PHYS 4410

Quantum Mechanics 2

Spring 2023

Lecture 25

Time-independent perturbation theory: first order

March 20

1 Perturbation theory: $H = \underbrace{H_0}_{\substack{\text{exactly} \\ \text{solved}}} + \underbrace{\lambda V}_{\substack{\text{small} \\ \text{perturbation}}}$

$H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle \leftarrow$

exact eigenstates/values: $H|n\rangle = E_n|n\rangle$:

$$\begin{array}{lcl} \begin{array}{l} E_n = E_n^{(0)} + \\[1em] |n\rangle = |n^{(0)}\rangle + \end{array} & \boxed{\begin{array}{c} \lambda E_n^{(1)} + \\[1em] \lambda |n^{(1)}\rangle \end{array}} & \begin{array}{l} \lambda^2 E_n^{(2)} + \cdots \\[1em] + \lambda^2 |n^{(2)}\rangle + \cdots \end{array} \end{array}$$

Goal today.

<u>First-order</u> perturbation theory.

$$H|n\rangle = E_n|n\rangle$$

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

Order λ^0: $H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle \rightarrow \langle n^{(0)}|H_0 = E_n^{(0)}\langle n^{(0)}|$

Order λ:

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

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

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

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

$m \neq n$

- Calculate $|n^{(1)}\rangle$: $\langle m^{(0)}|\left[\text{order } \lambda \text{ eqn}\right] = ?$

$$\langle m^{(0)}|V|n^{(0)}\rangle + \langle m^{(0)}|H_0|n^{(1)}\rangle = E_n^{(1)}\cancel{\langle m^{(0)}|n^{(0)}\rangle} + E_n^{(0)}\langle m^{(0)}|n^{(1)}\rangle.$$

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

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

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

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

no n in the sum: b/c $\langle n|n\rangle = 1$.

$H = H_0 + \lambda V$

$$H_0 = \begin{array}{c} \begin{array}{ccc} 1 & 2 & 3 \end{array} \\ \begin{pmatrix} A & 0 & 0 \\ 0 & 2A & 0 \\ 0 & 0 & 3A \end{pmatrix} \end{array} ; \quad \lambda V = \begin{pmatrix} \underline{0} & 0 & \lambda \\ 0 & \underline{\lambda} & 0 \\ \lambda & 0 & \underline{0} \end{pmatrix}$$

E_n to first order in λ?

$E_1 = A + \lambda \, \underline{0}$

$= A$

$E_2 = 2A + \lambda \, \underline{1}$

$= 2A + \lambda$

$E_3 = 3A + \lambda \, \underline{0}$

$= 3A$

$|1^{(0)}\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$ $\quad |2^{(0)}\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$ $\quad |3^{(0)}\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

$$E_1^{(1)} = \langle 1^{(0)} | V | 1^{(0)} \rangle = (1 \quad 0 \quad 0) \, \lambda V \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

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$H = H_0 + \lambda V$

$$H_0 = \begin{pmatrix} A & 0 & 0 \\ 0 & 2A & 0 \\ 0 & 0 & 3A \end{pmatrix} ; \quad \lambda V = \begin{pmatrix} 0 & 0 & \lambda \\ 0 & \lambda & 0 \\ \lambda & 0 & 0 \end{pmatrix}$$

Calculate:

$$|1\rangle = |1^{(0)}\rangle \quad \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

$$|2\rangle = |2^{(0)}\rangle \quad \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

$$|3\rangle = |3^{(0)}\rangle \quad \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$|1^{(0)}\rangle = -\frac{\lambda}{2A}|3^{(0)}\rangle$$

$$+ \lambda|1^{(1)}\rangle \quad \begin{pmatrix} 0 \\ 0 \\ \end{pmatrix}$$

$$+ \lambda|2^{(1)}\rangle \quad \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

$$+ \underbrace{\lambda|3^{(1)}\rangle}$$

$$+ \frac{\lambda}{2A}|1^{(0)}\rangle$$

$$+ \begin{pmatrix} \lambda/2A \\ 0 \\ 0 \end{pmatrix}$$

$\langle m^{(0)}|V|1^{(0)}\rangle$ $m \neq 1$

$\langle 3^{(0)}|V|1^{(0)}\rangle$

$$\frac{\lambda}{A - 3A}$$

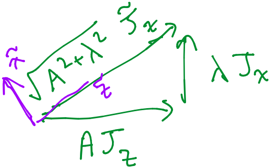
Recall:

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

$\boxed{5}$ $H_0 = A J_z$ $\qquad \lambda V = \lambda J_x$ $\qquad$ spin-1

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

$E_n^{(1)} = 0$ for $n = -1, 0, 1$



$$(\lambda \;\; 0 \;\; A) \cdot \begin{pmatrix} J_x \\ J_y \\ J_z \end{pmatrix} = H$$

If $H = \sqrt{A^2+\lambda^2}\; \tilde{J}_z$ then eigenvalues are:

$0, \pm\hbar$ for spin 1

$$E_1 = \sqrt{A^2+\lambda^2}\,\hbar \qquad E_0 = 0 \qquad E_{-1} = -\sqrt{A^2+\lambda^2}\,\hbar$$

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