Problem set for 2nd week of the course Quantum Physics 1

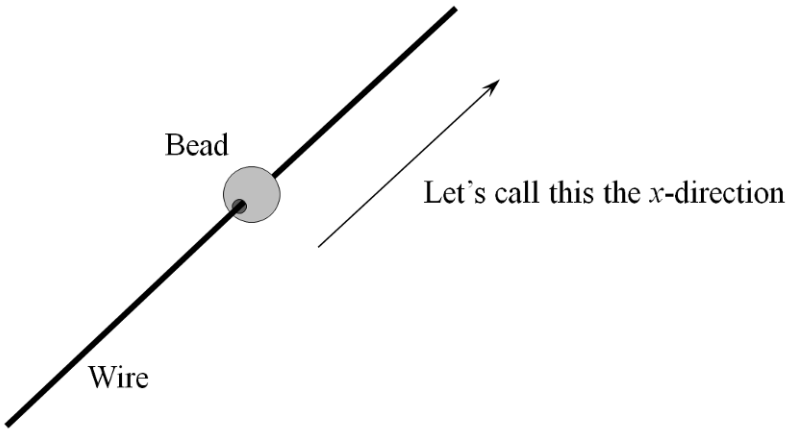
For the tutorial sessions of 10 and 12 September 2014

Homework, to be made before the werkcollege:
From the book (Griffiths 2nd Ed.) Chapter 2 - 2.1, 2.3, 2.4, 2.8 and 2.9

Problems to work on during werkcollege:
Problems W2.1 – W2.5 (this hand out), this is the minimal set you need to do.
Other good problems that we selected (we advise you to make these for the topics where you need or like to do extra training):
from the book Chapter 2 - 2.2, 2.5a-c (hint: draw the state for n=1, n=2), 2.6, 2.7, 2.15

Problem W2.1

When learning quantum mechanics, it very important to understand the difference between a *degree of freedom* and a *parameter* (with a fixed value) of a physical system. In classical mechanics, the state of each degree of freedom of a certain system is described by a coordinate (generalized coordinate) that can be represented by a number. In the quantum version of that system, however, the state of that degree of freedom must be described by a wavefunction. There is then a wavefunction for each degree of freedom. But what is the number of degrees of freedom for a single bead on a rigid wire (see figure)? One (only x coordinate) or three (x, y and z coordinate)? If we assume that the bead can only move along the wire, there is a *constraint* for the motion in the y and z direction, and the number of degrees of freedom is only one. In a description of the quantum version of the system, the x position is then described by a wavefunction, while the fixed y and z position (and the mass) are parameters (fixed numbers) for the system. Apply this idea in the remainder of this question.



For each of the following systems, specify the number of degrees of freedom and a set of good coordinates.

(a) A bead constrained to move on a closed circular hoop that is fixed in space.
(b) A bead constrained to move on a helix of constant pitch and constant radius.
(c) A particle on a right circular cylinder.
(d) A pair of scissors on a plane.
(e) A rigid rod in 3-space.
(f) A rigid cross in 3-space.
(g) A linear spring in 3-space.
(h) Any rigid body with one point fixed.
(i) A hydrogen atom.
(j) A lithium atom.
(k) A compound pendulum (two pendulums attached end to end).

Problem W2.2

One of the first expressions that we usually learn in quantum mechanics is an expression for the photon energy when a quantum system decays from a quantum level with energy E_n to a level with energy $E_{n'}$: $\hbar\omega = E_n - E_{n'}$ (but in Griffiths only at p. 158). This expression did not return in the first weeks at the hearing lectures (hoorcollege) as one of the postulates (most basic principles), so one should be able to derive it using the postulates. This problem illustrates how this comes about. Assume there is a simplified model for the electron dynamics in the hydrogen atom, which gives only three energy levels (eigenvalues for the total energy). This simple model is based on a time-independent Hamiltonian $\hat{H}$ (with only a term for kinetic energy $\hat{T}$, and a term for potential energy $\hat{V}_p$ that results from the Coulomb interaction with the nucleus). In this model, the time-independent Schrödinger equation (the eigenvalue equation for the system's energy levels) gives the following three solutions (with eigenvalues E_n and eigenfunctions φ_n):

$$\begin{cases} \hat{H}\,\varphi_1 = E_1\,\varphi_1 \\ \hat{H}\,\varphi_2 = E_2\,\varphi_2 \\ \hat{H}\,\varphi_3 = E_3\,\varphi_3 \end{cases} \quad , \quad \text{with } E_1 < E_2 < E_3.$$

Note that terms in a calculation of the expectation value of the total energy $<\hat{H}>$ obey (by definition of the eigenvalue):

$$\begin{cases} \int_V \varphi_n^* \hat{H}\,\varphi_n d\boldsymbol{r} = E_n \ , \\ \int_V \varphi_m^* \hat{H}\,\varphi_n d\boldsymbol{r} = 0 \ , \ \text{for } n \neq m \end{cases}$$

Here V is the total relevant volume, and $\boldsymbol{r}$ the position coordinate.

a) Assume that at $t = 0$, the system is in the ground state, $\Psi(t = 0) = \varphi_1$. What is now the expectation value for the total energy $<\hat{H}>$? Also calculate it for $\Psi(t = 0) = \varphi_2$.

b) Assume that at $t = 0$, the system is in the state $\Psi(t=0) = \frac{1}{\sqrt{2}}(\varphi_1 + \varphi_3)$.

What is now the expectation value for the total energy $<\hat{H}>$?

c) What is for the state as in **b)**, the uncertainty in the total energy $<\Delta\hat{H}>$.

d) Assume that at $t = 0$, the system is in the state $\Psi(t=0) = c_1\varphi_1 + c_2\varphi_2$. Consider c_1 and c_2 to be real numbers and the eigenfunctions φ_1 and φ_2 to be normalized. Also φ_1 and φ_2 obey the orthogonality condition: $\int_V \varphi_n^* \varphi_m dr = 0$ for n≠m. From the fact that $\Psi(t = 0)$ must also be normalized prove that $c_1^2+c_2^2=1$. Calculate the expectation value of Hamiltonian in the state $\Psi(t=0) = c_1\varphi_1 + c_2\varphi_2$. Explain the result of this last question in terms of the probability of finding the system in states φ_1 and φ_2.

This model system is time-independent, so we can use an operator $\hat{U} = e^{-\frac{i\hat{H}t}{\hbar}}$ (based on p. 24-26 of the book, see also the slides of the lectures) to calculate how its states evolve in time.

e) For the states as in **a)** and **b)**, write down an expression for $\Psi(t)$ for $t > 0$ in terms of φ_n and E_n.

f) For the initial states as in **a)** and **b)**, write down how the expectation value for the total energy $<\hat{H}>(t)$ depends on t .

Consider now the operator $\hat{A}$ for the electric dipole moment of this system, which is mainly responsible for the emission of optical fields. It obeys (note that the second equation is not zero because φ_n are eigenfunctions of $\hat{H}$, and not of $\hat{A}$):

$$\begin{cases} \int_V \varphi_n^* \hat{A} \varphi_n d\boldsymbol{r} = A_0 \quad , \quad \text{for } n = 1,2,3 \\ \int_V \varphi_m^* \hat{A} \varphi_n d\boldsymbol{r} = A_1 \quad , \quad \text{for all cases } n \neq m \end{cases} .$$

g) For the states as in **a)** and **b)**, write down how the expectation value for the electric dipole moment $<\hat{A}>(t)$ depends on t. What is the frequency of the electric dipole oscillation for state of **b)**?

h) Now assume that at $t = 0$, the system is in the state $\Psi(t = 0) = \alpha\ \varphi_1 + \beta\ \varphi_3$. Note that α and β are in general complex constants, but assume them real and $0 \leq \alpha \leq 1$ for this problem. This initial state is normalized, and therefore α and β obey $|\alpha|^2 + |\beta|^2 = 1$. Calculate how the amplitude of the oscillating dipole moment $<\hat{A}>(t)$ at some $t > 0$ depends on α. Express the answer on a scale compared to A_1.

i) For the state in **h)**, note that the expression $|\alpha|^2 + |\beta|^2 = 1$ invites us to express α and β as $\alpha = \sin(\theta/2)$ and $\beta = \cos(\theta/2)$. We use as most text books the angle as $\theta/2$, because decay from the excited state to the ground state can then be pictured as some rotation from top to bottom, with θ running from 0 to π. Make a sketch of how α, β and the amplitude of the oscillating dipole moment at $t > 0$ depend on θ (assume $0 \leq \theta \leq \pi$). Express the number for the amplitude on a scale compared to A_1.

j) How much energy does the system loose when it decays from the state φ_3 to the ground state φ_1? How many photons are emitted, what is the photon energy?

k) Note that in classical physics an electromagnetic field is radiated from an oscillating dipole as in **g)** and **h)**. However for the state $\Psi(t = 0) = \frac{1}{\sqrt{2}}(\varphi_1 + \varphi_3)$ (that is $\theta = \pi/2$), the result of **f)** shows that $<\hat{H}>(t)$ is constant. In terms of the sketch for **i)**, this means $d\theta/dt = 0$. The system does not decay! Explain why this is, for the model used here.

l) A second problem with the model is the following. If the system is at $t = 0$ in the excited state, $\Psi(t = 0) = \varphi_3$, it has no observable property that depends on time (see **g)** and **i)**). One could argue, that (besides the problem of **k)**) the system will therefore never start with its radiative decay to the ground state. Why does in practice an atom in the state $\Psi(t = 0) = \varphi_3$ nevertheless always start its decay to the ground state immediately?

Problem W2.3
Consider the following quantum system: a particle with mass m that can only move in the x-direction. It is not a free particle, it experiences a position-dependent potential that is constant in time. This is a system with one degree of freedom and with a stationary Hamiltonian.

a) Derive for this system the time-independent Schrödinger equation from the time-dependent Schrödinger equation. Use the x-representation.

b) Write down (once more) the time-independent Schrödinger equation. Explain for what physical property it is an eigenvalue equation. What is the meaning of the eigenvalues and eigenstates of this equation?

c) Now assume that the quantum system is a particle that moves in a potential $V(x) = B_0 \cos(3x)$. Write down the time-independent Schrödinger equation for this case, using a representation where all states and operators are expressed as functions of x. That is, you must write it out in a form that shows each term of the equation, and work out each term as a function of x in as much detail as possible with the information that is given.

Problem W2.4
This problem continues on the derivation of the states for a particle in a box (infinite square well) in the Griffiths book (2nd ed.), and uses similar notation as on p. 30-32.

a) What are the energy eigenfunctions for n=1 and n=2?

b) Calculate $\langle p_x \rangle$ and Δp_x for n=1 and n=2.

c) The value of the energy of the ground state E_1 is higher than the lowest potential (the bottom) of the box: $E_1>0$. Is it possible to reduce this ground state energy by reducing the uncertainty Δx? Explain qualitatively why it is not possible to reduce this ground state energy by reducing the uncertainty Δx. Hint: use the Heisenberg uncertainty relation, and use the answer for Δp_x in **b)** and a quick rough estimate for Δx and assume that the width a cannot be changed.

d) The same question as **c)**, but now for Δp_x. Explain qualitatively that this does not work out either.

e) Calculate for the ground state the expectation value for the particle's kinetic energy.

f) By definition, an energy eigenvalue of a time-independent Hamiltonian has a well-defined energy, with zero uncertainty: ΔH=0. The expression for E_1 with the momentum expressed in terms of $k_1=p_x/\hbar$ suggests that also k_1 must have a well-defined value (with zero uncertainty) for the energy eigenstate $|\varphi_1\rangle$. However, the answer on **b)** gives $\Delta p_x > 0$ and seems to contradict this. Explain why there is no contradiction, and why $\langle p_x \rangle = 0$.

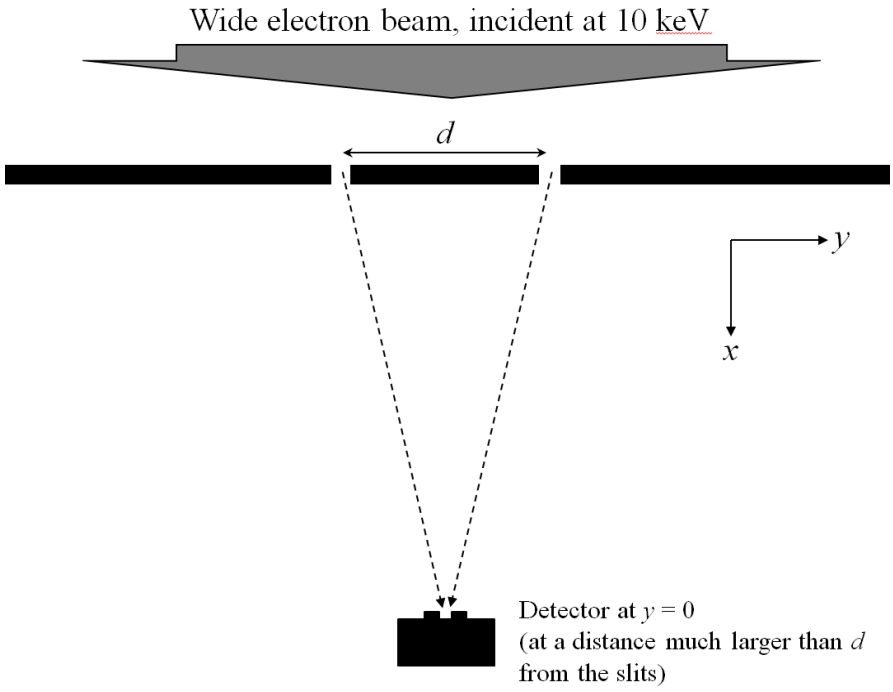
P.S. Some useful integrals solved:

$$\int \sin(Ax)\cos(Ax)\,dx = \frac{-1}{2A}\left(\cos^2(Ax) - 1\right)$$

$$\int \sin^2(Ax)\,dx = \frac{1}{2A}\left(Ax - \sin(Ax)\cos(Ax)\right)$$

Problem W2.5 *(first skip this problem until double-slit interference was treated in a lecture)*
In an electron microscope, electrons are accelerated to a high velocity such that they get a very small De Broglie wavelength, much smaller than the wavelength of optical waves. This allows for making images with much higher resolution than can be obtained with optical microscopes. One of the ways to get contrast in the images made with an electron microscope relies on interference between different partial electron waves that go through a sample (this has similarity with optical phase contrast microscopy, discovered by Prof. Frits Zernike from Groningen, for which he won the Nobel Prize in Physics in 1953).

To study the basic principles of such electron wave interference we will perform a double slit experiment with electrons. The figure illustrates the setup, with a beam of electrons that is incident on a screen with a double slit in it. The width of the slits is a, and they have very sharp edges. The distance between the slits (center to center) is d. The incoming electron flux (a very wide bundle much wider than d) is hitting the two slits at an equal rate. You can also assume that the plate that contains the slits is very thin (less than a, but thick enough to block electrons).



a) Sketch a probability density for the wavefunction that describes the y-position of the electrons, for the moment they just come out of the slits (assume that the plane with the slits is very thin, that is, the electrons spend almost zero time between the walls of the slits). Write down a normalized wavefunction that is in agreement with it.

b) The electrons that fly through the slits have been accelerated (starting with zero velocity) over 10 kV, in a region with an electric field. What is the De Broglie wavelength of the electrons?

c) We will now assume that $d >> a$, and that a and d are both much smaller than the distance from the slits to the electron detector. This detector has a very narrow opening and is positioned at the symmetry axis at $y = 0$. Inside one of the slits (the left one in the figure, named slit A, the other one is slit B), we will build a device that can be used for changing the phase of the complex *wavefunction that describes the x-position of each electron*. If an electron passes through slit A, the only change to its wavefunction is that the phase of the wavefunction $\Psi(x,t)$ increases by a controllable amount φ. Consequently, for an electron that went through slit A, the phase of its wavefunction is still increased by an amount φ. by the time it arrives at the detector (with respect to the case that it did not get any additional phase while going through slit A). The electrons arrive at the detector at time t_D (on a time scale for which we set the time they leave the source equal to $t = 0$, for each electron). Thus, the effect of the phase-changing device is that it changes the wavefunction of electrons that went through slit A according to

$$\Psi_0(x,t_D) \rightarrow \Psi_0(x,t_D)e^{i\varphi} = \Psi(x,t_D) \ ,$$

Where $\Psi(x,t)$ is the actual wavefunction at the detector and $\Psi_0(x,t)$ is this wavefunction for the case that $\varphi = 0$. With a constant electron flux going towards the slits, we count the number electron clicks per second that is observed at the detector. Analyze and sketch how this count rate varies as a function of φ, with slit B closed (only A open).

d) The same as for c), but now with both slits open.

e) How rapidly the phase of electron wavefunctions evolve in time depends on the material that surrounds the electron. Explain using the answers on the previous questions how one can build an electron microscope with a double-slit setup.