PHYS 5002: Homework 7

1 Perturbed two-level system

Consider a general two-level system with a Hamiltonian:

$$\hat{H}_0 = \begin{pmatrix} E_0^0 & 0 \\ 0 & E_1^0 \end{pmatrix}, \; \hat{V} = \begin{pmatrix} V_{00} & V_{01} \\ V_{10} & V_{11} \end{pmatrix}$$

where $E_0^0 \leq E_1^0$ and $V_{01} = V_{10}$.

a.) Find the exact eigenvalues of $\hat{H} = \hat{H}_0 + \hat{V}$

b.) Expand both energies to order V^2.

c.) <u>No Crossing Theorem:</u> As V increases, one might expect the lower level to become higher than the higher level. Show this cannot occur if $V_{01} \neq 0$.

d.) Specialize to the degenerate case $E_0^0 = E_1^0$. Can you expand the energies for small V? To what order in V are the corrections to E_0?

e.) Now consider also $V_{00} = V_{11} = 0$. Compare the exact result to an incorrect application of Rayleigh-Schrödinger perturbation theory to first order. Compare to Wigner-Brillouin perturbation theory at second order.

2 More degenerate perturbation theory

In the case where $\hat{P}_k \hat{V} \hat{P}_k = \hat{V}_k = 0$, the degeneracy is not lifted at all to first order in degenerate perturbation theory. Then, all $E^{(1)}_{k,n_k} = 0$ and $|k, n_k\rangle^{(1)}_{\|}$ are undetermined.

a.) Show that second order perturbation theory gives another eigenvalue problem for $|k, n_k\rangle^{(2)}_{\|}$.

b.) Show the equation for the energy shift is $\det(V_k - E_k^{(2)}) = 0$ with

$$V^k_{ij} = \sum_{k', n_{k'}} \frac{\left\langle ki \middle| \hat{V} \middle| k' n_{k'} \right\rangle \left\langle k' n'_k \middle| \hat{V} \middle| kj \right\rangle}{E_k^0 - E_{k'}^0}$$

where $|\cdot\rangle$ refers to the unperturbed kets. Here k denotes the degenerate subspace and i runs through all of its members, while k' is an energy eigenstate that is not degenerate with the k states, but could be degenerate itself.This is known as the matrix of second order matrix elements. Note that it takes a moment to really follow how to calculate this.

c.) Consider the Hamiltonian:

$$\hat{H}_0 = \begin{pmatrix} E_0^0 & 0 & 0 \\ 0 & E_0^0 & 0 \\ 0 & 0 & E_1^0 \end{pmatrix}, \; \hat{V} = \begin{pmatrix} 0 & 0 & a \\ 0 & 0 & b \\ a^* & b^* & 0 \end{pmatrix}$$

Use perturbation theory to compute **all three** energies to $O(V^2)$ and determine $|k, n_k\rangle^{(2)}_{\|}$ for the 2×2 degenerate space.

d.) Compute the energies of the Hamiltonian in (c) exactly. Compare the energies to the perturbative expansion by plotting on the same plot. Choose $E_0^0 = 0$ and $E_1^0 = 1$ and $a = b$ with $0 < a < 5$ and $a = \frac{1}{2}b$ with $0 < a < 2.5$.

3 Hyperfine splitting

We want to consider the effect of nuclear spins on the atomic energy levels. In particular, we will work with hydrogen taking into account that the nucleus is a proton with spin one half and has a magnetic moment.

Let $\hat{\mathbf{S}}$ be the electron spin operator and $\hat{\mathbf{I}}$ be the proton spin operator. The magnetic moment of the proton is

$$\mathbf{m}_p = g_p \frac{e\hbar}{2Mc}\mathbf{I}$$

where M is the mass of the proton and $g_p = 5.56$ and of the electron is

$$\mathbf{m}_e = -g_e \frac{e\hbar}{2mc}\mathbf{S}$$

where m is the mass of the electron and $g_e = 2$.

If we start analyzing classically, we imagine the proton moment provides a magnetic field

$$\mathbf{B} = \nabla \times \mathbf{A}, \text{ with } \quad \mathbf{A} = -\mathbf{m}_p \times \nabla\left(\frac{1}{r}\right)$$

The electron experiences an interaction with this field.

$$\hat{H}' = -\mathbf{m}_p \cdot \mathbf{B} = \mathbf{m}_e \cdot \mathbf{m}_p \nabla^2\left(\frac{1}{r}\right) + (\mathbf{m}_e \cdot \nabla)(\mathbf{m}_p \cdot \nabla)\left(\frac{1}{r}\right)$$

or

$$\hat{H}' = \frac{e^2 g_e g_p \hbar^2}{4nMc^2}\left\{-\mathbf{S}\cdot\mathbf{I}\,\nabla\left(\frac{1}{r^2}\right) + \mathbf{S}\cdot\nabla\,\mathbf{I}\cdot\nabla\,\left(\frac{1}{r}\right)\right\}.$$

We will treat this to first order as a perturbation of the $l = 0$ levels of hydrogen (ignoring fine structure). For $l = 0$ wavefunctions, the spatial wavefunction is symmetric, so

$$\int d\Omega\;\mathbf{S}\cdot\nabla\,\mathbf{I}\cdot\nabla\,\left(\frac{1}{r}\right) = \frac{\mathbf{S}\cdot\mathbf{I}}{3}\nabla^2\left(\frac{1}{r}\right)\int d\Omega$$

So we write

$$\hat{H}' = -\frac{2}{3}\frac{e^2 g_e g_p \hbar^2}{4mMc^2}\nabla^2\left(\frac{1}{r}\right)\;\mathbf{S}\cdot\mathbf{I}.$$

But, $\nabla^2\left(\frac{1}{r}\right) = -4\pi\delta(\mathbf{r})$ so

$$\hat{H}' = \frac{4\pi}{3}\frac{e^2 g_e g_p \hbar^2}{2mMc^2}\delta(\mathbf{r})\mathbf{S}\cdot\mathbf{I}.$$

In the absence of the perturbation, the $l = 0$ states are fourfold degenerate (electron spins up and down and proton spins up and down). Work on the ground state $n = 1$. The perturbation will split the levels into two different levels. Compute the energy separation of these levels to lowest order in $\hat{H}'$.

Express your answer analytically in terms of $e, g_e, g_p, m, M, c,$ etc. Numerically determine the wavelength (in cm) of a photon with ΔE. This photon is very important in radio astronomy. Note that it is very easy to make a mistake in your numerical calculation, so work carefully and check things frequently. Your final answer will be on the order of a foot.