The Simple Harmonic Oscillator, Part 2

Meet! What meet? Might as well be a track meet as far as I'm concerned...maybe my man will come through...at least the pigeons seem to be enjoying this popcorn...I should be in Atlantic City where the slots are friendly and...Charles! "Gave the case to another gal. Black, average height, slender like the mark, dressed in a brown business suit, no purse, no hat. Drove off in a gold Mercedes. Had a New York vanity plate." "A gold Mercedes with a vanity plate, wow, not exactly low profile. What did the plate say Charles?" "HERMEET."

1. Show that Schrodinger's equation in position space can be written

$$\frac{d^2\psi(x)}{dx^2} + \left(\lambda - \alpha^2 x^2\right)\psi(x) = 0 \quad \text{for an SHO in one dimension.}$$

Part 2 should amplify and reinforce the results of part 1, however, it emphasizes the procedures for solving an ordinary differential equation (ODE) using power series. The SHO potential is only the first ODE that we will solve with a power series solution. Further, power series solutions to ODE's are useful in numerous areas of physics.

The Schrodinger equation for the SHO potential in one dimension in position space is

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + \frac{1}{2} kx^2 \right) \psi\left(x\right) = E \psi\left(x\right) \quad \Rightarrow \quad \frac{d^2 \psi\left(x\right)}{dx^2} + \frac{2m}{\hbar^2} \left(E - \frac{1}{2} kx^2\right) \psi\left(x\right) = 0 \,.$$

$$\text{Let } \lambda = \frac{2mE}{\hbar^2} \text{ and } \alpha^2 = \frac{mk}{\hbar^2} \quad \Rightarrow \quad \frac{d^2 \psi\left(x\right)}{dx^2} + \left(\lambda - \alpha^2 x^2\right) \psi\left(x\right) = 0 \,.$$

2. Discuss the procedures for solving an ODE using a power series solution.

Power series solutions to ODE's are longer problems. Breaking longer problems into smaller segments will often make the overall solution more accessible, so here is a six step procedure.

Power Series Solution Road Map

- 1. Find the solution as x approaches infinity, *i.e.*, the asymptotic solution.
- 2. Assume that the product of the asymptotic solution and an arbitrary function, f(x),
- is a solution. Use this solution in the homogeneous ODE and simplify.
- 3. Assume the arbitrary function can be expressed as an infinite power series, *i.e.*,

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \dots = \sum_{i=0}^{\infty} a_i x^i.$$

4. Evaluate the derivatives where f(x) is expressed as the power series of step 3, and substitute these into the ODE.

5. Group like powers of x such that each power of x has its own coefficient.

6. The expressions that are the coefficients must vanish individually. Express this fact as a recursion relation in closed form if possible.

Postscript: The fact given in step 6 "The expressions that are the coefficients must vanish individually," is not obvious. Each power of x may be viewed as a basis vector. The different basis vectors cannot mix, so in the homogeneous series $a_0 + a_1x + a_2x^2 + a_3x^3 + \cdots = 0$, each a_i must be zero individually. The coefficients are usually expressions and not individual scalars, like $(\lambda - n)$ or more sophisticated expressions, so that each coefficient can vanish individually. Arfken³ provides a more formal discussion. Problem 7 will likely be illustrative.

3. Find the asymptotic solution to $\frac{d^{2}\psi(x)}{dx^{2}} + (\lambda - \alpha^{2}x^{2})\psi(x) = 0.$

An asymptotic solution means the solution as $|x| \gg 0$. The solution that is sought is a wavefunction. A wavefunction must be normalizable so must approach zero as $|x| \gg 0$.

$$|x| \gg 0 \Rightarrow \alpha^2 x^2 \gg \lambda$$
, so at large x the ODE approaches $\frac{d^2 \psi(x)}{dx^2} - \alpha^2 x^2 \psi(x) = 0$. (1)

The solution to this asymptotic form of the rearranged time independent Schrodinger equation is

$$\psi(x) = A e^{-\alpha x^2/2} + B e^{\alpha x^2/2} = A e^{-\alpha x^2/2}, \qquad (2)$$

where B = 0 because the exponential term with the positive argument approaches infinity so is not normalizable and is discarded. To show that equation (2) is a solution to equation (1),

$$\frac{d}{dx}\psi(x) = -\alpha x A e^{-\alpha x^2/2} \quad \Rightarrow \quad \frac{d^2}{dx^2}\psi(x) = \frac{d}{dx}\left(-\alpha x A e^{-\alpha x^2/2}\right) = \alpha^2 x^2 A e^{-\alpha x^2/2} - \alpha A e^{-\alpha x^2/2}$$

where the last term is struck because it is negligible under the assumption $x \gg 0$. Substituting into equation (1) yields $\alpha^2 x^2 A e^{-\alpha x^2/2} - \alpha^2 x^2 A e^{-\alpha x^2/2} = 0$, so equation (2) is the asymptotic form sought. Now we know the "long distance" behavior. Step 1 of the road map is complete.

Postscript: Other terminology used to convey the fact that a function is not normalizable is that it is not square integrable or that the function is non-physical.

4. Reduce $\frac{d^2 \psi(x)}{dx^2} + (\lambda - \alpha^2 x^2) \psi(x) = 0$ to an equivalent ODE valid over the entire domain.

The domain is $-\infty < x < \infty$. Step 2 is substitute $\psi(x) = A e^{-\alpha x^2/2} f(x)$ and reduce.

 $^{^3\,}$ Arfken Mathematical Methods for Physicists (Academic Press, New York, 1970, 2nd ed.), pp 267–270.

$$\frac{d^2}{dx^2} e^{-\alpha x^2/2} f(x) + \left(\lambda - \alpha^2 x^2\right) e^{-\alpha x^2/2} f(x) = 0, \qquad (1)$$

where we have divided both sides by the constant A so it does not appear. The second derivative of the composite function is required, so

$$\frac{d^2}{dx^2} e^{-\alpha x^2/2} f(x) = \frac{d}{dx} \left(-\alpha x e^{-\alpha x^2/2} f(x) + e^{-\alpha x^2/2} \frac{d}{dx} f(x) \right)$$
$$= -\alpha e^{-\alpha x^2/2} f(x) + \alpha^2 x^2 e^{-\alpha x^2/2} f(x) - \alpha x e^{-\alpha x^2/2} f'(x) - \alpha x e^{-\alpha x^2/2} \frac{d}{dx} f(x) + e^{-\alpha x^2/2} f''(x).$$

Using this in equation (1),

$$\begin{aligned} -\alpha \, e^{-\alpha x^2/2} f\left(x\right) + \alpha^2 x^2 e^{-\alpha x^2/2} f\left(x\right) - \alpha x \, e^{-\alpha x^2/2} \frac{d}{dx} \, f\left(x\right) - \alpha x \, e^{-\alpha x^2/2} \frac{d}{dx} \, f\left(x\right) \\ &+ e^{-\alpha x^2/2} \frac{d^2}{dx^2} \, f\left(x\right) + \left(\lambda - \alpha^2 x^2\right) e^{-\alpha x^2/2} f\left(x\right) = 0 \end{aligned}$$

Each of the six terms on the left contains the same exponential. Dividing both sides by the exponential and striking terms that sum to zero,

$$-\alpha f(x) + \alpha^2 \not x^2 f(x) - 2\alpha x \frac{d}{dx} f(x) + \frac{d^2}{dx^2} f(x) + \lambda f(x) - \alpha^2 \not x^2 f(x) = 0$$

$$\Rightarrow \quad \frac{d^2}{dx^2} f(x) - 2\alpha x \frac{d}{dx} f(x) + (\lambda - \alpha) f(x) = 0, \quad \text{and that concludes step 2.}$$

5. Change the variable in
$$\frac{d^2}{dx^2} f(x) - 2\alpha x \frac{d}{dx} f(x) + (\lambda - \alpha) f(x) = 0$$
 to $\xi = \sqrt{\alpha} x$.

A change of variables is used to caste an expression or equation into a more favorable form. This is an optional technique prior to step 3 that should expose some of the existing body of mathematics.

$$\begin{split} \xi &= \sqrt{\alpha} \ x \quad \Rightarrow \quad d\xi = \sqrt{\alpha} \ dx \quad \Rightarrow \quad \frac{d\xi}{dx} = \sqrt{\alpha} \ . \end{split}$$
To change variables, also needed is $\frac{d}{dx} f(x) = \frac{d}{d\xi} \frac{d\xi}{dx} f(\xi) = \frac{d}{d\xi} \sqrt{\alpha} \ f(\xi) = \sqrt{\alpha} \ \frac{d}{d\xi} f(\xi)$

$$\Rightarrow \quad \frac{d^2}{dx^2} f(x) = \frac{d}{dx} \sqrt{\alpha} \ \frac{d}{d\xi} f(\xi) = \frac{d}{d\xi} \frac{d\xi}{dx} \sqrt{\alpha} \ \frac{d}{d\xi} f(\xi) = \frac{d}{d\xi} \alpha \ \frac{d}{d\xi} f(\xi) = \alpha \ \frac{d^2}{d\xi^2} f(\xi) , \end{split}$$
therefore, $\frac{d^2}{dx^2} f(x) - 2\alpha x \ \frac{d}{dx} f(x) + (\lambda - \alpha) f(x) = 0$ becomes

$$\alpha \frac{d^2}{d\xi^2} f(\xi) - 2\alpha \frac{\xi}{\sqrt{\alpha}} \sqrt{\alpha} \frac{d}{d\xi} f(\xi) + (\lambda - \alpha) f(\xi) = 0$$

$$\Rightarrow \quad \frac{d^2}{d\xi^2} f(\xi) - 2\xi \frac{d}{d\xi} f(\xi) + \left(\frac{\lambda}{\alpha} - 1\right) f(\xi) = 0$$

and this is **Hermite's equation**. The arbitrary function $f(\xi)$ is often represented $H_n(\xi)$, or

$$\frac{d^2}{d\xi^2} H_n(\xi) - 2\xi \frac{d}{d\xi} H_n(\xi) + \left(\frac{\lambda}{\alpha} - 1\right) H_n(\xi) = 0.$$

The solutions to Hermite's equation are the Hermite polynomials denoted $H_{n}(\xi)$.

6. Express Hermite's equation in terms of an infinite power series.

Solutions to Schrödinger's equation with the SHO potential are $\psi(x) = H_n(\xi)$ where a normalization constant A and an exponential factor $e^{-\alpha x^2/2}$ have been divided from the ODE. The $H_n(\xi)$ are the solutions so the rest of the road map is unnecessary. We continue the process only to illustrate the further procedures of completing a power series solution. Generally, we assume

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \dots = \sum_{i=0}^{\infty} a_i x^i, \text{ but in terms of } \xi,$$
$$f(\xi) = a_0 + a_1 \xi + a_2 \xi^2 + a_3 \xi^3 + \dots = \sum_{i=0}^{\infty} a_i \xi^i.$$

$$\frac{d}{d\xi}f(\xi) = a_1 + 2a_2\xi + 3a_3\xi^2 + 4a_4\xi^3 + \dots = \sum_{i=1}^{\infty} i a_i\xi^{i-1},$$
$$\frac{d^2}{d\xi^2}f(\xi) = 1 \cdot 2a_2 + 2 \cdot 3a_3\xi + 3 \cdot 4a_4\xi^2 + 4 \cdot 5a_5\xi^3 + \dots = \sum_{i=2}^{\infty} (i-1)i a_i\xi^{i-2}.$$

Inserting these derivatives into Hermite's equation,

 $1 \cdot 2a_2 + 2 \cdot 3a_3 \xi + 3 \cdot 4a_4 \xi^2 + 4 \cdot 5a_5 \xi^3 + \dots - 2\xi \left(a_1 + 2a_2 \xi + 3a_3 \xi^2 + 4a_4 \xi^3 + \dots\right) \\ + \left(\frac{\lambda}{\alpha} - 1\right) \left(a_0 + a_1 \xi + a_2 \xi^2 + a_3 \xi^3 + \dots\right) = 0,$

is the power series form of Hermite's equation, completing steps 3 and 4.

7. Find the coefficient of each power of ξ in the power series form of Hermite's equation then develop a recursion relation summarizing all coefficients.

Steps 5 and 6 in the power series solution road map follows.

 $1 \cdot 2a_2 + 2 \cdot 3a_3\xi + 3 \cdot 4a_4\xi^2 + 4 \cdot 5a_5\xi^3 + \cdots$

$$-2\xi a_{1} - 2\xi 2a_{2}\xi - 2\xi 3a_{3}\xi^{2} - 2\xi 4a_{4}\xi^{3} - \cdots + \left(\frac{\lambda}{\alpha} - 1\right)a_{0} + \left(\frac{\lambda}{\alpha} - 1\right)a_{1}\xi + \left(\frac{\lambda}{\alpha} - 1\right)a_{2}\xi^{2} + \left(\frac{\lambda}{\alpha} - 1\right)a_{3}\xi^{3} + \cdots = 0$$

$$\Rightarrow \quad 1 \cdot 2a_{2} + 2 \cdot 3a_{3}\xi + 3 \cdot 4a_{4}\xi^{2} + 4 \cdot 5a_{5}\xi^{3} + \cdots - 2a_{1}\xi - 2 \cdot 2a_{2}\xi^{2} - 2 \cdot 3a_{3}\xi^{3} - 2 \cdot 4a_{4}\xi^{4} - \cdots + \left(\frac{\lambda}{\alpha} - 1\right)a_{0} + \left(\frac{\lambda}{\alpha} - 1\right)a_{1}\xi + \left(\frac{\lambda}{\alpha} - 1\right)a_{2}\xi^{2} + \left(\frac{\lambda}{\alpha} - 1\right)a_{3}\xi^{3} + \cdots = 0.$$

Examining each power of ξ reveals

coefficient of
$$\xi^{0}$$
: $1 \cdot 2a_{2} + \left(\frac{\lambda}{\alpha} - 1\right)a_{0}$
coefficient of ξ^{1} : $2 \cdot 3a_{3} + \left(\frac{\lambda}{\alpha} - 1 - 2\right)a_{1}$
coefficient of ξ^{2} : $3 \cdot 4a_{4} + \left(\frac{\lambda}{\alpha} - 1 - 2 \cdot 2\right)a_{2}$
coefficient of ξ^{3} : $4 \cdot 5a_{5} + \left(\frac{\lambda}{\alpha} - 1 - 2 \cdot 3\right)a_{3}$
 \vdots \vdots

The pattern can be written $(n+1)(n+2)a_{n+2} + \left(\frac{\lambda}{\alpha} - 1 - 2 \cdot n\right)a_n$ for $n = 0, 1, 2, 3, \dots$ Each coefficient must vanish individually, or $(n+1)(n+2)a_{n+2} + \left(\frac{\lambda}{\alpha} - 1 - 2 \cdot n\right)a_n = 0$

$$\Rightarrow \quad a_{n+2} = -\frac{\left(\lambda/\alpha - 1 - 2 \cdot n\right)}{(n+1)(n+2)} a_n \quad \text{for} \quad n = 0, \ 1, \ 2, \ 3, \ \dots$$

is the recursion relation that completes step 6.

Postscript: The statement that says each coefficient must vanish individually is

$$(n+1)(n+2)a_{n+2} + \left(\frac{\lambda}{\alpha} - 1 - 2 \cdot n\right)a_n = 0.$$

8. Find the eigenenergies of the SHO from the recursion relation.

The eigenfunctions do not approach zero at $|x| \gg 0$ quickly enough to be normalizable if the series does not terminate⁴, so termination is a requirement. It follows that $\lambda/\alpha - 1 - 2n = 0$, as can be seen from the recursion relation found in the previous problem.

⁴ Gasiorowicz Quantum Physics (John Wiley & Sons, New York, 1974), pp 101–105.

$$\frac{\lambda}{\alpha} - 1 - 2n = 0 \quad \Rightarrow \quad \lambda_n = (2n+1) \alpha . \quad \text{Also} \quad \lambda = \frac{2mE}{\hbar^2} \quad \text{and} \quad \alpha^2 = \frac{mk}{\hbar^2} \quad \text{from problem 1}$$
$$\Rightarrow \quad \frac{2mE_n}{\hbar^2} = (2n+1) \frac{\sqrt{mk}}{\hbar} \quad \Rightarrow \quad E_n = (2n+1) \frac{1}{\hbar} \frac{\hbar^2}{2m} \sqrt{mk}$$
$$\Rightarrow \quad E_n = \left(n + \frac{1}{2}\right) \hbar \sqrt{\frac{k}{m}} , \quad \text{or} \quad E_n = \left(n + \frac{1}{2}\right) \hbar \omega .$$

Practice Problems

9. Consider the three-dimensional SHO with the potential $V(r) = \frac{1}{2}m\omega^2 r^2$. Separate the three-dimensional, time-dependent Schrodinger equation into time and spatial variables in (a) spherical coordinates, (b) Cartesian coordinates, and then (c) solve the time-dependent portion of the separated equation. Discuss the meaning of the differential equation dependent only on time.

10. Solve the time-independent Schrodinger equation in Cartesian coordinates by separating spatial variables. Find the eigenenergies and the degree of degeneracy for a three-dimensional SHO in the arbitrary excited state n.

11. Solve the time-independent Schrodinger equation in spherical coordinates in three dimensions for the SHO. Separate radial and angular dependence. Solve the radial equation using a power series solution. Find the eigenenergies a three-dimensional SHO in the arbitrary excited state n.

12. Compare your solutions for the Cartesian and spherical models by showing that the eigenenergies and total degeneracy are the same. Relate the eigenstates expressed in Cartesian coordinates and the eigenstates expressed in spherical coordinates.

We are going to address these four problems as one problem with 21 parts. This problem set is designed to guide you through two different differential equation solutions to the three-dimensional harmonic oscillator problem, namely the solution in Cartesian coordinates which is precisely like solving the one-dimensional problem three times, and the solution in spherical coordinates which involves a separation of the radial and angular degrees of freedom which is very similar to our solution of the hydrogen atom—specifically, there is an effective radial potential governing the radial dependence, and the spherical harmonics govern the angular dependence. This problem contains several important pedagogical issues:

(1) You should be able to separate the time and space dependence of the wavefunction. You should understand how the energy eigenvalues emerge as the separation constant during this separation of time and space, and how this separation of variables leads from the time-dependent Schrodinger equation to the time-independent Schrodinger equation. As we saw for the one-dimensional harmonic oscillator, only special values of the separation constant terminate the power series—these special solutions to the time-independent Schrodinger equation are the "stationary states". When you solve the time-independent Schrodinger equation to get the stationary states, remember that there are only a few special values of the separation constant (the energy eigenvalues) that produce these very special time and space separated stationary solutions. For an arbitrary energy, you cannot separate the wavefunction into a single function of space times a single function of time! In fact, there are infinitely many linear combinations of the stationary states with any given expectation value of the energy. However, you can always uniquely separate any given initial state (which will always have a definite expectation value of its energy E at t = 0) into a sum of the stationary states times their respective time dependences. Of course, that's why we spent so much time expanding the initial t = 0 wavefunction in terms of the energy eigenstates...

- (2) You should be able to separate three-dimensional problems in Cartesian coordinates or in spherical coordinates. The 3D SHO is one of the few problems that is so easily soluble in both coordinate systems, and it gives us a good chance to compare the two approaches.
- (3) You should be able to make the separated differential equation dimensionless. Once you have a dimensionless equation, you should be able to solve it in the asymptotic limit. Then you should be able to separate the asymptotic behavior. Finally, you must be able to solve for the dimensionless asymptotic-behavior-removed stationary state wavefunctions. Of course, the point is that by making the equation dimensionless, and by removing the asymptotic behavior, you will find a complete set of finite polynomials that solve your problem. The special values of the separation constant that terminate these otherwise infinite series solutions are the dimensionless energy eigenvalues. And, of course, you must be able to use the recursion relations you obtain to deduce the polynomials and the corresponding energy eigenvalues.
- (4) Finally, you should realize that no matter what set of coordinates you use to solve the problem, you must get the same answer! For this problem your answers will look very different, but there is nevertheless a fairly simple way to relate them to each other: linear combinations of the Cartesian stationary states are the energy eigenfunctions of the radial and angular momentum description, and, of course, linear combinations of the radial and angular momentum stationary states are the energy eigenfunctions of the radial and angular momentum stationary states are the energy eigenfunctions of the radial and angular momentum stationary states are the energy eigenfunctions of the Cartesian description...

9. Separating Variables for the 3d SHO

- (a) Write down the time-dependent Schrodinger equation in the position space representation using $V(r) = \frac{1}{2}m\omega^2 r^2$. Then separate the time and space dependence of this equation using separable product eigenfunctions of the form $\Psi_n(\vec{\mathbf{r}},t) = \psi_n(\vec{\mathbf{r}}) g_n(t)$.
- (b) Use $r^2 = x^2 + y^2 + z^2$ and the Cartesian form of the Laplacian to express the time-dependent Schrödinger equation in Cartesian coordinates. Then separate the time and space dependence using separable product eigenfunctions of the form $\Psi_n(x, y, z, t) = \psi_n(x, y, z) g_n(t)$. The resulting time dependent $g_n(t)$ must be the same as part (a).

Parts (a) and (b) illustrate how the time-independent Schrodinger equation can be constructed from the time-dependent Schrodinger equation in a position representation. The time-independent Schrodinger equation only applies to the stationary states—all wavefunctions obey the time-dependent Schrodinger equation, but only the stationary states obey the time-independent Schrodinger equation!

(c) Show that the time-dependent functions are given by $g_n(t) = e^{-iE_nt/\hbar}$ by solving the differential equation that you obtained for $g_n(t)$ when you separated the time and space dependence. This is the differential equation version of the origin of the exponential phase describing time-dependence of the stationary states!

10. The 3d SHO in Cartesian Coordinates

(d) Express your time-independent Schrodinger equation in Cartesian coordinates, *i.e.*, in terms of x, y, z, p_x, p_y , and p_z , and then separate the x, y, and z dependence of this equation with eigenfunctions of the form $\psi_n(\vec{\mathbf{r}}) = \psi_n(x, y, z) = f(x) g(y) h(z)$. This is a little trickier than parts (a) and (b) since we considered only two degrees of freedom but have three degrees of freedom and a constant term here. Consider the Hamiltonian for the SHO

$$\mathcal{H} = \mathcal{H}_x + \mathcal{H}_y + \mathcal{H}_z = \left(\frac{\mathcal{P}_x^2}{2m} + \frac{1}{2}m\omega^2 x^2\right) + \left(\frac{\mathcal{P}_y^2}{2m} + \frac{1}{2}m\omega^2 y^2\right) + \left(\frac{\mathcal{P}_z^2}{2m} + \frac{1}{2}m\omega^2 z^2\right)$$

and you should be able to conclude what the separation constants must be. The final form of your separated equations for f(x), g(y), and h(z) are time-independent Schrödinger equations for the one-dimensional SHO.

(e) Show that the eigenenergies for the three-dimensional harmonic oscillator are just the sum of the eigenenergies for the three separated directions, *i.e.*, show that

$$E_n = E(n_x, n_y, n_z) = \left(n + \frac{3}{2}\right) \hbar\omega, \quad \text{where} \quad n = n_x + n_y + n_z.$$

(f) Make a table of all possible combinations of the component and total quantum numbers for the ground state and for the first three excited states. Show that the degeneracy of the *n*-th state is $d(n) = \frac{1}{2}(n+1)(n+2)$ and list n_x , n_y , and n_z . This can be tricky. You may want to use form 1.2.2.1 in the Handbook of Mathematical Formulas and Integrals by Jeffrey,

$$\sum_{k=0}^{m-1} (a+kd) = \frac{m}{2} \left[2a + (m-1)d \right].$$

11. The 3d SHO in Spherical Coordinates

(g) Express your time-independent Schrödinger equation in spherical coordinates, *i.e.*, in terms of r, θ , and ϕ . Use the Laplacian in spherical coordinates,

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

Separate the radial dependence and the angular dependence of this equation using product eigenfunctions consisting of radial wavefunctions times the spherical harmonics, *i.e.*,

$$\psi_{klm}\left(\vec{\mathbf{r}}\right) = \psi_{klm}\left(r,\theta,\phi\right) = R_{kl}\left(r\right)Y_{lm}\left(\theta,\phi\right).$$

The subscripts are important but not particularly useful at this point so just use $\psi = RY$. Spherical harmonics are another family of orthogonal polynomials dependent only on polar and azimuthal angle for the moment. We will discuss the spherical harmonics in chapter 8. Use l(l+1) as the separation constant. The reason for this choice should become clear in chapters 8 and 9.

(h) Show that your separated radial equation has the form

$$\left[-\frac{\hbar^2}{2m}\frac{1}{r}\frac{d^2}{dr^2}r + \frac{1}{2}m\omega^2r^2 + \frac{l(l+1)\hbar^2}{2mr^2}\right]R_{kl}(r) = E_{kl}R_{kl}(r).$$

Again, the subscripts are important but since we have placed little emphasis on their meaning to this point, they are largely cosmetic.

(i) Set $R_{kl}(r) = r^{-1} u_{kl}(r)$ and $\epsilon_{kl} = 2m E_{kl}/\hbar^2$ to obtain the corresponding dimensionless energy version of the time-independent Schrödinger equation

$$\left[\frac{d^2}{dr^2} - \beta^4 r^2 - \frac{l(l+1)}{r^2} + \epsilon_{kl}\right] u_{kl}(r) = 0, \quad \text{where} \quad \beta = \sqrt{\frac{m\omega}{\hbar}}.$$

(j) Show that at large r, your asymptotic differential equation becomes

$$\left[\frac{d^2}{dr^2} - \beta^4 r^2\right] u_{kl}(r) = 0$$

Solve this asymptotic differential equation to obtain the asymptotic solutions $e^{\beta^2 r^2/2}$ and $e^{-\beta^2 r^2/2}$. Discard the solution that diverges at infinity since the wavefunction must go to zero at infinity. It is likely easiest to "guess" a proposed solution and differentiate to show that it is, in fact, a solution. See problem 3.

(k) Separate variables again to remove the Gaussian asymptotic behavior by substituting

$$u_{kl}(r) = e^{-\beta^2 r^2/2} y_{kl}(r)$$

into the differential equation for u_{kl} to obtain the corresponding differential equation for y_{kl} ,

$$\left[\frac{d^2}{dr^2} - 2\beta^2 r \frac{d}{dr} + \epsilon_{kl} - \beta^2 - \frac{l(l+1)}{r^2}\right] y_{kl}(r) = 0.$$

Again, it is good that you see the subscripts, but they are still cosmetic at this point.

- (1) Now substitute the power series $y_{kl}(r) = r^s \sum a_q r^q$ into the differential equation to obtain the recursion relation for the coefficients. See problem 6.
- (m) Show that $[s(s-1) l(l+1)]a_0 = 0$, and that this requires s = l+1 so that $a_0 \neq 0$.
- (n) Show that $[s(s+1) l(l+1)]a_1 = 0$, and that this requires $a_1 = 0$.
- (o) Show that for the coefficient of the r^{q+s} term to be equal to zero we must have

$$\left[\left(q+s+2\right) \left(q+s+1\right) - l\left(l+1\right) \right] a_{q+2} + \left[\epsilon_{kl} - \beta^2 - 2\beta^2 \left(q+s\right) \right] a_q = 0$$

or equivalently, after using s = l + 1, that

$$\left[(q+2)(q+2l+3) \right] a_{q+2} = \left[(2q+2l+3)\beta^2 - \epsilon_{kl} \right] a_q.$$

- (p) Show that all the coefficients with odd subscripts q are zero.
- (q) Explain why the interesting values of the separation constants are those that terminate the series. Then show that the series terminates when $\epsilon_{kl} = (2k + 2l + 3)\beta^2$ where k and l are non-negative integers.
- (r) Show that the eigenenergies are given by

$$E_{kl} = \left(k + l + \frac{3}{2}\right)\hbar\omega = \left(n + \frac{3}{2}\right)\hbar\omega.$$

(s) Show that the allowed values of $\{k, l\}$ for a given n depend on whether n is even or odd and are given by

For *n* even: $\{k, l\} = \{0, n\}, \{2, n - 2\}, \dots, \{n - 2, 2\}, \{n, 0\}.$ For *n* odd: $\{k, l\} = \{0, n\}, \{2, n - 2\}, \dots, \{n - 3, 3\}, \{n - 1, 1\}.$

12. Comparison of the Cartesian and Spherical Solutions

(t) Show that when the 2l+1 degeneracy of the angular momentum states is included, the total degeneracy of each state of the three-dimensional harmonic oscillator described in spherical coordinates is exactly the same as the degeneracy that you already calculated in Cartesian coordinates, $g(n) = \frac{1}{2}(n+1)(n+2)$. Use the formula for a finite arithmetic progression given in part (f). You must cast these sums into the same form where the index starts at zero and is consecutive. The forms that are comparable to the given finite arithmetic sum are

$$\sum_{l \text{ even}}^{n} (2l+1) = \sum_{i}^{n/2} (4i+1) \quad \text{and} \quad \sum_{l \text{ odd}}^{n} (2l+1) = \sum_{i}^{(n-1)/2} (4i+3).$$

(u) We would like to have you show that you can form a linear combination of the Cartesian stationary states to produce one of the spherical stationary states and vice versa, but we will not ask that here. We will ask you to do this problem after we have discussed spherical harmonics. In the interim, please be assured that the Cartesian stationary states are simply a linear combination of the spherical stationary states and vice versa. Not surprisingly, likely the easiest way to show this is using Dirac notation...