PHY 456 Lecture 4

Time-Independent Degenerate Perturbation Theory

Nondegenerate summary:

$$(H_0 + \lambda H_1)|n\rangle = E_n |n\rangle$$

$$|n\rangle = \sum_{k=0}^{\infty} \lambda^k |n^k\rangle \qquad \text{and} \qquad H_0|n^0\rangle = E_n^0|n^0\rangle$$

$$E_n = \sum_{k=0}^{\infty} E_n^k$$

Sol:

$$E_n = E_n^0 + \lambda \langle n^0|H_1|n^0\rangle + \lambda^2 \sum_{n\neq m} \frac{|\langle m^0|H_1|n_0\rangle|^2}{E_n^0 - E_m^0}$$

matrix element in unperturbed state

2nd order Ground State correction < 0

$$|n\rangle = |n^0\rangle + \sum_{n\neq m} |m^0\rangle \frac{\langle m^0|\lambda H_1|n^0\rangle}{E_n^0 - E_m^0} + O(\lambda^2)$$

DIY

Under assumption that $\forall E_n^0 \; \exists |n^0\rangle$ s.t. nondegenerate spectrum.

Motivation TI OPT

$$H_0 = \frac{\hat{p}^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2$$ System w/ ∞-dimensional H-space

$$\lambda H_1 = \lambda \hat{x}^4$$

$\rightarrow$ Reduce to finite-dimensional Hilbert space "Qubit" $|\psi\rangle = \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}$

2-level system

Let $H_0 = \begin{pmatrix} a+b & 0 \\ 0 & a-b \end{pmatrix}$ $a, b \in \mathbb{R}$

$$\equiv a\sigma_0 + b\sigma_3$$

and $\lambda H_1 = \lambda \sigma_1$ (simplicity, could be more general)

Then $H_0 + \lambda H_1 = \begin{pmatrix} a+b & \lambda \\ \lambda & a-b \end{pmatrix}$

whose trace is $\mathrm{tr}(H_0 + \lambda H_1) = 2a \equiv E_+ + E_-$,

$$\det(H_0 + \lambda H_1) = a^2 - b^2 - \lambda^2 \equiv E_+ \cdot E_-$$

which implies

$$E_\pm = a \pm \sqrt{b^2 + \lambda^2}$$ (2 energy states)

Since any vector is an eigenvector of $a\sigma_0$, we find the eigenvectors

$$\begin{pmatrix} b & \lambda \\ \lambda & -b \end{pmatrix} \begin{pmatrix} \alpha_\pm \\ \beta_\pm \end{pmatrix} = \pm\sqrt{b^2 + \lambda^2} \begin{pmatrix} \alpha_\pm \\ \beta_\pm \end{pmatrix}$$

and we find that

$$E_\pm = a \pm \sqrt{b^2+\lambda^2}$$

$$|\pm\rangle = \begin{pmatrix} b \pm \sqrt{b^2+\lambda^2} \\ \lambda \end{pmatrix} \quad \text{unnormalized}$$

$$H = \underbrace{\begin{pmatrix} a+b & 0 \\ 0 & a-b \end{pmatrix}}_{H_0} + \lambda \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{H_1}$$

For $b \neq 0$, this is a nondegenerate H_0

and $E_\pm^0 = a \pm b$,

$$E_\pm^1 = 0$$

$$E_\pm^2 = \pm \frac{1}{2b}$$

If $b=0$, $H = \underbrace{\begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix}}_{H_0} + \lambda \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{H_1}$ which now has a

degenerate unperturbed spectrum in H_0. We find

$$E_\pm = a \pm \lambda,$$

$$|\pm\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} \pm 1 \\ 1 \end{pmatrix}$$ as $b \to 0$, which is smooth as $\lambda \to 0$

as well.

What's special:

1) Unperturbed H_0 eigenvectors

2) The perturbation of H_1 is diagonal in $\begin{pmatrix} \pm 1 \\ 1 \end{pmatrix}$ basis.

Time Independent Perturbation Theory

Ex. 1 : $n > 1$ H-atom states all have degeneracies...

Ex. 2 : Spherical SHO $H = -\frac{\hbar^2 \nabla^2}{2m} + \frac{m\omega^2}{2} \vec{r}^{\,2}$ in spherical basis $|\ell, m\rangle$

or in Cartesian basis $n_x + n_y + n_z =$ constant.

In the spherical symmetry of 3D SHO, there's a freedom to choose

$\{|n, k_n\rangle, \ k_n = 1, \ldots, r_n\}$ states : any $\mathcal{U}(r_n)$ unitary transformation

is as good. *I don't understand what any of this means

Suppose H_0 has degenerate spectrum in unperturbed states.

[1] $$\hat{H}_0 |n, k_n\rangle = E_n^0 |n, k_n\rangle$$ k_n: degeneracy of n^{th}-level

and we want to solve for E, ψ :

[2] $$(\hat{H}_0 + \lambda \hat{H}_1) |\psi\rangle = E|\psi\rangle.$$

The values of E will be determined, but we will expand $|\psi\rangle$ in terms of $|n, k_n\rangle$ states (which is complete)

[3] $$|\psi\rangle = \sum_{n, k_n} c_{n, k_n} |n, k_n\rangle.$$

[3] → [2] implies

$$\sum_{n,k_n} \left(E_n^0 |n,k_n\rangle c_{n,k_n} + \lambda \hat{H}_1 |n,k_n\rangle c_{n,k_n} \right) = \sum_{n,k_n} E\, c_{n,k_n} |n,k_n\rangle$$

$$\Longrightarrow \sum_{n,k_n} |n,k_n\rangle (E - E_n^0) c_{n,k_n} = \sum_{n,k_n} \hat{H}_1 |n,k_n\rangle \lambda\, c_{n,k_n}$$

$\langle m,k_m|$ where $\langle m,k_m|n,k_n\rangle = \delta_{mn}\delta_{k_m k_n}$ by completeness

$$\Longrightarrow (E - E_m^0) c_{m,k_m} = \lambda \sum_{n,k_n} \langle m,k_m| \hat{H}_1 |n,k_n\rangle c_{n,k_n}$$

Still general, but we can look for a solution in series of λ:

$$E = E^0 + \lambda E^1 + \lambda^2 E^2 + \dots$$

$$c_{m,k_m} = c^0_{m,k_m} + \lambda c^1_{m,k_m} + \dots$$

[4]

$$\rightarrow (E^0 - E_m^0) c^0_{m,k_m} + \lambda E^1 c^0_{m,k_m} + \dots$$

$$= \lambda \sum_{n,k_n} \langle m,k_m| \hat{H}_1 |n,k_n\rangle c^0_{n,k_n} + \dots$$

∞-many equations
for each $m, k_m \dots$

which, at $\mathcal{O}(\lambda^0)$, says $0 = (E^0 - E^0_{m^0}) c^0_{m,k_m} \quad \forall m, k_m$.

Let's instead focus on one of the E_m^0 levels, denote it with

the energy expansions can be different for each $m, k_m \dots$

m^* : $E^0 = E^0_{m^*}$.

and let $C^0_{m\neq m^*,\, k_{m^*}} = 0$,

$C^0_{m^*,\, k_{m^*}}$ undetermined.

Hence only $m = m_*$ term remains from [4] at $O(\lambda)$

Thus from [4] we obtain

$$E^1 C^0_{m^*,\, k_{m^*}} = \sum_{k'_{m^*}} \langle m^*, k_{m^*} | \hat{H}_1 | m^*, k'_{m^*} \rangle \, C^0_{m^*,\, k'_{m^*}}$$

an $r_{m^*} \times r_{m^*}$ matrix, where r_{m^*} indicates the maximum degree of degeneracy of m^* state.

Invoke notation $(\hat{H}_1)_{k,k'} \equiv \langle m^*, k_{m^*} | \hat{H}_1 | m^*, k_{m^*}' \rangle$

$$C^0_{m^*,\, k_{m^*}} = C^0_k$$

$$\sum_{k'=1}^{r_{m^*}} \left[E^1 \delta_{kk'} - (\hat{H}_1)_{k,k'} \right] C^0_{k'} = 0$$

which only has solutions if $\det\left(E^1 \delta_{kk'} - (\hat{H}^1)_{k,k'} \right) = 0$

or that E^1 are the eigenvalues of $(\hat{H}_1)_{k,k'}$.

The first order corrections to the m^*-th degenerate level (degeneracy k_{m^*}) are the eigenvalues of the perturbation $\hat{H}_1$ in the basis of unperturbed states $|m^*, k_{m^*}\rangle$ of energy $E^0_{m^*}$.

$\Rightarrow$ We can choose $|m^*, K_{m^*}\rangle$ such that $\hat{H}_1$ is diagonal in the $E^0_{m^*}$ - subspace [since $(\hat{H}_1)_{K,K'}$ is Hermitian $r_{m^*} \times r_{m^*}$ matrix, this is always possible] and therefore

$$E_{m^*, K_{m^*}} = E^0_{m^*} + \lambda \overbrace{\langle m^*, K_{m^*} | \hat{H}_1 | m^*, K_{m^*}\rangle}^{E_1}$$

provided $\langle m^*, K_{m^*} | \hat{H}_1 | m^*, K'_{m^*}\rangle$ is diagonal.

Finding a diagonal basis may not always be obvious; if so we can take any basis and compute the $\langle m^*, K_{m^*} | \hat{H}_1 | m^*, K'_{m^*}\rangle$ matrix and find E' by solving

$$\det\left(E' \delta_{KK'} - \langle m^*, K_{m^*} | \hat{H}_1 | m^*, K'_{m^*}\rangle\right) = 0$$

If one works in the basis where $\hat{H}_1$ is diagonal, we find

$$E_{m,K_m} = E^0_m + \lambda \langle m, K_m | \hat{H}_1 | m, K_m\rangle + \lambda^2 \sum_{\substack{K_n\ (n \neq m) \\ n=m\ (K_n \neq K_m)}} \frac{|\langle m, K_m | \hat{H}_1 | n, K_n\rangle|^2}{E^0_m - E^0_n}$$

given w/o proof

First order wavefunction left for DIY.

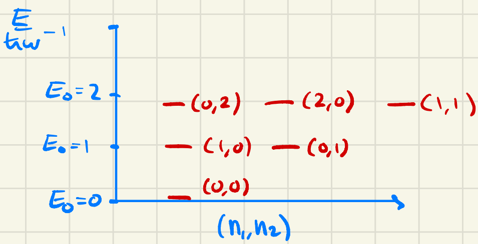
Note: to $\mathcal{O}(\lambda)$ the perturbation may lift all the degeneracy

Ex. 2d SHO

$$\hat{H}_0 = \frac{\hat{P}_x^2}{2m} + \frac{m\omega^2}{2}\hat{x}^2 + \frac{\hat{P}_y^2}{2m} + \frac{m\omega^2}{2}\hat{y}^2$$

$$= -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) + \frac{m\omega^2}{2}(\hat{x}^2 + \hat{y}^2)$$

$$E^0(n_1, n_2) = \hbar\omega(n_1 + n_2 + 1) \; ; \quad H^0|n_1, n_2\rangle = E^0|n_1, n_2\rangle$$



Degeneracy increases as E increases.

Let $\hat{H}_1 = 4\varepsilon\hat{x}^2\hat{y}^2$, how to solve now?

In perturbation theory, $\mathcal{O}(\varepsilon)$ and E' ?

$N=1$: unique (00)

$N=2$: two states (01) (10)

$N=3$: three states (20) (11) (02)

For generality set $\hbar = m = \omega = 1$ so

$$\hat{H}_0 = (a_x^\dagger a_x + a_y^\dagger a_y + 1) \qquad [a_i, a_j^\dagger] = \delta_{ij}$$

$$\hat{H}_1 = \varepsilon(a_x^\dagger + a_x)^2(a_y^\dagger + a_y)^2$$

then $\langle n' | (a_x^\dagger + a_x)^2 | n \rangle = \delta_{nn'} (2n+1) + \delta_{n-2,n'} \sqrt{n(n-1)} + \delta_{n+2,n'} \sqrt{(n+1)(n+2)}$ $\Big\}$ $(*)$

Consider the $N=2$ level where $|0,1\rangle$, $|1,0\rangle$ are degenerate unpertubed states. We need

$$(\hat{H}')_{kk'} \equiv \begin{pmatrix} \langle 0,1 | H_1 | 0,1 \rangle & \langle 0,1 | H_1 | 1,0 \rangle \\ \langle 1,0 | H_1 | 0,1 \rangle & \langle 1,0 | H_1 | 1,0 \rangle \end{pmatrix}$$

by $(*)$ this $(\hat{H}')_{kk'}$ is diagonal.

$$\langle 1,0 | H' | 0,1 \rangle = \varepsilon \langle 1 | (a_x^\dagger + a_x)^2 | 0 \rangle \cdot \underbrace{\langle 0 | (a_y^\dagger + a_y)^2 | 1 \rangle}_{0}$$

$$= 0$$

by raising / lowering

similarly for $\langle 0,1 | H' | 1,0 \rangle \ldots$

So $$(H')_{k,k'} = \varepsilon \begin{pmatrix} (2 \cdot 1 + 1) \cdot 1 & 0 \\ 0 & 1 \cdot (2 \cdot 1 + 1) \end{pmatrix}$$

$$= 3\varepsilon \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Diagonal and degeneracy isn't lifted to $O(\varepsilon)$ ... Try $N=3$.

Here we have 3 degeneracies

$|0,2\rangle \quad |2,0\rangle \quad |1,1\rangle$

$$(\hat{H})_{k,k'} = \begin{pmatrix} \langle 0,2|H'|0,2\rangle & \langle 0,2|H'|2,0\rangle & \underset{0}{\langle 0,2|\cancel{H'}|1,1\rangle} \\ \langle 2,0|H'|0,2\rangle & \langle 2,0|H'|2,0\rangle & \underset{0}{\langle 2,0|\cancel{H'}|1,1\rangle} \\ \underset{0}{\langle 1,1|\cancel{H'}|0,2\rangle} & \underset{0}{\langle 1,1|\cancel{H'}|2,0\rangle} & \langle 1,1|H'|1,1\rangle \end{pmatrix}$$

$$\langle 1,1|H'|1,1\rangle = \varepsilon \cdot 3 \cdot 3 = 9\varepsilon$$

$$\langle 0,2|H'|0,2\rangle = \langle 2,0|H'|2,0\rangle = 5\varepsilon$$

$$\langle 0,2|H'|2,0\rangle = \langle 2,0|H'|0,2\rangle = 2\varepsilon$$

So $$(H')_{k,k'} = \varepsilon \begin{pmatrix} 5 & 2 & 0 \\ 2 & 5 & 0 \\ 0 & 0 & 9 \end{pmatrix}$$

$\begin{pmatrix} 5 & 2 \\ 2 & 5 \end{pmatrix}$ has $\lambda_1 \cdot \lambda_2 = 21$, $\lambda_1 + \lambda_2 = 10$ $\Rightarrow$ $\lambda_1 = 7$, $\lambda_2 = 3$

$$\text{diag}(H')_{k,k'} = \begin{pmatrix} 7 & & \\ & 3 & \\ & & 9 \end{pmatrix}$$

which has eigenvectors.

$\therefore$ Choice of basis isn't arbitrary, we need to choose a basis that diagonalizes $\hat{H}_1$.

We Start in the degenerate subspace of $\hat{H}$ which makes the perturbation diagonal.