Supplementary Notes for lecture 34 for McGill Phys 357.

1. Comments on Power Series Solutions to SHO

If we switch to dimensionless units, the Schrodinger equation for the simple harmonic oscillator (SHO) becomes:

$$\frac{d^2\Psi}{dy^2} + (\epsilon - y^2)\Psi = 0 \tag{1}$$

where $y = \sqrt{\frac{m\omega}{\hbar}}x$ and $\epsilon = \frac{2E}{\hbar\omega}$. We want to get the rough behavior of solutions, as getting that overall behavior will make it much easier to get exact solution. The best way to start is to let y become very large, in which case we can ignore the ϵ term, and we have

$$\frac{d^2\Psi}{dy^2} - y^2\Psi = 0 \tag{2}$$

The book claims that the solutions to this are $A\exp(-y^2/2) + B\exp(y^2/2)$. This is not correct, but we'll it is incorrect in an interesting way. However, if we're at large enough y that we can treat y locally as constant, then the solutions do become Gaussians/inverse Gaussians.

If we set $\Psi = A\exp(-y^2/2)$ and plug it into our original Equation 1, something interesting happens. We have

$$\frac{d\Psi}{dy} = -yA\exp(-y^2/2) \tag{3}$$

$$\frac{d^2\Psi}{dy^2} = A(y^2-1)\exp(-y^2/2) \tag{4}$$

With the second derivative, Equation 1 become:

$$A(y^2-1)\exp(-y^2/2) + (\epsilon - y^2)A\exp(-y^2/2) = A\exp(-y^2/2)(\epsilon - 1)0 \tag{5}$$

We can divide out by A and $\exp(-y^2/2)$ to get

$$(y^2-1) + (\epsilon - y^2) = \epsilon - 1 = 0 \tag{6}$$

So the Gaussian *is* a solution, but only if $\epsilon = 1$. Since $\epsilon = 2E/\hbar\omega$, then $\epsilon = 1$ means $2E/\hbar\omega = 1$ or $E = \hbar\omega/2$ - we've found the ground state, and the ground-state energy. This isn't a *complete* solution - there's another linearly independent solution that we haven't found, but we *have* found one valid, normalizeable solution (the other is an erf times a Gaussian, which diverges). A Gaussian isn't generally a solution to Equation 1, unless we've picked our ϵ with exquisite care.

Now that we know a Gaussian is a solution for one particular value of ϵ, let's try some related functions. The absolute easiest thing we can try is y times a Gaussian. If we try that, we get

$$\Psi = y\exp(-y^2/2) \tag{7}$$

$$\frac{d\Psi}{dy} = A\exp(-y^2/2) - Ay^2\exp(-y^2/2) \tag{8}$$

$$\frac{d^2\Psi}{dy^2} = A\exp(-y^2/2)\left(-y + y^3 - 2y\right) = A\exp(-y^2/2)\left(y^3 - 3y\right) \tag{9}$$

We can clean this up by pulling a y out front, which leaves

$$\frac{d^2\Psi}{dy^2} = (y^2 - 3)\Psi \tag{10}$$

Plug this into Equation 1, and we get:

$$(y^2 - 3 + \epsilon - y^2)\Psi = (\epsilon - 3)\Psi = 0 \tag{11}$$

Once again, we have that our guess for the wave function is a solution, but this time it only works if $\epsilon = 3$, or $E = \frac{3}{2}\hbar\omega$.

Before moving on, notice that for both $\exp(-y^2/2$ and $y\exp(-y^2/2$, the leading order term once we plug Ψ into Equation 1 goes away. That's because generically, if I have $\Psi(y) = h(y)\exp(-y^2/2)$, when I differentiate twice, one of the terms will be $hy^2\exp(-y^2/2) = y^2\Psi$. That's because when I apply the product rule, one of the pieces will come from differentiating $\exp(-y^2/2$ twice, which picks up a $-y$ each time, for a total of y^2 in the second derivative. This term *always* cancels out the $-y^2\Psi$ term in Equation 1, which is why Gaussians times things are good guesses for solutions.

The next case is to try $\Psi = Ay^2\exp(-y^2/2)$. When we differentiate twice, we get

$$\frac{d\Psi}{dy} = A\exp(-y^2/2)\left(-y^3 + 2y\right) \tag{12}$$

$$\frac{d^2\Psi}{dy^2} = A\exp(-y^2/2)\left(y^4 - 2y^2 - 3y^2 + 2\right) \tag{13}$$

$$= A\exp(-y^2/2)\left(y^4 - 5y^2 + 2\right) \tag{14}$$

When we put this into the left-hand side of Equation 1, we get

$$A\exp(-y^2/2)\left(y^4 - 5y^2 + 2 + \epsilon y^2 - y^4\right) = A\exp(-y^2/2)\left((\epsilon - 5)y^2 + 2)\right) \tag{15}$$

Pretty clearly, we want to pick $\epsilon = 5$ to kill the y^2 term. This leaves that pesky 2, though, so $x^2\exp(-x^2/2)$ is *not* a solution, on its own, to the SHO. However, we know how to patch this up. From Equation 5, we know if we put in $A\exp(-y^2/2)$, the left-hand side becomes $A\exp(-y^2/2)(\epsilon - 1)$. Since $\epsilon = 5$, adding $A\exp(-y^2/2)$ gives us $4A\exp(-y^2/2)$. If we set $A = -1/2$ and add that to $y^2\exp(-y^2/2)$, the 2 in Equation 15 will get cancelled, and the total solution will be

$$\Psi = A\left(y^2 - \frac{1}{2}\right)\exp(-y^2/2) \tag{16}$$

This now is a valid solution to the simple harmonic oscillator, with $\epsilon = 5$, and $E = \frac{5}{2}\hbar\omega$.

Finally, since polynomials times Gaussians have been working out, let's plug in $\Psi = Ay^n\exp(-y^2/2)$ and see what happens. We get

$$\frac{d\Psi}{dy} = A\exp(-y^2/2)\left(ny^{n-1} - y^{n+1}\right) \tag{17}$$

$$\frac{d^2\Psi}{dy^2} = A\exp(-y^2/2)\left(n(n-1)y^{n-2} - ny^n + y^{n+2} - (n+1)y^n\right) \tag{18}$$

$$= A\exp(-y^2/2)\left(y^{n+2} - (2n+1)y^n + n(n-1)y^{n-2}\right) \tag{19}$$

Put this into Equation 1, and we get

$$A\exp(-y^2/2)\left(y^{n+2}-(2n+1)y^n+n(n-1)y^{n-2}-y^{n+2}+\epsilon y^n\right) \tag{20}$$
$$=A\exp(-y^2/2)\left((\epsilon-2n-1)y^n+n(n-1)y^{n-2}\right) \tag{21}$$

In general, a y^n term gives a y^n term and a y^{n-2} term. If we want the whole thing to be zero, and to have a highest-order term of y^n, then we need $\epsilon-2n-1=0$, or $\epsilon=2n+1$. Plugging in the definition of ϵ, we have $E_n=\hbar\omega(n+1/2)$ - our general solution for the energy eigenvalues. Note that if we don't have $\epsilon=2n+1$, then we'll need a higher-order y^{n+2} term to cancel out our y^n term, and that will need a y^{n+4} *etc.*, and our polynomial will keep going to arbitrarily high order. That leads to diverging solutions, so we're forced to pick $\epsilon=2n+1$ to get physical solutions.

We can use Equation 21 to work out solutions in general. Let's do the y^4 solution as an example. With $n=4$, we need $\epsilon=9$. Put $\Psi=y^4\exp(-y^2/2)$ into Equation 1, and we get $12y^2\exp(-y^2/2)$. If we put $Ay^2\exp(-y^2/2)$ with $\epsilon=9$ in, we get

$$A\exp(-y^2/2)\left(4y^2+2\right) \tag{22}$$

so we'll need $A=-3$ to cancel out the y^2 term. With $A=-3$, we get a $-6\exp(-y^2/2)$. We've only got one term to go, and we already know putting in $A\exp(-y^2/2)$ gives $A\exp(-y^2/2)(\epsilon-1)$. Since $\epsilon=9$, we get $8A\exp(-y^2.2)$. To cancel out the -6, we need $A=6/8=3/4$, giving us our final wave function:

$$|4\rangle=A\exp(-y^2/2)\left(y^4-3y^2+3/4\right) \tag{23}$$

We can do this even more generally. We'll let n be the leading order (so we're looking for state $|n\rangle$ with energy $\hbar\omega(n+1/2)$. We want to work out c_k where $k=n-2,n-4...[1,0]$ and $|n\rangle=\left(y^n+\sum c_k y^k\right)\exp(-y^2/2)$. With n referring to the max index and k the intermediate indices, we can re-write Equation 21 with $k's$ in place of $n's$, and set $\epsilon=2n+1$. That leaves

$$A\exp -y^2/2\left((2n-2k)y^k+k(k-1)y^{k-2}\right) \tag{24}$$

If we have a c_k, then we need the c_{k-2} term to cancel the y^{k-2} term from c_k, so $k(k-1)c_k=-(2n-2(k-2))c_{k-2}$. If we solve explicitly for c_{k-2}, we get

$$c_k=\frac{-(k+2)(k+1)}{2(n-k)}c_{k+2} \tag{25}$$

This gives us everything we need to make the eigenfunctions of the SHO. We'll get the same answer as with the raising/lowering operators (with a lot more math!), but we didn't have to psychically guess the magic operators that just solve the problem for us.

These polynomials are called the Hermite polynomials, with the n^{th} order polynomial labelled H_n. It's customary to have the leading coefficient $c_n=2^n$. Under that convention, the normalization is $\int_{-\infty}^{\infty}H_nH_m\exp(x^2)dx=\sqrt{\pi}\delta_{nm}2^nn!$. We can use this to write down the properly normalized eigenstates. Our final states are:

$$|n\rangle=H_n(y)\exp(-y^2/2)/\sqrt{\sqrt{\pi}2^nn!} \tag{26}$$