Exercises to Advanced Quantum Mechanics **Sheet 3**

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Exercise 3.1 *Virial theorem* (1 point)

Consider a spinless particle of mass m in a potential $V(\vec{x})$. Show the relation

$$2\langle T\rangle_{\phi_n} = \langle\hat{\vec{x}}\cdot\nabla V\rangle_{\phi_n} \tag{1}$$

for expectation values $\langle ...\rangle_{\phi_n}$ in (stationary) energy eigenstates $|\phi_n\rangle$, where $T = \hat{\vec{p}}^2/(2m)$ is the operator for the kinetic energy of the particle. What does this relation imply for the expectation values $\langle T\rangle_{\phi_n}$ and $\langle V\rangle_{\phi_n}$ for central potentials of the type $V(\vec{x}) \propto r^s$, where $r = |\vec{x}|$?

(Hint: Evaluate $\langle[\hat{\vec{x}}\cdot\hat{\vec{p}}, \hat{H}]\rangle_{\phi_n}$ is two different ways.)

Exercise 3.2 *Electromagnetic gauge transformations* (3 points)

The Hamiltonian of a non-relativistic, spinless particle of mass m and electric charge q in a classical electromagnetic field is given by

$$\hat{H}(\hat{\vec{x}},\hat{\vec{p}}) \;=\; \frac{1}{2m}\left(\hat{\vec{p}} - q\vec{A}(\hat{\vec{x}},t)\right)^2 + q\Phi(\hat{\vec{x}},t), \tag{2}$$

where $\vec{A}(\vec{x},t)$ and $\Phi(\vec{x},t)$ are the classical vector and scalar potentials of the electromagnetic field, respectively. Here, $\hat{\vec{x}}$ is the usual position operator and $\hat{\vec{p}}$ its canonical conjugate momentum.

a) The electric and magnetic field strengths $\vec{E} = -\nabla\Phi - \dot{\vec{A}}$ and $\vec{B} = \nabla\times\vec{A}$ are invariant under the gauge transformation:

$$\vec{A} \;\to\; \vec{A}' = \vec{A} + \nabla\chi, \qquad \Phi \;\to\; \Phi' = \Phi - \dot{\chi}, \tag{3}$$

where $\chi = \chi(\vec{x},t)$ is an arbitrary real function of space and time. Show that the Hamilton operator transforms as

$$\hat{H} \;\to\; \hat{H}' = U\hat{H}U^\dagger + \mathrm{i}\hbar\dot{U}U^\dagger, \tag{4}$$

with the operator $U(\hat{\vec{x}},t) = \exp\{\mathrm{i}q\chi(\hat{\vec{x}},t)/\hbar\}$. Is U unitary?

b) Show that $|\psi'(t)\rangle = U|\psi(t)\rangle$ obeys the time-dependent Schrödinger equation with Hamiltonian $\hat{H}'$ if $|\psi(t)\rangle$ obeys the Schrödinger equation with Hamiltonian $\hat{H}$.

c) Identify the operator $m\hat{\vec{v}}$ corresponding to the cartesian momentum $m\dot{\vec{x}}$ as the operator that produces the expectation value $m\frac{\mathrm{d}}{\mathrm{d}t}\langle\hat{\vec{x}}\rangle$. What are the commutators $[\hat{x}_k, m\hat{v}_l]$? Consider the two momentum expectation values $\langle\hat{\vec{p}}\rangle$ and $\langle m\hat{\vec{v}}\rangle$. Which of the two is invariant under gauge transformations (3) ?

Please turn over!

Exercise 3.3 *Discrete rotations in two dimensions – the cyclic groups* (3 points)

For a given natural number n, consider the group of discrete rotations about integer multiples of the angle $\frac{2\pi}{n}$ in two dimensions, which are represented by the matrices

$$R(\phi_k) \;=\; \begin{pmatrix} \cos\phi_k & -\sin\phi_k \\ \sin\phi_k & \cos\phi_k \end{pmatrix}, \qquad \phi_k = \frac{2\pi k}{n} \qquad k = 0, 1, \ldots, n-1. \tag{5}$$

These matrices define a two-dimensional representation of the *cyclic group* C_n.

a) Determine the similarity transformation that reduces the representation (5) to two irreducible representations.

b) The "regular representation" of C_3 (and analogously for C_n) is defined by the following three matrices:

$$D(e) = \mathbf{1}, \qquad D(g) = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}, \qquad D(g^2) = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \tag{6}$$

where g is the *generating element* of the group. Similarly to a) fully reduce this representation.
(Hint: Introduce $\epsilon = \mathrm{e}^{2\pi \mathrm{i}/3}$, with $\epsilon^2 = \epsilon^*$, $1 + \epsilon + \epsilon^2 = 0$.)

c) C_n possesses n one-dimensional inequivalent representations. Guess them from the pattern observed for C_3 in b).

Exercise 3.4 *Parity operator* (2 points)

The parity operator $\mathcal{P}$ is linear and defined by the following action on position eigenstates:

$$\mathcal{P}|\vec{x}\rangle \;=\; |-\vec{x}\rangle. \tag{7}$$

(Spin will not be considered in this exercise.)

a) Show that $\mathcal{P}$ is unitary and acts on position-space wave functions as $\mathcal{P}\psi(\vec{x}) = \psi(-\vec{x})$. Derive the operators $\hat{\vec{x}}\,'$, $\hat{\vec{p}}\,'$, $\hat{\vec{L}}\,'$, where $A' = \mathcal{P}\,A\,\mathcal{P}^{-1}$ is the parity-transformed version of an operator A. Here $\hat{\vec{L}} = \hat{\vec{x}} \times \hat{\vec{p}}$ is the usual orbital angular momentum of a single particle.

b) Derive the parity-transformed operators of the electromagnetic potentials and field strengths $\vec{A}\,'(\hat{\vec{x}}, t)$, $\Phi\,'(\hat{\vec{x}}, t)$, $\vec{E}\,'(\hat{\vec{x}}, t)$, $\vec{B}\,'(\hat{\vec{x}}, t)$, upon analyzing Maxwell's equations and the fact that electric charges do not change under parity transformations.