PHYS 4410

Quantum Mechanics 2

Spring 2023

Lecture 24

Time-independent perturbation theory: introduction

March 17

$\boxed{1}$ Perturbation theory: suppose

$$H = \underbrace{H_0}_{\text{"unperturbed" exactly solved}} + \underbrace{\lambda V}_{\text{small perturbation}}$$

λ = "bookkeeping" device... sets $\lambda = 1$, but keep track of order

Goal: $\underbrace{H |n\rangle = E_n |n\rangle}_{\text{exact}}$. Perturbation theory: E_n, $|n\rangle$ as Taylor series in λ

$|n\rangle$: eigenstate; E_n: eigenvalue

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

$$|n\rangle = \underbrace{|n^{(0)}\rangle}_{\text{leading order}} + \lambda |n^{(1)}\rangle + \dots$$

perturbative corrections.

For Lec 24–26: assume H_0 is non-degen. $E_n^{(0)} \neq E_{n'}^{(0)}$ if $n \neq n'$.

If $\lambda = 0$: $H = H_0$,

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

$\boxed{2}$ Toy model: $H_0 = \begin{pmatrix} a & 0 \\ 0 & b \end{pmatrix}$ $\quad V = \begin{pmatrix} \alpha & \gamma \\ \gamma & \beta \end{pmatrix}$

$H_0 \begin{pmatrix} 1 \\ 0 \end{pmatrix} = a \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ e.g. $\quad a \neq b$

α, β, γ <u>small</u> vs. a & b?

all parameters real.

Find eigenvalues of $H = H_0 + \lambda V$ <u>exactly</u>.

$$\det(H - E\mathbb{1}) = 0 = \det(H_0 + \lambda V - E\mathbb{1})$$

$$= \det\begin{pmatrix} a + \lambda\alpha - E & \lambda\gamma \\ \lambda\gamma & b + \lambda\beta - E \end{pmatrix} = (a + \lambda\alpha - E)(b + \lambda\beta - E) - \lambda^2\gamma^2 = 0$$

$$0 = E^2 - E\left[a + \lambda\alpha + b + \lambda\beta\right] + \left[(a + \lambda\alpha)(b + \lambda\beta) - (\lambda\gamma)^2\right]$$

$$E = \frac{a + \lambda\alpha + b + \lambda\beta \pm \sqrt{(a + \lambda\alpha - b - \lambda\beta)^2 + 4\lambda^2\gamma^2}}{2}$$

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$$E = \frac{a + \underline{\lambda}\alpha + b + \underline{\lambda}\beta \pm \sqrt{(a+\lambda\alpha - b - \lambda\beta)^2 + 4\lambda^2\gamma^2}}{2}$$

Assume $a > b$: $\sqrt{1+x} \approx 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \cdots$

$$\sqrt{(a-b+\lambda(\alpha-\beta))^2 + 4\lambda^2\gamma^2} = (a-b)\sqrt{1 + 2\lambda\frac{\alpha-\beta}{a-b} + \lambda^2\frac{(\alpha-\beta)^2 + 4\gamma^2}{(a-b)^2}}$$

$$\approx (a-b)\left[1 + \lambda\frac{\alpha-\beta}{a-b} + \lambda^2\frac{\cancel{(\alpha-\beta)^2} + 4\gamma^2}{2(a-b)^2} + \cdots \cancel{- \frac{1}{8}\left(2\lambda\frac{\alpha-\beta}{a-b} + \cdots\right)^2}\right]$$

[accurate to order λ^2]: error is $\sim\lambda^3$.

$$\approx a - b + \lambda(\alpha-\beta) + \lambda^2 \cdot \frac{2\gamma^2}{(a-b)}$$

$$E_+ = \frac{1}{2}\left(a + \lambda\alpha + b + \lambda\beta + \left[a - b + \lambda(\alpha-\beta) + \lambda^2\frac{2\gamma^2}{(a-b)}\right]\right)$$

$$= a + \underline{\lambda\alpha} + \lambda^2\frac{\gamma^2}{a-\underline{b}}$$

$$E_- = b + \underline{\lambda\beta} - \lambda^2\frac{\gamma^2}{\underline{a-b}}$$

depends on diagonal entries in V

$\downarrow$

first order: $E_+^{(0)} = a$, $E_+^{(1)} = \alpha$

lec 26: always depend on off-diagonal

$\downarrow$

second order: $E_+^{(2)} = \dfrac{\gamma^2}{a-b}$

$\boxed{4}$ Claim: $\underline{E_n^{(1)} = \langle n^{(0)}|V|n^{(0)}\rangle}$ ($\underline{H_0 \text{ not degenerate}}$)

<u>Proof:</u>
$$H|n\rangle = E_n|n\rangle$$
$$(H_0+\lambda V)\left[|n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \cdots\right] = \left(E_n^{(0)} + \lambda E_n^{(1)} + \cdots\right)\left[|n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \cdots\right]$$

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

Order λ: $\quad V|n^{(0)}\rangle + H_0|n^{(1)}\rangle = E_n^{(1)}|n^{(0)}\rangle + E_n^{(0)}|n^{(1)}\rangle$

Inner product w/ $\langle n^{(0)}|$:
$$\langle n^{(0)}|V|n^{(0)}\rangle + \cancel{\underbrace{\langle n^{(0)}|H_0|n^{(1)}\rangle}_{= \langle n^{(0)}|\cdot E_n^{(0)}}} = E_n^{(1)}\cancelto{1}{\langle n^{(0)}|n^{(0)}\rangle} + \cancel{E_n^{(0)}\langle n^{(0)}|n^{(1)}\rangle}$$

$\boxed{5}$ Take H_0 to be harmonic oscillator:

$H_0|n^{(0)}\rangle = \hbar\omega(n+\tfrac{1}{2})|n^{(0)}\rangle$. $V = \frac{m}{2}\cdot \underset{\text{"small"}}{C} x^2$

Problems stated as follows.

$\boxed{\text{What is } E_n \text{ at first order in } C\text{?}}$

$$E_n = E_n^{(0)} + \cancel{\lambda} E_n^{(1)}$$

$$= \hbar\omega(n+\tfrac{1}{2}) + \frac{\hbar C}{2\omega}(n+\tfrac{1}{2})$$

What is $E_n^{(1)}$?

$$E_n^{(1)} = \langle n^{(0)}| \frac{m}{2} C x^2 |n^{(0)}\rangle$$

$$= \frac{mC}{2}\cdot\frac{\hbar}{2m\omega}\langle n^{(0)}|(a+a^\dagger)^2|n^{(0)}\rangle$$

$$\cancel{aa} + \underbrace{aa^\dagger}_{n+1} + \underbrace{a^\dagger a}_{n} + \cancel{a^\dagger a^\dagger}$$

$$= \frac{C\hbar}{2\omega}(n+\tfrac{1}{2})$$

PT when perturb. is small

Exact solution:

$$H = \frac{p^2}{2m} + \frac{m}{2}\omega^2 x^2 + \frac{m}{2}Cx^2 = \frac{p^2}{2m} + \frac{m}{2}\overbrace{(\omega^2+C)}^{\tilde{\omega}^2}x^2$$

$$E_n = \hbar\tilde{\omega}(n+\tfrac{1}{2}) = \hbar\sqrt{\omega^2+C}\,(n+\tfrac{1}{2})$$

$$= \hbar\omega(n+\tfrac{1}{2})\sqrt{1+C/\omega^2} \simeq \hbar\omega(n+\tfrac{1}{2})\left[1+\frac{C}{2\omega^2}\right]$$

good approx. $C \ll \omega^2$

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