

QUANTUM MECHANICS

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1 Three-dimensional isotropic harmonic oscillator

The isotropic¹ harmonic oscillator corresponds to the potential

$$V(\vec{x}) = \frac{1}{2}m\omega^2 r^2, \quad r = \|\vec{x}\|,$$

for which the time-independent Schrödinger equation thus is

$$\left(-\frac{\hbar^2}{2m}\nabla^2 + \frac{1}{2}m\omega^2\|\vec{x}\|^2 \right)\psi = E\psi. \quad (1)$$

In the following we first determine the eigenvalues, and next express the eigenfunctions in terms of spherical harmonics and radial functions.

- a) We begin by solving the eigenvalue problem by using the fact that the three-dimensional oscillator can be regarded as a sum of three independent one-dimensional oscillators. We make use of this by applying a separation of variables via the ansatz $\psi(\vec{x}) = \psi^{(1)}(x_1)\psi^{(2)}(x_2)\psi^{(3)}(x_3)$, for Cartesian coordinates $\vec{x} = (x_1, x_2, x_3)$. Use this ansatz in order to find the energy eigenvalues E_n and the corresponding degeneracies d_n . It is perfectly fine to look up the eigenvalues of a one-dimensional Harmonic oscillator.

Hint: Recall that the degeneracy is the number of linearly independent eigenfunctions corresponding to the same eigenvalue. In order to calculate the degeneracy, one can think of precisely n balls that should be distributed over three boxes. In how many ways can this be done? Suppose that we put n_1 balls in box 1. In how many ways can we then distribute the remaining balls over boxes 2 and 3?

(6 points)

- b) The Hamiltonian is spherically symmetric (rotation invariant). Hence, we should be able to express the eigenfunctions in terms of spherical harmonics and radial functions. In principle, we could proceed via the eigenfunctions of the one-dimensional harmonic oscillators in a). However, that would require us to calculate quite nasty integrals.² In spherical coordinates, (1) takes the form

$$\frac{1}{2m} \frac{1}{r^2} L^2 \psi(r, \theta, \phi) - \frac{\hbar^2}{2m} \frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} \psi(r, \theta, \phi) + \frac{1}{2} m \omega^2 r^2 \psi(r, \theta, \phi) = E_n \psi(r, \theta, \phi), \quad (2)$$

where we use the eigenvalues E_n that we already have obtained in a). The angular momentum L^2 becomes a minor monstrosity in spherical coordinates, but for our purposes it suffices to know that the normalised eigenfunctions of L^2 are the spherical harmonics Y_l^m , with $L^2 Y_l^m = l(l+1)\hbar^2 Y_l^m$. Make the ansatz $\psi(r, \theta, \phi) = R(r)Y_l^m(\theta, \phi)$ and show that the radial equation (the

¹Here, 'isotropic' means that spring constant is the same in all directions. In the case the spring constants would be different, then $V(\vec{x}) = \frac{1}{2}m(\omega_1^2 x_1^2 + \omega_2^2 x_2^2 + \omega_3^2 x_3^2)$.

²At least I believe that they would be nasty to calculate, but to be honest I have not tried.

equation for $R(r)$) can be cast in the form of an effective model of a particle moving in a one-dimensional potential

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dr^2} + V_{\text{eff}}(r)\right)u(r) = E_n u(r), \quad \text{for } u(r) = rR(r) \quad (3)$$

and determine the effective potential V_{eff} . Here, E_n are the eigenvalues that you obtained in **a**).

(3 points)

- c) We wish to find the eigenfunctions of the radial equation (3). One strategy for doing this is to rewrite the equation into a form that someone else already has solved. The point is that previous generations of physicists and mathematicians have worked like busy little beavers in order to work out ‘special functions’ from various characterising differential equations. In the following we shall employ this strategy, and rewrite (3) as a special case of the generalised Laguerre equation. The first step is to make the change of variables

$$x = \gamma r^2, \quad r = \sqrt{\frac{x}{\gamma}}, \quad \gamma = \frac{m\omega}{\hbar}$$

and define

$$f(x) = u\left(\sqrt{\frac{x}{\gamma}}\right).$$

Show that (3) can be rewritten as

$$2x \frac{d^2}{dx^2} f(x) + \frac{d}{dx} f(x) - \frac{l(l+1)}{2} \frac{1}{x} f(x) - \frac{1}{2} x f(x) + \left(\frac{3}{2} + n\right) f(x) = 0. \quad (4)$$

(4 points)

- d) As the next step, make the ansatz

$$f(x) = x^{(l+1)/2} e^{-x/2} g(x).$$

Show that (4) results in

$$x \frac{d^2 g}{dx^2} + \left(l + \frac{1}{2} + 1 - x\right) \frac{dg}{dx} + \frac{1}{2} (n - l) g(x) = 0. \quad (5)$$

(5 points)

- e) Now you might ask why one should be more happy about (6) than (2). The answer is that (6) belongs to those classes of equations where the solutions have been determined, namely the generalized Laguerre equation

$$\left(x \frac{d^2}{dx^2} + (\alpha + 1 - x) \frac{d}{dx} + k\right) L_k^{(\alpha)}(x) = 0, \quad (6)$$

which for non-negative integers k has the generalised Laguerre polynomials $L_k^{(\alpha)}$ as solutions. With $\alpha = l + \frac{1}{2}$ and $k = \frac{1}{2}(n - l)$ we can thus conclude that the solution to (6) is $g(x) = L_{\frac{1}{2}(n-l)}^{(l+\frac{1}{2})}(x)$. One could now look up the generalised Laguerre polynomials, if one wants to. However, here we simply keep $L_{\frac{1}{2}(n-l)}^{(l+\frac{1}{2})}$ as a symbol. What we nevertheless should do is to retrace our steps and obtain the solutions $R(r)$ of the radial equation (3). Express the solutions $R_{n,l}$ in terms of $L_{\frac{1}{2}(n-l)}^{(l+\frac{1}{2})}$. Just to be clear, you don't have to try to find explicit expressions for

$L_{\frac{1}{2}(n-l)}^{(l+\frac{1}{2})}$; it is enough to express $R_{n,l}$ in terms of $L_{\frac{1}{2}(n-l)}^{(l+\frac{1}{2})}$. Also, there is no need to normalise the wave-function.

(2 points)

Remark: Strictly speaking, there is a hole in our argument. As mentioned above, k has to be a non-negative integer. We know that n and l are integers, but that is not enough for $\frac{1}{2}(n-l)$ to be a non-negative integer. We furthermore need $n \geq l$. Moreover, if n is even, then l must be even, or if n is odd, then l also has to be odd. In principle we need to show this. However, we skip this here. One may note that (6) can have solutions even if k is not an integer. However, in these cases the solutions are typically not polynomials.