2^{nd} Exercise sheet for Advanced Quantum Mechanics in WS16

Symmetries in Quantum Mechanical Systems

Exercise 4 *Time reversal and spinor representation*

a) Let $\psi(\mathbf{x}, t)$ be the wave function of a (spinless) three-dimensional plane wave. Show that $\psi^*(\mathbf{x}, -t)$ then represents the wave function of a plane wave with reversed momentum.

b) Let $\chi(\hat{\mathbf{n}})$ be the two-component eigenspinor of $\boldsymbol{\sigma} \cdot \hat{\mathbf{n}}$ with eigenvalue $+1$. Using the spinor representation of $\chi(\hat{\mathbf{n}})$ verify that the eigenspinor with reversed spin direction can be written as $\eta(\hat{\mathbf{n}}) = -\mathrm{i}\sigma_2 \chi^*(\hat{\mathbf{n}})$.
Hint: Express the vector $\hat{\mathbf{n}}$ via spherical coordinates.

Exercise 5 *Time reversal*

a) Let $\hat{H}$ be the Hamiltonian of a system with non-degenerate eigenstates $|n\rangle$. Show that one can choose their position representation $\langle \mathbf{x}|n\rangle$ real-valued if $\hat{H}$ is invariant under time reversal.

b) The wave function of a plane wave for the time $t = 0$ is given by the complex function $\exp(\mathrm{i}\mathbf{p} \cdot \mathbf{x}/\hbar)$. Why does this not violate time-reversal?

Exercise 6 *Time reversal, rotations, and parity*

Let $\mathcal{T}_{\mathbf{d}}$ be the translation operator w.r.t. a translation along a vector $\mathbf{d}$, $\mathcal{D}(\mathbf{n}, \phi)$ the rotation operator (with rotation axis $\mathbf{n}$ and angle ϕ), and π the parity operator. Find out which pairs of operators commute:

1. $\mathcal{T}_{\mathbf{d}}$ and $\mathcal{T}_{\mathbf{d}'}$ (with $\mathbf{d}$ and $\mathbf{d}'$ linearly independent),
2. $\mathcal{D}(\mathbf{n}, \phi)$ and $\mathcal{D}(\mathbf{n}', \phi')$ (with $\mathbf{n}$ and $\mathbf{n}'$ linearly independent),
3. $\mathcal{T}_{\mathbf{d}}$ and π, and
4. $\mathcal{D}(\mathbf{n}, \phi)$ and π.

Exercise 7 *One-dimensional lattice and Bloch waves*

Consider a one-dimensional lattice with lattice sites at R_m and periodic potential $V(r) = V(r + R_m)$ (w.l.o.g. the origin of the coordinate system is at either one of the lattice sites). Due to Bloch's theorem the eigenfunctions of the Hamilton operator H can be written in the form $\psi_k(r) = e^{ikr} u_k(r)$, where $u_k(r)$ is lattice periodic (i.e. $u_k(r + R_m) = u_k(r)$) and k is located in the first Brillouin zone ($|k| \leq \pi/a$).

a) Show that, in the case of a lattice with $N \gg 1$ lattice sites, k has exactly N discrete values.

Hint: Exploit the periodic boundary conditions of $\psi_k(r)$.

b) Using Bloch's theorem first show that $E_k = E_{-k}$ and then that $\psi_k^*(r) = \psi_{-k}(r)$, where E_k are the corresponding energy eigenvalues of the Hamiltonian H.

c) Now assume that the length of the lattice tends to infinity. The Bloch wave functions then obey the orthogonality relation

$$\int dr\, \psi_k^*(r)\psi_{k'}(r) = \Omega_B \delta(k - k') \ ,$$

where Ω_B is the volume of the first Brillouin zone. Consider the expansion

$$\psi_k(r) = \sum_m w(r - R_m)e^{ikR_m} \ , \quad \text{with } w(r - R) = \frac{1}{\Omega_B} \int_{\Omega_B} dk\, \psi_k(r)e^{-ikR} \ ,$$

where the R-summation runs over all lattice sites and the k–integration extends along the Brillouin zone. Without using the definition of w, show that $\psi_k(r)$ in the given representation fulfils Bloch's theorem.

d) Show that for different R_m the functions w are orthogonal to each other (these functions, which are localized around the lattice sites R_m, are called *Wannier functions*).