PH 500 Problem Set #7

Since there are very few realistic problems in quantum mechanics that can be solved exactly, it is useful to develop *approximate* solutions to quantum mechanical problems. Again, the things I want you to do are in **bold**.

1. Suppose we have a Hamiltonian

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_0 + \epsilon\hat{\mathcal{H}}' \tag{1}$$

where $\mathcal{H}_0$ is a Hamiltonian we know how to solve, and $\epsilon\hat{\mathcal{H}}'$ is a modification to that Hamiltonian, which in this context is usually called a *perturbation*. I've put an explicit coefficient ϵ in front of $\hat{\mathcal{H}}'$ because will want to think of $\epsilon\hat{\mathcal{H}}'$ as a small correction to $\mathcal{H}_0$, so that we can find results as series expansions in powers of ϵ around $\epsilon = 0$.

We assumed we know how to solve $\mathcal{H}_0$. That is, we know how to find its eigenvalues $\{\lambda_i^{(0)}\}$ and the corresponding eigenstates $\{|\lambda_i^{(0)}\rangle\}$. The superscript zero here indicates that these states are the solutions at order zero in the expansion in ϵ around $\epsilon = 0$, that is, the solutions when $\epsilon = 0$ so we only have $\mathcal{H}_0$.

Now let's turn to the full Hamiltonian. Formally, both the eigenvectors and eigenvalues have a Taylor expansion around $\epsilon = 0$:

$$\begin{aligned} \lambda_i &= \sum_{n=0}^{\infty} \epsilon^n \lambda_i^n = \lambda_i^{(0)} + \epsilon\lambda_i^{(1)} + \epsilon^2\lambda_i^{(2)} + \dots \\ |\lambda_i\rangle &= \sum_{n=0}^{\infty} \epsilon^n |\lambda_i^n\rangle = |\lambda_i^{(0)}\rangle + \epsilon|\lambda_i^{(1)}\rangle + \epsilon^2|\lambda_i^{(2)}\rangle + \dots \end{aligned} \tag{2}$$

We know what $\lambda_i^{(0)}$ and $|\lambda_i^{(0)}\rangle$ are, that $\hat{\mathcal{H}}_0|\lambda_i^{(0)}\rangle = \lambda_i^{(0)}|\lambda_i^{(0)}\rangle$ and that $\hat{\mathcal{H}}|\lambda_i\rangle = \lambda_i|\lambda_i\rangle$. We won't be able to solve for λ_i or $|\lambda_i\rangle$ exactly, but we can use this information to find the first few terms in their expansions in ϵ, that is $\lambda_i^{(1)}$, $\lambda_i^{(2)}$, etc. and $|\lambda_i^{(1)}\rangle$, $|\lambda_i^{(2)}\rangle$, etc. The result is an *approximate* expression for λ_i and $|\lambda_i\rangle$, valid for small ϵ.

There is one more subtle thing that we also know. The full states are *orthonormal*, $\langle\lambda_i|\lambda_j\rangle = \delta_{ij}$. For this expansion to make sense, it must be orthonormal *at every step*. To zeroth order, this simply means that we should start from orthonormal states, $\langle\lambda_i^{(0)}|\lambda_j^{(0)}\rangle = \delta_{ij}$. At first order, we have

$$\begin{aligned} \delta_{ij} &= \left(\langle\lambda_i^{(0)}| + \epsilon\langle\lambda_i^{(1)}|\right)\left(|\lambda_j^{(0)}\rangle + \epsilon|\lambda_j^{(1)}\rangle\right) \\ &= \langle\lambda_i^{(0)}|\lambda_j^{(0)}\rangle + \epsilon\langle\lambda_i^{(1)}|\lambda_j^{(0)}\rangle + \epsilon\langle\lambda_i^{(0)}|\lambda_j^{(1)}\rangle \\ &= \delta_{ij} + \epsilon\langle\lambda_i^{(1)}|\lambda_j^{(0)}\rangle + \epsilon\langle\lambda_i^{(0)}|\lambda_j^{(1)}\rangle \end{aligned} \tag{3}$$

where we have dropped terms with ϵ^2 and higher powers. Thus

$$\langle \lambda_i^{(1)} | \lambda_j^{(0)} \rangle + \langle \lambda_i^{(0)} | \lambda_j^{(1)} \rangle = 0 \tag{4}$$

Show that

$$\lambda_i^{(1)} = \langle \lambda_i^{(0)} | \hat{\mathcal{H}}' | \lambda_i^{(0)} \rangle \tag{5}$$

Note that finding the *first*–order correction to the energy only required knowing the states to *zeroth* order.

Hint: Expand $\lambda_i = \langle \lambda_i | \hat{\mathcal{H}} | \lambda_i \rangle$ to first order.

2. Having found the leading correction to the energy, we would now like to find the leading correction to the state. This is a vector, so writing it down explicitly requires that we pick a basis. The natural choice is the basis of zeroth order states, $\{|\lambda_i^{(0)}\rangle\}$. So we write

$$|\lambda_i^{(1)}\rangle = \sum_j c_{ij}^{(1)} |\lambda_j^{(0)}\rangle \tag{6}$$

and we need to find the coefficients $c_{ij}^{(1)} = \langle \lambda_j^{(0)} | \lambda_i^{(1)} \rangle$.

Show that

$$|\lambda_i^{(1)}\rangle = \sum_{\lambda_j^{(0)} \neq \lambda_i^{(0)}} |\lambda_j^{(0)}\rangle \frac{\langle \lambda_j^{(0)} | \hat{\mathcal{H}}' | \lambda_i^{(0)} \rangle}{\lambda_i^{(0)} - \lambda_j^{(0)}} \tag{7}$$

Hint: To find $c_{ij}^{(1)}$ with $i \neq j$, consider the eigenvalue equation $\hat{\mathcal{H}}|\lambda_i\rangle = \lambda_i |\lambda_i\rangle$ to first order and act with $\langle \lambda_j^{(0)}|$ on the left. This should allow you to find $c_{ij}^{(1)}$ for all $i \neq j$, so you just have to find $c_{ii}^{(1)}$. Using Eq. (4) with $i = j$, we know that it is purely imaginary. But we could always rescale $|\lambda_i^{(0)}\rangle$ by a phase to absorb this term. Thus we can set it to zero.

Note that this formula only works if the original eigenvalues are *nondegenerate* — that is, no two eigenvalues are the same (otherwise the denominator blows up). In practice, degeneracy is extremely rare unless there is a *symmetry* guaranteeing the degeneracy. As we have seen, a symmetry corresponds to an operator $\hat{\mathcal{A}}$ that *commutes* with the Hamiltonian. So in that case we can diagonalize both operators at once and each eigenstate will be labelled by its energy eigenvalue and its eignvalue of $\hat{\mathcal{A}}$, and the states with the same energies will have different eigenvalues of $\hat{\mathcal{A}}$. Then we can show that the sum in Eq. (7) need only run over states with the same eigenvalue of $\hat{\mathcal{A}}$ as the original state (otherwise the matrix element in the numerator is zero), so the degeneracy can be avoided.

In the rare case of an *accidental* degeneracy not associated with symmetry, there is a slightly messier technique required to avoid this problem.

3. **Find the second–order correction to the energy.** Hint: It should only require the *first*–order states (which you now know from the previous problem). Expand the eigenvector equation to second order and act with $\langle\lambda_i^{(0)}|$ on both sides.

   When you do the Taylor expansion, you will get second–order terms in the states, but by extending Eq. (3) you can show they are zero.

4. Take a system of two spins with the Hamiltonian

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}_1 + \hat{\mathcal{H}}_2 \tag{8}$$

   where

$$\begin{aligned} \hat{\mathcal{H}}_1 &= -\gamma(\hat{\boldsymbol{S}}_{\mathbf{1}} \cdot \boldsymbol{B}_{\mathbf{1}} + \hat{\boldsymbol{S}}_{\mathbf{2}} \cdot \boldsymbol{B}_{\mathbf{2}}) \\ \hat{\mathcal{H}}_2 &= -g' \hat{\boldsymbol{S}}_{\mathbf{1}} \cdot \hat{\boldsymbol{S}}_{\mathbf{2}} \end{aligned} \tag{9}$$

   with $\boldsymbol{B}_{\mathbf{1}} = (0, 0, B_1)$ and $\boldsymbol{B}_{\mathbf{2}} = (0, 0, B_2)$.

   (a) **Treating $\hat{\mathcal{H}}_1$ exactly and $\hat{\mathcal{H}}_2$ as a perturbation, find the first–order eigenvalues of $\hat{\mathcal{H}}$.** Hint: work in the basis of eigenstates of $\hat{S}_{1z}$ and $\hat{S}_{2z}$.

   (b) **Treating $\hat{\mathcal{H}}_2$ exactly and $\hat{\mathcal{H}}_1$ as a perturbation, find the first–order eigenvalues of $\hat{\mathcal{H}}$.** Hint: work in the basis of eigenstates of $\hat{J}^2$.

   (c) **Find the eigenvalues exactly. Check that you can recover your results from each of the previous two parts by expanding this result as a Taylor series to first order in the appropriate parameter.**