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Group theory and symmetries in quantum mechanics
Summer semester 2016 - Exercise sheet 6
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Problem 18: Particle confined to a 2D-square.

Consider a particle of mass m confined to a square in two dimensions whose vertices are located at the following points of the xy-plane: (L, L), $(L, -L)$, $(-L, -L)$, and $(-L, L)$. The potential is assumed to be zero within the square and infinitely large at the edges of the square. The stationary eigenfunctions of the corresponding quantum-mechanical problem have the form:

$$\psi_{p,q}(x, y) = \frac{1}{L} \left\{ \begin{array}{c} \cos(k_p x) \\ \sin(k_p x) \end{array} \right\} \left\{ \begin{array}{c} \cos(k_q y) \\ \sin(k_q y) \end{array} \right\} ,$$

where $k_p = \frac{p\pi}{2L}$ and $k_q = \frac{q\pi}{2L}$, with p and q being positive integers. The notation with $\{\}$ in the equation above means that $\cos(k_p x)$ is taken if p is odd, $\sin(k_p x)$ is taken if p is even, and similarly for the other factor. The corresponding eigenvalues are

$$E_{p,q} = \frac{\hbar^2}{8mL^2}(p^2 + q^2) .$$

(a) What is the symmetry group of the Hamiltonian of this problem? Copy its character table here for the further steps.

(b) For which irreducible representations do the eigenfunctions $\psi_{1,1}(x, y)$ and $\psi_{2,2}(x, y)$ form bases?

(c) For which irreducible representation do the eigenfunctions $\psi_{1,2}(x, y)$ and $\psi_{2,1}(x, y)$ form a basis?

(d) What is the degeneracy corresponding to $(p = 6, q = 7)$ and $(p = 2, q = 9)$? Is this a normal or accidental degeneracy?

(e) Think of a modification of the system which does not destroy its symmetry but partly lifts this degeneracy.

(f) Check if all of the irreducible representations occur in the Hilbert space spanned by the eigenfunctions $\psi_{p,q}(x, y)$.

Problem 19: Selection rules for a system having the C_{6v} symmetry.

Consider a quantum-mechanical system which has the symmetry of a regular hexagon (cf. problems 8). The character table is given on the next sheet. Suppose there is a “vector” perturbation of this system, i.e. a perturbation that transforms as $\{x, y, z\}$. Determine the selection rules for transitions induced by this perturbation from the initial state that transforms according to the “parity” representation (i.e. the 1-dimensional representation with a sign change for the inversion, reflections and any improper rotations in general, contained in the symmetry group).

χ	E	C_2	$2C_3$	$2C_6$	$3\sigma_v$	$3\sigma_d$
Γ_1	1	1	1	1	1	1
Γ_2	1	1	1	1	-1	-1
Γ_3	1	-1	1	-1	1	-1
Γ_4	1	-1	1	-1	-1	1
Γ_5	2	-2	-1	1	0	0
Γ_6	2	2	-1	-1	0	0