Exercises to Advanced Quantum Mechanics — Sheet 4

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Exercise 4.1 *The dihedral groups* (3 points)

Enlarge the symmetry group of Exercise 3.3 by a reflection that reverses the x_2 axis, leaving the x_1 axis invariant. This construction defines a two-dimensional representation of the *dihedral group* D_n.

a) Determine all group elements of D_n in the two-dimensional representation given above. What is the order of D_n?

b) Show that the given two-dimensional representation of D_n is irreducible.

c) D_n has two one-dimensional inequivalent representations if n is odd and four one-dimensional inequivalent representations if n is even. Determine these representations.

   Remark: All other irreducible representations of D_n are two-dimensional. For a proof see, e.g., *Ramond: Group Theory – A Physicist's Survey, chap. 3.8.*

Exercise 4.2 *Symmetry group of the ozone molecule* (2 points)

Consider an electron in the field of three point particles carrying equal positive electric charge that are positioned at the vertices of an equilateral triangle.

a) What is the symmetry group of the Hamiltonian for the electron states? What kind of degeneracy can be expected for energy eigenstates (ignoring possible accidental degeneracies)?

b) What happens to the degenerate energy eigenstates if a homogeneous electric or magnetic field is applied perpendicular to the triangle spanned by the three positive charges?

Please turn over!

Exercise 4.3 *Kronig-Penney model* (3 points)

Consider the one-dimensional motion of a particle of mass m in a periodic potential of the form

$$V(x) = \frac{\hbar^2 P}{2ma} \sum_{n=-\infty}^{+\infty} \delta(x - na), \tag{1}$$

where P is a dimensionless constant quantifying the strength of the interaction and a the lattice constant.

a) Derive Bloch's theorem for any potential $V(x)$ with periodicity with respect to $x \to x + a$, i.e. that there is a basis of energy eigenfunctions $\psi(x)$ with the property

$$\psi_k(x) = \mathrm{e}^{\mathrm{i}kx} u_k(x), \qquad u_k(x+a) = u_k(x), \qquad k \in \mathbb{R}. \tag{2}$$

Do not use group-theoretical arguments here to handle the issue of degeneracy.

b) Solve the Schrödinger equation for $x \neq na$, $n \in \mathbb{Z}$, and derive the continuity conditions on $\psi(x)$ and $\psi'(x)$ at the positions $x = na$.

Hint: Integrate the Schrödinger equation in the intervals $na - \epsilon \leq x \leq na + \epsilon$ with some small parameter $\epsilon > 0$.

c) Use Bloch's theorem and the result from b) to find the equation that determines the allowed energy values E and show that solutions exist only in specific energy intervals ("energy bands"). Find an appropriate way to visualise this condition in a graph for fixed P from which the boundaries of the energy bands could be read. Calculate the upper boundaries of the energy bands analytically.