Due Friday October 10

**Problem 1.** We wish to use the variational principle to estimate the ground state energy of the Hydrogen atom.

1.1. Using the techniques we have previously studied, adimensionalize the time independent Schrodinger equation for the electron in a Hydrogen atom

\[ E\psi(r) = -\frac{\hbar^2}{2m} \nabla^2 \psi(r) - \frac{e^2}{4\pi\epsilon_0 r} \psi(r). \]  

Call your scaled coordinate \( s \).

1.2. Given an arbitrary normalized function of the scaled coordinate, \( \psi(s) \), we can use the variational principle to produce an upper bound to the ground state energy of Hydrogen. By normalized, I mean

\[ \int d^3s |\psi(s)|^2 = 1. \]  

Write an expression for this variational bound. The expression will have the form

\[ \frac{E}{E_0} = A \int d^3s |\nabla \psi(s)|^2 + B \int d^3s \frac{|\psi(s)|^2}{s}, \]  

where \( E_0 \) is the energy scale used in adimensionalizing the Schrodinger equation, \( A, B \) are dimensionless constants. Find \( A \) and \( B \).

1.3. We will try the following variational wavefunction

\[ \psi(s) = \frac{1}{\sqrt{8\pi\lambda^3}} e^{-s/(2\lambda)}, \]  

where \( \lambda \) is an undetermined variational parameter. This is is properly normalized as

\[ \int d^3s |\psi(s)|^2 = 4\pi \int ds \ s^2 |\psi(s)|^2 = 1. \]  

Calculate the variational energy \( E(\lambda) \) in Eq. (3). Just use the symbols, \( A, B, \) and \( E_0 \). Do not substitute your expressions for these parameters.

1.4. Minimize \( E(\lambda) \) with respect to \( \lambda \). Again, just use the symbols \( A, B, \) and \( E_0 \).

1.5. Substitute in your values for \( A, B, \) and \( E_0 \). What is your bound on the energy in eV.

**Problem 2. Angular momentum operator** The \( z \)-component of the angular momentum operator is

\[ L_z = xp_y - yp_x. \]  

Suppose we write \( \psi(x, y) \) in polar coordinates as \( \psi(r, \theta, \phi) \). Using the chain rule, show that

\[ L_z \psi = -i\hbar \partial_\phi \psi. \]
Problem 3. Degeneracies of the 2D Harmonic Oscillator

3.1. The eigenstates of the 2D harmonic oscillator can be labeled by 2 quantum numbers, \( n_x, n_y = 0, 1, \cdots \) corresponding to the number of quanta of excitation in each direction. What is the energy of the state with quantum numbers \( n_x, n_y \)?

3.2. Make a table that has three columns. In the first column put the energy \( E \). In the second column list all of the \( n_x, n_y \) combinations which make that energy. In the third column put the total degeneracy of the energy level. Fill in the first four energies.

3.3. What is the degeneracy of the \( n' \)th level? Note: this degeneracy is in many ways analogous to the large degeneracy in the Hydrogen spectrum. In both cases all classical trajectories are closed. Here we have the additional features that all classical orbits have the same period.

Julien Schwinger, one of the great physicists of the 20th century, came up with an ingenious way to map the symmetry in this problem onto something which looks like angular momentum. I should emphasize however that it is not angular momentum. He started with the ladder operators for the \( x \) and \( y \) oscillators:

\[
| n_x, n_y \rangle = \sqrt{n_x} | n_x - 1, n_y \rangle \quad (8)
\]
\[
| n_x, n_y \rangle = \sqrt{n_y} | n_x, n_y - 1 \rangle \quad (9)
\]

He then created the following combinations:

\[
\mathcal{L}_x = \frac{a_x^\dagger a_y + a_y^\dagger a_x}{2} \quad (10)
\]
\[
\mathcal{L}_y = \frac{a_x^\dagger a_y - a_y^\dagger a_x}{2i} \quad (11)
\]
\[
\mathcal{L}_z = \frac{a_x^\dagger a_x - a_y^\dagger a_y}{2} \quad (12)
\]

The first two are traditionally combined to make

\[
\mathcal{L}_+ = a_y^\dagger a_x \quad (13)
\]
\[
\mathcal{L}_- = a_x^\dagger a_y \quad (14)
\]

3.4. I would like you to prove that \( \mathcal{L} \) obeys the same commutation relations as angular momentum:

\[
[\mathcal{L}_\pm, \mathcal{L}_z] = \mp \mathcal{L}_\pm \quad (15)
\]
\[
[\mathcal{L}_+, \mathcal{L}_-] = 2 \mathcal{L}_z \quad (16)
\]
Tricks:
Use the identity


and the relations

\[
\begin{align*}
[a_x, a_y] &= [a_x, a_y^\dagger] = [a_x^\dagger, a_y] = [a_x^\dagger, a_y^\dagger] = 0 \\
[a_x, a_x^\dagger] &= [a_y, a_y^\dagger] = 1 \\
[a_x, a_x] &= [a_x^\dagger, a_x] = [a_y, a_y] = [a_y^\dagger, a_y^\dagger] = 0
\end{align*}
\]

Using these tricks, the identities should not take more than a few lines to prove. If you get stuck, skip it. I will give you full marks if you write "I spent 30 minutes on this part of the problem, and could not complete it." [Don’t forget to complete the other questions though – particularly the one at the end where you look at the anisotropic oscillator.]

3.5. Prove that \( \mathcal{L}_\pm \) and \( \mathcal{L}_z \) commute with the Hamiltonian – and hence are generators of a symmetry.

Again, using the tricks in 3.4, this should only take a couple lines. Again, don’t spend more than another 30 minutes on this one. You will get full marks if you write "I spent 30 minutes on this part of the problem, and could not complete it." [Don’t forget to complete the other questions though – particularly the one at the end where you look at the anisotropic oscillator.]

[As an aside – typically Schwinger’s trick is used in reverse: you map an angular momentum problem onto a constrained 2D harmonic oscillator. It typically goes under the name “method of Schwinger bosons.”]

[As an even more sophisticated aside – the rotations form a group structure. The group is often labeled SU(2) as it is locally isomorphic to the \(2 \times 2\) unitary, unimodular, matrices. One can do a similar trick of finding representations of \(SU(3)\) by looking at the the states of a 3-dimensional harmonic oscillator. The degeneracies of the 3D harmonic oscillator are: 1, 3, 6, 10, 15... and this construction explicitly produces representations of \(SU(3)\) with those dimension. It turns out that this trick does not exhaustively enumerate the representations of \(SU(3)\). For example, when we talk about Mesons, we will see that there are 8-dimensional representations of SU(3).]

3.6. Suppose we have a slightly anisotropic oscillator: \( \omega_x = \omega_0 + \delta, \omega_y = \omega_0 - \delta \). The energy \( \delta \) quantifies the breaking of the symmetry between \( x \) and \( y \). In particular, it means that classical trajectories are no longer closed.

Make a plot of \( E \) vs \( \delta \) for the 15 lowest energy states. Go from \( \delta = 0 \) to \( \delta = 0.2\omega_0 \). Properly label your axes. Describe qualitatively how the energy levels respond to breaking the symmetry.
**Problem 4.** Atomic physicists can excite atoms into very high energy orbits. These highly excited atoms are relatively stable, and are known as “Rydberg atoms.” Here you will estimate their size.

4.1. What is the degeneracy of the $n = 137$ level in Hydrogen? Show your reasoning.

4.2. What is the energy of a Hydrogen in the $n = 137$ level (in eV)? Take your origin of energy so that ionized Hydrogen has energy $E = 0$.

4.3. High energy states like this are quite “classical,” meaning one can understand them by classical reasoning. Consider a classical particle of mass $m_e$ executing a circular orbit in an energy potential $V(r) = -e^2/(4\pi\epsilon_0 r)$. What is the energy of such a classical particle with radius $r$. Choose the origin of energy so that a stationary electron at $r = \infty$ would have zero energy. [Don’t forget to include the kinetic energy from the orbiting.]

4.4. By comparing these expressions, estimate the size (in Angstroms) of a Rydberg atom in the $n = 137$ level.

4.5. This classical reasoning becomes less accurate for smaller values of $n$, but since it is dimensionally correct, it gives the right order of magnitude. What size (in Angstroms) do you get if you repeat with $n = 1$?

**Problem 5.** Consider the adimensionalized time independent Schrodinger equation for a particle in a double well potential

$$E\psi(x) = -\frac{1}{2}\frac{\partial^2}{\partial x^2}\psi(x) + V_0(x^2 - 1)^2\psi(x).$$

Take $V_0 = 20$.

5.1. Plot the potential. Label your graph.

5.2. Choose a reasonable spatial and temporal discretization (I took $dx = 0.05$ with $x$ running from $-5$ to $5$ and $dt = 0.01$, and it seemed to work for me). Make a stationary wave packet of width 0.3, centered at $x = -1$. Numerically integrate the time dependent Schrodinger equation until time $t = 600$. Make a properly labeled density plot where the horizontal axis is position, the vertical axis is time, and the brightness corresponds to $|\psi|^2$.

5.3. Describe in words what you observe. Is this result consistent with the modeling of Ammonia we used in terms of two-level systems?

**Problem 6. Feedback**

6.1. How long did this homework take?

6.2. Which of the following words come to mind when you think about this homework (feel free to add your own words if you have something better): frustrating, fun, tedious, insightful, hard, easy, useful, useless, fair, unfair

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