Problem set for Chapter 3 for werkcollege Kwantumfysica 1

For 2nd werkcollege of 2nd week and 1st werkcollege of 3rd week (Nov. 2010)

Problems (Homework, to be made before the werkcollege)
Book Chapter 3 - 3.1, 3.2, 3.3, 3.4, 3.5, 3.10,
3.11 (lots of algebra, use first X_o=0 and P_o=0 if you get stuck),

Problems to work on during werkcollege
Problems C3.1 – C3.4 (this handout) and Book Chapter 3 - 3.12, 3.15, 3.16, 3.20, 3.21

Problem C3.1

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 $E_{n'}$: $\hbar\omega = E_n - E_{n'}$ (see e.g. p. 41). This expression did not return this week as one of the postulates, 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):

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

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 expectation value of Hamiltonian in the state $\Psi(t=0) = c_1\varphi_1 + c_2\varphi_2$. Explain the last result obtained 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 the operator $\hat{U} = e^{-\frac{i\hat{H}t}{\hbar}}$ on p. 84 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 $\hat{A}$):

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

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 **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 $0 \le \alpha \le 1$ 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 $0 \le \theta \le \pi$). 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 C3.2

The problems **C3.2** and **C3.3** are meant to clarify how an operator works on a wavefunction, and to clarify the theory around Eq. (3.26) on p. 74 and Eq. (3.67) on p. 85 in the book. You will also get familiar with the properties of the Dirac delta function $\delta(x)$. We will consider here the operator $\hat{X}$ associated with the position x of a particle in one dimension (as Eq. (3.26), but we use slightly different notation here), defined by the following eigenvalue equation:

$$\hat{X}\,\delta(x - x_n) = x_n\,\delta(x - x_n) \quad ,$$

where $\delta(x\text{-}x_n)$ the eigenfunction for the associated eigenvalue x_n. We consider situations where the state of a particle is described by one of the following three time-independent wavefunctions that describe the position x (in problems **C3.2** and **C3.3**, assume that x is a dimensionless coordinate, the ratio of position to a certain length scale)

$$\varphi_1(x) = \delta(x+2) \quad ,$$
$$\varphi_2(x) = \frac{1}{\sqrt{2}}\left(\delta(x-1) + \delta(x-3) \right) \quad ,$$
$$\varphi_3(x) = \sum_n c_n \delta(x - x_n) \ , \qquad \text{with } \sum_n |c_n|^2 = 1 \quad .$$

a) For φ_1 and φ_2, describe what the possible outcomes are when we measure the position of the particle, and calculate the probabilities (give a number) for each of the measurement results. For each measurement outcome, give the state of the particle immediately after the measurement.

b) For φ_3, describe what the possible outcomes are when we measure the position of the particle, and calculate the probabilities for each of the measurement results (give the answer in terms of x_n, c_n).

c) Show that these three wavefunctions can*not* be normalized.

The fact that these wavefunctions cannot be normalized, is because in quantum mechanics the uncertainty Δx in the position of the particle can never be really zero (see also p. 164). Physically, a particle in the state $\delta(x\text{-}x_n)$ cannot exist. A state in the form of true plane wave (that runs by definition from $-\infty$ to $+\infty$) as used on p. 72, also cannot exist. However, it will turn out that the Dirac delta function and plane waves are very useful mathematical tools for calculating with wavefunctions.

Problem C3.3
Consider again the operator $\hat{X}$ of problem **C3.2**, and also the wavefunctions φ_1, φ_2 and φ_3.

a) Calculate the wavefunction that results if $\hat{X}$ operates on φ_1, φ_2, and φ_3 in terms of wavefunctions $\delta(x\text{-}x_n)$

b) Calculate the wavefunction that results if $\hat{X}^2$ operates on φ_1 and φ_2 in terms of wavefunctions $\delta(x\text{-}x_n)$.

c) Calculate the wavefunction that results if the operator $(\hat{X} + \hat{X}^2)$ operates on φ_1 and φ_2 in terms of wavefunctions $\delta(x\text{-}x_n)$.

d) Prove for φ_3 that $\hat{X}^2 \varphi_3(x) = \sum_n \left(c_n \, x_n^2 \, \delta(x - x_n) \right)$.

e) We now consider the operator $\hat{S} = e^{i\hat{X}}$. Write down the first three terms of the Taylor expansion of $\hat{S}$ in $\hat{X}$. Use for the notation of the identity operator in your answer $\hat{I}$.

f) Prove for φ_3 that $\hat{S}\,\varphi_3(x) = \sum_n \left(c_n \, e^{ix_n} \, \delta(x - x_n) \right)$.

Problem C3.4

a) Consider a free particle with mass m, with kinetic energy $E = p^2/2m$, moving in 1 dimension. The uncertainty in its location is Δx. Show that if $\Delta x \Delta p > \hbar/2$, its energy-time uncertainty then obeys $\Delta E \Delta t > \hbar/2$. Show first that $(p/m)\Delta t = \Delta x$.

One technique to study physical processes in solid state systems as a function of time, is making use of ultrafast pulsed lasers. Such lasers produce Heisenberg limited optical pulses with an energy spread ΔE and have a duration Δt. The duration Δt limits the resolution at which we can study processes in solid state systems. A typical spectrum of the laser pulses ranges from 780 to 820 nm.

b) Calculate the temporal resolution of such a laser.

For some systems, we do not only want to study certain properties in time, but we also like to know how they depend on the spectrum with which we excite the system.

c) Say we have a experiment in which we need to excite our system with 10 ps time resolution or better. To what spectral resolution are we limited in this case, if we need to study the system with pulses that have an average wavelength of 800 nm? Give the answer both in units nm and eV.