L67-Degenerate Perturbation Theory

Monday, March 7, 2016 08:08

* Review: Quantum Mechanical perturbation theory is a systematic method of diagonalizing matrices:

- decompose into diagonal + perturbation
- may be the only way of diagonalizing $\infty \times \infty$ matrix!

* Example: 3x3 matrix:

$$\begin{pmatrix} \lambda_1+\alpha & \delta & \varepsilon \\ \delta & \lambda_2+\beta & \zeta \\ \varepsilon & \zeta & \lambda_3+\gamma \end{pmatrix}\begin{pmatrix} V_1 \\ V_2 \\ V_3 \end{pmatrix} = \Lambda \begin{pmatrix} V_1 \\ V_2 \\ V_3 \end{pmatrix}$$

0) $\mathcal{H}^0 \psi_n^0 = E_n^0 \psi_n^0$: $\mathcal{H} = \begin{pmatrix} \lambda_1 & & \\ & \lambda_2 & \\ & & \lambda_3 \end{pmatrix}$

1a) $E_n^1 = V_{nn} = \langle \psi_n^0 | \mathcal{H}' | \psi_n^0 \rangle$ $\quad E_1^1 = \alpha \quad E_2^1 = \beta \quad E_3^1 = \gamma$

b) $|\psi_n^1\rangle = \sum_{m\neq n} \frac{V_{mn}}{\Delta_{nm}} |\psi_m^0\rangle = \sum_{m \neq n} \frac{|\psi_m^0\rangle\langle\psi_m^0|\mathcal{H}'|\psi_n^0\rangle}{E_n - E_m}$ $\quad \mathcal{H} V = V \Lambda$ to first order in $\alpha, \beta, \gamma, \delta, \varepsilon, \zeta$.

$$\vec{V}_1 = \begin{pmatrix}1\\0\\0\end{pmatrix} + \frac{\delta}{\lambda_1-\lambda_2}\begin{pmatrix}0\\1\\0\end{pmatrix} + \frac{\varepsilon}{\lambda_1-\lambda_3}\begin{pmatrix}0\\0\\1\end{pmatrix}$$

$$\vec{V}_2 = \frac{\delta}{\lambda_2-\lambda_1}\begin{pmatrix}1\\0\\0\end{pmatrix} + \begin{pmatrix}0\\1\\0\end{pmatrix} + \frac{\zeta}{\lambda_2-\lambda_3}\begin{pmatrix}0\\0\\1\end{pmatrix}$$

$$\vec{V}_3 = \frac{\varepsilon}{\lambda_3-\lambda_1}\begin{pmatrix}1\\0\\0\end{pmatrix} + \frac{\zeta}{\lambda_3-\lambda_2}\begin{pmatrix}0\\1\\0\end{pmatrix} + \begin{pmatrix}0\\0\\1\end{pmatrix}$$

$$\begin{pmatrix} \lambda_1+\alpha & \delta & \varepsilon \\ \delta & \lambda_2+\beta & \zeta \\ \varepsilon & \zeta & \lambda_3+\gamma \end{pmatrix}\begin{pmatrix} 1 & \frac{\delta}{\lambda_1-\lambda_2} & \frac{\varepsilon}{\lambda_1-\lambda_3} \\ \frac{\delta}{\lambda_2-\lambda_1} & 1 & \frac{\zeta}{\lambda_2-\lambda_3} \\ \frac{\varepsilon}{\lambda_3-\lambda_1} & \frac{\zeta}{\lambda_3-\lambda_2} & 1 \end{pmatrix} \overset{?}{\cong} \begin{pmatrix} 1 & \frac{\delta}{\lambda_1-\lambda_2} & \frac{\varepsilon}{\lambda_1-\lambda_3} \\ \frac{\delta}{\lambda_2-\lambda_1} & 1 & \frac{\zeta}{\lambda_2-\lambda_3} \\ \frac{\varepsilon}{\lambda_3-\lambda_1} & \frac{\zeta}{\lambda_3-\lambda_2} & 1 \end{pmatrix}\begin{pmatrix} \lambda_1+\alpha & & \\ & \lambda_2+\beta & \\ & & \lambda_3+\gamma \end{pmatrix}$$

$\vec{V}_1 \quad \vec{V}_2 \quad \vec{V}_3$ $\qquad +E_1^2 \quad +E_2^2 \quad +E_3^2$

2) $E_n^2 = \sum_{m\neq n} \frac{|V_{mn}|^2}{\Delta_{nm}} = \sum_{m\neq n} \frac{|\langle\psi_m^0|\mathcal{H}'|\psi_n^0\rangle|}{E_n - E_m}$

$E_1^2 = \frac{\delta^2}{\lambda_1-\lambda_2} + \frac{\varepsilon^2}{\lambda_1-\lambda_3} \qquad E_2^2 = \frac{\delta^2}{\lambda_2-\lambda_1} + \frac{\zeta^2}{\lambda_2-\lambda_3} \qquad E_3^2 = \frac{\varepsilon^2}{\lambda_3-\lambda_1} + \frac{\zeta^2}{\lambda_3-\lambda_2}$

- this fixes the diagonal entries, but adds extra terms to off-diagonal
- we need $|\psi_n^2\rangle$ to fix off-diagonal entries of $\mathcal{H}V = V\Lambda$

* What about the case where $\mathcal{H}^0$ is degenerate? $\mathcal{H} = \begin{pmatrix} \lambda+\alpha & \delta & \varepsilon \\ \delta & \lambda+\beta & \zeta \\ \varepsilon & \zeta & \mu+\gamma \end{pmatrix}$

- In this case, $|\psi_1^1\rangle$ and $|\psi_2^1\rangle$ explode! $\frac{1}{\lambda-\lambda}$ also E_1^2, E_2^2 by extension.

- the basis vectors $\begin{pmatrix}1\\0\\0\end{pmatrix}$ and $\begin{pmatrix}0\\1\\0\end{pmatrix}$ are degenerate, that means that even the energy E_1^1, E_1^2 depends on the arbitrary linear combination of these chosen on the arbitrary linear combination of these chosen

$$E_1^1 = (c_\theta\ s_\theta\ 0)\begin{pmatrix}\alpha & \delta & \varepsilon\\ \delta & \beta & \xi\\ \varepsilon & \xi & \gamma\end{pmatrix}\begin{pmatrix}c_\theta\\ s_\theta\\ 0\end{pmatrix} \qquad E_2^1 = (-s_\theta\ c_\theta\ 0)\begin{pmatrix}\alpha & \delta & \varepsilon\\ \delta & \beta & \xi\\ \varepsilon & \xi & \gamma\end{pmatrix}\begin{pmatrix}-s_\theta\\ c_\theta\\ 0\end{pmatrix}$$

$$= c_\theta^2\alpha + s_\theta^2\beta + s_{2\theta}\delta \qquad\qquad = -s_\theta^2\alpha + c_\theta^2\beta - s_{2\theta}\delta$$

- how do you know which values to use?

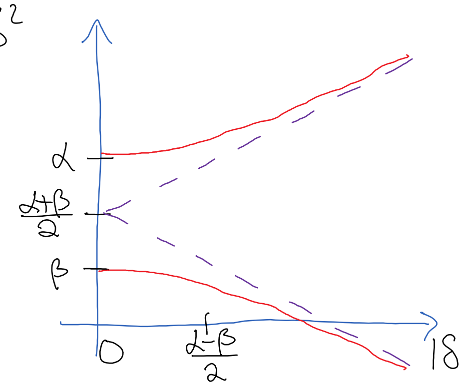
If $W = \begin{pmatrix}\alpha & \delta\\ \delta & \beta\end{pmatrix} \not\propto I$, ie if $\alpha \neq \gamma$ or $\beta \neq 0$, then we can use the eigenvectors of $\mathcal{H}'$ to break the degeneracy of $\mathcal{H}$ [only in this subspace]

$$|W - E^1 I| = \begin{vmatrix}\alpha - E^1 & \delta\\ \delta & \beta - E^1\end{vmatrix} = (\alpha - E^1)(\beta - E^1) - \delta^2$$

$$= E^{1\,2} - (\alpha+\beta)E^1 + \underbrace{(\alpha\beta - \delta^2)}_{|W|} = 0$$

$$E^1 = \frac{\alpha+\beta}{2} \pm \sqrt{\left(\frac{\alpha+\beta}{2}\right)^2 - (\alpha\beta - \delta^2)}$$

$$= \frac{1}{2}\left(\alpha + \beta \pm \sqrt{(\alpha-\beta)^2 + 4\delta^2}\right)$$

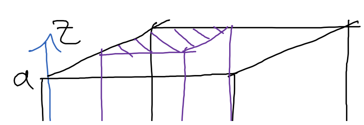


* Theorem: let A be a Hermitian operator that commutes with $\mathcal{H}_0$, $\mathcal{H}'$. If ψ_a^0, ψ_b^0, the degenerate eigenfunctions of $\mathcal{H}_0$ are also eigenfunctions of A with distinct eigenvalues, then $W_{ab} = 0$, and hence ψ_a^0, ψ_b^0 are good states to use in perturbation theory.

proof: $[\mathcal{H}_0, A]$ form a set of commuting observables (complete in this 2-d space). Since $[\mathcal{H}_0, \mathcal{H}'] = 0 = [A, \mathcal{H}']$, $\mathcal{H}'$ has the same eigenvectors and is diagonal in ψ_a^0, ψ_b^0.

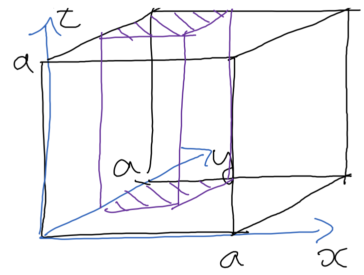
* How to avoid dividing by 0 in above formulas:
Divide by $\Delta_{nm}(E^0 + E^1)$ instead of $\Delta_{nm}(E^0)$, which are distinct.

* Example 6.2 3-d inf. square well



$V(x,y,z) = \{ 0 \quad 0 < x, y < a$

Example 6.2 3-d inf. square well



$$V(x,y,z) = \begin{cases} 0 & 0 < x,y,z < a \\ \infty & \text{otherwise} \end{cases}$$

$$E^0_{n_x n_y n_z} = \frac{\pi^2\hbar^2}{2ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

$$\psi^0_{n_x n_y n_z} = \left(\frac{2}{a}\right)^{3/2} \sin\left(\frac{n_x\pi}{a}x\right) \sin\left(\frac{n_y\pi}{a}y\right) \sin\left(\frac{n_z\pi}{a}z\right)$$

ground state: ψ^0_{111} nondegenerate $\rightarrow$ $E^0_0 = \frac{\pi^2\hbar^2}{2ma^2}\cdot 3$

$\psi_a = \psi^0_{112}$, $\psi_b = \psi^0_{121}$, $\psi_c = \psi^0_{211}$ tripply degenerate: $\rightarrow$ $E^0_1 = \frac{\pi^2\hbar^2}{2ma^2}\cdot 6$

Perturbation: $\mathcal{H}' = \begin{cases} V_0 & \text{if } 0 < x,y < a/2 \\ 0 & \text{otherwise} \end{cases}$

$$E^1_0 = \langle \psi^0_{111} | \mathcal{H}' | \psi^0_{111} \rangle = \frac{1}{4}V_0$$

$W_{aa} = \langle \psi_a | \mathcal{H}' | \psi_a \rangle = \frac{1}{4}V_0 = W_{bb} = W_{cc}$

$W_{ab} = \langle \psi_a | \mathcal{H}' | \psi_b \rangle = 0 = W_{ac}$

$W_{bc} = \langle \psi_b | \mathcal{H}' | \psi_c \rangle = \left(\frac{8}{3\pi}\right)^2 V_0$ (see 2-d example)

$$W = \frac{V_0}{4}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & \kappa \\ 0 & \kappa & 1 \end{pmatrix}$$

Apply above form on lower 2x2 matrix: $\alpha = \beta = 1$ $\delta = \kappa$

$$E_1(\lambda) = E^0_1 + \frac{1}{4}V_0\left(1,\ 1+\kappa,\ 1-\kappa\right)$$

$\underbrace{}_{\pm\kappa}$