2. Exercise Sheet, Theoretical Physics III (Quantum Mechanics)

Solutions to be handed in and class exercises to be discussed in the tutorials of the 3rd. week (2.11.07)

P2: Hamilton-Jacobi Equation (3 points)

Consider a system with N degrees of freedom in classical mechanics. The generalised coordinates are $\mathbf{q} = (q_1, \dots, q_N)$ and the canonical momenta are $\mathbf{p} = (p_1, \dots, p_N)$. The Hamiltonian is $H(\mathbf{q}, \mathbf{p}, t)$. A *canonical transformation* is a mapping $(\mathbf{q}, \mathbf{p}) \to (\mathbf{Q}, \mathbf{P})$ onto a new system of generalised coordinates and momenta, that fulfil Hamilton's principle (principle of stationary action) with the transformed Hamiltonian $K(\mathbf{Q}, \mathbf{P}, t)$:

$$0 = \delta \int dt\, (\mathbf{p} \cdot \dot{\mathbf{q}} - H(\mathbf{q}, \mathbf{p}, t)) = \delta \int dt\, \Big(\mathbf{P} \cdot \dot{\mathbf{Q}} - K(\mathbf{Q}, \mathbf{P}, t)\Big) .$$

a) Show that a function $F(\mathbf{q}, \mathbf{P}, t)$ (a *generating function*) defines a canonical transformation through the relations

$$\mathbf{p} = \frac{\partial F}{\partial \mathbf{q}}, \qquad \mathbf{Q} = \frac{\partial F}{\partial \mathbf{P}}, \qquad K = H + \frac{\partial F}{\partial t}.$$

Now given that $S(\mathbf{q}, \mathbf{P}, t)$ is a solution of the differential equation

$$H\left(\mathbf{q}, \frac{\partial S}{\partial \mathbf{q}}, t\right) + \frac{\partial S}{\partial t} = 0 \qquad \text{(Hamilton-Jacobi equation)},$$

then the Hamiltonian K which is obtained by taking S as generating function is identically zero. Thus the equations of motion are trivial: $\mathbf{P}$ und $\mathbf{Q}$ are constant.

b) Show that the following holds for the Lagrangian L:

$$\frac{dS\left(\mathbf{q}(t), \mathbf{P}, t\right)}{dt} = L\left(\mathbf{q}(t), \dot{\mathbf{q}}(t), t\right).$$

So that, as shown in the lecture, S is (up to a constant) equal to the action:

$$S\left(\mathbf{q}(t), \mathbf{P}, t\right) = \int^t dt'\, L\left(\mathbf{q}(t'), \dot{\mathbf{q}}(t'), t'\right).$$

c) Consider a solution $\psi(\mathbf{x}, t)$ of the time-dependent Schrödinger equation with an arbitrary potential in three dimensions. We define the real functions $S(\mathbf{x}, t)$ and $A(\mathbf{x}, t)$ by

$$\psi(\mathbf{x}, t) = A(\mathbf{x}, t) \exp\left(\frac{i}{\hbar} S(\mathbf{x}, t)\right).$$

Show that, on domains where A does not vanish, S satisfies the Hamilton-Jacobi equation for the corresponding classical Hamiltonian, up to terms of order $\hbar^2$ (compare the eikonal approximation from the lecture).

H2: Tunnelling effect (8 points)

Consider a one-dimensional potential

$$V(x) = \begin{cases} V_0, & 0 \le x \le a \\ 0, & \text{otherwise} \end{cases}$$

with $V_0 > 0$. Now consider a plane wave incident from the left (x negative) with energy $E < V_0$. Determine the wavefunction in the three regions (I) $x < 0$, (II) $0 \le x \le a$ and (III) $x > a$ taking into account the boundary conditions, as demonstrated in the lecture for the potential step. How large is the probability of tunnelling? What is the result in the classical limit $\hbar \to 0$?

H3: Infinite potential well (6 points)

Consider a one-dimensional potential

$$V(x) = \begin{cases} 0, & 0 \le x \le a \\ \infty, & \text{otherwise} \end{cases}$$

Find all (correctly normalized) solutions of the Schrödinger equation. Consider initially what are the boundary conditions that the wavefunction must fulfil at $x = 0$ und $x = a$. Which energies are possible?