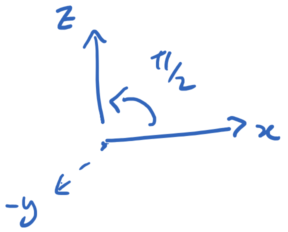
PC3130 W9L1 AY24

Tuesday, 15 October 2024 9:57 am

Tutorial 3

Q1. $|x;+\rangle \longrightarrow |z;+\rangle$

$e^{ik}|x;+\rangle = |z;+\rangle$



Anticlockwise rotation (+ve angle.)

$\measuredangle \ \frac{\pi}{2}$

axis $-\hat{y}$.

Transformation operator: $e^{\frac{-i\left(\frac{\pi}{2}\right)(\hat{S})\cdot(-\hat{y})}{\hbar}}$

$$= e^{\frac{-i\left(\frac{\pi}{2}\right)(-S_y)}{\hbar}}$$

Perturbation theory – time-independent.

$\Rightarrow$ eigenvalues ; eigenstates

Non-degenerate Degenerate

Non-degenerate perturbation theory (continued)

$$\left.\begin{aligned} |\psi_n\rangle &= |\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \lambda^2|\psi_n^2\rangle + \dots \\ E_n &= E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots \qquad , \lambda \ll 1. \end{aligned}\right\} (*)$$

(smooth functions of λ

As $\lambda \to 0$, $|\psi_n\rangle \to |\psi_n^0\rangle$, $E_n \to E_n^0$)

Sub. $(*)$ in $H|\psi_n\rangle = E_n|\psi_n\rangle$

Compare coeff of λ^n.

Compare coeff. of λ^1 :

$$\hat{H}_0|\psi_n^1\rangle + \hat{V}|\psi_n^0\rangle = E_n^0|\psi_n^1\rangle + E_n^1|\psi_n^0\rangle \quad — (1)$$

Last time, we showed that $\boxed{E_n^1 = \langle \psi_n^0 | V | \psi_n^0 \rangle}$ using (1)

Next, how about $|\psi_n^1\rangle = \sum_{m\neq n} \underbrace{\frac{\langle \psi_m^0 | V | \psi_n^0 \rangle}{E_n^0 - E_m^0}}_{\langle \psi_m^0 | \psi_n^1 \rangle,\ m\neq n} |\psi_m^0\rangle$

To get $\langle \psi_m^0 | \psi_n^1 \rangle$, $m \neq n$,

Using (1): Operate $\langle \psi_m^0 |$ on LHS and RHS:

$m\neq n$: $\langle \psi_m^0 | \hat{H}_0 | \psi_n^1 \rangle + \langle \psi_m^0 | \hat{V} | \psi_n^0 \rangle = E_n^0 \langle \psi_m^0 | \psi_n^1 \rangle + E_n^1 \underbrace{\langle \psi_m^0 | \psi_n^0 \rangle}_{0}$

eigenstate of $\hat{H}_0$

$m \neq n$ orthonormality

$$E_m^0 \langle \psi_m^0 | \psi_n^1 \rangle + \langle \psi_m^0 | \hat{V} | \psi_n^0 \rangle = E_n^0 \langle \psi_m^0 | \psi_n^1 \rangle$$

$$\langle \psi_m^0 | \psi_n^1 \rangle = \frac{\langle \psi_m^0 | \hat{V} | \psi_n^0 \rangle}{E_n^0 - E_m^0}, \quad E_n^0 \neq E_n^0.$$

state n is (ok - non-degenerate)

$$\text{So } |\psi_n^1\rangle = \sum_{m\neq n} \langle \psi_m^0 | \psi_n^1 \rangle |\psi_m^0\rangle$$

$$= \sum_{m\neq n} \frac{\langle \psi_m^0 | \hat{V} | \psi_n^0 \rangle}{E_n^0 - E_m^0} |\psi_m^0\rangle$$

From here, $|\langle \psi_m^0 | \hat{V} | \psi_n^0 \rangle| \ll |E_n^0 - E_m^0|$.

Now for $E_n^{(2)} = \sum_{m\neq n} \frac{|V_{mn}|^2}{E_n^0 - E_m^0}$ where $V_{mn} = \langle \psi_m^0 | V | \psi_n^0 \rangle$

$$(H_0 + \lambda V)\,|\psi_n(\lambda)\rangle = E_n(\lambda)\,|\psi_n(\lambda)\rangle$$

$$(H_0 + \lambda V)\left(|\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \lambda^2|\psi_n^2\rangle + \dots\right)$$

$$= \left(E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots\right)\left(|\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \lambda^2|\psi_n^2\rangle + \dots\right)$$

Compare coeff of λ^2:

$$H_0|\psi_n^2\rangle + V|\psi_n^1\rangle = E_n^0|\psi_n^2\rangle + E_n^1|\psi_n^1\rangle + E_n^2|\psi_n^0\rangle$$

Operate $\langle\psi_n^0|$ on LHS and RHS:

$$\langle\psi_n^0|\hat{H}_0|\psi_n^2\rangle + \langle\psi_n^0|\hat{V}|\psi_n^1\rangle$$

eigenstate of $\hat{H}_0$.

$$= E_n^0\underbrace{\langle\psi_n^0|\psi_n^2\rangle}_{0} + E_n^1\underbrace{\langle\psi_n^0|\psi_n^1\rangle}_{0} + E_n^2\underbrace{\langle\psi_n^0|\psi_n^0\rangle}_{1}$$

$$E_n^0\underbrace{\cancel{\langle\psi_n^0|\psi_n^2\rangle}}_{0} + \langle\psi_n^0|\hat{V}|\psi_n^1\rangle = E_n^2$$

$$E_n^2 = \langle\psi_n^0|\hat{V}|\psi_n^1\rangle, \quad |\psi_n^1\rangle = \sum_{m\neq n}\frac{\langle\psi_m^0|V|\psi_n^0\rangle}{E_n^0 - E_m^0}|\psi_m^0\rangle$$

complex no. / scalar

$$= \langle\psi_n^0|\hat{V}\left(\sum_{m\neq n}\frac{\langle\psi_m^0|\hat{V}|\psi_n^0\rangle}{E_n^0 - E_m^0}|\psi_m^0\rangle\right)$$

$$= \sum_{m\neq n}\frac{\langle\psi_m^0|\hat{V}|\psi_n^0\rangle}{E_n^0 - E_m^0}\underbrace{\langle\psi_n^0|\hat{V}|\psi_m^0\rangle}_{\langle\psi_m^0|\hat{V}|\psi_n^0\rangle^*}$$

$$= \sum_{m\neq n}\frac{|\langle\psi_m^0|\hat{V}|\psi_n^0\rangle|^2}{E_n^0 - E_m^0}$$

On λ:

Recall we defined $H = H_0 + \underbrace{V'}_{\text{perturbation}}$.

$$V' = \lambda V \quad , \quad V = \frac{1}{\lambda} V'.$$

$$E_n = E_n^0 + \underbrace{\lambda E_n^1}_{\uparrow} + \underbrace{\lambda^2 E_n^2} + \ldots$$

But at the beginning we wrote

$$E_n = E_n^0 + E_n^1 + E_n^2 + \ldots$$

E_n^1: 1st order correction to E_n^0

E_n^2: 2nd correction to E_n^0

What is E_n to 1st order in the perturbation?

Ans: $E_n = E_n^0 + E_n^1$

What is the 1st order correction to E_n^0?

Ans: E_n^1.

$$H = H_0 + \lambda V$$

Compare coeff of λ: $E_n^1 = \langle \psi_n^0 | V | \psi_n^0 \rangle$

$$\lambda E_n^1 = \lambda \langle \psi_n^0 | V | \psi_n^0 \rangle = \langle \psi_n^0 | \lambda V | \psi_n^0 \rangle$$
$$= \langle \psi_n^0 | V' | \psi_n^0 \rangle$$

$$H = H_0 + V'$$

$$E_n^1 = \langle \psi_n^0 | V' | \psi_n^0 \rangle$$

↑ "λE_n^1" in the notation with λ.

$$H = H_0 + \text{perturbation}$$

$$\text{Perturbation} = H - H_0$$

↑ V

$$E_n^1 = \langle \psi_n^0 | \overset{(H-H_0)}{V} | \psi_n^0 \rangle$$

$$|\psi_n^1\rangle = \sum \frac{\langle \psi_m^0 | \overset{(H-H_0)}{V} | \psi_n^0 \rangle}{E_n^0 - E_m^0} |\psi_m^0\rangle$$

$$E_n = E_n^0 + E_n^1 + E_n^2 + \ldots$$

$$|\psi_n^1\rangle = \sum_{m\neq n} \frac{\langle\psi_m^0|V|\psi_n^0\rangle}{E_n^0 - E_m^0}|\psi_m^0\rangle$$

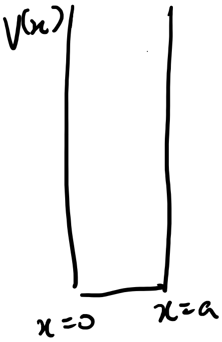
$$E_n^2 = \sum_{m\neq n} \frac{|\langle\psi_m^0|\overset{H-H_0}{V}|\psi_n^0\rangle|^2}{E_n^0 - E_m^0}$$

$E_n = E_n^0 + E_n^1 + E_n^2 \ldots$

$|\psi_n\rangle = |\psi_n^0\rangle + |\psi_n^1\rangle + \ldots$

Example.

Infinite square well with two identical bosons.



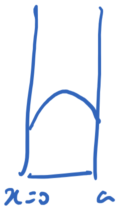
Perturbation $\tilde{V} = -aV_0\,\delta(x_1 - x_2)$

Dirac delta function.

$$H_0 = h_1 \otimes \mathbb{1}_2 + \mathbb{1}_1 \otimes h_2$$

$$h_1 = \frac{p^2}{2m} + V(x_1)$$

$$h_2 = \frac{p^2}{2m} + V(x_2)$$



$\psi_1^{0\,(s\text{-}p)}(x) = \sqrt{\frac{2}{a}}\sin\frac{\pi x}{a}$ $\quad 0\le x\le a$.

$E_1^0 = \frac{\hbar^2\pi^2}{2ma^2}$

Ground state for single particle.

Find the 1st order change in the ground state energy of H_0, due to $\tilde{V}$.

$$E_1^1 = \langle\psi_1^{0,2\text{-}b}|\tilde{V}|\psi_1^{0,2\text{-}b}\rangle \quad (2\text{-}b:\ 2\text{-body})$$

Ground state $|\psi_1^{0,2\text{-}b}\rangle = |\psi_1^{0,s\text{-}p}\rangle \otimes |\psi_1^{0,s\text{-}p}\rangle$ (symmetric)

$$\underbrace{\langle x_1, x_2|}_{\langle x_1|\otimes\langle x_2|}\psi_1^{0,2\text{-}b}\rangle = \langle x_1|\psi_1^{0,s\text{-}p}\rangle\langle x_2|\psi_1^{0,s\text{-}p}\rangle$$

particle

$$\psi_1^{0,2\text{-}b}(x_1, x_2) = \psi_1^{0,s\text{-}p}(x_1)\,\psi_1^{0,s\text{-}p}(x_2)$$

"ground state"

$$= \frac{2}{a}\sin\frac{\pi x_1}{a}\sin\frac{\pi x_2}{a}$$

$$= \frac{2}{a} \sin\frac{\pi x_1}{a} \sin\frac{\pi x_2}{a}$$

$$E_1' = \langle \psi_1^{0,2-b} | \tilde{V} | \psi_1^{0,2-b} \rangle \quad , \quad \tilde{V} = -aV_0\,\delta(x_1 - x_2)$$

$$= -aV_0\left(\frac{2}{a}\right)^2 \int_0^a dx_1 \int_0^a dx_2 \, \sin^2\frac{\pi x_1}{a} \sin^2\frac{\pi x_2}{a} \, \delta(x_1 - x_2)$$

$$= -aV_0\left(\frac{2}{a}\right)^2 \int_0^a dx_1 \sin^2\frac{\pi x_1}{a} \underbrace{\int_0^a dx_2 \sin^2\frac{\pi x_2}{a} \, \delta(x_1 - x_2)}_{\sin^2\frac{\pi x_1}{a}}$$

$$= -aV_0\left(\frac{2}{a}\right)^2 \int_0^a dx_1 \sin^4\frac{\pi x_1}{a}$$

$$= -aV_0\left(\frac{2}{a}\right)^2 \int_0^a dx \sin^4\frac{\pi x}{a}$$

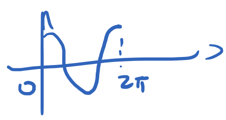
$$\sin^2 x = \frac{1 - \cos 2x}{2}$$

$$\sin^4 x = \left(\frac{1 - \cos 2x}{2}\right)^2$$

$$= \frac{1}{4}\left(1 - 2\cos 2x + \underbrace{\cos^2 2x}_{\frac{1 + \cos 4x}{2}}\right)$$

$$= \frac{1}{4}\left(\frac{3}{2} - 2\cos 2x + \frac{1}{2}\cos 4x\right)$$

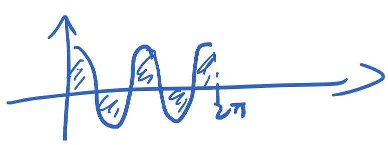
$$\int_0^a dx \cos\frac{2\pi x}{a} = 0$$



Let $u = \frac{2\pi x}{a}$

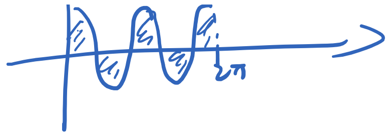
$x = \frac{a}{2\pi} u$

$$\frac{a}{2\pi}\int_0^{2\pi} du \cos u = 0$$



Likewise $\int^a dx \cos\frac{4\pi x}{a} = 0$

Likewise $\int_0^a dx \cos\frac{4\pi x}{a} = 0$



$$E_1^1 = -\frac{4V_0}{a}\int_0^a dx \ \sin^4\frac{\pi x}{a}$$

$$= -\frac{4V_0}{a}\cdot\frac{1}{4}\cdot\frac{3}{2}\int_0^a dx$$

$$= -\frac{V_0}{a}\cdot\frac{3}{2}\cdot a$$

$$= -\frac{3}{2}V_0$$

//

($E_1^0 = \frac{\hbar^2\pi^2}{2ma^2} + \frac{\hbar^2\pi^2}{2ma^2} = \frac{\hbar^2\pi^2}{ma^2}$

Perturbation theory is valid if

$$|E_1^1| \ll |E_1^0|$$

$$\left|\frac{3}{2}V_0\right| \ll \frac{\hbar^2\pi^2}{ma^2}$$

$$|V_0| \ll \frac{2}{3}\frac{\hbar^2\pi^2}{ma^2}.$$)

__Example__

__Harmonic oscillator__

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2x^2,$$

Perturbation $V = -qEx$ (Stark effect) (Electric field effect of an external)

Find the 1st and 2nd order corrections to the eigenvalues E_n^0.

—

$E_n^0 = (n + \frac{1}{2})\hbar\omega$

$E_n = (\quad 2) \ldots$

$$E_n^1 = \langle \psi_n^0 | V | \psi_n^0 \rangle$$

$$= -qE \langle \psi_n^0 | x | \psi_n^0 \rangle$$

$= 0$ because $\psi_n^0(x)$ is either even or odd about $x = 0$.

(or $\psi_n^0(x)$ has definite parity)

Recall from lecture on symmetries:

Parity operator $\hat{\pi}$: $x \longrightarrow -x$

(inversion)

if $[H_0, \hat{\pi}] = 0$ (H_0 is invariant wrt inversion)

then $\exists$ common eigenstates of H_0 and $\hat{\pi}$.

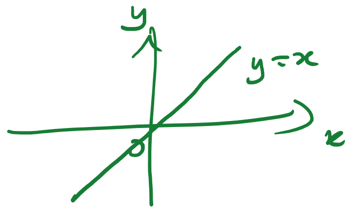
$\Rightarrow$ If the eigenstates are non-degenerate, these must be eigenstates of $\hat{\pi}$.

ie. The eigenstates of H_0 have definite parity.

$$\int_{-\infty}^{\infty} dx \; \psi_n^*(x) \; x \; \psi_n(x)$$

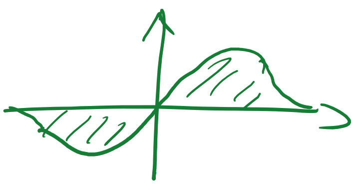
Case 1: $\psi_n(x)$ is even. $\Rightarrow$ $\psi_n^*(x)$ is also even

$$\underbrace{\int_{-\infty}^{\infty} dx \; \text{even} \, . \, \underset{\substack{\uparrow \\ \text{odd}}}{x} \, . \, \text{even}}_{\text{overall odd}}$$



odd

$$\therefore \int_{-\infty}^{\infty} dx \; \psi_n^*(x) \; x \; \psi_n(x) = 0$$



Case 2: $\psi_n(x)$ is odd $\Rightarrow$ $\psi_n^*(x)$ is also odd

$$\int_{-\infty}^{\infty} dx \; \underbrace{\text{odd} \cdot \text{odd} \cdot \text{odd}}_{\text{overall odd}} = 0$$

(odd $\times$ odd $\to$ even
even $\times$ odd $\to$ odd)

Math:

$$\langle \psi_n^0 | x | \psi_n^0 \rangle = \int_{-\infty}^{\infty} \psi_n^{0*}(x) \; x \; \psi_n^0(x) \, dx$$

$$\underset{\substack{x \to -x \\ u = -x}}{=} \int_{\infty}^{-\infty} \psi_n^{0*}(-x) \, (-x) \, \psi_n^0(-x) \, d(-x)$$

$$= - \int_{-\infty}^{\infty} dx \; \psi_n^{0*}(-x) \, x \, \psi_n^0(-x)$$

$\psi_n^0(-x) = \pm \psi_n^0(x)$
$\psi_n^{0*}(-x) = \pm \psi_n^{0*}(x)$

$$= - \int_{-\infty}^{\infty} dx \; \psi_n^{0*}(x) \, x \, \psi_n^0(x)$$

$$= - \langle \psi_n^0 | x | \psi_n^0 \rangle$$

Since $\langle \psi_n^0 | x | \psi_n^0 \rangle = - \langle \psi_n^0 | x | \psi_n^0 \rangle$,
$\langle \psi_n^0 | x | \psi_n^0 \rangle = 0$

The expectation value of odd operators vanishes for states with definite parity (either even or odd).

Another way to show that $E_n' = 0$.
uses $\hat{a}, \hat{a}^+$.