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Höhere Quantenmechanik

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Exercise sheet 4

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Exercise 1: Group theory, reducible and irreducible representations *(12 Points)*

We have seen what groups and representations are in the previous exercise sheet. In this exercise, we introduce the concepts of reducible and irreducible representations, and how to recognize them. The ideas are once more quite abstract, but we try to keep them simple and use an example. As in the previous sheet, we denote the group by $\mathcal{G}$, a generic element of the group by g and the operation of the group by $\circ$. Note: we again restrict our discussion to the case of a finite group.

Let us consider the $C_{3\text{v}}$ group, which contains 6 elements. A practical way to visualize them is considering the symmetries of the ammonia molecule (NH_3). We can use the website https://symotter.org/gallery for this purpose. In the menu on the left, you can select the entry "pyramidal (C_{nv})" and then the entry "$C_{3\text{v}}$ – ammonia". You'll have a three dimensional picture of the molecule that you can freely rotate. The menu on the right lists all the symmetries of NH_3 (the identity, 2 three-fold rotations and 3 reflections with respect to different planes). Just click on the play buttons to see their effects on the molecule.

	E	C_3^+	C_3^-	σ_v	σ_v'	σ_v''
E	E	C_3^+	C_3^-	σ_v	σ_v'	σ_v''
C_3^+	C_3^+	C_3^-	E	σ_v''	σ_v	σ_v'
C_3^-	C_3^-	E	C_3^+	σ_v'	σ_v''	σ_v
σ_v	σ_v	σ_v'	σ_v''	E	C_3^+	C_3^-
σ_v'	σ_v'	σ_v''	σ_v	C_3^-	E	C_3^+
σ_v''	σ_v''	σ_v	σ_v'	C_3^+	C_3^-	E

Figure 1: Multiplication table of the $C_{3\text{v}}$ group.

Let us denote the elements of the group as E (the identity), C_3^+ and C_3^- (the two rotations), σ_v, σ_v' and σ_v'' (the three reflections). A possible way to define the group is using its *multiplication table*, reported in Fig. 1, in which each row and column corresponds to a certain element of the group. If we denote by A the row element and by B the column element, the corresponding entry of the table contains the result of the operation $A \circ B$.

We introduce a three-dimensional representation of $C_{3\mathrm{v}}$:

$$\rho_1(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \rho_1(C_3^+) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \rho_1(C_3^-) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\rho_1(\sigma_v) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \rho_1(\sigma_v') = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} & 0 \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \rho_1(\sigma_v'') = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} & 0 \\ \frac{\sqrt{3}}{2} & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{1}$$

(i) Show that $\rho_1(C_3^+)\rho_1(\sigma_v) = \rho_1(\sigma_v'')$ (as we expected from the multiplication table, Fig. 1). *(1 Point)*

In general, two representations ρ_1 and ρ_2 are said to be *equivalent* if there is a non-singular matrix A such that

$$\rho_2(g) = A\rho_1(g)A^{-1}, \ \forall g \in \mathcal{G} \tag{2}$$

This is called a *similarity transformation.* We introduce a second three-dimensional representation for the $C_{3\mathrm{v}}$ group:

$$\rho_2(E) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \qquad \rho_2(C_3^+) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{4} & -\frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{2} & \frac{1}{4} & -\frac{3}{4} \\ \frac{\sqrt{3}}{2} & -\frac{3}{4} & \frac{1}{4} \end{pmatrix} \qquad \rho_2(C_3^-) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{4} & \frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{2} & \frac{1}{4} & -\frac{3}{4} \\ -\frac{\sqrt{3}}{2} & -\frac{3}{4} & \frac{1}{4} \end{pmatrix}$$

$$\rho_2(\sigma_v) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{pmatrix} \qquad \rho_2(\sigma_v') = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{4} & -\frac{\sqrt{3}}{4} \\ -\frac{\sqrt{3}}{2} & \frac{3}{4} & -\frac{1}{4} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{4} & \frac{3}{4} \end{pmatrix} \qquad \rho_2(\sigma_v'') = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{4} & \frac{\sqrt{3}}{4} \\ \frac{\sqrt{3}}{2} & \frac{3}{4} & -\frac{1}{4} \\ \frac{\sqrt{3}}{2} & -\frac{1}{4} & \frac{3}{4} \end{pmatrix} \tag{3}$$

(ii) Take one g element at your choice (not E) and show that the two representations ρ_1 and ρ_2 are equivalent for that element if we take

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 1 \\ 0 & 1 & -1 \end{pmatrix} \qquad A^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1/2 & 1/2 \\ 0 & 1/2 & -1/2 \end{pmatrix}$$

in the similarity transformation of Eq. (2). *(1 Point)*

(iii) An important property of two equivalent representations, ρ_1 and ρ_2, is the fact that the traces of the matrices representing each element are equal in the two representations, i.e.

$$\rho_1 \text{ and } \rho_2 \text{ are equivalent } \Rightarrow \ \mathrm{Tr}(\rho_1(g)) = \mathrm{Tr}(\rho_2(g)), \ \forall g \in \mathcal{G}$$

Can you prove this statement (for a generic similarity transformation)? *(1 Point)*
Note: the arrow is actually true also in the opposite direction, i.e.

$$\mathrm{Tr}(\rho_1(g)) = \mathrm{Tr}(\rho_2(g)), \ \forall g \in \mathcal{G} \ \Rightarrow \ \rho_1 \text{ and } \rho_2 \text{ are equivalent}$$

but this is much harder to prove.

The invariance of the trace for two equivalent representations is a very important property. Let use introduce the following notation for the traces of the matrices forming a certain representation ρ:

$$\chi_\rho(g) = \mathrm{Tr}(\rho(g)) \tag{4}$$

The set of traces $\{\chi_\rho(g)\}_{g\in\mathcal{G}}$ is known as the **character** of the representation ρ. We also define a scalar product between characters of two generic representations ρ and ρ' as

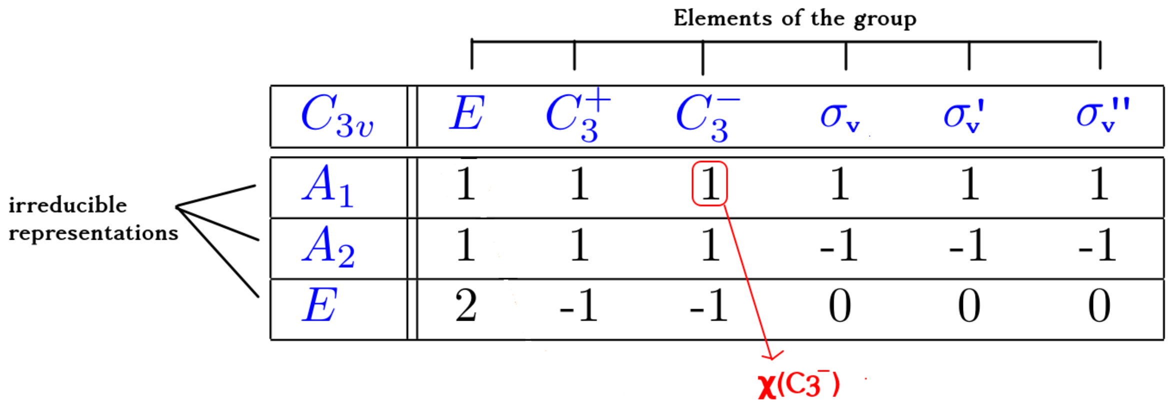
$$(\rho, \rho') = \frac{1}{N} \sum_{g\in\mathcal{G}} \chi_\rho^*(g)\chi_{\rho'}(g). \tag{5}$$

Here N the denotes the total number of elements in the group ($N = 6$ for $C_{3\mathrm{v}}$) and * is a complex conjugation. This scalar product will be useful in the following.

We can now introduce the concept of reducible and irreducible representations, by using our example. Let's take a closer look at the representation ρ_1 in Eq. (1). All the matrices are block-diagonal, with a 2×2 block in the upper-left corner and a 1×1 block in the lower-right corner. Interestingly, if we isolate the 2×2 blocks themselves, we can see that they form a valid representation of the group. The same happens for the 1×1 blocks (it is just the trivial representation). Therefore, we say that ρ_1 is a **reducible** representation. The same statement applies to ρ_2, although it is not immediately clear from the form of the matrices. It is reducible because we can find a similarity transformation like the one of Eq. (2) that brings it to a block-diagonal form (e.g., to ρ_1, in this case). By contrast, when this is not possible, we say that the representation is **irreducible**. For example, the 2×2 and 1×1 blocks that we can read off from the matrices of ρ_1 form two irreducible representations of $C_{3\mathrm{v}}$ (one is two-dimensional, the other is one-dimensional).

We are skipping a lot of mathematical details here, for simplicity. The important thing to learn is that *the number of irreducible representations of a finite group is finite.* For the $C_{3\mathrm{v}}$ group that we are considering, there exist only three irreducible representations, called A_1, A_2 and E in Mulliken's notation (please, don't confuse this E with the identity element!). A_1 and A_2 are one-dimensional, while E is two-dimensional. Any other representation is reducible and can be *decomposed* into a combination of these irreducible representations. In other words, its matrices can be made block diagonal by a transformation like the one in Eq. (2), such that each of the blocks corresponds to one of the irreducible representations.

The irreducible representations of a certain finite group are listed in the so-called **character tables**. In these tables the traces $\chi_\rho(g)$ are reported, for each element g of the group and for each irreducible representations ρ. The character table of $C_{3\mathrm{v}}$ is shown in Fig. 2.



C_{3v}	E	C_3^+	C_3^-	σ_v	σ_v'	σ_v''
A_1	1	1	1	1	1	1
A_2	1	1	1	-1	-1	-1
E	2	-1	-1	0	0	0

Figure 2: Character table of the $C_{3\mathrm{v}}$ group. The rows correspond to the irreducible representations. The columns correspond to the group elements. The entries of the table are the traces of the matrices in the given representation. As an example, we highlight the trace of the matrix for the element C_3^- in the A_1 irreducible representation. Note: the trace of the identity element (first column) always gives the dimension of the representation.

(iv) Take the 2×2 blocks in the upper-left corner of the matrices of ρ_1 (Eq. (1)) and show that their traces are equal to the ones in the character of the irreducible representation E. Do the same for the 1×1 blocks. What irreducible representation is formed by the 1×1 blocks, A_1 or A_2? *(1 Point)*

(v) Take the character table of Fig. 2 and show that, for each pair of irreducible representation ρ and ρ', the following property holds

$$\begin{cases} (\rho, \rho') = 0 & \text{if } \rho \neq \rho' \\ (\rho, \rho') = 1 & \text{if } \rho = \rho' \end{cases}$$

Use the scalar product defined in Eq. (5). *(2 Points)*
Hint: you can see the rows of the character table as vectors and do a scalar product between them (and divide by N). Convince yourself that this is equivalent to the product in Eq. (5)*.*

(vi) The property discussed in the previous point is peculiar of irreducible representations. Now try to compute (ρ_1, ρ_1) for the representation ρ_1 (Eq. (1)). You can conclude from the result that ρ_1 is not an irreducible representation. *(1 Point)*

In the case of ρ_1, we could convince ourselves that it is reducible and decompose it by seeing that it is block-diagonal. For ρ_2 the story is more complicated if we don't know how to make it block-diagonal. We surely know that it is reducible, since it is three-dimensional, and the irreducible representations of $C_{3\text{v}}$ are either one- or two-dimensional. Can we find the irreducible representations in which ρ_2 can be decomposed? There is a simple way to identify them. As we will see, they turn out to be equal to the ones we obtained for ρ_1, since ρ_1 and ρ_2 are equivalent.

(vii) The trick to decompose a reducible representation ρ into irreducible representations is the following. For each irreducible representation ρ_i ($i = A_1, A_2, E$ for $C_{3\text{v}}$), compute (ρ, ρ_i). You'll get an integer number m_i. If it is zero, the irreducible representation ρ_i is not part of the decomposition of ρ. If it is finite, it tells you how many times ρ_i appears in the decomposition of ρ.

Use the trick outlined above to explicitly show that ρ_1 and ρ_2 are both decomposable into A_1 "plus" E (i.e., $m_{A_1} = 1$, $m_{A_2} = 0$ and $m_E = 1$). *(2 Points)*

(viii) Consider now the four-dimensional representation of $C_{3\text{v}}$ reported in Fig. 3 (denoted by Γ). Use the trick described in the previous point to decompose it into irreducible representations. Is some irreducible representation appearing more than once in the decomposition? *(2 Points)*

$$\Gamma(E) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \Gamma(C_3^+) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} \quad \Gamma(C_3^-) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

$$\Gamma(\sigma_v) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad \Gamma(\sigma_v') = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad \Gamma(\sigma_v'') = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

Figure 3: Four-dimensional representation of the $C_{3\text{v}}$ group.

In conclusion of the exercise: if you try to solve all of the points (i-viii), even if some are wrong, you get 1 extra point for the patience of having read all the text up to here. *(1 Point)*

Exercise 2: Time reversal ***(8 Points)***

(i) Let H be a Hamiltonian with a *nondegenerate* discrete spectrum (eigenstates $|n\rangle$ with energies E_n), which is invariant under time-reversal transformation Θ, i.e.

$$[H, \Theta] = 0. \tag{6}$$

Show that the wave functions of the eigenstates of the Hamiltonian can be chosen to be real for any instant of time (i.e., $\phi_n(\vec{x}, t) \in \mathbb{R}$). *(4 Points)*
Hints: First figure out what the stationary state $\Theta|n\rangle$ is (using the time-independent Schrödinger equation). Then study how the operator Θ acts on the time-dependent eigenstates of the Hamiltonian (use the real space representation and the Schrödinger picture).

(ii) Let $|n\rangle$ be a nondegenerate eigenstate of a time-reversal-invariant Hamiltonian.
Show that $\langle n|\vec{\mathbf{L}}|n\rangle = 0$. *(2 Points)*

(iii) Let $\phi_\alpha(\vec{p}) = \langle \vec{p}|\alpha\rangle$ be a momentum-space representation of a state $|\alpha\rangle$.
Show that $\langle \vec{p}|\Theta\alpha\rangle = \phi^*_\alpha(-\vec{p})$. *(2 Points)*