NAME:

To be returned until Tuesday, April 16, 10.00 h to the Departmental Office. This is the first of two courseworks, each having 30 MARKS. The second coursework will be handed out in the first week after the Easter vacations.

Answer question 1.1 AND 1.2 or, alternatively, question 1.3.

1.1 The Infinite Potential Well (15 MARKS)

Consider the motion of a particle of mass m within the infinitely high potential well

$$V(x) = \begin{cases} \infty, & -\infty < x \le -L/2 \\ 0, & -L/2 < x \le L/2 \\ \infty & L/2 < x < \infty \end{cases}$$

Determine the eigenfunctions $\psi_n(x)$ of energy E_n , and find the eigenvalues of the energy E_n . You do not need to determine the normalization factor of the wave functions $\psi_n(x)$. What are the symmetry properties of the eigenfunctions?

1.2 The Schrödinger Equation (15 MARKS)

a) (10 MARKS)

We consider a one-dimensional potential V(x) and a stationary wave function $\psi(x)$ at energy E,

$$V(x) = \begin{cases} V_1, & -\infty < x \le 0\\ V_2 & 0 < x \le \infty \end{cases} \quad \psi(x) = \begin{cases} a_1 e^{ik_1 x} + b_1 e^{-ik_1 x}, & -\infty < x \le 0\\ a_2 e^{ik_2 x} + b_2 e^{-ik_2 x}, & 0 < x \le \infty \end{cases}$$

We consider the case $E > V_1$ and $E > V_2$ such that k_1 and k_2 are real wave vectors and $\psi(x)$ describes running waves. By consideration of the boundary conditions at x = 0, show that the arbitrary constants a_i and b_i can be related by a matrix equation

$$\mathbf{u}_1 = \begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} \mathbf{u}_2, \quad \mathbf{u}_i = \begin{pmatrix} a_i \\ b_i \end{pmatrix}, \quad i = 1, 2,$$

by explicitly calculating the 2 by 2 matrix.

b) (5 MARKS)

Consider the matrix equation from part a) for the coefficients of the wave functions on both sides of the potential step from part a). (You don't need the solution from a) to answer this part). We set $b_2 = 0$ and define the transmission coefficient $T = k_2 |a_2|^2 / (k_1 |a_1|^2)$. Show that $T = k_2 / (k_1 |M_{11}|^2)$. If we consider T(E) as a function of energy, what is the limiting value $T(E \to \infty)$ for very high energies?

1.3 The Time–Dependent Schrödinger Equation (30 MARKS)

In this problem, we solve the time–dependent Schrödinger equation for the wave function $\Psi(x, t > 0)$ of a free particle in one dimension (zero potential) with the initial condition

$$\Psi(x, t = 0) = C \exp(-x^2/(2\sigma^2)).$$

by Fourier transformation. The Fourier transformation f(k) of a function f(x) is defined by the equations

$$f(k) = \int_{-\infty}^{\infty} dx e^{-ikx} f(x), \quad f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk e^{ikx} f(k).$$

a) (10 MARKS) By performing a Fourier transformation with respect to the xcoordinate, write down the time-dependent Schrödinger equation (V=0) in k-space
and solve the k-space equation for $\Psi(k, t)$.

b) (10 MARKS)

Perform an inverse Fourier transformation on $\Psi(k, t)$, using the relation

$$\int_{-\infty}^{\infty} dx e^{-ax^2 + bx} = \sqrt{\frac{\pi}{a}} e^{b^2/4a}$$

Show that the final result takes the form

$$\Psi(x,t) \propto \exp\left(-\frac{x^2}{2\sigma^2 + 2i\hbar t/m}\right),$$
(1.1)

where \propto means 'proportional to'.

c) (10 MARKS)

Calculate the absolute square $|\Psi(x,t)|^2$, Eq.(1.1), neglecting all prefactors. From this you can read off how the wave packet broadens as a function of time. Calculate this width as a function of time t explicitly and compare it to the original width σ^2 of the wave packet at time t = 0.