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

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 3×3 matrix, and then Taylor expand the eigenvalues to first and second order in λ (see `tutorial3_v3.nb`, but do not look at that yet, all required results from it are provided on this sheet).

(i) **Non-degenerate case:** Find the first and second order energy correction for the three states, if the Hamiltonian is $\hat{H} = \hat{H}^{(0)} + \hat{H}'$ with ($\Delta_2 \neq \Delta_3$, λ 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
$\{E_1 = -\frac{\Delta_2+\Delta_3}{\Delta_2\Delta_3}\lambda^2,\ E_2 = \Delta_2 + \frac{\lambda^2}{\Delta_2},\ E_3 = \Delta_3 + \frac{\lambda^2}{\Delta_3}\} + \mathcal{O}(\lambda^3)$.
Solution: Using Eq. (7.12), we directly see that all first order corrections $E_n^{(1)} = \langle\, n\,|\hat{H}'|\,n\,\rangle$ *are zero, since* $\hat{H}'$ *does not contain any diagonal elements. Proceeding to second order with Eq. (7.23), for the present case we can explicitly write*

$$E_1^{(2)} = \underbrace{|\langle\, 2\,|\hat{H}'|\,1\,\rangle|^2}_{=\lambda^2} / \underbrace{(E_1^{(0)} - E_2^{(0)})}_{=-\Delta_2} + \underbrace{|\langle\, 3\,|\hat{H}'|\,1\,\rangle|^2}_{=\lambda^2} / \underbrace{(E_1^{(0)} - E_3^{(0)})}_{=-\Delta_3} = -\frac{\Delta_2+\Delta_3}{\Delta_2\Delta_3}\lambda^2 \tag{2}$$

$$E_2^{(2)} = \underbrace{|\langle\, 1\,|\hat{H}'|\,2\,\rangle|^2}_{=\lambda^2} / \underbrace{(E_2^{(0)} - E_1^{(0)})}_{=\Delta_2} = \lambda^2/\Delta_2 \tag{3}$$

$$E_3^{(2)} = \underbrace{|\langle\, 1\,|\hat{H}'|\,3\,\rangle|^2}_{=\lambda^2} / \underbrace{(E_3^{(0)} - E_1^{(0)})}_{=\Delta_3} = \lambda^2/\Delta_3 \tag{4}$$

Adding these to the unperturbed energies, we recover the Taylor expansion of the exact energies.

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

$$\hat{H}^{(0)} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \Delta_0 & 0 \\ 0 & 0 & \Delta_0 \end{bmatrix}, \qquad \hat{H}' = \begin{bmatrix} 0 & \lambda & 0 \\ \lambda & 0 & \lambda \\ 0 & \lambda & 0 \end{bmatrix}. \tag{5}$$

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

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.
Solution: All first order contributions are zero, since the diagonal of the matrix $\hat{H}'$ contains only zeros. Comparison with the exact eigenvalues tells us that this result is already wrong, since there should be contributions linear in λ. Similar to the calculation in (i), the energy eigenvalues up to the second order of λ using non-degenerate PT theory are:

$$\begin{aligned} E_1^{(2)} &= \underbrace{|\langle\,2\,|\hat{H}'|\,1\,\rangle|^2}_{=\lambda^2} / \underbrace{(E_1^{(0)} - E_2^{(0)})}_{=-\Delta_0} + \underbrace{|\langle\,3\,|\hat{H}'|\,1\,\rangle|^2}_{=0} / \underbrace{(E_1^{(0)} - E_3^{(0)})}_{=-\Delta_0} \\ &= -\frac{\lambda^2}{\Delta_0} \end{aligned} \tag{6}$$

$$\begin{aligned} E_2^{(2)} &= \underbrace{|\langle\,1\,|\hat{H}'|\,2\,\rangle|^2}_{=\lambda^2} / \underbrace{(E_2^{(0)} - E_1^{(0)})}_{=\Delta_0} + \underbrace{|\langle\,3\,|\hat{H}'|\,2\,\rangle|^2}_{=\lambda^2} / \underbrace{(E_2^{(0)} - E_3^{(0)})}_{=0} \text{“} = \infty'' \\ E_3^{(2)} &= \underbrace{|\langle\,1\,|\hat{H}'|\,3\,\rangle|^2}_{=0} / \underbrace{(E_3^{(0)} - E_1^{(0)})}_{=\Delta_0} + \underbrace{|\langle\,2\,|\hat{H}'|\,3\,\rangle|^2}_{=\lambda^2} / \underbrace{(E_3^{(0)} - E_2^{(0)})}_{=0} \text{“} = \infty'' \end{aligned} \tag{7}$$

We see that while the formula works OK for the first eigenvalue E_1, we cannot successfully apply the second order formula to the degenerate eigenvalues, since for those it contains diverging terms.
For the two unperturbed eigenstates $|\,2\,\rangle$ and $|\,3\,\rangle$, we thus have to use degenerate perturbation theory. For that we extract the perturbation Hamiltonian in the degenerate subspace, which is the bottom right 2×2 submatrix of $\hat{H}'$:

$$\hat{H}' = \begin{bmatrix} 0 & \lambda \\ \lambda & 0 \end{bmatrix}. \tag{8}$$

Diagonalizing this gives an eigenstates $|+\rangle = (|\,2\,\rangle + |\,3\,\rangle)/\sqrt{2}$ with eigenvalue $E_+^{(1)} = +\lambda$ and $|-\rangle = (|\,2\,\rangle - |\,3\,\rangle)/\sqrt{2}$ with eigenvalue $E_-^{(1)} = -\lambda$ [2pts] . Thus here the leading nonvanishing order is found at first order in $\hat{H}'$. The complete energies are $E_\pm = \Delta_0 \pm \lambda$, which captures the correct values up to order λ (and we did not learn any second order degenerate PT, so we stop here [2]).

[2]Note the question did not ask you to do second order degenerate PT. Setting that up involves the use of projection operators, see e.g. Sakurai section 5.2

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

$$\hat{H}^{(0)} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \Delta_0 & 0 \\ 0 & 0 & \Delta_0 \end{bmatrix}, \qquad \hat{H}' = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & \lambda \end{bmatrix}. \tag{9}$$

Use non-degenerate PT to first order, and compare with the true eigenvalues. Discuss.
Solution: Here we can read the true energies off from the total Hamiltonian as $\{0, \Delta_0, \Delta_0 + \lambda\}$. *We can also safely use first order non-degenerate perturbation theory to predict these.*

Stage 2 Variational method: Consider the simple harmonic oscillator with

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2 x^2. \tag{10}$$

(a) Use the variational method with the normalized trial function $\varphi(x) = (2\beta/\pi)^{1/4}e^{-\beta x^2}$ with variational parameter β. Find the value of β 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

Solution:

(a) Let $|\,\Psi_g\,\rangle$ *be the true ground-state of a Hamiltonian* $\hat{H}$ *with energy* E_g. *Then for all other quantum states we have that* $E[\Psi] = \langle\,\Psi\,|\hat{H}|\,\Psi\,\rangle > E_g$. *Proof, see Eq. (7.90) and below: Let us order eigenstates of* $\hat{H}$ *such that their energy increases with n, hence* $E_{gs} = E_0 \le E_1 \le E_2 \cdots$. *Then we can expand the state* $\Psi(x) = \sum_n c_n\phi_n(x)$, *and*

$$\begin{aligned} \langle\,\hat{H}\,\rangle &= \int dx \left(\sum_k c_k^*\phi_k^*(x)\right)\left(\sum_n c_n \underbrace{\hat{H}\phi_n(x)}_{=E_n\phi_n(x)}\right) \\ &= \sum_{kn} c_k^* c_n E_n \underbrace{\int dx \phi_k^*(x)\phi_n(x)}_{\delta_{n,k}} = \sum_n |c_n|^2 E_n. \end{aligned} \tag{11}$$

Since all $E_n \ge E_{gs}$ *we can write* $\sum_n |c_n|^2 E_n \ge E_{gs}\underbrace{\sum_n |c_n|^2}_{=1} = E_{gs}$.

(b) We have to find the energy functional

$$E[\varphi] = \underbrace{\int dx\ \varphi^*(x)\frac{\hat{p}^2}{2m}\varphi(x)}_{=E_{kin}} + \underbrace{\int dx\ \varphi^*(x)\frac{m\omega^2 x^2}{2}\varphi(x)}_{=E_{pot}} \tag{12}$$

Using the integrals provided we can read off:

$$\begin{aligned}
E_{kin} &= -\frac{\hbar^2}{2m}(2\beta/\pi)^{1/2}\int dx\ e^{-\beta x^2}\frac{\partial^2}{\partial x^2}e^{-\beta x^2} \\
&= -\frac{\hbar^2}{2m}(2\beta/\pi)^{1/2}\left(-\sqrt{\frac{\pi\beta}{2}}\right) = \frac{\hbar^2\beta}{2m}, \\
E_{pot} &= \frac{m\omega^2}{2}(2\beta/\pi)^{1/2}\int dx\ e^{-2\beta x^2}x^2 \\
&= \frac{m\omega^2}{2}(2\beta/\pi)^{1/2}\sqrt{\pi}/(2(2\beta)^{3/2}) = \frac{m\omega^2}{8\beta}, \\
E &= \frac{\hbar^2\beta}{2m} + \frac{m\omega^2}{8\beta}.
\end{aligned} \tag{13}$$

Now solving $\frac{d}{d\beta}E[\varphi] = 0$ *to find the minimum we have*

$$\begin{aligned}
\frac{\hbar^2}{2m} - \frac{m\omega^2}{8\beta^2} &= 0, \\
\beta &= \frac{m\omega}{2\hbar}.
\end{aligned} \tag{14}$$

such that our optimal trial wavefunction is $\varphi_{trial}(x) = \varphi(x) = (2\frac{m\omega}{2\hbar}/\pi)^{1/4}e^{-\frac{m\omega}{2\hbar}x^2}$.

(c) Insertion of this β *into* $E[\beta]$ *and some simplification gives*

$$E[\varphi] = \frac{\hbar^2}{2m}\frac{m\omega}{2\hbar} + \frac{m\omega^2}{8}\frac{2\hbar}{m\omega}, \Leftrightarrow E = \hbar\omega/2, \tag{15}$$

which is the true ground-state energy. Also $\varphi_{trial}(x)$ *was the true ground-state wavefunction. This is expected if the family of trial functions contains the correct solution for the right choice of* β.