MAS 217 **Quantum Theory**

Exam Paper

Wednesday, 17th May 2006, 10:00h **Duration: 2 hours**

You should attempt all questions. Marks awarded are shown next to the question. Calculators are NOT permitted in this examination. The unauthorised use of a calculator constitutes an examination offense.

You are NOT permitted to start reading the following question paper until instructed to do so by an invigilator.

1. *Classical mechanics* (total: 30 marks)
Consider a classical dynamical system of N degrees of freedom with Hamiltonian $H(\underline{q}, \underline{p}) = H(q_1, q_2, \ldots, q_N, p_1, p_2, \ldots, p_N)$. Let $A(\underline{q}, \underline{p})$ and $B(\underline{q}, \underline{p})$ be two dynamical variables of this system. The Poisson bracket $\{A, B\}$ is defined by

$$\{A, B\} := \sum_{i=1}^{N} \left(\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right)$$

(a) (3 marks) Let $C(\underline{q}, \underline{p})$ be a third dynamical variable. Prove that

$$\begin{aligned} \{A, B\} &= -\{B, A\} \\ \{A, \beta B + \gamma C\} &= \beta\{A, B\} + \gamma\{A, C\} \end{aligned}$$

where β, γ are real constants.

(b) (7 marks) Let $N = 3$ with $q_1 = x$, $q_2 = y$, $q_3 = z$, $p_1 = p_x$, $p_2 = p_y$, $p_3 = p_z$. Calculate the two Poisson brackets $\{x^2, x\}$ and $\{z, p_y\}$. Define the components L_x, L_y, L_z of the classical angular momentum vector $\underline{L}$ and calculate the Poisson bracket $\{L_x, p^2\}$, where $p^2 = p_x^2 + p_y^2 + p_z^2$.

(c) (2 marks) For (c) to (e) let us restrict to $N = 1$ with $q_1 = x$ and $p_1 = p_x$. Assume we have a potential $V(x)$. What is the definition of the Hamiltonian $H(x, p_x)$ for a point mass m moving in this potential? Write down Hamilton's equations of motion for this Hamiltonian.

(d) (8 marks) Let $A(x, p_x)$ be a dynamical variable of the Hamiltonian system defined under (c). What does it mean to say that A is conserved? Derive an equation that expresses the rate of change of A in terms of a Poisson bracket. By using this equation, show that the Hamiltonian $H(x, p_x)$ defined under (c) is a conserved dynamical variable.

(e) (10 marks) Consider a point mass m moving along the x-axis in a potential defined by

$$V(x) = -5x^2 + \frac{1}{4}x^4 \ , \ x \in \mathbb{R} \, .$$

This is called a *double-well potential*, since it has two local minima positioned symmetrically around a local maximum. Calculate the positions of the minima and of the maximum. Discuss all possible types of motion in this potential by drawing $V(x)$ as a function of x and considering all values for the total energy E of the particle.

2. *Wave functions, operators and the Schrödinger equation* (total: 30 marks)

   (a) (2 marks) State de Broglie's relations and explain their meaning.

   (b) (2 marks) Suppose that $\hat{A}$ is a linear operator on a linear vector space H. Define what it means to say that $\alpha_i \in \mathbb{C}$, $i \in \mathbb{N}$, is an eigenvalue and $\phi_i \in H$ an eigenvector of $\hat{A}$.

   (c) (6 marks) The wave function $\phi(x,t) \in \mathbb{C}$ of a free particle in one dimension traveling in the positive x-direction is given by

   $$\phi(x,t) = c \exp\left[i(kx - \omega t)\right]$$

   with a constant c and $k, x, \omega \in \mathbb{R}, t \geq 0$. Show that the eigenvalue of the momentum operator $\hat{p}_x := -i\hbar\frac{\partial}{\partial x}$ applied onto ϕ is the particle's momentum. Likewise, show that the eigenvalue of the energy operator $\hat{E} := i\hbar\frac{\partial}{\partial t}$ applied onto ϕ is the particle's energy.

   (d) (10 marks) Write down the *time-independent* one-dimensional Schrödinger equation for a quantum mechanical wave function $\psi(x)$ in a potential $V(x)$. Solve it for the free particle case where $V(x) = 0$. Normalisation of your solution is not necessary. By using $\Psi(x,t) = c\psi(x)\exp(-i\omega t)$, construct the wave function of the corresponding *time-dependent* one-dimensional Schrödinger equation, where c is a real constant. The quantum mechanical wave function of a free particle bears a specific name. What is this name?

   (e) (10 marks) Consider a quantum state $\Phi(x) = c\exp(-2|x|)$, $x \in \mathbb{R}$. Determine the constant c such that the wave function is normalised. Define the probability to find the particle in the region $|x| \leq 1$ and calculate it. Define the mean value of the operator $\hat{D} = i\frac{\partial}{\partial x}$ and calculate it.

3. *Particle in an infinite potential well* (total: 20 marks)
   A particle of mass m is confined in a three-dimensional infinite potential well given by

   $$V(x,y,z) = \begin{cases} 0 \quad , & 0 < x < a \ , \ 0 < y < b \text{ and } 0 < z < c \\ \infty & \text{otherwise} \end{cases} ,$$

   where a, b, c are real constants.

   (a) (4 marks) Write down the three-dimensional time-independent Schrödinger equation for this problem. What are the boundary conditions for the wave function $\psi(x,y,z)$ in this case?

   (b) (16 marks) By separation of variables, solve this Schrödinger equation for $\psi(x,y,z)$ under these boundary conditions. Normalisation is not necesary. Calculate the energy E_{n_x,n_y,n_z} corresponding to your solution, where n_x, n_y, n_z are quantum numbers associated with x, y, z.

4. *Commutators and Hermitian operators* (total: 20 marks)

   (a) (3 marks) Let $\hat{A}, \hat{B}, \hat{C}$ be linear operators on a linear vector space H. Define the commutator $[\hat{A}, \hat{B}]$ and prove that

   $$[\hat{A}\hat{B}, \hat{C}] = \hat{A}[\hat{B}, \hat{C}] + [\hat{A}, \hat{C}]\hat{B}\,.$$

   (b) (10 marks) Consider a single particle in three dimensions, where $\hat{x}$ and $\hat{p}_x$ are the position and momentum operators. Evaluate the commutators $[\hat{p}_x, \hat{x}]$ and $[\hat{p}_x^2, \hat{x}]$. Define the x-component of the angular momentum operator $\hat{L}_x$ and evaluate the commutator $[\hat{L}_x, \hat{x}]$.

   (c) (7 marks) Let the wave functions $\phi(x), \psi(x)$ be elements of a linear vector space H such that they are bounded and sufficiently differentiable. Let $(\phi, \psi) := \int_{-\infty}^{\infty} dx\ \phi^*(x)\psi(x)$ be a scalar product on H. With respect to this scalar product, define what it means to say that a linear operator $\hat{A}$ on H is Hermitian. Determine whether the operator $\hat{E} := \frac{\partial^2}{\partial x^2}$ is Hermitian (note that the wave functions $\phi, \psi \in H$ vanish at $\pm\infty$).