20190507 CH4 particle dynamics in 3D space

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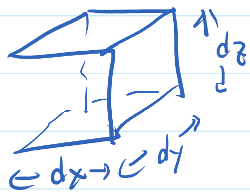
we live in a 3D space x, y, z. t time.

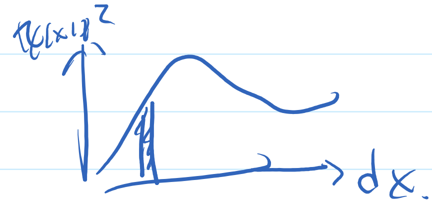
in 3-D, probability of finding a particle



$\leftarrow$ cube 立方块.

$$dP = |\psi(x,y,z)|^2 \, dx\,dy\,dz$$

recap of 1D. $dP = \underbrace{|\psi(x)|^2}_{\text{probability density}} dx$.



$\boxed{\text{specical case}}$

if $\psi(x,y,z) = \phi_1(x)\,\phi_2(y)\,\phi_3(z)$

$$dP = \underbrace{|\phi_1(x)|^2 dx}_{dP_x} \cdot \underbrace{|\phi_2(y)|^2 dy}_{dP_y} \cdot \underbrace{|\phi_3(z)|^2 dz}_{dP_z}.$$

example. 3-D harmonic oscillator. a particle in potential

$$V(x,y,z) = V_x + V_y + V_z = \frac{1}{2} m\omega^2 (x^2+y^2+z^2)$$

$$H = T_{\text{kinetic}} + V$$

$$= \frac{P_x^2}{2m} + \frac{P_y^2}{2m} + \frac{P_z^2}{2m} + V_x + V_y + V_z.$$

Schrödinger's equation $H|\psi\rangle = i\hbar\frac{\partial}{\partial t}|\psi\rangle$

$$\left[\left(\frac{P_x^2}{2m} + V_x\right) + \left(\frac{P_y^2}{2m} + V_y\right) + \left(\frac{P_z^2}{2m} + V_z\right)\right]|\psi\rangle$$

$$= i\hbar\frac{\partial}{\partial t}|\psi\rangle.$$

$\partial_t |\psi\rangle$

if $|\psi\rangle = |\psi_x\rangle |\psi_y\rangle |\psi_z\rangle$, where $|\psi_i\rangle$ is eigenstate along i-direction.

$$\left(\frac{P_i^2}{2m} + V_i\right)|\psi_i\rangle = E_i|\psi_i\rangle.$$

$$H|\psi_x\rangle|\psi_y\rangle|\psi_z\rangle = (H_x + H_y + H_z)|\ \rangle|\ \rangle|\ \rangle$$
$$= H_x|\psi_x\rangle|\psi_y\rangle|\psi_z\rangle + H_y|\ \rangle|\ \rangle|\ \rangle + H_z|\ \rangle|\ \rangle|\ \rangle$$
$$= E_x|\ \rangle|\ \rangle|\ \rangle + E_y|\ \rangle|\ \rangle|\ \rangle + E_z|\ \rangle|\ \rangle|\ \rangle$$
$$= (E_x + E_y + E_z)|\psi_x\rangle|\psi_y\rangle|\psi_z\rangle.$$

for each direction, $E_i = \hbar\omega(n_i + \frac{1}{2})$

eigen energy $E = \hbar\omega(n_x + n_y + n_z + \frac{3}{2})$

and the eigenstate $|n_x\rangle|n_y\rangle|n_z\rangle$.

digeneracy. $n_i = 0, 1, 2, \cdots$

total energy. E groundstate all n_i's $= 0$

$E_0 = \hbar\omega\frac{3}{2}$

1^{st} excited state. $E_1 = \hbar\omega\, 5/2$

choices $\underline{3}$

	E	n_x	n_y	n_z
gnd	$\hbar\omega\frac{3}{2}$	0	0	0
1^{st} excited	$\hbar\omega\frac{5}{2}$	1	0	0
		0	1	0
		0	0	1

3-fold degenerate
三重简并
defined by orthogonality of states.

2^{nd} excited $\hbar\omega\frac{7}{2}$

$$\left.\begin{array}{ccc} 2 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 2 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{array}\right\} \text{6-fold degen.}$$

$\vdots$

n^{th} excited $\hbar\omega(n+\frac{3}{2})$, $n = n_x + n_y + n_z$

question: how many degenerate states?

隔板法 method like inserting spacers.

$\underline{\underline{n}} = n_x + n_y + n_z$, n_i's ≥ 0

$\underbrace{\circ \circ \circ}_{n_x \text{ balls}} \Big| \underbrace{\circ - - - \circ}_{n_y} \Big| \underbrace{\circ \circ}_{n_z} \rightarrow n$ balls

spacers / panels

$n+2$ objects, including balls + panels.

$$\binom{n+2}{2} = \frac{(n+2)(n+1)}{2} \longrightarrow \begin{array}{l} n=0 \rightarrow 1\text{-fold} \\ n=1 \rightarrow 3\text{-fold} \\ n=2 \rightarrow 6\text{-fold} \checkmark \end{array}$$

teaser: $V = V(r)$.