# PHY 304, II-Semester 2023/24, Tutorial 3

8. Feb. 2024

*Discuss on your table in AIR. When all teams finished a stage, make sure all students at your table understand the solution and agree on one by using the board.*

**Stage 1 Degenerate versus non-degenerate perturbation theory** Let us see some pitfalls in improperly using non-degenerate PT when one should use degenerate one with a toy example, similar to tutorial 2, stage 3. Consider an abstract three-level system[1] in dimensionless units, with Hamiltonians in matrix form given below, using the basis $\{|1\rangle, |2\rangle, |3\rangle\}$ in that order. The sheet provides the splitting into unperturbed Hamiltonian $\hat{H}^{(0)}$ and perturbed Hamiltonian $\hat{H}'$.

In all cases, we can avoid perturbation theory and just diagonalize the $3 \times 3$ matrix, and then Taylor expand the eigenvalues to first and second order in $\lambda$ (see `tutorial3_v1.nb`, but do not look at that yet, all required results from it are provided on this sheet).

(i) **Non-degenerate case:** Find all first and second order energy corrections, for Hamiltonian $\hat{H} = \hat{H}^{(0)} + \hat{H}'$ with ($\Delta_2 \neq \Delta_3$, $\lambda$ small):

$$\hat{H}^{(0)} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \Delta_2 & 0 \\ 0 & 0 & \Delta_3 \end{bmatrix}, \qquad \hat{H}' = \begin{bmatrix} 0 & \lambda & \lambda \\ \lambda & 0 & 0 \\ \lambda & 0 & 0 \end{bmatrix}. \tag{1}$$

*Hint, the final energies to second order are*
$\{E_1 = -\frac{\Delta_2+\Delta_3}{\Delta_2\Delta_3}\lambda^2,\ E_2 = \Delta_2 + \frac{\lambda^2}{\Delta_2},\ E_3 = \Delta_3 + \frac{\lambda^2}{\Delta_3}\} + \mathcal{O}(\lambda^3)$.

(ii) **Degenerate case:** Now let $\Delta_2 = \Delta_3 \to \Delta_0$, and change the perturbation as shown below.

$$\hat{H}^{(0)} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \Delta_0 & 0 \\ 0 & 0 & \Delta_0 \end{bmatrix}, \qquad \hat{H}' = \begin{bmatrix} 0 & \lambda & 0 \\ \lambda & 0 & \lambda \\ 0 & \lambda & 0 \end{bmatrix}. \tag{2}$$

Calculate (or attempt to calculate) again the perturbed energies to order $\mathcal{O}(\lambda^2)$ using non-degenerate perturbation theory. Discuss what happens separately for perturbations of the state $|1\rangle$ versus states $|2,3\rangle$. Then compare with the correct values: $\{E_1 = -\lambda^2/\Delta_0,\ \tilde{E}_2 = \Delta_0 + \lambda + \lambda^2/(2\Delta_0),\ \tilde{E}_3 = \Delta_0 - \lambda + \lambda^2/(2\Delta_0)\}$. (Here $\tilde{E}$ indicates that you cannot directly associate these eigenvalues with any of the unperturbed eigenstates). Now redo the calculation using degenerate perturbation theory and compare again.

(iii) **Degenerate case, perturbation diagonal in unperturbed basis:** Now let's look at a simpler case

$$\hat{H}^{(0)} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \Delta_0 & 0 \\ 0 & 0 & \Delta_0 \end{bmatrix}, \qquad \hat{H}' = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \lambda \end{bmatrix}. \tag{3}$$

[1] Abstract means we don't care about the underlying physical system for now, because it does not matter.

Use non-degenerate PT to first order, and compare with the true eigenvalues. Discuss.

**Stage 2 Variational method:** Consider the simple harmonic oscillator with

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 x^2. \tag{4}$$

(a) Use the variational method with the normalized trial function $\varphi(x) = (2\beta/\pi)^{1/4} e^{-\beta x^2}$ with variational parameter $\beta$. Find the value of $\beta$ that gives the best approximation of the ground-state and ground-state wavefunction. *Hint: You may use* $\int_{-\infty}^{\infty} dx\, e^{-\alpha x^2} x^2 = \sqrt{\pi}/(2\alpha^{3/2})$, *for real* $\alpha > 0$ *(in all the following), and* $\int_{-\infty}^{\infty} dx\ e^{-\alpha x^2} \frac{\partial^2}{\partial x^2} e^{-\alpha x^2} = -\sqrt{\frac{\pi\alpha}{2}}$.

(b) Using that result, also find the variational value for the ground-state energy. Discuss the reason for the accuracy of the answers that you find