Physics 3220 – Quantum Mechanics 1 – Spring 2009
Problem Set #5

Due Wednesday, February 11 at 9am

Problem 5.1: Analytic solution of simple harmonic oscillator. (20 points)

There are two ways to solve the harmonic oscillator. In class we pursued the method using raising and lowering operators, which is more powerful but difficult to guess if you didn't already know about it. In this problem we go through the method of solving the differential equation directly.

Recall that the TISE for the simple harmonic oscillator is

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dx^2} + \frac{1}{2}m\omega^2 x^2 u = Eu\,. \tag{1}$$

a) It is convenient to simplify the problem by introducing a dimensionless variable. To define $\xi \equiv x/\bar{x}$ with ξ dimensionless, we must construct $\bar{x}$ with units of length. What are the units of the constants $\hbar$, m and ω? What is the unique combination (without any extra pure numbers) that gives a unit of length? Define this as $\bar{x}$ and switch variables to $\xi \equiv x/\bar{x}$. Show that the equation can be written

$$\frac{d^2u}{d\xi^2} = (\xi^2 - K)u\,, \tag{2}$$

where $K \equiv 2E/\hbar\omega$ contains the energy E. What are the units of $\hbar\omega/2$?

b) Consider the limit of the equation far from the center, $|x| \to \infty$. Explain why $\xi^2 \gg K$ in this limit, leading to the approximate equation

$$\frac{d^2u}{d\xi^2} \approx \xi^2 u\,. \tag{3}$$

Show that *in this limit*, an approximate solution is

$$u \approx Ae^{-\xi^2/2} + Be^{\xi^2/2}\,. \tag{4}$$

Be sure to explain any terms you neglect. We have to contstrain one of A and B to make sure that u can be normalized; what is this constraint? Explain why. (Don't actually try to normalize the function.)

c) The original equation turns out to simplify if we "extract" the asymptotic (large $|x|$) behavior of u and solve for what's left. Accordingly, define $h(\xi)$ by means of

$$u(\xi) \equiv h(\xi)e^{-\xi^2/2}\,. \tag{5}$$

Substitute this back into the full TISE (not just the asymptotic version) and show that it is equivalent to

$$h''(\xi) - 2\xi h'(\xi) + (K-1)h(\xi) = 0\,. \tag{6}$$

d) To solve this differential equation, postulate a series solution for h:

$$h(\xi) = \sum_{j=0}^{\infty} a_j \xi^j\,, \tag{7}$$

where the a_j are constants. Show that the result of part c) implies the *recursion relation* for the constants:

$$a_{j+2} = \frac{(2j+1-K)}{(j+1)(j+2)} a_j\,. \tag{8}$$

If we had tried to do this for u directly, we would have obtained a more complicated recursion relation.

e) Normalizability of the wavefunction implies that the series (7) can't go on forever. Thus to ensure we can normalize our wavefunction, the series must stop at some point. Assume that there exists a value n such that $a_n \neq 0$ but $a_{n+2} = 0$, and find the resulting constraint on the energy E_n associated with this wavefunction.

The SHO wavefunctions are thus of the form

$$\begin{aligned} u_n &= (n^{th} \text{ order polynomial in } \xi) \times e^{-\xi^2/2}\,, & (9)\\ &= (n^{th} \text{ order polynomial in } x) \times e^{-m\omega x^2/2\hbar}\,, & (10) \end{aligned}$$

where the polynomials are determined by the recursion relation (8) and are called (up to an overall constant) *Hermite polynomials.* This agrees with the results dervied using raising and lowering operators.

These sorts of methods are common in solving differential equations, and also show up in solving the radial part of the hydrogen wavefunction.

Problem 5.2: Finding quantized energies numerically. (20 points)

Only certain values of the energy E lead to normalizable solutions of the TISE for the simple harmonic oscillator. If a different E is picked, solutions exist, but they cannot be normalized – they blow up at large $|x|$. They can blow up either to positive or negative infinity; the allowed values of E "thread the needle" in between blowing up to plus infinity or to minus infinity by going to zero instead.

One can thus numerically determine the allowed energies for the simple harmonic oscillator (or a different potential) by guessing values of E and trying to find solutions that don't blow up at large $|x|$, tweaking your guess of E each time to get closer. Even if you don't guess the *exact* value of E, if you can find the cross-over region where the wavefunction switches from blowing up to positive infinity to blowing up to negative infinity, the allowed value of E must be in between.

a) Consider the version of the simple harmonic oscillator TISE derived in the previous problem,

$$\frac{\partial^2 u}{\partial \xi^2} = (\xi^2 - K)u\,, \tag{11}$$

where $K = 2E/\hbar\omega$ contains the energy and $\xi \equiv x/\bar{x}$ is the rescaled position variable.

Numerically solve and graph this equation for various values of K to find the ground state energy and plot the results. Use the initial conditions: $u(0) = 1$, $u'(0) = 0$. What property of the ground state are we assuming in order to set the first derivative equal to zero at the origin? (The choice $u(0) = 1$ is for convenience; we won't worry about actually normalizing the answer.)

If you use Mathematica, some useful code might be

```
K = 1.1; a = 0; b = 10; c = -10; d= 10;
Plot[ Evaluate[u[z] /.  NDSolve[{u''[z] - (z^2 - K)*u[z] == 0, u[0] == 1, u'[0]
== 0}, u[z], {z, .000000001, 10}, MaxSteps -> 10000]], {z, a, b}, PlotRange ->
{c, d}, PlotStyle -> Thick]
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Here we used z instead of ξ for convenience. (a, b) and (c, d) are the ranges on the two axes of the plot; feel free to tweak these to get a better view.

We already know the answer: $K = 1$. Try values like $K = 1.1$ and $K = 0.9$ and see how the asymptotic (large-$|x|$) behavior flips between these values; by tuning the guesses for K one can get closer and closer to the correct value. In your write-up, give plots for the result for one choice just above $K = 1$ and one choice just below $K = 1$.

(Note that by numerically solving, you are only working to a finite precision, and so even $K = 1$ may seem to blow up; this is because not enough significant digits are being kept. This is okay because we can still see that the asymptotic behavior flips right around $K = 1$, and hence the allowed energy is there to within the precision of the solution.)

b) Now consider the second-lowest energy state of the SHO, the so-called "first-excited state". How must you change the initial condition in the numerical evaluation to find this state? What value of K corresponds with this state? Check that you've chosen the right initial conditions by doing the numerical solution and seeing that the asymptotic behavior flips at this value of K. (You don't need to include the plots in your write-up.)

c) Now let's do something new: consider a different system, with potential energy

$$V(x) = \frac{1}{2}\alpha x^4\,. \tag{12}$$

What are the units of α? We would like to write the TISE for this potential with a dimensionless variable; show that the unique combination of α, m and $\hbar$ that gives a unit of length is of the form

$$\bar{x} = \left(\frac{\hbar^2}{\alpha m} \right)^{\gamma}, \tag{13}$$

and determine the power γ. Now define $\xi \equiv x/\bar{x}$ as before and rewrite the TISE as

$$\frac{\partial^2 u}{\partial \xi^2} = (\xi^4 - K)u\,, \tag{14}$$

where K will be different from the SHO case, of the form $K = E/\bar{E}$; what is $\bar{E}$?

d) Now find to three significant digits the values of K and the corresponding energies of both the ground state and first excited state of this system using the numerical method, assuming that $\alpha = 1$ in the appropriate MKS units. Don't forget to think about initial conditions as in the SHO case.

This method helps make explicit the mechanics of why only certain energies are allowed in bound state problems in quantum systems. The method gets very useful for cases where the potential is too complicated to solve analytically, as $V = \alpha x^4/2$ begins to show.

Problem 5.3: Properties of the simple harmonic oscillator. (20 points)

Some of these results are discussed in class or in the book, but it's quite useful to work through them.

a) Given the definitions

$$a_+ \equiv \frac{1}{\sqrt{2\hbar m\omega}}(-ip + m\omega x) \qquad a_- \equiv \frac{1}{\sqrt{2\hbar m\omega}}(ip + m\omega x)\,, \tag{15}$$

demonstrate that the simple harmonic oscillator Hamiltonian $\hat{H} = -(\hbar^2/2m)(\partial^2/\partial x^2) + (1/2)m\omega^2 x^2$ can be written in two ways,

$$\hat{H} = \hbar\omega \left(a_+ a_- + \frac{1}{2} \right) = \hbar\omega \left(a_- a_+ - \frac{1}{2} \right)\,. \tag{16}$$

b) Use the energy formula $E_n = \hbar\omega(n + 1/2)$ along with part a) to demonstrate that

$$a_- a_+ u_n = (n+1)u_n\,, \qquad a_+ a_- u_n = n u_n\,, \tag{17}$$

where $u_n(x)$ are the normalized stationary state wavefunctions.

c) Use equation (15) and integration by parts to demonstrate that

$$\int_{-\infty}^{\infty} f^*(a_\pm g)\, dx = \int_{-\infty}^{\infty} (a_\mp f)^* g\, dx\,, \tag{18}$$

for any functions $f(x)$, $g(x)$ that go to zero at infinity, $f(\pm\infty) = g(\pm\infty) = 0$; for example, they could be normalizable wavefunctions. (As we will discuss more later, this implies that a_+ and a_- are *adjoints* or *Hermitian conjugates* of each other.)

d) The raising and lowering operators must take one stationary state to the next, times an overall constant:

$$a_+ u_n = c_n u_{n+1}\,, \qquad a_- u_n = d_n u_{n-1}\,, \tag{19}$$

where c_n and d_n are constants to be determined. Consider the expression $\int_{-\infty}^{\infty}(a_+u_n)^*(a_+u_n)dx$. Evaluate it using both equation (19) and the results from parts b) and c), to solve for c_n. Now consider $\int_{-\infty}^{\infty}(a_-u_n)^*(a_-u_n)dx$ and do something similar to solve for d_n. You should find:

$$a_+ u_n = \sqrt{n+1}\,u_{n+1}\,, \qquad a_- u_n = \sqrt{n}\,u_{n-1}\,. \tag{20}$$

By using the formulas demonstrated in this problem, you will be able to evaluate a lot of things about the SHO without ever having to "get your hands dirty" with the explicit forms of the wavefunctions. You will see this in the next couple problems.

Problem 5.4: Expectation values in the SHO. (20 points)

a) Find an expression for the operators $\hat{x}$ and $\hat{p}$ in terms of the raising and lowering operators a_+ and a_- as well as constants.

b) Calculate $\langle x\rangle$, $\langle p\rangle$, $\langle x^2\rangle$ and $\langle p^2\rangle$ in the n^{th} stationary state *using the expressions from part a).* Hint: You don't ever need to write out the functional form of the u_n if you use results from the previous problem.

c) How must $\langle H\rangle$ be related to the expectation values you calculated in the previous part? Check that this relationship works given what you know $\langle H\rangle$ must be for a stationary state. How much do the kinetic and potential energies each contribute to the total expectation value $\langle H\rangle$?

d) Calculate the product of uncertainties $\sigma_x\sigma_p$ for the n^{th} stationary state and verify the Heisenberg Uncertainty Principle $\sigma_x\sigma_p \geq \hbar/2$. For which values of n is the minimum possible uncertainty achieved?

Besides learning some basic properties of the stationary states, here you get to practice with the algebraic method of using operators. These sorts of techniques will come up again when we study angular momentum in three dimensions.