

# Group representation theory and quantum physics\*

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## Abstract

This is a basic tutorial on the use of group representation theory in quantum physics, in particular for such systems as molecules and crystals, which forms the basis of spectroscopic studies in physics and chemistry. Note that, despite the now venerable character of the aforementioned scientific endeavors, group representation theory still finds interesting and novel applications, such as the hidden subgroup problem in quantum computing, which will be presented elsewhere.

## 1 Introduction

### 1.1 Preamble

Although seldom taught to physics students these days, group theory remains the method of choice for simplifying the physical analysis of systems possessing some degree of symmetry. Group theory is of course ubiquitous in high energy physics. In other areas of physics and chemistry, its uses have been predominantly confined to spectroscopic studies of atoms, molecules, and materials, which are now well established and not considered so new any more. The power, generality, and elegance of the method, however, do remain, as illustrated by new applications of group theory that have been discovered in the novel research field of quantum information. Thus, as group theory becomes trendy again via, for example, the hidden subgroup problem in quantum computing [1], I thought it might be of interest to first revisit the “old” use of group theory in quantum mechanics. Because this is a mathematics seminar, I will spend more time describing quantum mechanics than group theory, as the latter is already well known to the audience. I will also ask for your indulgence for my approximate wording and possible lacks of mathematical rigor, which I hope will remain limited.

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## 1.2 The Postulates of Quantum Mechanics

Nobody knows why quantum mechanics works, but it indeed does. There hasn't yet been an experiment invalidating the predictions of quantum theory. Such a day might eventually come, or not. In the meantime, I make the Copenhagen interpretation of quantum mechanics my own, and merely apply myself to understanding and applying its postulates, as stated for example in the textbook of Cohen-Tannoudji, Diu, and Laloë [2]. While recalling them, I will also try to translate the physicists' vocabulary into more mathematical terms.

### Postulate 1

At a fixed time  $t_0$ , the state of a quantum system is defined by the ket  $|\psi(t_0)\rangle$  (in Dirac's notation), which is a vector (or, better, a ray) of a Hilbert space  $\mathcal{E}$ .

### Postulate 2

Every measurable physical quantity  $\mathcal{A}$  is described by a Hermitian operator  $A$ , called an *observable*, and acting in  $\mathcal{E}$ .

### Postulate 3

The only possible result of a measurement of  $\mathcal{A}$  is one of the eigenvalues  $a_n$  of  $A$  (which are of course real). If an eigenvalue  $a_n$  has multiplicity  $g_n > 1$  (i.e. corresponds not to a single eigenvector  $|\varphi_n\rangle$  but to several ones  $\{|\varphi_n^j\rangle\}_{j=1\dots g_n}$ ), it is said to be *degenerate* or  *$g_n$ -fold degenerate*.

### Postulate 4

For a system initially in state  $|\psi\rangle$ , the probability that a measurement of  $\mathcal{A}$  yield the result  $a_n$  is given by:

- if  $a_n$  is nondegenerate,

$$\mathcal{P}(a_n) = |\langle \varphi_n | \psi \rangle|^2 \quad (1)$$

- if  $a_n$  is  $g_n$ -fold degenerate,

$$\mathcal{P}(a_n) = \sum_{j=1}^{g_n} |\langle \varphi_n^j | \psi \rangle|^2 \quad (2)$$

- if  $A$  has a continuous spectrum (e.g. position or linear momentum observables),

$$\mathcal{P}(a \leq \text{result} \leq a + da) = |\langle \varphi_a | \psi \rangle|^2 da. \quad (3)$$

### Postulate 5

The state after a measurement  $\mathcal{M}(a_n)$  of result  $a_n$  is obtained by application of a projection operator on the corresponding eigenstate

$$|\psi\rangle \xrightarrow{\mathcal{M}(a_n)} \frac{|\varphi_n\rangle \langle \varphi_n|}{|\langle \varphi_n | \psi \rangle|} |\psi\rangle. \quad (4)$$

Equivalently,

$$|\psi\rangle = \sum_n c_n |\varphi_n\rangle \xrightarrow{\mathcal{M}(a_n)} |\varphi_n\rangle. \quad (5)$$

If  $a_n$  is  $g_n$ -fold degenerate, we have

$$|\psi\rangle = \sum_n \sum_{j=1}^{g_n} c_n^j |\varphi_n^j\rangle \xrightarrow{\mathcal{M}(a_n)} \sum_{j=1}^{g_n} c_n^j |\varphi_n^j\rangle. \quad (6)$$

### Postulate 6

The evolution of  $|\psi(t)\rangle$  is given by the *Schrödinger equation*

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H |\psi(t)\rangle \quad (7)$$

where  $H$  is the observable corresponding to the total energy of the system, and is called the Hamiltonian.

## 1.3 Energy levels of a quantum system

From the postulates of quantum mechanics, it is clear that diagonalizing the Hamiltonian  $H$

$$H |\varphi_n\rangle = E_n |\varphi_n\rangle \quad (8)$$

not only gives the energy levels  $E_n$  and the stationary states  $|\varphi_n\rangle$  of the system (if  $H$  is independent of  $t$ ), but is also key to knowing its temporal evolution. Indeed, if we decompose  $|\psi(t)\rangle$  on the orthonormal basis of these states,

$$|\psi(t)\rangle = \sum_n c_n(t) |\varphi_n\rangle, \quad (9)$$

then the Schrödinger equation becomes, for example for  $\dim \mathcal{E} = N$  (but an infinite and even continuous Hilbert space may be considered as well),

$$i\hbar \frac{d}{dt} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} = \begin{pmatrix} E_1 & 0 & \dots & 0 \\ 0 & E_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & E_N \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{pmatrix} \quad (10)$$

$$c_n(t) = c_n(t_0) e^{-\frac{i}{\hbar} E_n(t-t_0)} \quad (11)$$

$$|\psi(t)\rangle = e^{-\frac{i}{\hbar} H(t-t_0)} |\psi(t_0)\rangle \quad (12)$$

The problem is, for example in atomic and molecular physics, that diagonalizing the Hamiltonian becomes quickly very complicated and intractable as the number of electrons increases and no analytical solutions are known beyond the Hydrogen atom. One is thus led to consider other ways of gaining information, such as using the symmetries of the system, which is the subject of this seminar.

Before moving on, I would like to make one remark about the use of quantum computers to simulate quantum physics. In a now well-known 1982 paper [3], Richard Feynman suggested that quantum systems could be used to simulate quantum physics, i.e. perform analog

implementations of Schrödinger equation, with an exponential speedup over classical computations of Schrödinger equation: consider, for example,  $p$  quantum systems with 2 states each. The Hamiltonian is a  $N \times N$  matrix, with  $N = 2^p$ , and has to be diagonalized. If one had a quantum computer, one could clearly evolve a superposition of all  $2^p$  quantum states in but a single shot. In theory, that would represent an exponential speedup.

## 2 Symmetry and the Hamiltonian

In order to help with the diagonalization of a complicated Hamiltonian, it is useful to seek the operators that commute with it. In fact, it also makes sense to look for the biggest group that commutes with the Hamiltonian, i.e. that leaves it invariant. Indeed, consider a symmetry operation  $\Gamma$  acting on the coordinates (e.g. an isometry)

$$\vec{r}' = \Gamma \vec{r}, \quad (13)$$

then the equivalent operator on  $\mathcal{E}$ ,  $G$ , is such that [4]

$$H'(\vec{r}) = GH(\vec{r})G^{-1} = H(\Gamma^{-1}\vec{r}). \quad (14)$$

It is then straightforward to see that, if  $H$  is invariant under  $G$ , then it commutes with  $G$

$$GHG^{-1} = H \Leftrightarrow GH = HG \Leftrightarrow [G, H] = 0. \quad (15)$$

The symmetry group of a Hamiltonian commutes with it. Let us now establish a few useful theorems.

### 2.1 First theorem (precursor of Wigner's theorem)

*If  $A$  and  $B$  are two operators that commute with each other, then every degenerate eigensubspace of  $A$  is globally invariant under  $B$  — and vice versa.*

*Proof:* Let  $|\varphi_n\rangle$  be an eigenvector of  $A$ , of eigenvalue  $a_n$ . Then,  $A(B|\varphi_n\rangle) = BA|\varphi_n\rangle = Ba_n|\varphi_n\rangle = a_n(B|\varphi_n\rangle)$ , i.e.  $B|\varphi_n\rangle$  is also an eigenvector of  $A$ , with the same eigenvalue. Two cases can then be considered:

(i)  $a_n$  is nondegenerate

Then  $|\varphi_n\rangle$  and  $B|\varphi_n\rangle$  must be parallel vectors in  $\mathcal{E}$  (i.e. be the same ray):

$$B|\varphi_n\rangle = b_n|\varphi_n\rangle, \quad (16)$$

which means that  $|\varphi_n\rangle$  is an eigenvector of  $B$  as well.

(ii)  $a_n$  is degenerate

The eigenvectors of  $a_n$   $\{|\varphi_n^j\rangle\}_{j=1,\dots,g_n}$  form an orthonormal basis of the degenerate eigensubspace  $\mathcal{E}_n$  of  $\mathcal{E}$ . We still have  $A(B|\varphi_n^j\rangle) = a_n(B|\varphi_n^j\rangle)$ , but now there is no *a priori* constraint for  $|\varphi_n^j\rangle$  and  $B|\varphi_n^j\rangle$  to be parallel. In fact, one can very well have

$$B|\varphi_n^j\rangle = \sum_{k=1}^{g_n} c_{nj}^k |\varphi_n^k\rangle, \quad (17)$$

but note that it is not necessary.

By virtue of the above and the orthonormality of the bases of  $\mathcal{E}$ , we can deduce that all matrix elements of  $B$  between eigenvectors of  $A$  corresponding to different eigenvalues are identically zero, thereby completing the proof of the theorem.

## 2.2 “Great theorem” of quantum mechanics

*If  $A$  and  $B$  are two operators that commute with each other, then one can always find an eigenbasis common to  $A$  and  $B$ .*

*Proof:* This is already proven by the first theorem in the nondegenerate case. In the degenerate case, it suffices to notice that, in a degenerate eigensubspace  $\mathcal{E}_n$ , the restriction of  $A$ ,  $A_n = a_n I$ , where  $I$  is the identity matrix. Therefore, if  $B$  is nondiagonal in  $\mathcal{E}_n$ , it can be directly diagonalized as  $A_n$  won't change. This proves the theorem.

This theorem is very important in physics, and the most used case by far is when  $A$  is the Hamiltonian and  $B$  is an observable, as it relates directly to conservation laws and constants of motion, which leads to the notion of Lie symmetry groups. Indeed, the Schrödinger equation may be rewritten in the Heisenberg picture, where the states are time-independent and the operators undergo time evolution, as the Heisenberg equation

$$i\hbar \frac{d\tilde{B}}{dt} = [\tilde{B}, H] \quad (18)$$

where  $B$  is an observable that doesn't depend on time in the Schrödinger picture and

$$\tilde{B} = e^{\frac{i}{\hbar}Ht} B e^{-\frac{i}{\hbar}Ht} \quad (19)$$

is the same observable in the Heisenberg picture. Now, if  $[\tilde{B}, H] = 0$ ,  $\tilde{B}$  is indeed a constant of motion, and  $H$  is invariant under any unitary operator  $\exp[-\frac{i}{\hbar}\beta B]$ , where  $\beta$  is an arbitrary c-number.

## 2.3 Complete Sets of Commuting Observables

The “great theorem” is particularly handy to label degenerate energy levels without knowing the eigenvectors. Consider, for example, the following diagonal matrices of a degenerate Hamiltonian restriction  $H_n$  and two observables  $A$  and  $B$  that commute with  $H_n$ :

$$H_n = \begin{pmatrix} E_n & 0 & 0 \\ 0 & E_n & 0 \\ 0 & 0 & E_n \end{pmatrix}; \quad A = \begin{pmatrix} a & 0 & 0 \\ 0 & a' & 0 \\ 0 & 0 & a' \end{pmatrix}; \quad B = \begin{pmatrix} b & 0 & 0 \\ 0 & b & 0 \\ 0 & 0 & b' \end{pmatrix}. \quad (20)$$

It is clear that the 3 degenerate energies  $E_n$  can now be distinguished from one another by using the eigenvalues of  $A$  and  $B$  as quantum labels, or *quantum numbers*. When the labeling is complete, we say that the set  $\{H, A, B\}$  is a *complete set of commuting observables*. Note that, if  $H$  is modified, say by turning on an external field or an interaction of the system

with another system, then the commutation relations with  $A$  and  $B$  may not hold any more, in which case the corresponding quantum numbers are said to not be *good* any more.

Physical quantities such as the orbital and spin angular momentums are therefore frequently used to label atomic and molecular energy spectra and identify physical interactions that condition the choices of good quantum numbers that best describe experimental observations. Let us now see how the use of group theory brings all this a big step further.

## 2.4 Wigner's Theorem

*If  $\mathcal{G}$  is the symmetry group of a Hamiltonian  $H$ , then every degenerate eigensubspace of  $H$  is globally invariant under  $\mathcal{G}$  i.e. constitutes a representation of the group  $\mathcal{G}$ .*

Note that the representation is not necessarily irreducible. However, it will be in the vast majority of practical cases. To prove Wigner's theorem, we use the first theorem and generalize it from the case  $A = H$  and a single operator  $B = G$  to  $A = H$  and a group  $\mathcal{G}$ .

Consider the matrices of  $\mathcal{G}$  in  $\mathcal{E}$ : they realize a representation of  $\mathcal{G}$ . Reducing this representation into a direct sum of irreducible representations (IR) of  $\mathcal{G}$  is equivalent to finding a basis change that simultaneously diagonalizes all matrices of  $\mathcal{G}$  (if  $\mathcal{G}$  is Abelian), or simultaneously block-diagonalizes them into the same smallest block structure (if  $\mathcal{G}$  is not Abelian).

We now turn to  $H$ . Because the matrix of  $H$  commutes with all the matrices of  $\mathcal{G}$ , it will also have the same block structure. This follows from the first theorem. Then we consider each individual IR block: by **Schur's lemma**, if a matrix commutes with all the group matrices of an irreducible representation, then this matrix must be proportional to the identity. This proves that

*All IR's of the symmetry group  $\mathcal{G}$  of a Hamiltonian  $H$  correspond to degenerate eigensubspaces of  $H$ .*

The reverse is not true: in a given degenerate eigensubspace, the matrices of a nonAbelian  $\mathcal{G}$  may or may not be completely diagonalizable. However, it turns out that the diagonalizable case is extremely rare in experimental observations, and that there is a *de facto* equivalence between energy degeneracies and IR's of the symmetry group, which yield what are called the *essential* degeneracies. Direct use can therefore be made of the extensive knowledge of the IR's of the group to label the energy levels of a system and predict its degeneracies.

Then, the extremely rare occurrence of a reducible degenerate subspace is usually the sign of an overlooked larger symmetry, and this case is called *accidental* degeneracy. Indeed, if  $\mathcal{G}$  is but a subgroup of a larger symmetry group of the Hamiltonian, then the IR of this larger group, which give the energy degeneracies, can be reducible in  $\mathcal{G}$ . One well-known example is the energy spectrum of the Hydrogen atom, in which some degenerate energies do belong to different IR's of SO(3). As it turns out, these IR's are in fact the reduction in SO(3) of an IR of SO(4), which happens to be the actual symmetry group of spherically symmetric Hamiltonians comprising only  $1/r$  potential terms.

### 3 More “quantum” applications of group theory

In addition to predicting degeneracies and labeling degenerate levels, group representation theory provides a powerful tool to predict the consequences of a symmetry-breaking perturbation, represented by an additional term in the Hamiltonian:  $H \rightarrow H + V$ , with  $\langle V \rangle \ll \langle H \rangle$ <sup>1</sup>. If  $V$  has a lower symmetry  $\mathcal{G}' \subset \mathcal{G}$ , then an IR  $D^{(\rho)}$  of  $\mathcal{G}$  may be reducible in  $\mathcal{G}'$  and the simple decomposition  $D^{(\rho)} \downarrow \mathcal{G}'$  will give direct information on the new energies (without calculating them!). For example, a tetrahedral molecule ( $\mathcal{G} = T_d$ ) will have nondegenerate energy levels ( $A_{1,2}$ ) as well as doublets ( $E$ ) and triplets ( $F_{1,2}$ ). If the molecule is placed in an external static electric or magnetic field, and we assume the field is aligned with one of the 3-fold symmetry axes of the tetrahedron, then  $\mathcal{G}' = C_{3v}$  and a triplet, say  $F_2$ , *disintegrates* or *splits* into  $F_2 \downarrow C_{3v} = A_1 + E$ , that is one singlet and one doublet. If the field is along a two-fold symmetry axis, we have  $F_2 \downarrow C_{2v} = A_1 + B_1 + B_2$ , i.e. three different energies. One says, in these two respective cases, that the initial  $F_2$  degeneracy has been *partially* or *completely lifted*.

Other powerful and interesting applications concern coupling schemes (when  $\langle V \rangle \sim \langle H \rangle$ ) and the Wigner-Eckart theorem, a very powerful tool that enables one to find *selection rules* (zero matrix elements of interaction terms in the Hamiltonian) with no calculations besides elementary considerations on Kronecker products of IR's. These are out of the scope of this short presentation.

## References

- [1] M.A. Nielsen and I.L. Chuang, *Quantum computation and quantum information*, Cambridge University Press (2000).
- [2] C. Cohen-Tannoudji, B. Diu, and F. Laloë, *Quantum mechanics*, Wiley (1977). 2 volumes.
- [3] R.P. Feynman, *Simulating physics with computers*, Int. J. Theor. Phys. **21**, 467 (1982).
- [4] M. Hamermesh, *Group theory and its application to physical problems*, Addison-Wesley (1962).

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<sup>1</sup>More trouble ought, of course, to be expected if  $V$  is not perturbative and does not commute with  $H$ .