Quantum Mechanics 115C: Homework 5

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5.1 Stability of the hydrogen ion H^-

The ground state energy of the hydrogen atom is -13.6 eV. However, it turns out that it is possible to add another electron to this system to form a stable negatively charged hydrogen ion, H^- with energy -14.36 eV. Therefore, despite only having one proton, hydrogen prefers to have *two* electrons.[1] In contrast, a negatively charged helium ion, He^-, is *not* stable.

(a) How much energy does it take to remove one of the two electrons from the H^- ion to recover the neutral hydrogen atom?

(a) Were we to ignore the electron-electron repulsion, what would be the ground state energy for the negatively charged H^- ion? How much energy would it take to remove an electron were electron-electron repulsion not present?

(b) Ignoring electron-electron repulsion, what would be the ground state energy for the negatively charged He^- ion?

(c) Can you explain qualitatively why hydrogen would prefer two electrons instead of one, while helium would not prefer three electrons instead of two? What are the competing physical effects/ energy scales?

Hint: It may be helpful to think about the variational solution to the He atom and about the energies involved.

5.2 Variational method for quartic potential

In this problem, you will use a trial wavefunction to solve for an oscillator in a quartic potential. Consider the following one dimensional potential:

$$V(x) = kx^4$$

This potential is similar to that of the harmonic oscillator, but with a "flatter" bottom. When comparing to the harmonic oscillator potential, we may then guess that the frequency will be affected. Remember that the ground state wavefunction for the harmonic oscillator is:

$$\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-m\omega x^2/2\hbar}$$

With the reasoning above, a good trial wavefunction might then be:

$$\psi_{trial}(x;\lambda) = \left(\frac{m\lambda}{\pi\hbar}\right)^{1/4} e^{-m\lambda x^2/2\hbar}$$

[1] Some of you may be familiar with this idea from physical chemistry – it is often referred to as "electron affinity".

where λ is the variational parameter. Note that because this wavefunction is identical in form to the ground state of the harmonic oscillator, it is automatically normalized.

Now, we need to calculate $\bar{H} = \langle\psi_{trial}| \frac{p^2}{2m} + V(x) |\psi_{trial}\rangle$.

(a) First, calculate $\langle\psi_{trial}| \frac{p^2}{2m} |\psi_{trial}\rangle$.

Hint: You don't have to perform the full integral. Think about the Problem 4.1 from the previous homework.

(b) Calculate $\langle\psi_{trial}| V(x) |\psi_{trial}\rangle$. You can use the following integral without proof:

$$\int_{-\infty}^{\infty} x^{2n} e^{-ax^2}\, dx = \frac{(2n-1)(2n-3)\cdots 3\cdot 1}{(2a)^n}\sqrt{\frac{\pi}{a}}$$

Optional: Prove the above integral formula.

(c) Calculate the value of λ that minimizes $\bar{H}$, i.e. obtain λ_{min}.

(d) Although the quartic potential has no known analytic solution, it has been calculated numerically with the following parameters: $\hbar = m = 1$ and $k = 1/2$. The numerical ground state energy is $E_0 \approx 0.53$. What do you obtain for $\bar{H}_{min}$ using the same parameter values? How close are you to the numerically calculated ground state (in terms of percent)?

5.3 Rabi oscillations at slight detuning

In class, we solved the Rabi flopping problem at perfect resonance. In this problem, we will look at what happens when the driving frequency is slightly off resonance (what atomic physicists often refer to as slightly detuned).

(a) If the driving frequency is off resonance, such that $\delta\omega = \omega_{21} - \omega$, write down the coupled first order differential equations for $\dot{c}_1$ and $\dot{c}_2$.

(b) Show that the coefficient c_2 now obeys the equation:

$$\ddot{c}_2 - i\delta\omega\dot{c}_2 + \frac{\gamma^2}{4\hbar^2}c_2 = 0$$

(c) Show that the general solution to this differential equation is of the form:

$$c_2(t) = C_+ e^{i\xi_+ t} + C_- e^{i\xi_- t}$$

where $\xi_\pm = (\delta\omega \pm \Omega)/2$ where $\Omega^2 = \delta\omega^2 + \gamma^2/\hbar^2$, and C_+ and C_- are constants.

(d) If the system starts out with $c_1(0) = 1$ and $c_2(0) = 0$, show that:

$$|c_2(t)|^2 = \frac{\gamma^2}{\hbar^2\Omega^2}\sin^2(\Omega t/2)$$

(e) What is the maximum value of $|c_2(t)|^2$? Show that this number does not exceed 1.

(f) How long does it take for the system to reach an equal superposition of the ground state and excited state (for the first time)? Compare this to the answer to the one we got in class for the case of perfect resonance. Does it now take a longer or shorter time?

5.4 Two-level system

Imagine a two dimensional system with Hilbert space spanned by states $|0\rangle$ and $|1\rangle$. In this basis, the matrix elements of the unperturbed Hamiltonian, H_0 can be written as:

$$\begin{pmatrix} \langle 0|\, H_0\, |0\rangle & \langle 0|\, H_0\, |1\rangle \\ \langle 1|\, H_0\, |0\rangle & \langle 1|\, H_0\, |1\rangle \end{pmatrix} = \begin{pmatrix} 2\hbar\omega & 0 \\ 0 & 0 \end{pmatrix}$$

where ω is real. At time $t = 0$ the system is in state $|0\rangle$, and a perturbation, H_1, is switched on. The matrix elements of H_1 are:

$$\begin{pmatrix} \langle 0|\, H_1\, |0\rangle & \langle 0|\, H_1\, |1\rangle \\ \langle 1|\, H_1\, |0\rangle & \langle 1|\, H_1\, |1\rangle \end{pmatrix} = \begin{pmatrix} 0 & \hbar\lambda \\ \hbar\lambda & 0 \end{pmatrix}$$

(a) Show that the eigenvalues and eigenvectors of $H_0 + H_1$ are respectively given by $E_\pm = \hbar(\omega \pm \Delta)$ and:

$$v_+ = d\begin{pmatrix} \omega + \Delta \\ \lambda \end{pmatrix} \qquad \text{and} \qquad v_- = d\begin{pmatrix} -\lambda \\ \omega + \Delta \end{pmatrix}$$

where $\Delta^2 \equiv \omega^2 + \lambda^2$ and $d^{-2} \equiv 2\Delta(\omega + \Delta)$.

(b) Show that the probability of finding the system in state $|1\rangle$ at time t, given that it was in state $|0\rangle$ at time $t = 0$, is given by $(\lambda^2/\Delta^2)\sin^2(\Delta t)$

(c) By using time-dependent perturbation theory to first order, find an approximate expression for the probability in part (b).

(d) By Taylor expanding the exact probability in part (b), recover the perturbative result of part (c) in the limit that $\omega \gg \lambda$.