16.2 Problem Set II

1. **Perturbation theory:** This question provides a very instructive application of approximation methods in quantum mechanics. The first part of the problem is straightforward and addresses the perturbative series expansion of the anharmonic oscillator. However, the same problem can be used to illustrate the failure of perturbation theory. The second part of the problem demands an application of the WKB method and illustrates the origin of the limitations of the perturbative scheme.

   Briefly summarize how perturbation theory can be used to obtain approximate values for the energy of a non-degenerate state when an exact solution of the Schrödinger equation is unavailable.

   (a) An anharmonic one-dimensional oscillator for a particle of mass m has potential $V(x) = \frac{1}{2}m\omega^2x^2 + \lambda x^4$, where $\lambda > 0$ is small. Using perturbation theory, determine the ground state energy to first order in λ. Consider how your result can be obtained using the ladder operator formalism.

   The ground state of the unperturbed oscillator is given by $\psi_0(x) = (\frac{m\omega}{\pi\hbar})^{1/4}\exp(-\frac{m\omega x^2}{2\hbar})$.

   †**(b)** When $\lambda < 0$, the anharmonic oscillator provides an instructive example illustrating the failure of perturbation theory. No matter how small is the value of λ, the potential minimum at $x = 0$ can only be metastable: For x large enough, the potential eventually turns negative providing an escape route for the particle from the harmonic potential. For this *tunneling* problem, make use of the WKB method to estimate (roughly) the tunneling probability and thereby elucidate the origin of the failure of the perturbation series expansion in λ.

   You may note that

   $$\int_0^b dx\, x(b^2 - x^2)^{1/2} = \frac{b^3}{3}\,.$$

2. **Perturbation theory:** In addition to relativistic corrections, the Hamiltonian of the hydrogen atom is also perturbed by the finite range of the nucleus. The following problem exploits perturbation theory to explore the scale of such corrections.

   The fact that the proton is not a point charge influences the energy levels of the hydrogen atom. This problem may be treated (for simplicity) by regarding the proton as a uniformly charged hollow spherical shell of radius $b = 5 \times 10^{-16}$m. Show that the change in the electrostatic potential energy corresponds to introducing a perturbation

   $$\hat{H}^{(1)}(x) = \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{r} - \frac{1}{b}\right), \qquad r < b\,,$$

   into the normal Schrödinger equation for the hydrogen atom. Using first order perturbation theory, estimate the energy shifts of the hydrogen $2s$ and $2p$ states and comment on your findings. Suggest why measurement of such energy shifts is not a good way of studying the proton charge distribution.

   Hint: You can, and should, simplify the integrals considerably by noting that the size of the nucleus is much smaller than the atomic Bohr radius, i.e. $b \ll a_0$. You may note that,
   $\psi_{2s} = \sqrt{\frac{1}{8\pi a_0^3}}\left(1 - \frac{r}{2a_0}\right)e^{-r/2a_0}$,
   $\psi_{2p_0} = \frac{re^{-r/2a_0}}{\sqrt{32\pi a_0^5}}\cos\theta$,
   $\psi_{2p_{\pm1}} = \frac{re^{-r/2a_0}}{\sqrt{64\pi a_0^5}}e^{\pm i\phi}\sin\theta$.

3. **Perturbation Theory:** This problem shows how perturbation theory may be used to estimate the polarizibility of the hydrogen atom in its ground state. (The induced dipole moment in an applied electric field $\mathbf{E}$ is $\alpha\epsilon_0\mathbf{E}$ where α is the polarizibility.)

Working to second order in field, **E**, show that induced polarization of the ground state $|0\rangle$ is given by $\alpha = \frac{2e^2}{\epsilon_0}\sum_{k\neq 0}\frac{|\langle k|z|0\rangle|^2}{E_k - E_0}$, where E_k is the unperturbed energy of state $|k\rangle$. Show that the same result may be obtained from the perturbed wavefunction to first order in **E** and evaluating the expectation value of the induced electric dipole moment.

To derive the matrix element, $\langle 0|z^2|0\rangle$, you will need the ground state of the hydrogen atom, $|0\rangle = (\frac{1}{\pi a_0^3})^{1/2} e^{-r/a_0}$.

Evaluation of α is tedious, but a useful upper bound may be obtained by noting that $E_k \geq E_1$, where E_1 is the energy of the first excited. Using this result, show that $\alpha \leq \frac{64\pi a_0^3}{3}$. Compare this with the experimental value of $\alpha = 8.5 \times 10^{-30}\text{m}^3$.

Variational method: The following three problems involve straightforward applications of the variational state analysis.

4. Give an account of the variational method for estimating the ground state energy of a quantum mechanical system. Explain how the method may also be applied to excited states.

   Use a trial wavefunction of the form,

$$\psi(x) = \begin{cases} A(a^2 - x^2) & -a < x < a \\ 0 & \text{otherwise} \end{cases},$$

   to place an upper bound on the ground state energy of the one-dimensional harmonic oscillator with potential $V(x) = m\omega^2 x^2/2$ where m is the mass of the particle and ω the oscillator frequency. Compare your answer with the exact result, and comment.

5. By taking a trial wavefunction proportional to $\exp(-\beta r)$ where β is a variational parameter, obtain an upper limit for the ground state energy of the H atom in terms of atomic constants. Comment on your result.

6. (a) E_1 and E_2 are the ground state energies of a particle moving in attractive potentials $V_1(\mathbf{r})$ and $V_2(\mathbf{r})$. Using the variational method, show that $E_1 \leq E_2$ if $V_1(\mathbf{r}) \leq V_2(\mathbf{r})$.

   Hint: Use the wavefunction of a particle moving in $V_2(\mathbf{r})$ as a trial wavefunction for potential $V_1(\mathbf{r})$.

   (b) Consider a particle moving in a one-dimensional attractive potential $V(x)$, i.e. a potential such that $V(x) \leq 0$, for all x and $V(x) \to 0$, as $|x| \to \infty$. Use the variational principle with trial function $A\exp(-\lambda x^2)$ to show that the upper bound on the ground state energy is negative, and hence that for any such potential at least one bound state must exist.

7. The following question addresses the constraints imposed by particle indistinguishability on the allowed spin and spatial states of a two-particle quantum mechanical system.

   Discuss the special considerations which apply to systems of indistinguishable particles in quantum mechanics, giving examples where they lead to observable consequences.

   Two non-interacting particles of mass m move in one dimension, their positions given by x_1 and x_2. The potential is given by

$$V(x) = \begin{cases} 0 & 0 < x < L \\ \infty & \text{otherwise} \end{cases}.$$

Show that the energy of the system is of the form $E = (n_1^2 + n_2^2)\varepsilon$ where n_1 and n_2 are integers and find an expression for ε. Consider the state with $E = 5\varepsilon$ for each of the following three cases:

(a) spin-zero particles;

(b) spin-1/2 particles in a spin singlet state;

(c) spin-1/2 particles in a spin triplet state.

In each case, what is the symmetry of the spin and spatial parts of the wavefunction? Hence write down the spatial wavefunction, and sketch the probability density $|\psi(x_1, x_2)|^2$ in the (x_1, x_2) plane.

Describe qualitatively how the energies of these states would change if the particles carried electric charge and hence interacted with each other (an example of the **exchange** interaction).

8. Together with the constraints imposed by particle indistingishability, a second feature of many-body problem in quantum mechanics is their typical analytical intractability! In the vast majority of interacting problems, some approximation is necessary. The following question involves an application of perturbation theory to a two particle system.

   Two identical spin-zero bosons are placed in a one-dimensional square potential well with infinitely high walls; $V = 0$ for $0 < x < L$, otherwise $V = \infty$. The normalized single-particle energy eigenstates are given by $u_n = (2/L)^{1/2} \sin(n\pi x/L)$.

   (a) Find the wavefunctions and energies for the ground state and the first two excited states of the system.

   (b) Suppose that the two bosons interact with each other through the perturbative "contact interaction",

   $$\hat{H}'(x_1, x_2) = -V_0 L \delta(x_1 - x_2)\,.$$

   Compute the the ground state energy to first order in V_0.