Symmetry in Condensed Matter Physics

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Exercises - part 1

1. Show that the identity operation and rotations through 180° about three mutually perpendicular axes form a group and construct the multiplication table.

2. The Hamiltonian for the 2 electrons in a hydrogen (H_2) molecule, considering the two protons to be fixed, is

$$H = -\frac{\hbar^2}{2m}\left(\nabla_1^2 + \nabla_2^2\right) - \frac{e^2}{4\pi\epsilon_0}\left(\frac{1}{|\mathbf{r_1}-\mathbf{a}|} + \frac{1}{|\mathbf{r_2}-\mathbf{a}|} + \frac{1}{|\mathbf{r_1}+\mathbf{a}|} + \frac{1}{|\mathbf{r_2}+\mathbf{a}|} - \frac{1}{|\mathbf{r_1}-\mathbf{r_2}|}\right)$$

   where $\mathbf{r_1}$ and $\mathbf{r_2}$ are the position vectors of the two electrons and $\pm\mathbf{a}$ are the displacements of the two protons relative to the centre of the molecule. Show that if $\mathbf{a} = [0, 0, a]$ then the Hamiltonian is invariant under any rotation about the z-axis, but only invariant under 180° rotations about the x- or the y- axes.

3. Show that the functions $\phi_1 = x + y$ and $\phi_2 = x - y$ transform according to a representation of the group 32. Write down the matrices of this representation, and verify that they multiply according to the group multiplication table.

4. This problem is designed to demonstrate how a group of rotations in ordinary space maps onto a set of linear transformations in the space of functions, defining a matrix representation of the group.

   (a) Consider the set of quadratic polynomials in two dimensions (see also Lecture 1):

$$f(x, y) = c_1 + c_2 x + c_3 y + c_4 x^2 + c_5 y^2 + c_6 xy \qquad (1)$$

   write a generic rotation by an angle ϕ of these polynomials, using the rules discussed in lecture 1:

   - define the dummy variables X and Y by back-rotating x and y, using 2×2 matrices.
   - replace x and y with X and Y.
   - Re-write the rotated polynomials as a function of the original variables x and y.

   (b) Write the generic rotation in the 'space' of polynomials as a 6×6 matrix acting on the coefficients c_i of the basis functions $1, x, y, x^2, y^2, xy$.

(c) Repeat this for the matrix corresponding to the mirror operation K of the group 32 (the matrix can be found in the notes for Lecture 4). You can also repeat this for the L and M matrices if you have time.

(d) Sketch the process to obtain the matrix representation of the group 32 onto the space of quadratic polynomials in two dimensions for the basis set given above. Each of the 6 operations of the group will map onto a 6×6 matrix. Write down at least one matrix for each of the three classes of the group 32.

(e) Write down the characters of the full representation and decompose it into irreducible representations.

5. Show that the functions $\phi_1 = 2xy$ and $\phi_2 = x^2 - y^2$ transform as one of the irreducible representations of the group 32. Show likewise for $\phi_1 = yz$ and $\phi_2 = -xz$. If $\phi_2 = xyz$ and ϕ_1 and ϕ_2 transform according to the same irreducible representation as the previous pairs of functions, what is ϕ_1?