PHYS 4410

Quantum Mechanics 2

Spring 2023

Lecture 26

Time-independent perturbation theory: second order

March 24

1 Review: $H = \underbrace{H_0}_{\text{unperturbed}} + \underbrace{\lambda V}_{\text{small perturbation}}$

If $H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle$ and $H|n\rangle = E_n |n\rangle$

non-degenerate

exact eigenval/vectors.

$$|n\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \cdots$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \boxed{\lambda^2 E_n^{(2)}} + \cdots$$

Today!

lec 25:

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

$$E_n^{(1)} = \langle n^{(0)}|V|n^{(0)}\rangle$$

$\boxed{2}$ To derive $E_n^{(2)}$: $\quad H|n\rangle = E_n|n\rangle$

$$(H_0 + \lambda V)\left[|n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \cdots\right] = \left(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)}\right)\left(|n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \cdots\right)$$

Collect terms at λ^2:

$$V|n^{(1)}\rangle + H_0|n^{(2)}\rangle = E_n^{(2)}|n^{(0)}\rangle + E_n^{(1)}|n^{(1)}\rangle + E_n^{(0)}|n^{(2)}\rangle$$

Inner product w/ $\langle n^{(0)}|$:

$$\langle n^{(0)}|V|n^{(1)}\rangle + \underbrace{\cancel{\langle n^{(0)}|H_0|n^{(2)}\rangle}}_{\cancel{E_n^{(0)}\langle n^{(0)}|n^{(2)}\rangle}} = E_n^{(2)}\cancelto{1}{\langle n^{(0)}|n^{(0)}\rangle} + E_n^{(1)}\cancelto{0}{\langle n^{(0)}|n^{(1)}\rangle} + \cancel{E_n^{(0)}\langle n^{(0)}|n^{(2)}\rangle}$$

$$E_n^{(2)} = \langle n^{(0)}|V|n^{(1)}\rangle = \sum_{m\neq n} \underbrace{\frac{|\langle m^{(0)}|V|n^{(0)}\rangle|^2}{E_n^{(0)} - E_m^{(0)}}}_{\text{off diagonal terms in } V.}$$

$\boxed{3}$ $H_0 = \begin{pmatrix} A & 0 & 0 \\ 0 & 2A & 0 \\ 0 & 0 & 3A \end{pmatrix}$ $|1^{(0)}\rangle \; |2^{(0)}\rangle \; |3^{(0)}\rangle$

$\lambda V = \begin{pmatrix} \cancel{\lambda} & 0 & \lambda \\ 0 & \lambda & 0 \\ \lambda & 0 & 0 \end{pmatrix}$ cf lec 25

Find eigenvalues of H upto second order in λ?

- Start w/ order λ: $E_1^{(1)} = E_3^{(0)} = 0$, and $E_2^{(1)} = \lambda$.

Then to order λ^2: $E_1^{(2)} = \sum_{m=2}^{3} \frac{|\langle m^{(0)}|V|1^{(0)}\rangle|^2}{E_1^{(0)} - E_m^{(0)}} = \frac{0^2}{A-2A} + \frac{\lambda^2}{A-3A} = -\frac{\lambda^2}{2A}$

$E_2^{(2)} = 0$; $E_3^{(2)} = \frac{\lambda^2}{3A-A} = +\frac{\lambda^2}{2A}$

When will perturbation theory fail?

if $E_n^{(0)} \lesssim E_n^{(2)}$ or $E_n^{(1)} \ldots$

$E_n^{(0)} - E_m^{(0)} \lesssim E_n^{(2)} - E_m^{(2)}$ or $E_n^{(1)} - E_m^{(1)}$

In this problem,

$E_3 - E_1 = 2A + \underbrace{\frac{\lambda^2}{A}}_{\text{small}}$

$\lambda \lesssim A$

$\boxed{4}$ $H_0 = A J_z$ $\lambda V = \lambda J_x$ (cf lec 25)

$$H_0 = A\hbar \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix} \qquad \lambda V = \frac{\lambda\hbar}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ \boxed{1} & 0 & 1 \\ \boxed{0} & 1 & 0 \end{pmatrix}$$

zero first

$$E_1 = A\hbar + 0\cdot\lambda + \frac{1}{A\hbar - 0}\left(\frac{\lambda\hbar}{\sqrt{2}}\right)^2 + 0 = \hbar\left(A + \frac{\lambda^2}{2A} + \cdots\right)$$

$$E_0 = 0 + 0\cdot\lambda + \cancel{\frac{1}{0 - A\hbar}\left(\frac{\lambda\hbar}{\sqrt{2}}\right)^2 + \frac{1}{0-(-A\hbar)}\left(\frac{\lambda\hbar}{\sqrt{2}}\right)^2} = 0$$

$$E_{-1} = -A\hbar + 0\cdot\lambda + \frac{1}{-A\hbar - 0}\left(\frac{\lambda\hbar}{\sqrt{2}}\right)^2 = \hbar\left(-A - \frac{\lambda^2}{2A} + \cdots\right)$$

$H = H_0 + \lambda V$ was exactly solvable:

$$E = 0,\ \pm \underbrace{\sqrt{A^2 + \lambda^2}}_{A\sqrt{1 + \lambda^2/A^2}} = A\left(1 + \frac{1}{2}\frac{\lambda^2}{A^2} + \cdots\right)$$

5 Two distinguishable spin-1/2 particles

$$H_0 = \underbrace{h_1 \sigma_{z,1}}_{\sigma_z \otimes 1} + \underbrace{h_2 \sigma_{z,2}}_{1 \otimes \sigma_z} \qquad h_1 > 0, \quad h_2 > 0$$

$\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$

$$\text{“}\lambda V\text{''} = \underbrace{g\,\sigma_{x,1}\sigma_{x,2}}_{\sigma_x \otimes \sigma_x} \qquad g \ll h_1, h_2 \qquad \sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

interaction

Zeroth order: $|\uparrow\uparrow^{(0)}\rangle$, $|\uparrow\downarrow^{(0)}\rangle$, $|\downarrow\uparrow^{(0)}\rangle$, $|\downarrow\downarrow^{(0)}\rangle$

$E^{(0)}$: $h_1 + h_2$, $h_1 - h_2$, $-h_1 + h_2$, $-h_1 - h_2$

First order: $E^{(1)}_{\uparrow\uparrow} = g\langle\uparrow\uparrow^{(0)}|\sigma_x \otimes \sigma_x|\uparrow\uparrow^{(0)}\rangle = \cancel{g\langle\uparrow\uparrow^{(0)}|\downarrow\downarrow^{(0)}\rangle} \to 0$

all $E^{(1)} = 0$.

Second order: $\lambda V|\uparrow\uparrow^{(0)}\rangle = g\,\sigma_x \otimes \sigma_x|\uparrow\uparrow^{(0)}\rangle = g|\downarrow\downarrow^{(0)}\rangle$

$$E^{(2)}_{\uparrow\uparrow} = \frac{|\langle\uparrow\uparrow^{(0)}|V|\downarrow\downarrow^{(0)}\rangle|^2}{E^{(0)}_{\uparrow\uparrow} - E^{(0)}_{\downarrow\downarrow}} = \frac{g^2}{2(h_1+h_2)}, \quad E^{(2)}_{\uparrow\downarrow} = \frac{g^2}{2(h_1-h_2)}, \quad E^{(2)}_{\downarrow\uparrow} = -E^{(2)}_{\uparrow\downarrow}$$

$$E^{(2)}_{\downarrow\downarrow} = -E^{(2)}_{\uparrow\uparrow}$$

PT fails if: $g \gtrsim h_1 - h_2$: H_0 becoming degenerate.

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