Final exam for Kwantumfysica 1 - 2006-2007

Friday 27 April 2007, 9:00 - 12:00

<u>**READ THIS FIRST:**</u>

- Clearly write your name and study number on each answer sheet that you use.
- On the first answer sheet, write clearly the total number of answer sheets that you turn in.
- Note that this exam has 3 questions, it continues on the backside of the papers!
- Start each question (number 1, 2, 3) on a new answer sheet.
- The exam is open book within limits. You are allowed to use the book by Liboff, and one A4 sheet with notes, but nothing more than this.
- If it says "make a rough estimate", there is no need to make a detailed calculation, and making a simple estimate is good enough. If it says "calculate" or "derive", you are supposed to present a full analytical calculation.
- If you get stuck on some part of a problem for a long time, it may be wise to skip it and try the next part of a problem first.
- If you are ready with the exam, please fill in the **course-evaluation question sheet**. You can keep working on the exam until 12:00, and fill it in shortly after 12:00 if you like.

Useful formulas and constants:

Electron mass	m_e	$= 9.1 \cdot 10^{-31}$ kg
Electron charge	$-e$	$= -1.6 \cdot 10^{-19}$ C
Planck's constant	h	$= 6.626 \cdot 10^{-34}$ Js $= 4.136 \cdot 10^{-15}$ eVs
Planck's reduced constant	$\hbar$	$= 1.055 \cdot 10^{-34}$ Js $= 6.582 \cdot 10^{-16}$ eVs

Fourier relation between x-representation and k-representation of a state

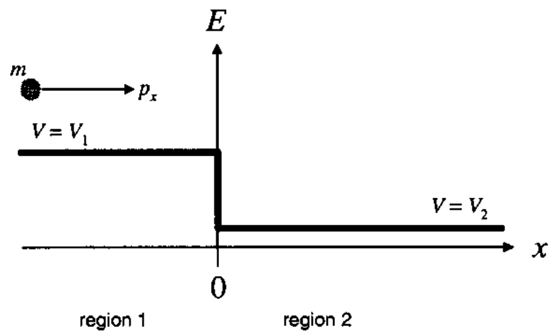
$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \overline{\Psi}(k) e^{ikx}\, dk$$

$$\overline{\Psi}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \Psi(x) e^{-ikx}\, dx$$

Z.O.Z.

Problem 1

A one-dimensional quantum particle with mass m, is propagating through space (position x, wavenumber k), and feels the potential $V(x)$ as in the sketch of the particles energy E below. The particle is approaching $x = 0$ coming from the left. The particle has negligible uncertainty in its velocity, and total energy E_0.



a) Derive an expression for k_i (where i is 1 or 2, referring to the regions) from the time-independent Schrödinger equation.

b) At some time the particle will reach $x = 0$, where it can scatter on the change in the potential $V(x)$. Derive an expression for the reflection coefficient R for this scatter event in terms of the parameters E_0, V_1 and V_2 only.

c) Show that the reflection coefficient R depends only on the differences $(E_0 - V_1)$ and $V_0 = V_1 - V_2$.

d) Assume that in an experiment the energies E_0 and V_1 are fixed (with $E_0 = 2\cdot V_1$), and that V_2 can be varied. Calculate R for the cases $V_2 = 0.5\cdot V_1$, $V_2 = V_1$, $V_2 = 1.5\cdot V_1$.

Problem 2

Consider an electron, that behaves as a one-dimensional quantum particle.

a) At some time t_0 the electron is in the state $\Psi(x) = Ae^{\frac{-|x|}{a}}$, where A real and positive. For which value of A is this state normalized?

b) Derive an expression that describes this state as a superposition of plane waves with wavenumber k.

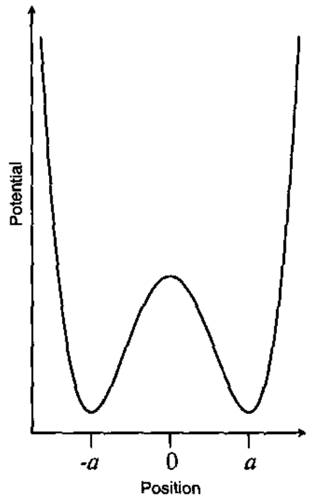
c) *Roughly estimate* Δx and Δp_x for the state of question **a)**, and check whether it violates the Heisenberg uncertainty relation.

d) One wants to measures the velocity of this particle at time t_0. Calculate the probability for getting a result between 40 km/s and 50 km/s. Calculate a numerical result, use $a = 1$ nm. You may need to use this solution to the following integral,

$$\int \left(\frac{1}{1+b^2y^2}\right)^2 dy = \frac{1}{2}\left(\frac{y}{1+b^2y^2} + \frac{\arctan(by)}{b}\right).$$

Problem 3

In a molecule, an electron is tightly bound to the other particles in the system. In one direction, it can be in either in one of two positions, because the electron experiences in this direction a one-dimensional potential as in the following sketch.



The barrier between the two wells is so high, that the tunneling between the left and right well is negligible. In this situation, the system has two energy eigenstates with the same energy E_0. One of these states, denoted as $|\varphi_L\rangle$, corresponds to the particle being localized at $-a$ in the left well. The other energy eigenstate, denoted as $|\varphi_R\rangle$, corresponds to the particle being localized at $+a$ in the right well. All other energy eigenstates are so high in energy that they do not need to be considered. The system can therefore be described as a two-state system. It is then convenient to use matrix and vector notation in the basis spanned by $|\varphi_L\rangle$ and $|\varphi_R\rangle$, which gives the following relations ($\hat{H}_0$ is the Hamiltonian)

$$\hat{H}_0 \leftrightarrow \begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix}, \quad |\varphi_L\rangle \leftrightarrow \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |\varphi_R\rangle \leftrightarrow \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

When the molecule is placed in a static electric field of 1 V/mm, the only effect on the potential for the electron is that barrier between the two wells becomes lower. In that case tunneling between the two wells can no longer be neglected when describing the dynamics of the electron. Using the same matrix notation as before (also in the same basis), the Hamiltonian of the system is now (here T is a real and negative number)

$$\hat{H} \leftrightarrow \begin{pmatrix} E_0 & T \\ T & E_0 \end{pmatrix}.$$

For the rest of the problem, assume that the static electric field is on!

a) From symmetry arguments it is known that the energy eigenstates of the Hamiltonian $\hat{H}$ are symmetric and anti-symmetric superpositions of $|\varphi_L\rangle$ and $|\varphi_R\rangle$, which are (using the same basis and vector notation as in the above expression)

$$\begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}.$$

Here one of these vectors is the ground state $|\varphi_g\rangle$ and the other the excited state $|\varphi_e\rangle$ Calculate the energy eigenvalues E_g and E_e that belong to these energy eigenvectors, and show which eigenvector is the ground state and which one is the excited state.

b) Proof that these energy eigenstates of $\hat{H}$ are normalized and orthogonal.

c) There is an operator (observable) $\hat{A}$ for the position of the electron in this double well system,

$$\hat{A} \leftrightarrow \begin{pmatrix} -a & 0 \\ 0 & a \end{pmatrix}.$$

Calculate whether $\hat{A}$ commutes with $\hat{H}_0$, and whether $\hat{A}$ commutes with $\hat{H}$.

d) What are the eigenvectors and eigenvalues of $\hat{A}$?

e) There is an experimental apparatus that can measure physical property described by $\hat{A}$ (determine whether the electron is in the left or the right well by performing a measurement of a short time). For the case that the system is in the ground state of $\hat{H}$, discuss what the possible measurements outcomes are, derive the probability for each of the measurement outcomes, and what the state is immediately after the measurement for each of the measurement outcomes.

f) Repeat question **e)**, but know for the case that the system is at the moment of measurement in the state

$$|\Psi\rangle = \sqrt{\frac{1}{3}}|\varphi_g\rangle + \sqrt{\frac{2}{3}}|\varphi_e\rangle.$$

g) The outcome of a measurement of $\hat{A}$ (which ended at time $t = 0$) is that the particle is in the left well. Express the state at $t = 0$ in terms of state $|\varphi_g\rangle$ and $|\varphi_e\rangle$.

h) Calculate the value of the four quantities

$$\langle\varphi_g|\hat{A}|\varphi_g\rangle,\ \langle\varphi_e|\hat{A}|\varphi_e\rangle,\ \langle\varphi_g|\hat{A}|\varphi_e\rangle \text{ and } \langle\varphi_e|\hat{A}|\varphi_g\rangle.$$

Describe in words what these quantities represent.

i) Following up on question **g)** and **h)**, calculate how $\langle\hat{A}\rangle$ depends on time for $t > 0$. Describe in words what the calculation represents.