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Exercise 1: Fourier transform (Oral)

a) Consider a finite system of length L, with periodic boundary conditions (PBC) and a continuous function $f(x)$ defined on it, $f(x+L) = f(x)$. Its decomposition in the Fourier space implies a discrete sum over $\mathbb{Z}$,

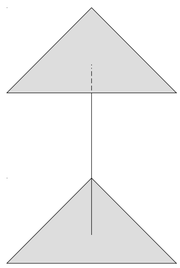
$$f(x) = \frac{1}{L}\sum_{n=-\infty}^{\infty} \tilde{f}_n e^{\mathrm{i}k_n x}, \text{ where } \tilde{f}_n = \int_0^L dx\, f(x) e^{-\mathrm{i}k_n x}, \quad k_n = \frac{2\pi n}{L}, \tag{1}$$

and where we have used the convention of concentrating the $1/L$ weight in just the direct transformation. Show that when $L \to \infty$ the sum transforms into an integral with measure $\int \frac{dk}{2\pi}$.

b) Now consider the same system but with a lattice support defined by a lattice spacing a, i.e. $f(x+a) = f(x)$. Show that the allowed k values in the sum reduce to the first Brillouin Zone (BZ), $-\pi/a \leq k < \pi/a$, and that when taking the limit $L \to \infty$ the measure is given by $\int_{BZ} \frac{dk}{2\pi}$.

Exercise 2: Groups and representations (Oral)

The 3D shape shown in the figure is invariant under the group D_{3h}.



Use the following procedure to construct its character table,

a) Determine the number of elements (symmetry operations), g, and the number of classes, k, with n_i elements each. (Hint: do not forget the improper rotations).

b) The number of irreducible representations k is the same as the number of equivalence classes. Create a table as shown below. The first representation is the identity, which is a 1-dimensional representation. It provides the first line of the table.

c) The character of the 1-dimensional representation is defined by making use of the relation

$$\chi(R_i)\chi(R_j) = \chi(R_i R_j), \tag{2}$$

and the properties defining a class of equivalence.

d) Use $\sum_{\mu=1}^{k} l_\mu^2 = g$, where l_μ are the dimensions of the irreducible representation μ. (This helps you to determine the first column of the table.)

e) Find the characters by determining the trace of the matrices in an explicit representation.

The above rules can be derived from the orthogonality and completeness relations,

$$\sum_{\mathcal{C}_i} n_i \chi^{\mu *}(\mathcal{C}_i)\chi^{\nu}(\mathcal{C}_i) = g\delta_{\mu\nu}, \tag{3}$$

and

$$\sum_{\mu} \chi^{\mu}(\mathcal{C}_i)\chi^{\mu *}(\mathcal{C}_j) = g/n_i \delta_{ij}, \tag{4}$$

where n_i is the number of elements in the class $\mathcal{C}_i$, and μ, ν refer to irreducible representations.

For higher dimensional representations, it is necessary to choose a suitable set of functions as a basis and to determine the matrices of the representation (one for each equivalence class).

D_{3h}	E	$2C_3$	$\dots$
Γ_1	1	$\dots$	
Γ_2	1	$\dots$	
$\vdots$	$\vdots$		

Exercise 3: Energy splitting of the f-orbitals (Written)

Show how the energy levels of an f-orbital is splitted when the symmetry is reduced in the sequence,

$$O(3) \rightarrow O_h \rightarrow D_{4h} \rightarrow D_{2h}. \tag{5}$$