

HARMONIC OSCILLATOR IN 3-D: SPHERICAL COORDINATES

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Problem 4.39.

The 3-d harmonic oscillator can also be solved in spherical coordinates. Since the potential is a function of r only, the angular part of the solution is a spherical harmonic.

To solve the radial equation we substitute the potential $V(r) = \frac{1}{2}m\omega^2 r^2$.

$$(1) \quad -\frac{\hbar^2}{2m} \frac{d^2 u}{dr^2} + \left(\frac{1}{2} m \omega^2 r^2 + \frac{\hbar^2}{2m} \frac{l(l+1)}{r^2} \right) u = E u$$

Using the treatment of the hydrogen atom as a guide we can proceed as follows. First, define $\kappa^2 = 2mE/\hbar^2$ (note that E is positive for all states, and κ has dimensions of length⁻¹) and divide through to get

$$(2) \quad \frac{1}{\kappa^2} \frac{d^2 u}{dr^2} - \left(\frac{l(l+1)}{(\kappa r)^2} + \frac{m^2 \omega^2}{\hbar^2 \kappa^4} (\kappa r)^2 \right) u = -u$$

We now define

$$(3) \quad \rho \equiv \kappa r$$

$$(4) \quad \rho_0 \equiv \frac{m\omega}{\hbar \kappa^2}$$

Note that both ρ and ρ_0 are dimensionless. With these definitions, we get

$$(5) \quad \frac{d^2 u}{d\rho^2} = \left(-1 + \frac{l(l+1)}{\rho^2} + \rho_0^2 \rho^2 \right) u$$

Now we need to investigate the behaviour of u for $\rho \rightarrow \infty$ and $\rho \rightarrow 0$. From ??, as $\rho \rightarrow \infty$, the ρ^2 term dominates and the equation becomes

$$(6) \quad \frac{d^2 u}{d\rho^2} \approx \rho_0^2 \rho^2 u$$

We can get the solution to this approximate equation

$$(7) \quad u \approx Ae^{-\rho_0\rho^2/2} + Be^{\rho_0\rho^2/2}$$

for some constants A and B . The second term is not normalizable, so we take $B = 0$.

This works as an approximate solution because

$$(8) \quad \frac{du}{d\rho} = -\rho_0\rho Ae^{-\rho_0\rho^2/2}$$

$$(9) \quad \frac{d^2u}{d\rho^2} = Ae^{-\rho_0\rho^2/2}(-\rho_0 + \rho_0^2\rho^2)$$

For large ρ , the last term is approximately $A\rho_0^2\rho^2e^{-\rho_0\rho^2/2} = \rho_0^2\rho^2u$.

For $\rho \rightarrow 0$, the ρ^{-2} term dominates and we get

$$(10) \quad \frac{d^2u}{d\rho^2} \approx \frac{l(l+1)}{\rho^2}u$$

which has the normalizable solution

$$(11) \quad u \approx C\rho^{l+1} + D\rho^{-l}$$

for some constants C and D . Again, we can set $D = 0$ to prevent the solution from becoming infinite at $\rho = 0$.

We therefore propose that the exact solution will have the form

$$(12) \quad u(\rho) = \rho^{l+1}e^{-\rho_0\rho^2/2}v(\rho)$$

for some function $v(\rho)$.

To proceed, we must substitute ?? into ??, so we need to calculate $d^2u/d\rho^2$ in terms of $v(\rho)$ and its derivatives.

(13)

$$\frac{du}{d\rho} = (l+1)\rho^l e^{-\rho_0\rho^2/2} v(\rho) - \rho_0\rho^{l+2} e^{-\rho_0\rho^2/2} v(\rho) + \rho^{l+1} e^{-\rho_0\rho^2/2} \frac{dv}{d\rho}$$

$$(14) \quad = \rho^l e^{-\rho_0\rho^2/2} \left(v(l+1 - \rho_0\rho^2) + \rho \frac{dv}{d\rho} \right)$$

(15)

$$\frac{d^2u}{d\rho^2} = l\rho^{l-1} e^{-\rho_0\rho^2/2} \left(v(l+1 - \rho_0\rho^2) + \rho \frac{dv}{d\rho} \right) -$$

$$(16) \quad \rho_0\rho^{l+1} e^{-\rho_0\rho^2/2} \left(v(l+1 - \rho_0\rho^2) + \rho \frac{dv}{d\rho} \right)$$

$$(17) \quad + \rho^l e^{-\rho_0\rho^2/2} \left((-2\rho_0\rho)v + (l+2 - \rho_0\rho^2) \frac{dv}{d\rho} + \rho \frac{d^2v}{d\rho^2} \right)$$

We can now substitute the second derivative and ?? into ?? and collect terms.

(18)

$$(l - \rho_0\rho^2) \left(v(l+1 - \rho_0\rho^2) + \rho \frac{dv}{d\rho} \right) +$$

(19)

$$\rho \left((-2\rho_0\rho)v + (l+2 - \rho_0\rho^2) \frac{dv}{d\rho} + \rho \frac{d^2v}{d\rho^2} \right) = \left(-1 + \frac{l(l+1)}{\rho^2} + \rho_0^2\rho^2 \right) \rho^2 v$$

(20)

$$\rho^2 \frac{d^2v}{d\rho^2} + 2((l+1)\rho - \rho_0\rho^3) \frac{dv}{d\rho} + \rho^2(1 - \rho_0(2l+3))v = 0$$

(21)

$$\rho \frac{d^2v}{d\rho^2} + 2(l+1 - \rho_0\rho^2) \frac{dv}{d\rho} + \rho(1 - \rho_0(2l+3))v = 0$$

We can now seek a solution where $v(\rho) = \sum c_j \rho^j$ as was done for the hydrogen atom. Substituting the series gives

(22)

$$\sum c_j j(j-1)\rho^{j-1} + 2(l+1) \sum c_j j\rho^{j-1} - 2\rho_0 \sum c_j j\rho^{j+1} + (1 - \rho_0(2l+3)) \sum c_j \rho^{j+1} = 0$$

We need to equate the coefficient of each power of ρ to zero separately, so we can redefine the index of summation in each case to make all the exponents of ρ the same:

$$(23) \quad \sum c_{j+1}(j+1)j\rho^j + 2(l+1)\sum c_{j+1}(j+1)\rho^j - 2\rho_0\sum c_{j-1}(j-1)\rho^j + (1-\rho_0(2l+3))\sum c_{j-1}\rho^j = 0$$

Consider first the term with $j = 0$. This gives:

$$(24) \quad 2(l+1)c_1 + (2\rho_0 + 1 - \rho_0(2l+3))c_{-1} = 0$$

Since the series starts with the $j = 0$ term, $c_{-1} = 0$, so we must have $c_1 = 0$ as well.

Considering the general case gives the recurrence relation:

$$(25) \quad c_{j+1} = \frac{\rho_0(2j+2l+1) - 1}{(j+1)(j+2(l+1))}c_{j-1}$$

Since we know that $c_1 = 0$ this relation tells us that *all* odd powers in the series must be zero: $c_{2k+1} = 0$ for all $k = 0, 1, 2, \dots$

We can alter the recursion relation slightly to make it look more natural by defining a new index variable $q \equiv j - 1$. Substituting this into ?? gives

$$(26) \quad c_{q+2} = \frac{\rho_0(2q+2l+3) - 1}{(q+2)(q+2l+3)}c_q$$

where $q = 0, 2, 4, 6, \dots$. The coefficient c_0 must of course be determined by normalization, which we won't bother with here.

For large q this has the asymptotic behaviour:

$$(27) \quad c_{q+2} \approx \frac{2\rho_0}{q+2}c_q$$

This is the same sort of asymptotic behaviour considered in the derivation of the radial function for the hydrogen atom, so if the series was infinite, it would lead to an exponential that blows up at infinite values of ρ . Thus we must require the series to terminate at some point, so from ?? we must have for some q_{max} :

$$(28) \quad \rho_0 = \frac{1}{2q_{max} + 2l + 3}$$

If we recall the original definitions of ρ_0 and κ this translates into a condition on the energy:

$$(29) \quad E = \hbar\omega \left(q_{max} + l + \frac{3}{2} \right)$$

This is valid for all non-negative values of l but only for even q_{max} , so we can make the formula a bit more explicit by introducing a new parameter k such that $q_{max} = 2k$ and $k = 0, 1, 2, 3, \dots$ thus we have

$$(30) \quad E = \hbar\omega \left(2k + l + \frac{3}{2} \right)$$

If we define a final quantum number $n \equiv 2k + l$ we get the well-known formula for the energies of the 3-d harmonic oscillator:

$$(31) \quad E_n = \hbar\omega \left(n + \frac{3}{2} \right)$$

Finally, we should check that the degeneracies of E_n match those for the solution where we solved the system in rectangular coordinates. To do this, we need to calculate how many ways each level n can be formed.

We know that $n = 2k + l$, and also that the number l relates to the spherical harmonic that is the solution of the angular part of the Schrödinger equation. For each value of l there are $2l + 1$ spherical harmonics with different values of m . So we need to figure out first, how many combinations of k and l can add up to $n = 2k + l$ and, second, how many states in total does this amount to when we take into consideration the $2l + 1$ states for each value of l ?

It is easiest to consider these questions for even and odd values of n separately. First, consider the case of n odd. In that case, $k = 0, 1, 2, \dots, (n-1)/2$ and $l = 1, 3, 5, \dots, n$ are the possible values of k and l . For example, we could have $l = 1; k = (n-1)/2$ or $l = 3; k = (n-1)/2 - 1$ and so on. Thus we can write that $l = 2a + 1$ where $a = 0, 1, 2, \dots, (n-1)/2$. Since each value of l has a degeneracy of $2l + 1$ the total degeneracy of level n is:

$$(32) \quad d(n) = \sum_{a=0}^{(n-1)/2} (2(2a+1) + 1)$$

$$(33) \quad = 4 \left(\frac{1}{2} \frac{(n-1)}{2} \frac{(n+1)}{2} \right) + 3 \left(\frac{n-1}{2} + 1 \right)$$

$$(34) \quad = \frac{1}{2} (n+1)(n+2)$$

which agrees with the value of $d(n)$ from our previous solution.

For even n the ranges are $k = 0, 1, 2, \dots, n/2$ and $l = 0, 2, 4, \dots, n$ so we can write $l = 2a$ for $a = 0, 1, 2, 3, \dots, n/2$. The degeneracy in this case is

$$(35) \quad d(n) = \sum_{a=0}^{n/2} (2(2a) + 1)$$

$$(36) \quad = 4 \frac{1}{2} \frac{n}{2} \left(\frac{n}{2} + 1 \right) + \frac{n}{2} + 1$$

$$(37) \quad = \frac{1}{2} (n+1)(n+2)$$

which again agrees with the earlier solution.

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