for } y \le 0 \text{ and } y \ge a \\ = 0 & \text{for } 0 < y < a \end{cases}$$

$$\hat{H}_{\mathrm{2D}} = \hat{H}_x + \hat{H}_y$$

This problem is simple because we can separate the Hamiltonian into two parts, and the parts commute with each other:

$$\left[\hat{H}_x, \hat{H}_y\right] = 0$$

The Schrödinger equation solution is a product:

$$\hat{H}\psi_{n1n2}\left(x, y\right) = E_{n1n2}\psi_{n1n2}\left(x, y\right)$$

$$\psi_{n1n2}\left(x, y\right) = \psi_{n1}\left(x\right)\psi_{n2}\left(y\right)$$

$$\hat{H}\psi_{n1}\left(x\right)\psi_{n2}\left(y\right) = E_{n1n2}\psi_{n1}\left(x\right)\psi_{n2}\left(y\right)$$

eigenfunction: $\psi_{n1n2}\left(x, y\right) = \tfrac{2}{a}\sin\left(\tfrac{n_1\pi x}{a}\right)\sin\left(\tfrac{n_2\pi y}{a}\right)$

$n_1 = 1, 2, 3, \ldots \quad n_2 = 1, 2, 3, \ldots$

eigenvalue: $E_{n1n2} = \tfrac{\hbar^2\pi^2}{2ma^2}\left(n_1^2 + n_2^2\right)$

3-D Infinite Potential Box

$$\hat{H}\psi_{n1n2n3}(x,y,z) = E_{n1n2n3}\psi_{n1n2n3}(x,y,z)$$

$$\psi_{n1n2n3}(x,y,z) = \psi_{n1}(x)\psi_{n2}(y)\psi_{n3}(z)$$

$$\hat{H}\psi_{n1}(x)\psi_{n2}(y)\psi_{n3}(z) = E_{n1n2n3}\psi_{n1}(x)\psi_{n2}(y)\psi_{n3}(z)$$

eigenfunction: $\psi_{n1n2n3}(x,y,z) = \sqrt[3]{\frac{2}{a}}\sin\left(\frac{n_1\pi x}{a}\right)\sin\left(\frac{n_2\pi y}{a}\right)\sin\left(\frac{n_3\pi z}{a}\right)$

$n_1 = 1,2,3,\ldots \quad n_2 = 1,2,3,\ldots \quad n_3 = 1,2,3,\ldots$

eigenvalue: $E_{n1n2} = \frac{\hbar^2\pi^2}{2ma^2}\left(n_1^2 + n_3^2 + n_3^2\right)$

n-D Infinite Potential Box

Use these 3 models to calculate complex systems. Harmonic oscillators – can solve it totally. Hydrogen H-H molecule – use Hamiltonian. If you want He, you have to use the Hamiltonian for Hydrogen to model. The quantum dot, box, wire and well, etc.

Degeneracy

Next let's look at degeneracy.

$$\left.\begin{array}{l} E_{n1n2} = \frac{\hbar^2\pi^2}{2ma^2}\left(n_1^2 + n_2^2\right) = E_1\left(n_1^2 + n_2^2\right) \\ E_{1,2} = E_{2,1} \\ \psi_{1,2} = \psi_{2,1} \end{array}\right\} \begin{array}{l} \text{true if and only if} \\ 0 < x < a \\ 0 < y < a \end{array}$$

3-D Harmonic Oscillator Degeneracy

$$\hat{H} = \frac{p_r^2}{2m} + \frac{k^2r^2}{2}$$

$$\hat{H} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{p_z^2}{2m} + \frac{k^2\left(x^2+y^2+z^2\right)}{2}$$

$$\hat{H} = \hat{H}_x + \hat{H}_y + \hat{H}_z$$

$$\psi_{n1n2n3} = \psi_{n1}\psi_{n2}\psi_{n3} = \left|n_1, n_2, n_3\right\rangle$$

$$E_{n1n2n3} = \hbar\omega_0\left(n_1 + n_2 + n_3 + \tfrac{3}{2}\right)$$

Degeneracy of E_{n1n2n3} S=4		
1	2	1
2	1	1
1	1	2
0	4	0
4	0	0
0	0	4
2	2	0
2	0	2
0	2	2

2-D Harmonic Oscillator Degeneracy

Qualifier – show that S has S+1 Degeneracy.

$$\hat{H} = \frac{p_r^2}{2m} + \frac{k^2 r^2}{2}$$

$$\hat{H} = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{k^2\left(x^2+y^2\right)}{2}$$

$$\hat{H} = \hat{H}_x + \hat{H}_y$$

$$\psi_{n1n2} = \psi_{n1}\psi_{n2} = \left|n_1, n_2\right\rangle$$

$$E_{n1n2} = \hbar\omega_0\left(\underbrace{n_1 + n_2}_{S} + 1\right) = \hbar\omega_0\left(S+1\right)$$

Degeneracy of E_{n1n2} S=3	
1	2
2	1
0	3
3	0

Prove that $\psi \Rightarrow \psi_1\psi_2$

$$\hat{H}\psi_{n1}\psi_{n2} = \left(\hat{H}_x + \hat{H}_y\right)\psi_{n1}\psi_{n2}$$

$$= \psi_{n2}(y)\hat{H}_x\psi_{n1}(x) + \psi_{n1}(x)\hat{H}_y\psi_{n2}(y)$$

$$= \psi_{n2}(y)E_{n1}\psi_{n1}(x) + \psi_{n1}(x)E_{n2}\psi_{n2}(y)$$

$$= \left(E_{n1} + E_{n2}\right)\psi_{n1}(x)\psi_{n2}(y)$$

2 Particles

We always talk about 1 particle, and in many dimensions. Now we talk about 2 particles. These are 2 identical, non-interacting particles.

$$\hat{H}(x_1,x_2)=\hat{H}(x_1)+\hat{H}(x_2)+\underbrace{V(x_1,x_2)}_{=0}$$

$$\left[\hat{H}(x_1),\hat{H}(x_2)\right]=0$$

$$\psi_{n1n2}=\tfrac{2}{a}\sin\left(\tfrac{n_1\pi x_1}{a}\right)\sin\left(\tfrac{n_2\pi x_2}{a}\right)$$

$$E_{n1n2}=\tfrac{\hbar^2\pi^2}{2ma^2}\left(n_1^2+n_2^2\right)\qquad n=1,2,\ldots$$

$$\psi_{n1n2}=A\psi_{n1n2}+B\psi_{n2n1}\quad\text{has same eigenenergy}$$

If ψ_{n1n2} is an eigenfunction, then ψ_{n2n1} is also an eigenfunction.

$\psi_{n1n2}=A\psi_{n1n2}+B\psi_{n2n1}$ is also an eigenfunction.

$$\left.\begin{aligned}\psi_{\substack{\text{Symmetric}\\\text{State}}}&=\frac{1}{\sqrt{2}}\left[\psi_{n1}(x_1)\psi_{n2}(x_2)+\psi_{n1}(x_2)\psi_{n2}(x_1)\right]\\ \psi_{\substack{\text{Antisymmetric}\\\text{State}}}&=\frac{1}{\sqrt{2}}\left[\psi_{n1}(x_1)\psi_{n2}(x_2)-\psi_{n1}(x_2)\psi_{n2}(x_1)\right]\end{aligned}\right\}\text{Two Special Eigenfunctions}$$

$$\psi_{\substack{\text{Symmetric}\\\text{State}}}(x_1,x_2)=\psi_{\substack{\text{Symmetric}\\\text{State}}}(x_2,x_1)\qquad\leftarrow\text{Boson}$$

$$\psi_{\substack{\text{Antisymmetric}\\\text{State}}}(x_1,x_2)=-\psi_{\substack{\text{Antisymmetric}\\\text{State}}}(x_2,x_1)\qquad\leftarrow\text{Fermion}$$

Hydrogen Atom

The molecular rotation spectrum – absorption of light scattering can be explained by a rotation spectrum. The rotation inertia becomes an operator $E=L^2/2I\to\hat{H}$. Here quantized L can explain the rotation spectrum. Be able to estimate the Hydrogen meV, μeV.

Spectral Lines
The defined separation ΔE
doesn't change

Angular Momentum

From classical mechanics:

$$\vec{L} = \vec{r} \times \vec{p}$$

We can write it in Cartesian coordinates:

$$\vec{L} = \begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ x & y & z \\ p_x & p_y & p_z \end{vmatrix}$$

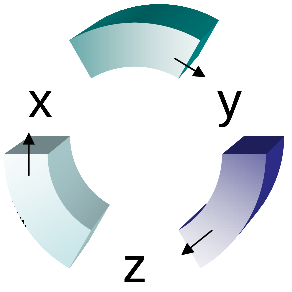
$$\boxed{\begin{aligned} \hat{L}_x &= yp_z - zp_y = -i\hbar\left(y\tfrac{\partial}{\partial z} - z\tfrac{\partial}{\partial y}\right) \\ \hat{L}_y &= zp_x - xp_z = -i\hbar\left(z\tfrac{\partial}{\partial x} - x\tfrac{\partial}{\partial z}\right) \\ \hat{L}_z &= xp_y - yp_x = -i\hbar\left(x\tfrac{\partial}{\partial y} - y\tfrac{\partial}{\partial x}\right) \end{aligned}}$$

Generally you can write:

$$\vec{p} = -i\hbar\vec{\nabla} \qquad \vec{L} = i\hbar\vec{r} \times \vec{\nabla}$$

The commutation relation is very important! Remember them by the cyclic x,y,z order.

$$\boxed{\begin{aligned} \left[\hat{L}_x, \hat{L}_y\right] &= i\hbar\hat{L}_z \\ \left[\hat{L}_y, \hat{L}_z\right] &= i\hbar\hat{L}_x \\ \left[\hat{L}_z, \hat{L}_x\right] &= i\hbar\hat{L}_y \end{aligned}}$$



We can prove this very easily. We have already proved the position and momentum commutation relations.

$$
\begin{aligned}
\left[\hat{x}, \hat{p}_x\right] &= i\hbar \\
\left[\hat{y}, \hat{p}_y\right] &= i\hbar \\
\left[\hat{z}, \hat{p}_z\right] &= i\hbar
\end{aligned}
$$

Now, we can show these angular momentum commutations in the same way we proved:

$$
\begin{aligned}
\left[\hat{L}_x, \hat{L}_y\right] &= \hat{L}_x\hat{L}_y - \hat{L}_y\hat{L}_x \\
&= \left(yp_z - zp_y\right)\left(zp_x - xp_z\right) - \left(zp_x - xp_z\right)\left(yp_z - zp_y\right) \\
&= \left(yp_z zp_x - yp_z xp_z - zp_y zp_x + zp_y xp_z\right) - \left(zp_x yp_z - zp_x zp_y - xp_z yp_z + xp_z zp_y\right) \\
&= z^2\,\cancel{\left(-p_x p_y - p_y p_x\right)} + yz\left(p_z p_x - p_x p_z\right) + xy\,\cancel{\left(p_z p_z - p_z p_z\right)} + xz\left(p_y p_z - p_z p_y\right) \\
&= yz\left(p_z p_x - p_x p_z\right) + xz\left(p_y p_z - p_z p_y\right) \\
&= xp_y\left(zp_z - p_z z\right) - yp_x\left(zp_z - p_z z\right) \\
&= i\hbar\left(xp_y - yp_x\right) \\
&= i\hbar\hat{L}_z
\end{aligned}
$$

Eigenvalues of Angular Momentum

Finding the eigenvalue of L is nearly impossible – it is very difficult. So, we look for $\hat{L}^2 = \hat{L}_x{}^2 + \hat{L}_y{}^2 + \hat{L}_z{}^2$. We want to prove this that L_z and L^2 commute with each other:

$$\left[\hat{L}_z, \hat{L}^2\right] = 0$$

This means that they have the same eigenfunction. We want to prove this:

$$\begin{aligned}
\left[\hat{L}_z, \hat{L}^2\right] &= \left[\hat{L}_z, \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2\right] \\
&= \left[\hat{L}_z, \hat{L}_x^2\right] + \left[\hat{L}_z, \hat{L}_y^2\right] + \cancelto{0}{\left[\hat{L}_z, \hat{L}_z^2\right]} \\
&= \hat{L}_z\hat{L}_x^2 - \hat{L}_x^2\hat{L}_z + \hat{L}_z\hat{L}_y^2 - \hat{L}_y^2\hat{L}_z \\
&= \hat{L}_z\hat{L}_x\hat{L}_x + \hat{L}_x\hat{L}_z\hat{L}_x - \hat{L}_x\hat{L}_x\hat{L}_z - \hat{L}_x\hat{L}_z\hat{L}_x + \hat{L}_z\hat{L}_y\hat{L}_y + \hat{L}_y\hat{L}_z\hat{L}_y - \hat{L}_y\hat{L}_y\hat{L}_z - \hat{L}_y\hat{L}_z\hat{L}_y \\
&= \hat{L}_x\left[\hat{L}_z, \hat{L}_x\right] + \left[\hat{L}_z, \hat{L}_x\right]\hat{L}_x + \hat{L}_y\left[\hat{L}_z, \hat{L}_y\right] + \left[\hat{L}_z, \hat{L}_y\right]\hat{L}_y \\
&= i\hbar L_x L_y + i\hbar L_y L_x - L_y i\hbar L_x - i\hbar L_x L_y \\
&= 0
\end{aligned}$$

This means that L_z and L^2 commute with each other which means that they have the same eigenfunctions.

To solve L_z and L^2 for the angular momentum, we solve:

$$\left.\begin{aligned} L^2\psi_{lm} &= \hbar^2 l(l+1)\psi_{lm} \\ L_z\psi_{lm} &= \hbar m\psi_{lm} \end{aligned}\right\} \quad \begin{aligned} l &= 0,1,2,... \\ m &= -l, -(l-1), -(l-2), ..., 0, ..., (l-1), l \end{aligned}$$

I hope you can remember this when you studied atomic physics. Next class we will learn the details of how to get this. Also, we have the spin momentum coupled together with the L. We got this all because of the commutation relation. We can't change the order of operators. Solve for the harmonic oscillator also become a commutator. This is the most fundamental relation: $\left[x, p_x\right] = i\hbar$. Even L is complicated.

Homework: 8.35 and 8.36 the Harmonic 2-D oscillator – on qualifier.