Symmetry group of a particle in an impenetrable cubic well potential

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Abstract. A quantum particle in a impenetrable cubic well potential presents accidental degeneracy when the $O_h$ group is considered to be the symmetry group of the system. This degeneracy becomes natural when a new symmetry group, embedding the $O_h$ group, is proposed. This new group turns out to be the semidirect product $G = T \ltimes O_h$, where $T$ is a two-dimensional compact continuous group whose generators correspond to linear combinations of the one-dimensional Hamiltonians. The systematic degeneracy is studied in detail, the new group is identified and its irreducible representations (irreps) are constructed by means of induction, an approach that allows the irreducibility and completeness to be assured. Pythagorean degeneracy as well as the one due to commensurable sides are not considered.

1. Introduction
The degeneracy degree is expected to correspond with the dimension of one of the symmetry group irreducible representations (irrep) [1]. When this is not the case the degeneracy is identified as accidental. Instances of accidental degeneracy are abundant in quantum mechanics [1], but in any case, according to the experience, the existence of this kind of degeneracy suggests an overlooked higher symmetry. The particle in a square or cubic box with impenetrable walls is the most simple quantum mechanical system where accidental degeneracy appears, however this systems receive a very brief mention in the literature[6, 7, 8], this may be explained by the fact that the natural language of symmetry is group theory, a specialized field not included in most textbooks of quantum mechanics. Though, in 1996 leyvraz et al [9] derived a new symmetry group to explain the accidental degeneracy of a square box from the group theory point of view.

A more interesting system presenting systematic degeneracy is a quantum particle in an impenetrable cubic well potential, because it provides a deeper insight into the mathematics and physics of the problem. The description of a particle in a cubic box allows the system of square and parallelepiped well potentials to be studied as a symmetry breaking process, in such a way that these cases can be analyzed as a mathematic subduction problem. The simultaneous analysis of these systems provides a clear example of the fact that the greater the symmetry the higher the degeneracy.

A free particle enclosed in an impenetrable three dimensional box of sides $a$, $b$ and $c$, as displayed in Figure 1, is described by the eigenstates $| \Psi_{n_1 n_2 n_3} \rangle = \psi_{n_1}(x) \psi_{n_2}(y) \psi_{n_3}(z)$, where $\psi_{n_1}(x) = \sqrt{\frac{2}{a}} \sin \left( \frac{n_1 \pi x}{a} \right)$; $\psi_{n_2}(y) = \sqrt{\frac{2}{b}} \sin \left( \frac{n_2 \pi y}{b} \right)$; $\psi_{n_3}(z) = \sqrt{\frac{2}{c}} \sin \left( \frac{n_3 \pi z}{c} \right)$; with $n_i$ positive integers. These states satisfy the condition $\Psi_{n_1 n_2 n_3}(x, y, z) = 0$ at the boundaries of the box.
The corresponding eigenvalues are given by

\[ E_{n_1 n_2 n_3} = \frac{\hbar^2 \pi^2}{2\mu} \left( \frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2} \right), \]  

(1)

where \( \mu \) is the reduced mass. The energies and eigenstates by itself does not provide information about the kind of degeneracy displayed, this should be established through the proposition of a symmetry group.

Figure 1. Impenetrable three-dimensional box. The origin \( \mathcal{O} \) taken to obtain the wave functions is displaced from the origin \( \mathcal{O}' \) where the symmetry elements converge.

When \( a = b = c \) we have a cubic box that presents three subspaces of degenerate funtions. For \( n_1 = n_2 = n_3 \) we have one-dimensional subspaces \( \mathcal{L}_1 = \{|\Psi_{nnn}\rangle\}; n_1 = n_2 = n_3 = n \), when only two quantum numbers are equal we have three-dimensional subspaces given by \( \mathcal{L}_3 = \{|\Psi_{nnn}\rangle, |\Psi_{nnm}\rangle, |\Psi_{nmn}\rangle\}; n_1 = n_2 = n \), and when all the quantum numbers are different, six dimensional subspaces are described by \( \mathcal{L}_6 = \{|\Psi_{n_1 n_2 n_3}\rangle; n_1 \neq n_2 \neq n_3 \} \).

2. New symmetry group

To identify the symmetry group we shall first consider the apparent geometrical symmetry of this system, such symmetry corresponds to the point group \( \mathcal{O}_h \), hence the eigenstates are expected to carry irreps of this group. The identification of the irreps, however, cannot be achieved straightforwardly since the eigenstates are given with respect to the origin \( O \), while the center of the parallelepiped is located at \( O' \). Both origins are related with the translation \( O_T \), with \( T \) defined by \( T(r_O) = r_{O'} = r_O - (\frac{a}{2}, \frac{b}{2}, \frac{c}{2}) \). Now, if \( O_R \), with \( R \in \mathcal{O}_h \), are operators respect to the origin \( O \), the corresponding operators \( O_R' \) are obtained through \( O_T O_R O_T^{-1} = O'R \) [14].

The character table for the geometrical symmetry group \( \mathcal{O}_h \) is displayed in Table 1 and the reduction assuming this group as the symmetry group is given in Table 2. For \( \mathcal{L}_3 \) systematic accidental degeneracy appears when \( n \) and \( m \) are both even or odd. Furthermore the six fold degeneracy appearing in the \( \mathcal{L}_6 \) subspaces cannot be explained in the context of the \( \mathcal{O}_h \) symmetry group [10], because, according to the character table, the expected larger degeneracy degree is three. An interesting peculiarity for this subspace is that a multiplicity of 2 appears for both representations \( E_g \) and \( E_u \), Table 2.
Table 1. Character table of the point group $O_h$. The assignment of the classes is indicated in the second row.

| $O_h$ | $E$ | $3C_3$ | $3C_2'$ | $6C_4$ | $6C_2$ | $I$ | $8S_6$ | $3\sigma_h$ | $6S_4$ | $6\sigma_d$ |
|-------|-----|--------|----------|--------|--------|-----|--------|-------------|-------|------------|
|       | $K_1$ | $K_2$ | $K_3$ | $K_4$ | $K_5$ | $K_6$ | $K_7$ | $K_8$ | $K_9$ | $K_{10}$ |
| $A_1g$ | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| $A_2g$ | 1 | 1 | 1 | -1 | -1 | 1 | 1 | 1 | -1 | -1 |
| $E_g'$ | 2 | -1 | 2 | 0 | 0 | 2 | -1 | 2 | 0 | 0 |
| $T_{1g}$ | 3 | 0 | -1 | 1 | -1 | 3 | 0 | -1 | 1 | -1 |
| $T_{2g}$ | 3 | 0 | -1 | -1 | 1 | 3 | 0 | -1 | -1 | 1 |
| $A_{1u}$ | 1 | 1 | 1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 |
| $A_{2u}$ | 1 | 1 | 1 | -1 | -1 | -1 | -1 | -1 | -1 | -1 |
| $E_u$ | 2 | -1 | 2 | 0 | 0 | -2 | 1 | -2 | 0 | 0 |
| $T_{1u}$ | 3 | 0 | -1 | 1 | -1 | -3 | 0 | 1 | -1 | 1 |
| $T_{2u}$ | 3 | 0 | -1 | -1 | 1 | -3 | 0 | 1 | -1 | -1 |

Table 2. Decomposition of the degenerate states associated with a particle in a cubic box with impenetrable walls. The $O_h$ irreducible representations contained in the degenerate subspaces are displayed explicitly.

| Dimension | Parity | Condition | Representation | Direct product |
|-----------|--------|-----------|----------------|---------------|
| 1(mm)     | $n = 2p$ | $n_x = n_y = n_z$ | $A_2u$ | $A_1g$ |
|           | $n = 2p + 1$ |              |               |               |
| 3(mm)     | $n = 2p$ | $n_x = n_y \neq n_z$ | $A_2u \oplus E_u$ | $A_2u \oplus E_g = E_u$ |
|           | $m = 2p$ | $n_x = n_y \neq n_z$ | $A_1g \oplus E_g$ | $A_1g \oplus E_g = E_g$ |
|           | $n = 2p + 1$ | $n_y = n_z \neq n_x$ | $T_{2g}$ |               |
|           | $n = 2p$ |               | $T_{1u}$ |               |
| 6(mm)     | $n = m = l = 2p$ | $n_x \neq n_y \neq n_z$ | $A_1u \oplus A_{2u} \oplus 2E_u$ | $E_g \oplus E_u = A_{1u} \oplus A_{2u} \oplus E_u$ |
|           | $n = m = l = 2p + 1$ |               | $A_{1g} \oplus A_{2g} \oplus 2E_g$ | $E_g \oplus E_g = A_{1g} \oplus A_{2g} \oplus E_g$ |
|           | $l = 2p + 1$ |               | $T_{1g} \oplus T_{2g}$ | $E_g \oplus T_{1g} = T_{1g} \oplus T_{2g}$ |
|           | $n = m = 2p + 1$ |               | $T_{1u} \oplus T_{2u}$ | $E_g \oplus T_{1u} = T_{1u} \oplus T_{2u}$ |

The first thing to establish a new symmetry group is identifying the operator or operators that connect the subspaces spanning $O_h$ irreps. To achieve this goal we look for an operator $F_r^{(\rho)}$, spanning the irrep $\rho$ and satisfies that $\langle \psi_{\gamma'}|F_r^{(\rho)}|\psi_{\gamma}\rangle$ vanish unless $\Gamma' \in \rho \otimes \Gamma = \sum_{\mu} \otimes \mu$ where $\Gamma'$ and $\Gamma$, with components $\gamma'$ and $\gamma$ respectively, are the irreps spanned by the kets. It is not difficult to check that such operator must hold the irrep $E_g$ and consequently $\rho = E_g$, [19]. From the $O_h$ character table [19] we notice that the following Cartesian Harmonics span the irrep $E_g$:

\[
Y_{\cos 2_\phi}^2(x', y', z') = \frac{1}{4} \sqrt{\frac{15}{\pi}} \frac{(x'^2 - y'^2)}{r'^2},
\]

\[
Y_0^2(x', y', z') = \frac{1}{4} \sqrt{\frac{5}{\pi}} \frac{(2x'^2 - x'^2 - y'^2)}{r'^2},
\]
The same linear combination in terms of the square momenta does transform according to \(E_g\) in both reference systems \([9, 10]\). We thus have the following operators

\[
\begin{align*}
F_{A_{1g}, A_g}^{(E_g)} &= \frac{1}{4} \sqrt{\frac{5}{\pi}} \left( 2 \frac{\partial^2}{\partial z^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right), \\
F_{B_{1g}, A_g}^{(E_g)} &= \frac{1}{4} \sqrt{\frac{15}{\pi}} \left( \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} \right),
\end{align*}
\]

where we have added the components according to the chain \(O_h \supset D_{4h} \supset D_{2h}\). The operators (3) explain the accidental degeneracy, because they connect degenerate states with different \(O_h\) irreps.

Once that the accidental degeneracy as well as the operators that connect the degenerate states have been identified, we are ready to propose a new symmetry group for this system. The operators generate the continuous group \(T\), whose elements are obtained by exponentiation and form a two dimensional group with elements

\[
U(\alpha, \beta) = U_1(\alpha) \otimes U_2(\beta) = e^{i\alpha F_{A_{1g}}^{(E_g)} + i\beta F_{B_{1g}}^{(E_g)}}.
\]

The corresponding Casimir operator of this group is the Hamiltonian itself.

Considering the transformation of the elements (4) under the action of \(R \in O_h\), we realize that the subgroup \(T\) is invariant in the context of the new group \(G\). This fact allows the new group to be expressed as

\[
G = T \wedge O_h,
\]

and in terms of left cosets

\[
G = \sum_{\lambda=1}^{|\lambda|} S_\lambda \ T; \quad |\lambda| = \frac{|G|}{|T|} = |O_h|; \quad S_\lambda \in O_h.
\]

Therefore all the elements \(g \in G\) can be written in the form

\[
g = \hat{O}_R \ U(\alpha, \beta); \quad R \in O_h, \quad g \in G,
\]

with the product of elements \(gg' = g''\).

3. Representations of the group \(G\)

Once we have identified the new symmetry group, we proceed to construct the irreps following the induction approach, this method will assure the irreducibility and completeness of the representations [11]. According to this, we have first to construct the irreps of the invariant subgroup \(T\). The representation of the \(T\) elements is diagonal in the basis of the cubic box eigenfunctions.

For the six dimensional space \(L_6 = \{|\Psi_{n_1n_2n_3}\rangle\}\). The action of the subgroup \(T\) elements over the state \(|\Psi_{n_1n_2n_3}\rangle\) is depicted by

\[
\hat{U}(\alpha, \beta)|\Psi_{n_1n_2n_3}\rangle = D^{(k_n)}(U(\alpha, \beta)) \ |\Psi_{n_1n_2n_3}\rangle,
\]

where

\[
D^{(k_n)}(U(\alpha, \beta)) = e^{i\alpha k_n^{(1)} + i\beta k_n^{(2)}},
\]

where we define the vectors,

\[
\begin{align*}
k_n &\equiv (k_{n_1n_2n_3}^{(1)}, k_{n_1n_2n_3}^{(2)}), \\
t &\equiv (\alpha, \beta),
\end{align*}
\]
The vectors (10) will be considered to be written in an orthonormal basis. It is appropriate to add the label $k_n$ to the state in the form $|\Psi_{k_n}^{n_1 n_2 n_3}\rangle$. If we apply the elements of $T$ to the other five states of $L_6$ we obtain five additional representations associated with the functions of permuted indices in accordance to the permutations of $S_3$. In this context, each function in the space $L_6$ span a different representation. These irreps are the starting point to obtain the irreps of the complete group $G$ by induction.

The $T$ irrep $k_1$ is invariant under the action of the elements of $T$ as well as the elements of the subgroup $D_{2h}$. This set of transformations form a group, the so called little group of $k_1$, denoted by $K(k_1)$, in this case given by

$$K(k_1) = T \lor D_{2h}. \tag{11}$$

The little group of $k_1$, however, is still infinite. To have a group of finite order we note that

$$\frac{K(k_1)}{T} \approx D_{2h} \tag{12}$$

On the other hand

$$\frac{G}{T} \approx O_h, \tag{13}$$

showing that the left coset expansion

$$O_h = \sum_{\lambda} p_\lambda \ D_{2h}; \quad |\lambda| = \frac{|O_h|}{|D_{2h}|} \tag{14}$$

is the relevant expansion in constructing the irreps, since the action of the elements of the group $T$ is diagonal over the basis $L_6$. The expression (14) indicates that every element $g \in O_h$, may be expressed in terms of a product of the form

$$g = p_\lambda \ h; \quad h \in D_{2h}, \tag{15}$$

in accordance with the explicit coset expansion

$$O_h = D_{2h} + C_4(x) \ D_{2h} + C_4(y) \ D_{2h} + C_4(z) \ D_{2h} + C_3^f \ D_{2h} + (C_3^f)^2 \ D_{2h}. \tag{16}$$

To obtain the irreducible representations by induction, we start projecting the state $|\phi_{k_1}\rangle$ to irreps of the little cogroup $D_{2h}$, giving rise to the states $|\phi_{k_1}; \Gamma, \gamma\rangle$. Finally, the induction is carried out and the representations so obtained are irreducible and complete with the form

$$\Gamma_{k_1} G = \Gamma K(k_1) T \uparrow G \tag{17}$$

There are two labels, the prong corresponding to the irrep $k_1$ of $T$, and the irrep $\Gamma$ of the little cogroup $k_1 K = D_{2h}$.

We now proceed to generate the irreps of the group $G$. For the elements of $T$ the matrix representation in the new basis is diagonal as we have already noted,
Let us now consider the point operations. In order to obtain the representation of the generator \(C_4(x)\), for instance, the basal representation should be obtained to generate:

\[
D(C_4(x)) = \begin{pmatrix}
0 & \chi^\mu(C_2(x)) & 0 & 0 & 0 & 0 \\
\chi^\mu(E) & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \chi^\mu(C_2(z)) & 0 \\
0 & 0 & 0 & 0 & 0 & \chi^\mu(C_2(z)) \\
0 & \chi^\mu(E) & 0 & 0 & 0 & 0 \\
0 & 0 & \chi^\mu(C_2(x)) & 0 & 0 & 0
\end{pmatrix}.
\]

(19)

where \(\chi^\mu(h)\) is the irrep, in this case the character, of the element \(h \in D_{2h}\). It should be clear that \(\chi^\mu(E) = 1\), \(\forall \mu\). In the same way we obtain for the generator \(C_4(y)\):

\[
D(C_4(y)) = \begin{pmatrix}
0 & 0 & \chi^\mu(C_2(y)) & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \chi^\mu(C_2(x)) \\
\chi^\mu(E) & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \chi^\mu(C_2(z)) & 0 \\
0 & 0 & 0 & \chi^\mu(E) & 0 & 0 \\
0 & \chi^\mu(C_2(y)) & 0 & 0 & 0 & 0
\end{pmatrix}.
\]

(20)

Finally, the representation \(D(I)\) is diagonal with elements \(\chi^\mu(I) = (-1)^{n_1+n_2+n_3+1}\). We have thus constructed the representation of the group \(G\) associated with the \(L_6\) subspaces. Formally we have induced the representations of \(T\) through the little cogroup [11].

Let us now consider the subspace \(L_3\). We proceed to identify the little group of \(k_1\). Besides the elements of the subgroups \(T\) and \(D_{2h}\), the transformation \(\sigma_d\) also keeps the irrep \(k_1\) invariant. We note that \(D_{4h} = D_{2h} + \sigma_d D_{2h}\), and consequently

\[
\mathcal{K}(k_1) = T \triangleleft D_{4h}.
\]

(21)

In explicit form we select the expansion

\[
\mathcal{O}_h = D_{4h} + C_4(x)D_{4h} + C_4(y)D_{4h}.
\]

(22)

Again, the basal representation is needed to obtain,

\[
D(C_4(x)) = \begin{pmatrix}
0 & \mathbf{D}^\mu(C_2(x)) & 0 \\
\mathbf{D}^\mu(E) & 0 & 0 \\
0 & \mathbf{D}^\mu(C_2(z)) & 0
\end{pmatrix},
\]

(23)

\[
D(C_4(y)) = \begin{pmatrix}
0 & 0 & \mathbf{D}^\mu(C_2(y)) \\
0 & \mathbf{D}^\mu(C_2^2(z)) & 0 \\
\mathbf{D}^\mu(E) & 0 & 0
\end{pmatrix},
\]

(24)

with a diagonal matrix for the representation \(D(I)\) with elements \(\chi^\mu(I) = (-1)^{m+1}\). Finally, for the representation of the elements of \(T\) we have the trivial result

\[
D(t) = \begin{pmatrix}
e^{it \cdot k_1} & 0 & 0 \\
0 & e^{it \cdot k_2} & 0 \\
0 & 0 & e^{it \cdot k_3}
\end{pmatrix}.
\]

(25)
Figure 2. Schematic energy diagram depicting the symmetry breaking from the cubic box to the parallelepiped box. Degenerate levels are shown together, the irreps associated with the symmetry group are indicated above each set. According to these groups the degeneracy of all these levels are natural. Notice that the greater the symmetry the higher the degeneracy. Here we have taken $c > b > a$.

We have also the one dimensional space, for this case the associated representation of $U(t)$ carries the irrep $k = 0$, which means that $\hat{U}(t)|\Psi^0_{nnn}\rangle = |\Psi^0_{nnn}\rangle$, and consequently the little group of $k$ coincides with the group $G$ itself. Then the little cogroup is given by $O_h$ with the basal representation given by the one dimensional unit matrix. Hence the states $|\Psi^0_{nnn}\rangle$ span the irreps of the octahedral group.

The analysis of the system when the symmetry is broken is presented in Figure 2. If in our previous analysis of the cubic box we introduce the condition $a = b \neq c$, then some of the transformations of the group $T \wedge O_h$ stop keeping invariant the Hamiltonian. We thus have to identify the new symmetry group by subduction. For a rectangular box the $z$-axis is not
equivalent anymore and the operator $\hat{F}^{E_0}_{\lambda\mu}$ is not relevant. On the other hand the symmetry is diminished from $O_h$ to $D_{4h}$. These considerations lead to the reduction

$$T \wedge O_h \supset T_1 \wedge D_{4h},$$

(26)

In the case of $a \neq b \neq c k = 0$ the states are labeled by the group $D_{2h}$.

4. Conclusions

The symmetry group of a particle inside an impenetrable cubic well potential has been identified to be $G = T \wedge O_h$, where $T$ is a compact continuous group. Reducing the representations generated by the eigenstates allowed us to identify the systematic degeneracy. The continuous group was obtained identifying the operators that connect degenerate states spanning different $O_h$ irreps, by means of the coupling coefficients. The elements of the group $T$ are constructed by exponentiation of the operators.

We have thus obtained the irreps of the symmetry group by the process of induction, an approach that assures the irreducibility and completeness of the representations as well as their completeness. From this perspective the systematic accidental degeneracy become natural, then by introducing the continuous group whose Casimir operator is the Hamiltonian all levels are distinguished, as can be observed in Figure 2.

The states of this system have been classified according with the chain of subgroups consistent with the reduction of symmetry to obtain the square and rectangular boxes, allowing us to analyze the symmetry breaking in a natural form [20].

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