Symmetry in Condensed Matter Physics

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Exercises - part 2

1. Consider the group $\bar{4}3m$ (its character table is on the web site). Verify that the rows of the character table are mutually orthogonal. The representation Γ has the following set of characters: $\chi(E) = 9$, $\chi(3) = 0$, $\chi(2_z) = 1$, $\chi(m_d) = 3$, $\chi(\bar{4}_z) = -1$. Decompose Γ into the irreducible representations of $\bar{4}3m$. Try first of all to do it by inspection, and then verify your answer with the orthogonality theorem.

2. The wavefunctions of the five degenerate d orbitals of a free ion are, in Cartesian coordinates,

   $$\phi_1 = 2(x+iy)zf(r),\ \phi_2 = 2(x-iy)zf(r),\ \phi_3 = (x+iy)^2f(r),\ \phi_4 = (x-iy)^2f(r),\ \phi_5 = (3z^2-r^2)f(r).$$

   where $f(r)$ is the radial wavefunction. Show that these functions transform into one another under the elements E, A and K representative of the classes of the group 32. Hence, deduce that the five-fold degeneracy of the d orbitals splits into two doublets and a singlet when the ion is placed in a site of symmetry 32.

3. Consider the four functions. $\phi_1 = (x+iy)yz$, $\phi_2 = (x-iy)yz$, $\phi_3 = -(x+iy)xz$, $\phi_4 = -(x-iy)xz$.

   a What is the dimensionality of the subspace of the cubic polynomials spanned by all linear combinations of these functions?

   b Having chosen a suitable basis set for this subspace, write the matrix representation of the (reducible) representation Γ of group 32 onto that subspace, and decompose Γ into irreducible representations.

   c Show that the space spanned by $\phi_1 \ldots \phi_4$ can be obtained as $[\{x,y\} \otimes \{x,y\}] \otimes \{z\}$, where the square brackets indicate the symmetrised tensor product, $\{x,y\}$ is the two-dimensional space of linear functions $ax+by$ and $\{z\}$ is the one-dimensional space of linear functions cz. Using the formula for symmetrised tensor products of representations, determine the characters of the representation Γ and show that the result is the same as in part **b**.