Exercício do CAP VI do Griffiths: Teoria de Perturbação

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∗**Problem 6.9** Consider a quantum system with just *three* linearly independent states. Suppose the Hamiltonian, in matrix form, is

$$\mathbf{H} = V_0 \begin{pmatrix} (1-\epsilon) & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix}.$$

where V_0 is a constant, and ϵ is some small number ($\epsilon \ll 1$).

(a) Write down the eigenvectors and eigenvalues of the *unperturbed* Hamiltonian ($\epsilon = 0$).

(b) Solve for the *exact* eigenvalues of $\mathbf{H}$. Expand each of them as a power series in ϵ, up to second order.

(c) Use first- and second-order *non*degenerate perturbation theory to find the approximate eigenvalue for the state that grows out of the nondegenerate eigenvector of H^0. Compare the exact result, from (a).

(d) Use *degenerate* perturbation theory to find the first-order correction to the two initially degenerate eigenvalues. Compare the exact results.

$$H = H^0 + H'$$

$$V_0 \begin{pmatrix} (1-\epsilon) & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix} = \underbrace{V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}}_{H^0} + \underbrace{\epsilon\, V_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}}_{H'}$$

$$H \quad \rightarrow \quad \{|1\rangle, |2\rangle, |3\rangle\}$$

$$H = \begin{pmatrix} \langle 1|H|1\rangle & \langle 1|H|2\rangle & \langle 1|H|3\rangle \\ \langle 2|H|1\rangle & \langle 2|H|2\rangle & \langle 2|H|3\rangle \\ \langle 3|H|1\rangle & \langle 3|H|2\rangle & \langle 3|H|3\rangle \end{pmatrix}$$

(a) Write down the eigenvectors and eigenvalues of the *unperturbed* Hamiltonian

- Hamiltoniano não perturbado:

$$H^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

- Autovetores normalizados:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

- Autovalores:

$$E_1^0 = V_0 \qquad E_2^0 = V_0 \qquad E_3^0 = 2V_0$$

(b) Solve for the *exact* eigenvalues of **H**. Expand each of them as a power series in ϵ, up to second order.

$$\mathbf{H}\,\psi = \lambda\,\psi$$

$$\mathbf{H} = V_0 \begin{pmatrix} (1-\epsilon) & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix}$$

- Equação característica:

$$\det(\boldsymbol{H} - \boldsymbol{I}\,\lambda) = 0$$

$$\begin{vmatrix} [V_0(1-\epsilon)-\lambda] & 0 & 0 \\ 0 & [V_0-\lambda] & \epsilon V_0 \\ 0 & \epsilon V_0 & [2V_0-\lambda] \end{vmatrix} = 0$$

- Polinômio característico:

$$[V_0(1-\epsilon)-\lambda][(V_0-\lambda)(2V_0-\lambda)-(\epsilon V_0)^2] = 0$$

$$\lambda_1 = V_0(1-\epsilon) \qquad \lambda^2 - 3V_0\lambda + (2V_0^2 - \epsilon^2 V_0^2) = 0$$

$$\lambda = \frac{3V_0 \pm \sqrt{9V_0^2 - 4(2V_0^2 - \epsilon^2 V_0^2)}}{2} = \frac{V_0}{2}\left[3 \pm \sqrt{1+4\epsilon^2}\right]$$

- Autovalores exatos de **H**:

$$\sqrt{1+4\epsilon^2} \sim 1+2\epsilon^2$$

$$\lambda_1 = V_0(1-\epsilon)$$

$$\lambda_2 = \frac{V_0}{2}\left(3-\sqrt{1+4\epsilon^2}\right) \approx V_0(1-\epsilon^2)$$

$$\lambda_3 = \frac{V_0}{2}\left(3+\sqrt{1+4\epsilon^2}\right) \approx V_0(2+\epsilon^2)$$

(c) Use first- and second-order *non*degenerate perturbation theory to find the approximate eigenvalue for the state that grows out of the nondegenerate eigenvector of H^0. Compare the exact result, from (a).

$$H^0 = V_0 \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

- Autoestado não degenerado de **H⁰** :

$$E_3^0 = 2V_0 \qquad |3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

- Correção de primeira ordem no autovalor:

$$\mathrm{H}' = \epsilon V_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \rightarrow E_3^1 = \langle 3|\, H' |3\rangle = \epsilon V_0 \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

$$= \epsilon V_0 \begin{pmatrix} 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0$$

- não temos correção $1^{\underline{a}}$ ordem

- Correção de segunda ordem no autovalor:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \quad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad \mathrm{H}' = \epsilon V_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

$$E_3^2 = \sum_{m=1,2} \frac{|\langle m| H' |3\rangle|^2}{E_3^0 - E_m^0}$$

$$\langle 1| H' |3\rangle = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = 0$$

$$\langle 2| H' |3\rangle = \epsilon V_0 \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \epsilon V_0$$

$$E_3^2 = \frac{|\langle 2|\, H' |3\rangle|^2}{E_3^0 - E_2^0}$$

$$\begin{cases} \langle 2|\, H' |3\rangle = \epsilon\, V_0 \\ E_3^0 - E_2^0 = 2V_0 - V_0 = V_0 \end{cases}$$

$$\therefore\; E_3^2 = (\epsilon V_0)^2 / V_0 = \epsilon^2 V_0$$

- Autovalor corrigido até segunda orderm em ϵ :

$$\Rightarrow E_3 = E_3^0 + E_3^1 + E_3^2 = 2V_0 + 0 + \epsilon^2 V_0 = V_0(2 + \epsilon^2)$$

resultado exato até segunda ordem em ϵ :

$$\lambda_3 \approx V_0(2 + \epsilon^2)$$

(d) Use *degenerate* perturbation theory to find the first-order correction to the two initially degenerate eigenvalues. Compare the exact results.

Teroria de perturbação - estados degenerados

- Estados degenerados de **H**^{0} ψ_a^0 , ψ_b^0

$$H^0\psi_a^0 = E^0\psi_a^0, \quad H^0\psi_b^0 = E^0\psi_b^0, \quad \langle\psi_a^0|\psi_b^0\rangle = 0$$

- Combinação linear desses estados:

$$\psi^0 = \alpha\psi_a^0 + \beta\psi_b^0$$

autoestado de **H**^{0}

$$H^0\psi^0 = E^0\psi^0$$

- Queremos resolver a equação de Schrodinger:

$$H\psi = E\psi \qquad H = H^0 + \lambda H'$$

$$\begin{cases} E = E^0 + \lambda E^1 \\ \psi = \psi^0 + \lambda \psi^1 \end{cases}$$

correções até a primeira ordem no espectro de energia e autoestado do **H** do problema perturbado.

$$H^0\psi^0 + \lambda(H'\psi^0 + H^0\psi^1) + \cdots = E^0\psi^0 + \lambda(E^1\psi^0 + E^0\psi^1) + \cdots$$

- ordem zero em λ:

$$H^0\psi^0 = E^0\psi^0$$

- ordem 1 em λ:

$$H^0\psi^1 + H'\psi^0 = E^0\psi^1 + E^1\psi^0$$

- ordem 1 em λ:

$$H^0\psi^1 + H'\psi^0 = E^0\psi^1 + E^1\psi^0$$

Produto escalar com ψ_a^0

$$\langle\psi_a^0|H^0\psi^1\rangle + \langle\psi_a^0|H'\psi^0\rangle = E^0\langle\psi_a^0|\psi^1\rangle + E^1\langle\psi_a^0|\psi^0\rangle$$

H^0 Hermitiano

Considerando a combinação linear $\psi^0 = \alpha\,\psi_a^0 + \beta\,\psi_b^0$ teremos:

$$\alpha\langle\psi_a^0|H'|\psi_a^0\rangle + \beta\langle\psi_a^0|H'|\psi_b^0\rangle = \alpha E^1$$

- ordem 1 em λ:

$$H^0\psi^1 + H'\psi^0 = E^0\psi^1 + E^1\psi^0$$

Produto escalar com ψ_b^0

$$\alpha\langle\psi_b^0|H'|\psi_a^0\rangle + \beta\,\langle\psi_b^0|H'|\psi_b^0\rangle = \beta E^1$$

- Sistema de equações

$$\alpha\langle\psi_a^0|H'|\psi_a^0\rangle + \beta\langle\psi_a^0|H'|\psi_b^0\rangle = \alpha E^1$$

$$\alpha\langle\psi_b^0|H'|\psi_a^0\rangle + \beta\langle\psi_b^0|H'|\psi_b^0\rangle = \beta E^1$$

$$\rightarrow\ W_{ij} \equiv \langle\psi_i^0|H'|\psi_j^0\rangle, \quad (i, j = a, b)$$

- Reescrevo em termos dos elementos da matriz **W**

$$\alpha W_{aa} + \beta W_{ab} = \alpha E^1$$

$$\alpha W_{ba} + \beta W_{bb} = \beta E^1$$

- Forma matricial do sistema de equações:

$$\begin{pmatrix} W_{aa} & W_{ab} \\ W_{ba} & W_{bb} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E^1 \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

$$\rightarrow \det(\boldsymbol{W} - \boldsymbol{I}\, E^1) = 0$$

- Polinômio característico: $(W_{aa} - E^1)(W_{bb} - E^1) - W_{ab}W_{ba} = 0$

$$(E^1)^2 - E^1(W_{aa} + W_{bb}) + (W_{aa}W_{bb} - W_{ab}W_{ba}) = 0$$

- Correção de primeira ordem para autovalor degenerado:

$$E^1_{\pm} = \frac{1}{2}\left[W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2}\,\right]$$

$$W_{ba} = W_{ab}^*$$

(d) Use *degenerate* perturbation theory to find the first-order correction to the two initially degenerate eigenvalues. Compare the exact results.

$$H' = \epsilon V_0 \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$$

- Autovetores degenerados $\mathbf{H}^0$:

$$|1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

Autovalor:

$$E_1^0 = E_2^0 = V_0$$

- Elementos da Matriz W

$$W_{aa} = \langle 1|\, H' |1\rangle = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 \\ 0 \\ 0 \end{pmatrix} = -\epsilon V_0$$

$$W_{bb} = \langle 2|\, H' |2\rangle = \epsilon V_0 \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \epsilon V_0 \begin{pmatrix} 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0$$

$$W_{ab} = \langle 1|\, H' |2\rangle = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} -1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \epsilon V_0 \begin{pmatrix} 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0$$

$$W_{ba} = 0.$$

- Solução para correção de primeira ordem dos autovalores degenereados:

$$E_{\pm}^{1} = \frac{1}{2}\left[W_{aa} + W_{bb} \pm \sqrt{(W_{aa} - W_{bb})^2 + 4|W_{ab}|^2}\right]$$

Teremos:

$$E_{\pm}^{1} = \frac{1}{2}\left[-\epsilon V_0 + 0 \pm \sqrt{\epsilon^2 V_0^2 + 0}\right] = \frac{1}{2}(-\epsilon V_0 \pm \epsilon V_0)$$

Finalmente: $E_1^0 = E_2^0 = V_0 \quad E_{-}^1 = -\epsilon V_0 \quad E_{+}^1 = 0$

➡ $E_1 = E_1^0 + E_{-}^1 = V_0 - \epsilon V_0$

➡ $E_2 = E_2^0 + E_{+}^1 = V_0$

resultado exato até primeira ordem em ϵ:

$$\lambda_1 = V_0(1-\epsilon) \qquad \lambda_2 = V_0$$