Quantum Mechanics Qualifier

August 2005

1. States of a Three Atom Molecule In this problem, consider the model of a simple 3-atom molecule with one valence electron. The electron can be bound to one of the three atoms, labeled by the three states $|L\rangle$, $|C\rangle$, and $|R\rangle$. These correspond to the electron being localized on the Left, Center, or Right atom respectively. Call this the LCR basis of states.

(a) (1 pt) If the eignenergies of the $|L\rangle$ and $|R\rangle$ states are equal to ϵ, and the eigenenergy of the $|C\rangle$ state is equal to 2ϵ, write down the Hamiltonian matrix (call it H_0) for the electron in the LCR basis.

(b) (1 pt) The Hamiltonian H_0 neglects all interactions between the atoms in the molecules. Let's assume that there is nearest neighbor coupling between the atoms described by the potential,

$$V|L\rangle = \gamma|C\rangle, \quad V|R\rangle = \gamma|C\rangle.$$

Write down the matrix for this potential in the LCR basis. Note that this potential is both Hermitian and purely off-diagonal ($\langle i|V|i\rangle = 0$) for $|i\rangle$ being any of the three basis states).

(c) (3 pts) What are the eigenenergies of the full Hamiltonian, $H_0 + V$? Show that your answer reduces to the correct result in the limit as $\gamma \to 0$.

(d) (3 pts) Consider the case were the coupling between the atoms is of the same magnitude as H_0, $\gamma = \epsilon$. What are the energy eigenvalues of the full Hamiltonian and the eigenstate in the LCR basis?

(e) (2 pts) For the case where $\gamma = \epsilon$, if the eletron is in the state $|C\rangle$ and the energy is measured, what are the possible outcomes of the measurement and their probabilities? Answer this same question for the state $|R\rangle$.

2. Square Well Oscillations

Consider a particle in a symmetric 1D square well of width L:

$$\begin{aligned} V(x) &= 0, \quad |x| \leq L/2 \\ V(x) &= \infty \quad |x| > L/2 \end{aligned}$$

(a) (1 pts.) What are the energy eigenvalues and eigenstates of the first three energy levels in the well? (You do not have to derive these, you may just state them.)

(b) (2 pts.) Assume a particle is, at time t = 0, in a linear combination of the ground and first excited states of the well:

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \left[|1\rangle + |2\rangle \right]$$

What is the expectation value of the position of the particle at time $t = 0$?

(c) (2 pts.) What is the expectation value of the momentum of the particle in the state given in (b)?

(d) (3 pts.) Starting at time $t = 0$ in the state given in (b), what are the time dependent expectation values, $\langle x \rangle(t)$ and $\langle p \rangle(t)$? Explain the relationship between these time dependent expectation values. In particular, explain the relation between the times when these expectation values are at their maximum, minimum, and are equal to zero.

(e) (2 pts.) Repeat the questions (b), (c), and (d) above for the case where the initial state of the particle is a linear combination of the ground and second excited state of the well:

$$|\Psi\rangle = \frac{1}{\sqrt{2}} \left[|1\rangle + |3\rangle \right].$$

3. 3D Square Well

Consider a 3D particle moving in a square well, given by the potential

$$\begin{aligned} V(\vec{r}) &= -V_0 \quad 0 \leq |\vec{r}| \leq a_0 \\ V(\vec{r}) &= 0 \quad |\vec{r}| > a_0. \end{aligned}$$

In this problem, only consider the bound states of this well, so that $-V_0 < E < 0$.

(a) (1 pt.) Explain why we can write the eigenstates of this potential as

$$\Psi_{k,l,m} = f_{k,l}(r) Y_l^m(\theta, \phi).$$

(b) (1 pt.) Defining the function $u_{k,l}(r) = r f_{k,l}(r)$, write the radial Schrödinger equation for $u_{k,l}(r)$.

(c) (2 pts.) For $l = 0$, write the form for the function $u_{k,0}(r)$ in the regions $0 \leq r \leq a_0$ and $r \geq a_0$. Define any constants that you use.

(d) (3 pts.) Using the boundary conditions on the function $u_{k,0}(r)$, derive an equation that gives the bound state energies for the $l = 0$ states. Hint: For $r = 0$ the function $f_{k,l}(r)$ must be finite.

(e) (2 pts.) For a fixed radius for the potential, a_0, calculate the minimum depth, $V_0 = V_{min}$, for which this potential has at least one a bound state.

(f) (2 pts.) Give a physical reason why there is always a bound state in a symmetric 1D square well, but not in a 3D square well.

Note: In spherical coordinates,

$$\nabla^2 \psi = \frac{1}{r} \frac{\partial^2}{\partial r^2} r\psi + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} (\sin\theta \frac{\partial \psi}{\partial \theta}) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\partial \phi^2} \psi.$$

4. Perturbations of the Harmonic Oscillator

Consider a particle of mass m and charge q moving in a one dimensional harmonic oscillator potential and an electric field E. The Hamiltonian for this system is

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

Use the usual notation $|n\rangle$ for the states of the harmonic oscillator without an external field.

(a) (2 pts.) Using perturbation theory, show that there is no change in the eigenenergies of the system to first order in qE.

(b) (2 pts.) Calculate the change in the energy eigenstate $|n\rangle$ to second order in E.

(c) (1 pt) Show, by rewriting the Hamiltonian in equation (1), that the result that you found in (b) is exact to all orders in E

(d) (3 pts.) Next, let's consider what happens to the harmonic oscillator if the electric field is turned on abruptly at time $t = 0$.

Assume the oscillator is initially in its ground state, $|0\rangle$ when the field is turned on. Using an expansion of the time-dependent state:

$$|\Psi(t)\rangle = \sum_n c_n(t)|n\rangle,$$

and the time-dependent Schrödinger Equation, derive an expression for $\frac{d}{dt}c_n(t)$ that is correct to first order in the electric field strength E.

Note: This expression should contain terms with the matrix elements of the form $\langle n|qEx|m\rangle$.

(e) (2 pts.) Calculate the probability of finding the oscillator in the first excited state at some time t assuming it was initially in the ground state and the field is turned on abruptly at $t = 0$,

$$\begin{aligned} E(t) &= 0, \quad t < 0 \\ E(t) &= E, \quad t > 0. \end{aligned}$$

Note: The problem is done most easily using the raising and lowering operators a, $a^\dagger$, and $n = a^\dagger a$, where $\left[a, a^\dagger\right] = 1$.

5. Rigid Rotor Molecular Model

Consider the rigid rotor model of a simple molecule, where

$$H = \frac{L^2}{2mR^2}$$

where m is the effective mass of the molecule and R is the (constant) orbital length. Because the radial coordinate is fixed, the states of this molecule can be written as functions of the angular coordinates $\psi(\theta, \phi)$.

(a) (1 pt) What are the energy eigenstate, eigenenergies, and degeneracies of these states?

(b) (2 pts.) Consider the molecule in the state:

$$\psi(\theta, \phi) = \frac{\sqrt{2}}{2\sqrt{\pi}} sin(\theta) sin(\phi)$$

If you perform a measurement of the energy of this state, what will be the results, and what are the probabilities? What are the results and probabilities of measurements of L^2 and L_z?

(c) (4 pts.) Repeat question (b) for the state

$$\psi(\theta, \phi) = \frac{\sqrt{5}}{2\sqrt{\pi}} cos^2(\theta).$$

(d) (2 pts.) Finally, consider the state

$$\psi(\theta, \phi) = \frac{\sqrt{5}}{4\sqrt{\pi}} sin(\theta) \left(e^{-i\phi} - cos(\theta) e^{i\phi}\right).$$

If you perform a measurement of L_z on the molecule, get the result of $\hbar$, and then measure the energy, what result will you get?

(e) (2 pts.) Repeat (d) for the case where the initial measurement of L_z gives a value of $-\hbar$.

6. 1D bound states

In the figures below are two different 1D potential wells. Your job is to make a fairly accurate sketch of the first three energy eigenstates of these wells, and answer the related questions.

You will need to be fairly accurate in your wavefunction sketches. In particular, the number of nodes of the wavefunctions must be correct as well as their approximate placement. You also need to be accurate as to the relative curvatures and amplitudes of different parts of the wavefunction. **For each wavefunction, explain briefly why you placed the nodes where you did and why you drew the relative amplitudes and curvatures.**

(a) (5 pts.) The potential shown below is an infinite square well with a tilt in the potential at the bottom of the well. The value of the potential is $-V_0$ at the left edge of the well, 0 at the center of the well, and V_0 at the right edge of the well. Assume the ground state energy eigenstate of this well has an energy $E = 0$, but the first and second excited states have energies greater than V_0.

Figure 1: a. Infinite Square Well with a Tilted Bottom

Sketch the energy eigenfunctions of this well for the first three energy states, as described above. For each of these states is the expectation of x less than, greater than, or equal to zero?

(b) (5 pts.) The potential shown below is a smooth double well. The potential far from $x = 0$ is approximately quadratic, but there is a potential barrier of height V_0 in the middle of the well. Assume the ground state and first excited state energies are less than V_0, but the second excited state energy is greater than V_0.

Figure 2: a. Infinite Square Well with a Tilted Bottom

Sketch the energy eigenfunctions of this will for the first three energy states, as described above. What would happen to the difference between the energies of the ground state and first excited state if V_0 became large? Explain.