Symmetry group of the 3D Harmonic Oscillator

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1 Quantum Harmonic Oscillator

The harmonic potential is a well-known quantum system of a great interest in the community. It is exactly solvable, so it is possible to find the complete set of eigenfunctions $|\Psi_n\rangle$ and eigenvalues E_n and accepts an algebraic representation of its solutions.

The main difference with the classical system is that the quantum particles presents a non-zero probability of trespass the harmonic barrier and the solutions are not continuous, they are discrete and depends on the energy level n. As can be seen on the right: the ground solution is the so-called vacuum state. The higher the energies are, the more nodes the wavefunction have. This potential is quite important in ultracold atoms due to optical lattices are commonly modeled as a harmonic potential or even as a periodic combination of harmonic potentials.

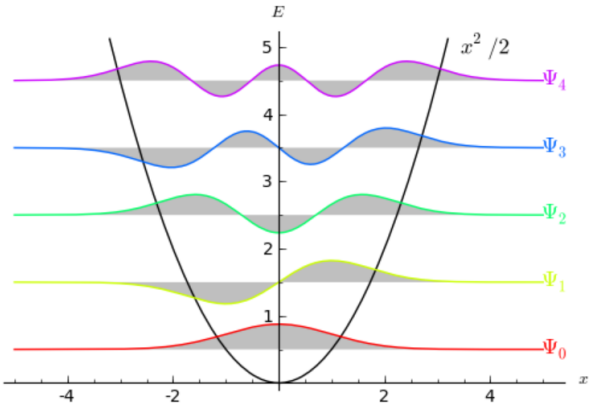

Figure 1: Harmonic potential and its quantized solutions.

In what concerns to this paper, a revision of the Schrödinger-equation solutions for the harmonic potential has been made as well as a deep discussion of the symmetry group that satisfies the wavefunctions.

The total Hamiltonian of a particle in a harmonic potential is:

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2 \tag{1}$$

The time-independent Schrödinger equation is then:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_n(x)}{dx^2} + \left[\frac{1}{2}m\omega^2 x^2 - E_n\right]\psi_n(x) = 0 \tag{2}$$

Due to the asymptotic behaviour of the potential ($\lim_{x\to\infty} V(x) \to \infty$) we expect to have bound states ($\lim_{x\to\infty} \psi_n(x) \to 0$). Firstly, let us write the Hamiltonian with dimensionless variables:

$$H = \frac{\hbar\omega}{2}(P^2 + Q^2) \tag{3}$$

$$P = \frac{p}{\sqrt{m\hbar\omega}} \tag{4}$$

$$Q = \sqrt{\frac{m\omega}{\hbar}}x \tag{5}$$

This choice of variables keeps the same canonical quantization, i.e. the commutation relation $[Q, P] = i$. To proceed, it is useful to factorize the Hamiltonian:

$$H = \frac{\hbar\omega}{2}\underbrace{(Q + iP)}_{\sqrt{2}a}\underbrace{(Q - iP)}_{\sqrt{2}a^\dagger} \tag{6}$$

Here, a and $a^\dagger$ are the annihilation and creation operators respectively:

$$Q = \frac{1}{\sqrt{2}}(a + a^\dagger) \tag{7}$$

$$P = \frac{1}{\sqrt{2}}(a^\dagger - a) \tag{8}$$

In terms of the original coordinates:

$$x = \sqrt{\frac{\hbar}{2m\omega}}(a + a^\dagger) \tag{9}$$

$$p = \sqrt{\frac{m\hbar\omega}{2}}(a^\dagger - a) \tag{10}$$

Plugging this definitions in Eq. (6):

$$\boxed{H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right) = \hbar\omega\left(N + \frac{1}{2}\right)} \tag{11}$$

Where N is the number operator. The basis that diagonalizes the Hamiltonian is represented by the energy level $|n\rangle$, the properties of this basis are:

$$\left.\begin{array}{rcl} N\,|n\rangle & = & n\,|n\rangle \\ \langle n|n'\rangle & = & \delta_{n,n'} \\ a\,|0\rangle & = & 0 \\ a^\dagger\,|n\rangle & = & \sqrt{n+1}\,|n+1\rangle \\ a\,|n\rangle & = & \sqrt{n}\,|n-1\rangle \end{array}\right\} \tag{12}$$

Thus, every general state can be expressed as the superposition of the basis vectors:

$$|\Psi\rangle = \sum_{n=0}^{\infty} c_n\,|n\rangle \tag{13}$$

The action of the annihilation and creation operators on the basis vectors are:

$$a^\dagger\,|n\rangle = \sqrt{n+1}\,|n+1\rangle \tag{14}$$

$$a\,|n\rangle = \sqrt{n}\,|n-1\rangle \tag{15}$$

These last equations suggests that given the vacuum state, the remaining states can be obtained applying the creation operator recursively:

$$|n\rangle = \frac{a^\dagger}{\sqrt{n}}\,|n-1\rangle = \frac{(a^\dagger)^2}{\sqrt{n(n-1)}}\,|n-2\rangle = ... = \frac{(a^\dagger)^n}{\sqrt{n!}}\,|0\rangle \tag{16}$$

The question now is how do we derive an expression for the vacuum state. In general, there is an arbitrariness in the election of vacuum state because it depends on the selected orthogonal basis. For the shake of clarity, let us remind that in every canonical quantization in the position representation the next equations are true:

$$Q\,|\Psi\rangle = q\,|\Psi\rangle \tag{17}$$

$$P\,|\Psi\rangle = -i\frac{d}{dQ}\,|\Psi\rangle \tag{18}$$

Hence, taking into account the destruction of the vacuum state:

$$\langle q|a|0\rangle = \frac{1}{\sqrt{2}}\,\langle q|Q+iP|0\rangle = \frac{1}{\sqrt{2}}\,\langle q|Q+\frac{d}{dQ}|0\rangle \tag{19}$$

$$= \left(Q+\frac{d}{dQ}\right)\langle q|0\rangle = \left(Q+\frac{d}{dQ}\right)\psi_0(Q) = 0 \tag{20}$$

The solution to this ode is:

$$\psi_0(Q) = Ae^{-\frac{1}{2}Q^2} \tag{21}$$

Normalizing the wavefunction yields:

$$\boxed{\psi_0(Q) = \pi^{-1/4} e^{-\frac{1}{2}Q^2} = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-\frac{m\omega}{2\hbar}x^2}} \tag{22}$$

Therefore:

$$\psi_n(Q) = \frac{\langle q|(a^\dagger)^n|0\rangle}{\sqrt{n!}} = \frac{(\pi)^{-1/4}}{\sqrt{2^n n!}} \left(Q + \frac{d}{dQ}\right)^n e^{-\frac{1}{2}Q^2} \tag{23}$$

The latter equation can be simplified with the Hermite polynomials:

$$H_n(Q) = (-1)^n e^{Q^2} \frac{d^n}{dQ^n} e^{-Q^2} \tag{24}$$

$$\psi_n(Q) = \frac{(\pi)^{-1/4}}{\sqrt{2^n n!}} H_n(Q) e^{Q^2/2} \tag{25}$$

As an example, the three lowest-lying states:

$$\psi_0(Q) = \pi^{-1/4} e^{Q^2/2} \ (even) \tag{26}$$

$$\psi_1(Q) = \frac{\pi^{-1/4}}{\sqrt{2}} 2Q e^{Q^2/2} \ (odd) \tag{27}$$

$$\psi_2(Q) = \frac{\pi^{-1/4}}{\sqrt{2}} (2Q^2 - 1) e^{Q^2/2} \ (even) \tag{28}$$

2 Energy degeneracy of the 3D model

In a 3D space:

$$\Psi_n(x, y, z) = \psi_n(x)\psi_n(y)\psi_n(z) \tag{29}$$

$$E_n = \hbar\omega(N + 3/2) \tag{30}$$

with $N = n_x + n_y + n_z$.

In the Table 1 we show the energy degeneracy:

Table 1: States with same energy value for different quantum numbers.

E_n	(n_x, n_y, n_z)	g_n
$3/2\hbar\omega$	$(0,0,0)$	1
$5/2\hbar\omega$	$(1,0,0), (0,1,0), (0,0,1)$	3
$3/2\hbar\omega$	$(2,0,0), (0,2,0), (0,0,2), (1,1,0), (1,0,1), (0,1,1)$	6

The general equation for compute the degeneracy on this system has been shown to be:

$$g_N = \frac{1}{2}(N + 1)(N + 2) \tag{31}$$

3 Symmetry group

The general 3D wavefunction is:

$$\psi_n(Q_x, Q_y, Q_z) = \left(\frac{(\pi)^{-1/4}}{\sqrt{2^n n!}}\right)^3 H_n(Q_x)H_n(Q_y)H_n(Q_z)e^{Q_x^2+Q_y^2+Q_z^2/2} \tag{32}$$

Let us check the groups of symmetries that they satisfy for states distinct than $|0,0,0\rangle$, which is completely symmetric:

- E: $+1$
- $C_2(x,y,z)$ (rotations of π rad): the angular momentum is the generator of the rotations:

$$R_z(\Delta\phi)|n_x,n_y,n_z\rangle = e^{-il_z\Delta\phi/\hbar}|n_x,n_y,n_z\rangle = e^{-im\Delta\phi/\hbar}|n_x,n_y,n_z\rangle \tag{33}$$

It is straightforward to see the angular momentum degeneracy:

$$N = 0 \rightarrow E = \frac{3}{2}\hbar\omega,\ |0,0,0\rangle \implies l = 0\ (singlet) \tag{34}$$

$$N = 1 \rightarrow E = \frac{5}{2}\hbar\omega,\ |1,0,0\rangle, |0,1,0\rangle, |0,0,1\rangle \implies l = 1\ (triplet) \tag{35}$$

$$N = 2 \rightarrow E = \frac{7}{2}\hbar\omega,\ 6\ total\ states\ 5(l=2)\ +1(l=0) \tag{36}$$

l jumps by steps of two. starting for the maximal l. In order to develop a mathematical explanation, let's start with the angular momentum algebra:

$$\left.\begin{array}{rcl} l_x &=& yp_z - p_z y \\ l_y &=& zp_x - p_x z \\ l_z &=& xp_y - p_y x \end{array}\right\} [l_i, l_j] = i\hbar\epsilon_{ijk}l_k \implies l_i = i\hbar\epsilon_{ijk}x_i p_j \tag{37}$$

Thus:

$$l_i = -i\frac{\hbar}{2}\epsilon_{ijk}a_j^\dagger a_k \tag{38}$$

We can define new creation-annihilation operators:

$$a_R = \frac{1}{\sqrt{2}}(a_x - ia_y), \quad a_L = \frac{1}{\sqrt{2}}(a_x + ia_y) \tag{39}$$

Acting on the basis $|n_z, N_R, N_L\rangle$, $a_{R,L}^\dagger$ increase the angular momentum in $\pm\hbar$. The Hamiltonian stands for:

$$H = \hbar\omega(N_R + N_L + N_z + 3/2) \tag{40}$$

$N = 1$ states are then presented by:

$$a_R^\dagger|0,0,0\rangle, \quad a_z^\dagger|0,0,0\rangle, \quad a_L^\dagger|0,0,0\rangle \tag{41}$$

The first one has $m = \hbar$, the second $m = 0$ and the third $m = -\hbar$, exactly the three expected values of the $l = 1$ multiplets identified before. For arbitrary positive integer number N, the state with highest m is $(a_R^\dagger)^N|0\rangle$ and it has $m = N\hbar$. This shows we must have $l = N$ multiplet.

Similar results are obtained in the other directions.

$$\begin{aligned} Even\ N &\implies even\ l \implies R_{x,y,z}(\pi)\Psi_{2N}(x,y,z) = -\Psi(x,y,z) \\ Odd\ N &\implies Odd\ l \implies R_{x,y,z}(\pi)\Psi_{2N+1}(x,y,z) = +\Psi(x,y,z) \end{aligned}$$

- $\sigma(x,y), \sigma(y,z), \sigma(z,x)$ (reflections): $\sigma(x,y)\Psi(x,y,z) = \Psi(x,y,-z)$. The change of sign only affects to the Hermite polynomials. It can be demonstrated the reflection property of $H_n(z)$ as follows:

$$H_n(-z) = (-1)^n e^{(-z)^2}\frac{d^n}{d(-z)^n}e^{-(-z)^2} = (-1)^n H_n(z) \tag{42}$$

The total sign aroused from the reflection depends on the order of the polynomial:

$$H_n(-z)\ (odd\ n) = -H_n(z) \tag{43}$$

$$H_n(-z)\ (even\ n) = H_n(z) \tag{44}$$

In this manner, the symmetry group is splitted in two different groups:

$$\begin{aligned} \sigma(x,y) = \sigma(y,z) = \sigma(z,x) &= +1\ (even\ n) \\ \sigma(x,y) = \sigma(y,z) = \sigma(z,x) &= -1\ (odd\ n) \end{aligned}$$

- i (complete relfection): $i\Psi(x,y,z) = \Psi(-x,-y,-z)$. Using the Hermite polynomials property showed before:

$$\Psi(-x,-y,-z) = (-1)^{3n}\Psi(x,y,z) \tag{45}$$

Once again, if n is a even number $i = +1$ if odd $i = -1$.

We can conclude that the groups of symmetry are:

Table 2: Symmetry groups for different states.

$\lvert n_x, n_y, n_z\rangle$	$C_2(z)$	$C_2(y)$	$C_2(x)$	i	$\sigma(xy)$	$\sigma(xz)$	$\sigma(yz)$	Group
$\lvert 0,0,0\rangle$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	A_g
$\lvert 0,0,1\rangle$	$+1$	-1	-1	-1	-1	$+1$	$+1$	B_{1u}
$\lvert 0,1,0\rangle$	-1	$+1$	-1	-1	$+1$	-1	$+1$	B_{2u}
$\lvert 1,0,0\rangle$	-1	-1	$+1$	-1	$+1$	$+1$	-1	B_{3u}
$\lvert 1,1,0\rangle = \lvert 1,0,0\rangle \otimes \lvert 0,1,0\rangle$	$+1$	-1	-1	$+1$	$+1$	-1	-1	B_{1g}
$\lvert 1,0,1\rangle = \lvert 1,0,0\rangle \otimes \lvert 0,0,1\rangle$	-1	$+1$	-1	$+1$	-1	$+1$	-1	B_{2g}
$\lvert 0,1,1\rangle = \lvert 0,0,1\rangle \otimes \lvert 0,1,0\rangle$	$+1$	-1	-1	-1	-1	$+1$	$+1$	B_{3g}
$\lvert 1,1,1\rangle = \lvert 0,1,1\rangle \otimes \lvert 1,0,0\rangle$	$+1$	$+1$	$+1$	-1	-1	-1	-1	A_u
$\lvert 2,0,0\rangle = \lvert 0,2,0\rangle = \lvert 0,0,2\rangle$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	$+1$	A_g

Going further on the levels is straightforward since $|2,0,0\rangle$ is A_g and $|1,1,1\rangle$ A_u. The next levels can be build computing tensor products between the states on Table 2. The tensor product by a gerade group keeps the original symmetry, in contrast with ungerade groups that changes the symmetry. $N = 0$ is group A_g, $N = 1$ B_u, $N = 2$ B_g, $N = 3$ will be B_u and $N = 4$ B_g.

This analysis can also be done in two-particle systems on a harmonic potential since the Schrödinger equation accepts a complete separation of the two independent Hamiltonians, obtaining what is shown in https://es.webqc.org/symmetrypointgroup-d2h.html.

4 Anisotropic or quasi-1D HO

An anisotropic HO is characterized by having at least one of the frequencies different to the others what causes a preferred spatial direction, in this case, the Z-axis, $\omega_z \neq \omega_x, \omega_y = \omega$. This causes a break of symmetry to the 3D harmonic oscillator having a direct effect on the energy levels.

Assuming $\omega_z = 0.01\omega$, the total energy is:

$$E_n = \hbar\omega(n_x + n_y + 0.01n_z + 1.005) \tag{46}$$

And the energy levels schema is presented in the next figure:

As expected, the degeneracy persist on the XY plane. 100 Z-levels will be found between each X and Y level. It is similar to hyperfine structure on atoms or more likely, the rotational and vibrational states of molecules.

This is the way quasi-1D harmonic oscillators are experimentally obtained: building an extreem anisotropy in one of the spatial directions. The gap between Z-levels is considerably smaller than for X or Y levels. For energies comparable to $\hbar\omega_z$ the system will behave like it lives in one-spatial dimension.

The symmetry groups are sorted as follows:

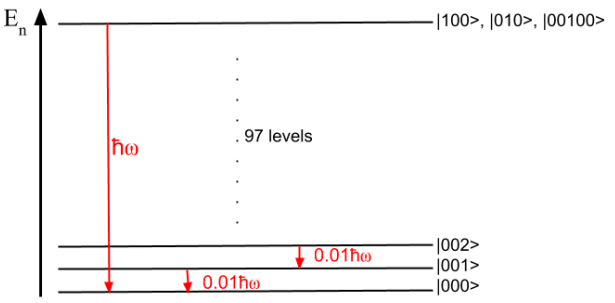

Figure 2: Energy levels in a anisotropic harmonic oscillator with $\omega_z = 0.01\omega$.

Table 3: Symmetry groups and energy degeneracy for the anisotropic harmonic oscillator

$E_n/\hbar\omega$	$\lvert n_x, n_y, n_z\rangle$	Group
1.005	$\lvert 0,0,0\rangle$	A_g
1.015	$\lvert 0,0,1\rangle$	B_{1u}
1.025	$\lvert 0,0,2\rangle$	A_g
$\vdots$	$\vdots$	$\vdots$
2.005	$\lvert 0,0,100\rangle, \lvert 0,1,0\rangle, \lvert 1,0,0\rangle$	A_g, B_{2u}, B_{3u}
2.015	$\lvert 0,1,1\rangle, \lvert 1,0,1\rangle$	B_{3g}, B_{2g}
2.025	$\lvert 0,1,2\rangle, \lvert 1,0,2\rangle$	B_{2u}, B_{3u}
$\vdots$	$\vdots$	$\vdots$
3.005	$\lvert 1,1,0\rangle, \lvert 2,0,0\rangle, \lvert 0,2,0\rangle, \lvert 0,1,100\rangle, \lvert 1,0,100\rangle$	$B_{1g}, A_g, A_g, B_{2u}, B_{3u}$
$\vdots$	$\vdots$	$\vdots$