Midterm -II - Homework

Phys4410, Spring 2013
DUE: Apr 29, Monday!

Some basic formulas for the simple harmonic oscillator:

\[ H = \frac{1}{2m} p^2 + \frac{1}{2} m\omega x^2 = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} m\omega^2 x^2 \]

The creation/annihilation operators are

\[ a_\pm = \frac{1}{\sqrt{2\hbar m\omega}} (\mp ip + m\omega x) \]

The ground state wave function is

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

while the first excited state is

\[ \psi_1(x) = \left( \frac{m\omega}{\pi\hbar} \right)^{1/4} \sqrt{\frac{2m\omega}{\hbar}} xe^{-\frac{m\omega}{2\hbar} x^2} \]

Observe the combination \( \frac{m\omega}{\hbar} \) always occurs together.

A few useful integrals

\[ \int_0^\infty e^{-\alpha x^2} dx = \frac{1}{\sqrt{\alpha}} \left( \frac{\pi}{4} \right) \]

\[ \int_0^\infty xe^{-\alpha x^2} dx = \frac{1}{2\alpha} \left( \frac{\pi}{4} \right) \]

\[ \int_0^\infty x^2 e^{-\alpha x^2} dx = \frac{1}{4\alpha^2} \left( \frac{\pi}{4} \right) \]

\[ \int_0^\infty x^3 e^{-\alpha x^2} dx = \frac{1}{4\alpha^2} \left( \frac{\pi}{4} \right) \]

A spin matrix element for last: \( <+|S_z|->=\hbar/2 \)
1) Consider a "half" harmonic oscillator, where the potential is

\[ V(x) = \begin{cases} \frac{1}{2}m\omega^2 x^2 & \text{if } x > 0 \\ \infty & \text{if } x < 0 \end{cases} \]

Determine the ground state energy using a variational wave function.

a) (10 pts) What qualitative wave function do you expect for the ground state? Sketch it. Choose as your trial wave function the one that matches your expectation the best from the following set:

\[ \psi_1(x) = e^{-\alpha x^2} \quad \text{if } x > 0; \quad 0 \quad \text{if } x < 0 \]
\[ \psi_2(x) = xe^{-\alpha x^2} \quad \text{if } x > 0; \quad 0 \quad \text{if } x < 0 \]
\[ \psi_3(x) = e^{-\alpha x} \quad \text{if } x > 0; \quad 0 \quad \text{if } x < 0 \]

b) (20 pts) Now calculate the variational energy. To make life easier assume \( \frac{m\omega}{h} = 1 \) and rescale the energy by \( \frac{2\pi}{h} \).

c) (10 pts) Bonus: Can you figure out the ground state energy exactly for this problem? Explain and compare to the variational value. Interpret your result.

*Unfortunately I had a misprint on this problem. I wanted a half-harmonic potential. Since I messed it up, I accepted any reasonable solution. For the extra credit, however, solve the intended problem. Before you do anything, think about it: can you relate the energy eigenstates and wave functions of the half harmonic potential to the full harmonic potential? Also, can the wave function be discontinuous at \( x = 0 \)? Do not forget the normalization!*
The energy

\[ \tilde{H}(a = \frac{1}{2}) = 3 \implies E_0 = 3 \cdot \frac{\hbar^2}{2m} = \frac{3}{2} \hbar \omega \]

This is the same as the \( n=1 \) level of \( \text{H}_2 \)

\( \checkmark \)
2) Two identical spin $1/2$ particles are in a 1-dimensional square well potential

\[ V(x) = \begin{cases} 
0 & \text{if } 0 < x < a \\
\infty & \text{otherwise}
\end{cases} \]

a) (5 pts) What is the energy and the wave function ground state? What is its spin?
b) (10 pts) What is the energy and the wave function of the first excited state? What is its spin? If there are degenerate states, state that clearly.
c)(5 pts) If the particles are charged and repel each other, how would the energy levels of the first excited state shift? You don't have to calculate it, just determine if there is any change and in what direction.

Hint: The wave function of a single particle in the square well is

\[ \psi_n(x) = \sqrt{\frac{2}{a}} \sin \left( \frac{\pi x}{a} \right) \]

and the corresponding energy is

\[ E_n = \frac{\hbar^2 \pi^2}{2ma^2 n^2} \]

More hints: you have 2 electrons. The total wave function is the product of the spin and spatial part and has to be antisymmetric. What are the possible spin states? Now sketch the possible states: 2 electrons in the square well. Can both be in the $n = 1$ level? With what wave function? How about one in $n = 1$, the other in $n = 2$? What could the wave function be now? Can it be symmetric? Antisymmetric?
The first excited state is quadrupole degenerate:

\[ S = 0 \quad 1 \text{ state} \]
\[ S = 1 \quad 3 \text{ states} \]

9) If the fermions repel each other, the state with larger \( \langle \alpha | x^2 | \beta \rangle \) is lower.

As spatial a triplet spin state

\[ E^+ - E_0 \quad \text{singlet} \]

\[ 2E_0 \quad \text{singlet} \]
3) (20 pts) A spin 1/2 particle is in a constant magnetic field, i.e.

\[ H_0 - \mu S_z. \]

A spatially uniform magnetic field in the x direction is turned on and off creating a time dependent potential

\[ V(t) = \begin{cases} 0 & t < 0, \quad t > T \\ V_0 S_z & 0 < t < T \end{cases} \]

Using first order perturbation theory calculate the probability that the system transits from the \( S_z = \hbar/2 \) state to the \( S_z = -\hbar/2 \) state. Just calculate the transition amplitude \( c_m \), and the probability \( P = |c|^2 \)

\[
c = -\frac{i}{\hbar} \int_0^T e^{i(\omega_m \cdot t) } \langle V(t) \rangle dt \approx -\frac{i}{\hbar} \langle V \rangle \frac{e^{i\omega_m T} - 1}{i\omega_m} \]

\[
\omega_m = \mu \cdot \frac{\hbar}{2} = \frac{\hbar}{m} \]

\[
\langle V \rangle = \frac{\hbar}{2} \]

\[
c = \frac{1}{2\mu} \left( e^{i\mu T} - 1 \right) \]

\[
P = \langle c \rangle^2 = \frac{1}{\mu^2} \left( 2 - 2 \cos \mu T \right) \]
4) A hydrogen atom is in the 2P, \( m = 0 \) (2,1,0) state. At \( t = 0 \) a spatially constant electric field

\[
\vec{E} = E_0 \hat{z} e^{-\alpha t}
\]

is turned on.

a) (10 pts) Derive the transition probability to the state \((n,l,m)\) at large times. Give a general expression here for an arbitrary final state.

b) (10 pts) Apply a) to find the transition rate at first order perturbation theory to the 2S (2,0,0) final state. Do not evaluate the radial integral but do the angular one. What value of the time constant \( \alpha \) would make this transition the most likely?

c) (10 pts) Repeat for the (2,1,1) and (1,0,0) final states. (Are any of these transitions forbidden by a selection rule? )

Some spherical harmonics:

\[
Y_{0,0} = \sqrt{\frac{1}{4\pi}} \\
Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos(\theta) \\
Y_{1,1} = -\sqrt{\frac{3}{8\pi}} \sin(\theta)e^{i\phi}
\]

For a) do the time integral for \( c \) and take into account that \( t \to \infty \). Take \( P = |c|^2 \).

That is the general result with some matrix element. For b) c) you know the selection rules but I want you to actually calculate the corresponding angular integrals. It is not complicated at all.

\[
a) \quad c = -\frac{i}{\hbar} \int_0^\infty e^{-\alpha t} e^{i\omega_{ni} t} \langle \chi_0 \mid \chi_{nl} \rangle \, dt
\]

\[
= -\frac{i}{\hbar} \langle \chi_0 \rangle E_0 \left. \frac{1}{i\omega_{ni} - \alpha} \left( e^{-\alpha t} + i\omega_{ni} t \right) \right|_0^\infty
\]

\[
= +\frac{i}{\hbar} \langle \chi_0 \rangle E_0 \left. \frac{1}{\omega_{ni} - i\omega_{ni}} \right|_0^\infty
\]

\[
P = |c|^2 = \frac{1}{\hbar} \frac{E_0^2}{\hbar} \left( \frac{1}{\alpha^2 + \hbar^2} \right) = \alpha \to 0 \text{ will maximize the transition rate.}
\]

b) \( \langle \chi_0 \rangle \): \( \langle 200|t \cos \theta|210\rangle = \int r^2 e^{-\alpha t} R_{20} R_{21} \left( \frac{1}{\sqrt{4\pi}} e^{i\phi} \right) e^{\frac{3}{4\pi} \cos^2 \theta} = \frac{\sqrt{\pi}}{\sqrt{4\pi}} \frac{2\pi}{3} \cdot 2 = \frac{\sqrt{3}}{2} \)
\[ \frac{d}{dt} \int \mathcal{L}(x,t) \left( \frac{d^2}{dt^2} + \frac{1}{c^2} \right) x^2 \sin t \, dt \]