Accidental Degeneracy in the Quantum Tridimensional Isotropic Harmonic Oscillator: a Clarification via Ladder Operators

STEFANO PATRI'

Department of
METHODS AND MODELS FOR TERRITORY, ECONOMICS AND FINANCE

Faculty of ECONOMICS - "SAPIENZA" University of Rome

101° Congress of the ITALIAN PHYSICAL SOCIETY

September 21-25, 2015
ROME

Contents

Schrödinger equation

The Schrödinger equation of the quantum Tridimensional Isotropic Harmonic Oscillator (TIHO) is

$$\left[-\frac{\hbar^2}{2m}\boldsymbol{\nabla}^2+\frac{m\omega^2\boldsymbol{r}^2}{2}\right]\Psi(x,y,z)=E\,\Psi(x,y,z). \qquad (1)$$

If we rewrite the eigenfunctions in the separated form $\Psi(x,y,z)=\phi(x)\,\eta(y)\,\chi(z)$, the equation (1) becomes

Separated Schrödinger equation

$$
\frac{1}{\phi(x)}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{m\omega^2 x^2}{2}\right]\phi(x)+
+\frac{1}{\eta(y)}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dy^2}+\frac{m\omega^2 y^2}{2}\right]\eta(y)+
+\frac{1}{\chi(z)}\left[-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}+\frac{m\omega^2 z^2}{2}\right]\chi(z)=E,
$$

that is

$$
\frac{H_x\,\phi(x)}{\phi(x)}+\frac{H_y\,\eta(y)}{\eta(y)}+\frac{H_z\,\chi(z)}{\chi(z)}=E.
$$

Separated Schrödinger equation

In the last equation each term in the left hand side has to be a constant because the terms depend on the different variables x, y, z and their sum is the constant E. Then we can write

$$\frac{H_x\,\phi(x)}{\phi(x)} = E_x\,, \qquad \frac{H_y\,\eta(y)}{\eta(y)} = E_y\,, \qquad \frac{H_z\,\chi(z)}{\chi(z)} = E_z\,,$$

which are three eigenvalue problems of unidimensional harmonic oscillator.

Eigenvalues and eigenfunctions

We then obtain the eigenvalues of the quantum TIHO

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

with $n_x + n_y + n_z = n$, and the corresponding eigenfunctions denoted by

$$\Psi_n(x, y, z) = \phi_{n_x}(x)\,\eta_{n_y}(y)\,\chi_{n_z}(z) \qquad \text{or} \qquad |\Psi_n\rangle = |n_x, n_y, n_z\rangle.$$

Polar Schrödinger Equation

If we write the Schrödinger equation (1)

$$\left[-\frac{\hbar^2}{2m}\nabla^2+\frac{m\omega^2\boldsymbol{r}^2}{2}\right]\Psi(x,y,z)=E\,\Psi(x,y,z)$$

in spherical polar coordinates and separate the eigenfunction as $\Psi(x,y,z)\equiv R(r)\,Y_{l,m}(\theta,\varphi)$, the radial equation for the function $R(r)\equiv R_{n,l}(r)$ is

$$\frac{d^2R(r)}{dr^2}+\frac{2}{r}\frac{dR(r)}{dr}+\left[\frac{2mE_n}{\hbar^2}-\frac{m^2\omega^2r^2}{\hbar^2}-\frac{l(l+1)}{r^2}\right]R(r)=0.$$

Polar eigenfunctions and Laguerre polynomials

If we solve the radial equation by power series expansion, we obtain the same eigenvalues

$$E_n = \hbar\omega \left(n_x + n_y + n_z + \frac{3}{2} \right) = \hbar\omega \left(n + \frac{3}{2} \right)$$

and the eigenfunctions in polar coordinates

$$\psi_{nlm}(\boldsymbol{r}) = R_{nl}(r)\, Y_{lm}(\theta, \phi) = N\, r^l\, e^{-\alpha r^2/2}\, \mathcal{L}_{n/2-l/2}^{(l+1/2)}(\alpha r^2)\, Y_{lm}(\theta, \phi),$$

Parity of the quantum numbers

where

1) the nonnegative quantum numbers n, l have the same parity, with $l \leq n$;

2) $\mathcal{L}_s^{(a)}(x)$ denotes the associated Laguerre polynomials whose expression for the real parameter $a > -1$ and the nonnegative integer parameter s is

$$\mathcal{L}_s^{(a)}(x) = \frac{e^x}{x^a} \frac{d^s}{dx^s} (x^{s+a} e^{-x}).$$

Dimension of the eigenspace of E_n

It is worth noting that the total degeneracy d_n of an eigenvalue E_n is

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

and that the number d_n is coincident with the total number $\mathcal{N}$ of spherical harmonics corresponding to all quantum numbers l having the same parity of n, with $l \leq n$.

Comparison with the spherical harmonics

In fact, for even $n = 2m$ we have $l = 2k$ and then

$$\mathcal{N} = \sum_{k=0}^{m} [2\,(2k)+1] = 2m^2+3m+1 = \frac{(2m+1)(2m+2)}{2} = d_{2m}\,;$$

while for odd $n = 2m+1$ we have $l = 2k+1$ and then

$$\mathcal{N} = \sum_{k=0}^{m} [2\,(2k+1)+1] = 2m^2+5m+3 = \frac{(2m+2)(2m+3)}{2} = d_{2m+1}.$$

Degeneracy: example with $n = 1$

For $n = 1$ we have the $d_1 = (1+1)(1+2)/2 = 3$ eigenfunctions denoted by $|n_x, n_y, n_z\rangle$ given by

$$|1,0,0\rangle, \qquad |0,1,0\rangle, \qquad |0,0,1\rangle$$

or the three eigenfunctions denoted by $|\psi_{n,l,m}\rangle$ given by

$$|\psi_{1,1,-1}\rangle, \qquad |\psi_{1,1,0}\rangle, \qquad |\psi_{1,1,1}\rangle,$$

corresponding to the same eigenvalue

$$E_1 = \frac{5}{2}\,\hbar\omega.$$

Degeneracy: example with $n = 2$

For $n = 1$ we have the $d_2 = (2 + 1)(2 + 2)/2 = 6$ eigenfunctions denoted by $|n_x, n_y, n_z\rangle$ given by

$$|2,0,0\rangle, \quad |0,2,0\rangle, \quad |0,0,2\rangle, \quad |1,1,0\rangle, \quad |1,0,1\rangle, \quad |0,1,1\rangle,$$

or the six eigenfunctions denoted by $|\psi_{n,l,m}\rangle$ given by

$$|\psi_{2,2,2}\rangle, \quad |\psi_{2,2,1}\rangle, \quad |\psi_{2,2,0}\rangle, \quad |\psi_{2,2,-1}\rangle, \quad |\psi_{2,2,-2}\rangle, \quad |\psi_{2,0,0}\rangle,$$

corresponding to the same eigenvalue

$$E_2 = \frac{7}{2}\,\hbar\omega.$$

Natural and accidental degeneracy

From the eigenfunctions $|\psi_{n,l,m}\rangle$ corresponding to the eigenvalue E_2 we see that the energy E_2 is independent from both the quantum numbers l, m.

The independence from the quantum number m is called *natural degeneracy* and is due, as it is well known, to the rotational invariance of the central hamiltonian (conservation of the angular momentum).

The independence from the quantum number l is called *accidental degeneracy* and is due to a second conservation law of the hamiltonian.

Degeneracy and ladder operators

Our aim is now to explain each degeneracy in terms of suitable *ladder operators*.

For the natural degeneracy, the corresponding ladder operator has to leave unchanged the quantum numbers n, l shifting the quantum number m by a unity. As it is well known, the *ladder operators* for the quantum number m are the operators L_+, L_-.

Also for the accidental degeneracy, we would like to give its clarification in terms of other *ladder operators* which leave unchanged the quantum number n (and then the energy) shifting the quantum number l.

Statement of the theorem

In order to obtain a ladder operator, we use an important general theorem of linear algebra which could be called *quantum shift theorem*.

Theorem: *given a hermitian operator B and an eigenvector* $|\bar{\mu}\rangle$ *of B corresponding to the eigenvalue* $\bar{\mu}$*, if another (not necessarily hermitian) operator* $\mathcal{O}$ *satisfies the relation*

$$[B, \mathcal{O}]|\bar{\mu}\rangle = \mu \mathcal{O}|\bar{\mu}\rangle, \quad \text{for a real number } \mu,$$

then it follows that either $\mathcal{O}|\bar{\mu}\rangle$ *is the null vector, or it is still an eigenvector of B, corresponding to the eigenvalue* $\bar{\mu} + \mu$.

Application to a non-degenerate spectrum

For the unidimensional harmonic oscillator we have

$$H = \hbar\omega \left(N + \frac{1}{2} \right), \quad \text{with } N = a^\dagger a.$$

Since $[N, a^\dagger] = a^\dagger = (+1)a^\dagger$, that is $\mu = 1$, it follows that for each eigenvector $|n\rangle$ of N, the vector $a^\dagger|n\rangle$ is the eigenvector of N corresponding to the shifted eigenvalue $n + \mu = n + 1$.

Analogously, since $[N, a] = -a = (-1)a$, that is $\mu = -1$, it follows that for each eigenvector $|n\rangle$ of N, the vector $a|n\rangle$ is either the null vector or is the eigenvector of N corresponding to the shifted eigenvalue $n + \mu = n - 1$.

Application to a non-degenerate spectrum

By virtue of these properties, the non-hermitian operators $a^\dagger$, a are called ***ladder operators*** of the unidimensional harmonic oscillator.

Application to a degenerate spectrum

By denoting with $|l, m\rangle$ the simultaneous eigenvectors of the hermitian operators $\boldsymbol{L}^2, L_z$, we have that the specification of the quantum number $m = -l, -l+1, -l+2, \ldots, l-2, l-1, l$ removes the degeneracy of the spectrum of $\boldsymbol{L}^2$.

Since $[\boldsymbol{L}^2, L_\pm] = 0$ and $[L_z, L_\pm] = \pm\hbar L_\pm$, that is $\mu = \pm\hbar$, then if $L_\pm|l, m\rangle$ is not the null vector, it follows

$$\boldsymbol{L}^2|l, m\rangle = \hbar^2\, l(l+1)|l, m\rangle,$$

$$\boldsymbol{L}^2 \left[L_\pm|l, m\rangle \right] = \hbar^2\, l(l+1) \left[L_\pm|l, m\rangle \right],$$

that is $|l, m\rangle$ and $L_\pm|l, m\rangle$ are eigenvectors of $\boldsymbol{L}^2$ corresponding to the same eigenvalue $\hbar^2\, l(l+1)$,

Application to a degenerate spectrum

and then

$$L_z \left[L_\pm |l, m\rangle \right] = \hbar \, (m \pm 1) \left[L_\pm |l, m\rangle \right] ,$$

that is, by virtue of the theorem with $\mu = \pm\hbar$, the vectors $L_\pm |l, m\rangle$ are eigenvectors of L_z corresponding to the shifted eigenvalues $m \pm 1$.

For these properties, the operators $L_\pm$ are called ***ladder operators*** of the angular momentum.

Statement of the problem

By denoting the eigenvectors of the hamiltonian $\mathcal{H}$ of the TIHO with $|\psi_{n,l,m}\rangle \equiv |n,l,m\rangle$, we look for a *raising operator*, denoted by $\mathcal{M}_+$, such that, in analogy with the degenerate case of the angular momentum, it yields

$$1) \quad \mathcal{H}|n,l,m\rangle = E_n\,|n,l,m\rangle,$$

$$2) \quad \mathcal{H}\left[\mathcal{M}_+|n,l,m\rangle\right] = E_n\left[\mathcal{M}_+|n,l,m\rangle\right],$$

that is $|n,l,m\rangle$ and $\mathcal{M}_+|n,l,m\rangle$ have the same energy E_n, and

$$3) \quad \boldsymbol{L}^2\left(\mathcal{M}_+|n,l,m\rangle\right) = \hbar^2[l(l+1)+(4l+6)]\left(\mathcal{M}_+|n,l,m\rangle\right),$$

Statement of the problem

because the difference between two consecutive eigenvalues of $\boldsymbol{L}^2$ (**having the same parity**) is

$$(l+2)(l+3) - l(l+1) = 4l+6.$$

As a consequence, the *raising operator* $\mathcal{M}_+$ has to satisfy, by virtue of the quantum shift theorem, the two commutation rules

$$[\mathcal{H}, \mathcal{M}_+] = 0$$

and

$$[\boldsymbol{L}^2, \mathcal{M}_+]|n, l, \bar{m}\rangle = \hbar^2(4l+6)\mathcal{M}_+|n, l, \bar{m}\rangle,$$

for some eigenvectors $|n, l, \bar{m}\rangle$ of $\boldsymbol{L}^2$, with $\mu = 4l+6$.

Conserved second order tensor

It is easy to prove that the second conservation law of the hamiltonian

$$\mathcal{H} = \frac{\boldsymbol{p}^2}{2m} + \frac{m\omega^2 \boldsymbol{r}^2}{2}$$

of the TIHO is the symmetric second order tensor

$$T_{ij} = \frac{p_i p_j + m^2\omega^2 x_i x_j}{2} ,$$

whose *trace* is coincident with the hamiltonian.

Construction of the ladder operators

With the conserved components

$$\mathcal{M}_x = \frac{p_x p_y}{2m\omega} + \frac{m\omega}{2}\, xy \qquad \text{and} \qquad \mathcal{M}_y = \frac{p_y^2 - p_x^2}{4m\omega} + \frac{m\omega}{4}\,(y^2 - x^2),$$

of the tensor T_{ij} we construct the operators $\mathcal{M}_\pm = \mathcal{M}_x \pm i\mathcal{M}_y$, which verify the commutation rules

$$[L_z, \mathcal{M}_\pm] = \pm 2\hbar \mathcal{M}_\pm \tag{2a}$$

and

$$[\boldsymbol{L}^2, \mathcal{M}_+] = 4\hbar \mathcal{M}_+ L_z + 6\hbar^2 \mathcal{M}_+ + \mathcal{O}(\boldsymbol{r}, \boldsymbol{p}) L_+ \,, \tag{2b}$$

where $\mathcal{O}(\boldsymbol{r}, \boldsymbol{p})$ is a differential operator depending on the components of $\boldsymbol{r}, \boldsymbol{p}$.

Construction of the ladder operators

From the relation (2b) it effectively follows, with $\mu = 4l + 6$

$$[\boldsymbol{L}^2, \mathcal{M}_+]|n, l, l\rangle = \hbar^2(4l + 6)\mathcal{M}_+|n, l, l\rangle. \tag{3}$$

At this point, the conservation of $\mathcal{M}_+$, that is $[\mathcal{H}, \mathcal{M}_+] = 0$, assures that the two vectors $|n, l, l\rangle$ and $\mathcal{M}_+|n, l, l\rangle$ have the same energy, that is they correspond to the same energy eigenvalue E_n.

Further, the relations (2a) and (3) give us, up to a normalization constant C, the operatorial action

$$\mathcal{M}_+|n, l, l\rangle = C\,|n, l + 2, l + 2\rangle$$

and then the operator $\mathcal{M}_+$ is the *raising operator* of $\boldsymbol{L}^2$.

Clarification of the accidental degeneration

By iterating the action of the *raising operator* $\mathcal{M}_+$ on the eigenvectors $|n, l, l\rangle$ starting from $l = 0$ or $l = 1$, we obtain all the eigenvectors of the degenerate eigenspace of E_n, because we get

$$|n, 0, 0\rangle \longrightarrow |n, 2, 2\rangle \longrightarrow |n, 4, 4\rangle \longrightarrow \dots \longrightarrow |n, n, n\rangle$$

for even n and

$$|n, 1, 1\rangle \longrightarrow |n, 3, 3\rangle \longrightarrow |n, 5, 5\rangle \longrightarrow \dots \longrightarrow |n, n, n\rangle$$

for odd n.

Clarification of the accidental degeneration

In order to terminate, we want to explain shortly why the *lowering operator* of $\boldsymbol{L}^2$ does not exist. Both the commutation rule

$$[\boldsymbol{L}^2, \mathcal{M}_-]|l, -l\rangle = \hbar^2(4l+6)\mathcal{M}_-|l, -l\rangle$$

and the relation (2a) give us the operatorial action of $\mathcal{M}_-$

$$\mathcal{M}_-|n, l, -l\rangle = \tilde{C}\,|n, l+2, -l-2\rangle,$$

from which we can realize that the action of $\mathcal{M}_-$ on $|n, l, -l\rangle$ can not give an eigenvector with a lower quantum number of the operator $\boldsymbol{L}^2$, because the quantum number $m = -l-2$ can not belong to the multiplet of $l-2$.

Clarification of the accidental degeneration

By iterating the action of the *lowering operator* $\mathcal{M}_-$ on the eigenvectors $|n, l, -l\rangle$ starting from $l = 0$ or $l = 1$, we then obtain

$$|n, 0, 0\rangle \longrightarrow |n, 2, -2\rangle \longrightarrow |n, 4, -4\rangle \longrightarrow \ldots \longrightarrow |n, n, -n\rangle$$

for even n and

$$|n, 1, -1\rangle \longrightarrow |n, 3, -3\rangle \longrightarrow |n, 5, -5\rangle \longrightarrow \ldots \longrightarrow |n, n, -n\rangle$$

for odd n.

THANK YOU VERY MUCH FOR YOUR ATTENTION