PHYS 4410

Quantum Mechanics 2

Spring 2023

Lecture 27

Time-independent perturbation theory: degenerate

April 3

$\boxed{1}$ Perturbation theory: $H = H_0 + \lambda \cdot V$

H_0: exactly solved; λ: "bookkeeping" $(\lambda = 1)$; V: Small perturbation

Goal: eigenstates/vals of H: (Taylor series in λ)

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

$$\left.\begin{aligned} |n\rangle &= |n^{(0)}\rangle + \lambda|n^{(1)}\rangle + \lambda^2|n^{(2)}\rangle + \cdots \\ E_n &= E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots \end{aligned}\right\} \quad H_0|n^{(0)}\rangle = E_n^{(0)}|n^{(0)}\rangle$$

When H_0 has degeneracy: (i.e degenerate)

$$E_n^{(2)} = \sum_{m \neq n} \frac{|\langle m^{(0)}|V|n^{(0)}\rangle|^2}{E_n^{(0)} - E_m^{(0)}} \rightarrow \text{if } E_n^{(0)} = E_m^{(0)} \text{ problem.}$$

$\boxed{2}$ $H_0 = A\vec{S}\cdot\vec{I}$

Add: $V = B\cdot S_z$

S, I : spin-1/2

unperturbed e-states:
coupled basis:

spin 1: $|11^{(0)}\rangle = |\uparrow\uparrow\rangle$

$|1-1^{(0)}\rangle = |\downarrow\downarrow\rangle$

$|10^{(0)}\rangle = \frac{1}{\sqrt{2}}\left[|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right]$

spin 0: $|00^{(0)}\rangle = \frac{1}{\sqrt{2}}\left[|\underset{SI}{\uparrow\downarrow}\rangle - |\underset{SI}{\downarrow\uparrow}\rangle\right]$

$$V + H_0 = \begin{array}{c} |11\rangle \quad\quad |1-1\rangle \quad\quad |10\rangle \quad\quad |00\rangle \\ \begin{pmatrix} A\hbar^2/4 + \frac{B\hbar}{2} & 0 & 0 & 0 \\ 0 & A\hbar^2/4 - \frac{B\hbar}{2} & 0 & 0 \\ 0 & 0 & A\hbar^2/4 & \frac{B\hbar}{2} \\ 0 & 0 & \frac{B\hbar}{2} & -\frac{3A\hbar^2}{4} \end{pmatrix} \end{array}$$

$V|11^{(0)}\rangle = BS_z|\uparrow\uparrow\rangle = B\left(S_z|\uparrow\rangle\right)\otimes|\uparrow\rangle = B\frac{\hbar}{2}|\uparrow\uparrow\rangle = B\frac{\hbar}{2}|11^{(0)}\rangle$

$V|1-1^{(0)}\rangle = -B\frac{\hbar}{2}|1-1^{(0)}\rangle$

$V|10^{(0)}\rangle = B\frac{1}{\sqrt{2}}\left[\underset{(+\hbar/2)}{S_z|\uparrow\downarrow\rangle} + \overset{(-\hbar/2)}{S_z|\downarrow\uparrow\rangle}\right] = B\frac{\hbar}{2}|00^{(0)}\rangle$

$V|00^{(0)}\rangle = B\frac{\hbar}{2}|10^{(0)}\rangle$

$\boxed{3}$

$$
V + H_0 = \begin{array}{c} \\ \\ \end{array}
\begin{array}{cccc}
|11\rangle & |1\,{-1}\rangle & |10\rangle & |00\rangle \\
\end{array}
$$

$$
V + H_0 = \left(\begin{array}{cccc}
\frac{A\hbar^2}{4} + \frac{B\hbar}{2} & 0 & 0 & 0 \\
0 & \frac{A\hbar^2}{4} - \frac{B\hbar}{2} & 0 & 0 \\
0 & 0 & \frac{A\hbar^2}{4} & \frac{B\hbar}{2} \\
0 & 0 & \frac{B\hbar}{2} & -\frac{3A\hbar^2}{4}
\end{array}\right)
$$

First-order PT:

$$E^{(1)}_{11} = \frac{B\hbar}{2} \qquad E^{(1)}_{1-1} = -\frac{B\hbar}{2}$$

$$E^{(1)}_{10} = E^{(1)}_{00} = 0$$

Second-order PT:

$$E^{(2)}_{10} = \frac{\left(\frac{B\hbar}{2}\right)^2}{\frac{A}{4}\hbar^2(1-(-3))} = \frac{B^2}{4A}$$

$$E^{(2)}_{00} = -\frac{B^2}{4A}$$

In this problem:

- each block is not degenerate
- all "off-block-diagonal" components of $V = 0$.

$\hookrightarrow$ use "non-degenerate" PT.

$\boxed{4}$ $\quad H_0 = A\vec{S}\cdot\vec{I} \qquad V = BS_x$

Recall: $S_x|\uparrow\rangle = \hbar/2\,|\downarrow\rangle \qquad S_x|\downarrow\rangle = \frac{\hbar}{2}|\uparrow\rangle$.

What are eigenvalues? [H_0 has rotational symmetry. V is "rotation of BS_z"].

$$V|11^{(0)}\rangle = BS_x|\uparrow\uparrow\rangle = \frac{B\hbar}{2}|\downarrow\uparrow\rangle = \frac{B\hbar}{2}\cdot\frac{1}{\sqrt{2}}\left[|10^{(0)}\rangle - |00^{(0)}\rangle\right]$$

$$V|1-1^{(0)}\rangle = BS_x|\downarrow\downarrow\rangle = \frac{B\hbar}{2}\frac{1}{\sqrt{2}}\left[|10\rangle^{(0)} + |00^{(0)}\rangle\right].$$

etc.

$$V = \frac{B\hbar}{2}\frac{1}{\sqrt{2}}\begin{array}{c} \begin{array}{cccc} |11\rangle & |1-1\rangle & |10\rangle & |00\rangle \end{array} \\ \begin{pmatrix} 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \end{pmatrix} \end{array}$$

} degenerate for H_0

~~no first order corr. $E^{(1)} = 0$??~~

$$\frac{|\langle m^{(0)}|V|n^{(0)}\rangle|^2}{E_n^{(0)} - E_m^{(0)}}$$

within degenerate subspace, off-diagonal V.

$\boxed{5}$

$$V = \frac{B\hbar}{2}\frac{1}{\sqrt{2}}\;\begin{array}{cccc} |11\rangle & |1{-1}\rangle & |10\rangle & |00\rangle \\ \end{array}$$
$$\left(\begin{array}{cc|c|c} 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 1 \\ \hline 1 & 1 & 0 & 0 \\ \hline -1 & 1 & 0 & 0 \end{array}\right)$$

Need to diagonalize V in top 3x3 block...

$$|b\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \\ 0 \end{pmatrix}$$

Let $|a\rangle = \dfrac{|11\rangle + |1{-1}\rangle}{\sqrt{2}} = \dfrac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \end{pmatrix}$

$$V = \begin{array}{cccc} |a\rangle & |b\rangle & |10\rangle & |00\rangle \end{array}$$
$$\left(\begin{array}{ccc|c} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ \hline 1 & 0 & 0 & 0 \end{array}\right)$$

$$|b'\rangle = \frac{1}{\sqrt{2}}\big[\,|b\rangle + |10\rangle\,\big]$$

$$|b''\rangle = \frac{1}{\sqrt{2}}\big[\,|b\rangle - |10\rangle\,\big]$$

up to rearranging row/col:

Same as bef.

$$V = \begin{array}{cccc} |a\rangle & |b'\rangle & |b''\rangle & |00\rangle \end{array}$$
$$\left(\begin{array}{ccc|c} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ \hline 1 & 0 & 0 & 0 \end{array}\right)$$

$\boxed{6}$ let $H_0 = \left(\begin{array}{cc|c} 0 & 0 & 0 \\ 0 & 0 & 0 \\ \hline 0 & 0 & 1 \end{array}\right)$ $V = \left(\begin{array}{cc|c} \boxed{\begin{matrix} 0 & \varepsilon \\ \varepsilon & 0 \end{matrix}} & & 0 \\ & & \varepsilon \\ \hline 0 & \varepsilon & 0 \end{array}\right)$

Eigenvalues of $H = H_0 + (\lambda) V$ to first order in ε?

$|b'\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} = \frac{|1\rangle + |2\rangle}{\sqrt{2}}$

$|b''\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} = \frac{|1\rangle - |2\rangle}{\sqrt{2}}$

$$V = \begin{array}{c} \begin{matrix} |b'\rangle & |b''\rangle & \end{matrix} \\ \left(\begin{array}{cc|c} 1 & 0 & 1/\sqrt{2} \\ 0 & -1 & -1/\sqrt{2} \\ \hline 1/\sqrt{2} & -1/\sqrt{2} & 0 \end{array}\right) \end{array} \varepsilon$$

since V is diagonal in top 2×2 block: $\varepsilon, -\varepsilon, 1$

Second order: eigenvalues

$|1\rangle = \frac{|b'\rangle + |b''\rangle}{\sqrt{2}}$

$$\varepsilon - \frac{\varepsilon^2}{2} + \dots, \quad -\varepsilon - \frac{\varepsilon^2}{2} + \dots, \quad 1 + \varepsilon^2 + \dots$$

$|2\rangle = \frac{|b'\rangle - |b''\rangle}{\sqrt{2}}$

$$V = \varepsilon|1\rangle\langle 2| + \varepsilon|2\rangle\langle 1| = \varepsilon\frac{(|b'\rangle + |b''\rangle)(\langle b'| - \langle b''|)}{2} + \dots = \varepsilon|b'\rangle\langle b'| - \varepsilon|b''\rangle\langle b''|$$