Problem set for 4th week of the course Quantum Physics 1

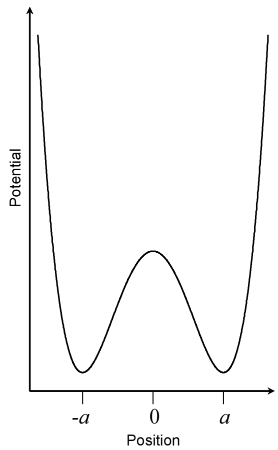
For the tutorial sessions of 24 and 26 September 2014

Homework, to be made before the werkcollege:
From the book (Griffiths 2nd Ed.) Chapter 3 - 3.7, 3.13, 3.17, 3.31.

Problems to work on during werkcollege:
Problems W4.1 – W4.4 (this hand out), and from the book Chapter 3 - 3.14, 3.15, 3.38, 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 3 - 3.8, 3.10, 3.12, 3.27.

Problem W4.1

In this problem you practice with quantum mechanical calculation on systems that can be represented by 2 x 2 matrix representations.
In a molecule, an electron is tightly bound to the other particles in the system. In one direction, it can be in either 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** (introduced in this week's lecture, also see the Griffiths book, Sec. 2.5, before Eq. [2.109] and after Eq. [2.141]) 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 around $-a$ in the left well. The other energy eigenstate, denoted as $|\varphi_R\rangle$, corresponds to the particle being localized around $+a$ 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 a matrix and vector representation that uses $|\varphi_L\rangle$ and $|\varphi_R\rangle$ as basis vectors, 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)

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

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) Prove 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 the 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 now 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.

Problem W4.2

This problem is meant to clarify the importance of symmetry in quantum mechanics. You will learn about an operator that can be used to characterize symmetry (parity operator), and why certain atomic transitions do not emit radiation at all because of symmetry while they are energetically allowed (so-called *forbidden transitions*, as opposed to *allowed transitions* , behavior that is summarized in *selection rules*).

Consider the following model system for an atom with one electron: a one-dimensional particle-in-a-box system, where the potential for the electron outside the box is infinite, and inside the box the potential $V = 0$. The position of the electron is described by a coordinate x. The width of the box is a, with the walls at $x = -a/2$ and $x = +a/2$. Eq. [2.28] of the Griffiths book gives the energy eigenstates for a particle this system, but for a box (or quantum well) that runs from x=0 to x=a. Here we use a description where the box runs from x=-a/2 to x=a/2 (and slightly different notation with $\varphi_n(x)$ for the energy eigen states, instead of $\Psi_n(x)$ as in the book). The eigen energies E_n are of course the same, but the eigenstates are now

$$\varphi_n(x) = \sqrt{\tfrac{2}{a}}\cos\left(\tfrac{n\pi x}{a}\right), \qquad \text{for } n = 1, 3, 5, 7,...$$
$$\varphi_n(x) = \sqrt{\tfrac{2}{a}}\sin\left(\tfrac{n\pi x}{a}\right), \qquad \text{for } n = 2, 4, 6, 8,...$$

Assume that this system has an electrical dipole moment that oscillates when the system is emitting a photon. This can occur when the system is in a superposition of two different energy eigenstates $|\varphi_m\rangle$ and $|\varphi_n\rangle$. The operator for this dipole moment is $\hat{D} = e\hat{X}$, where $\hat{X}$ the position operator and e the electron charge.

We introduce here the parity operator $\hat{P}$, which is defined by how it works on a function $f(x)$:

$$\hat{P} f(x) = f(-x).$$

It can be shown that $\hat{P}$ has two eigenvalues +1 (*even parity*) and -1 (*odd parity*). Any even function is an eigenfunction for the eigenvalue +1, while any odd function is an eigenfunction for the eigenvalue -1. $\hat{P}$ can also be used to characterize the symmetry (parity) of operators.

a) Evaluate $\hat{P}\,\varphi_n(x)$ and derive for which n the state $\varphi_n(x)$ has even or odd parity.

b) What is the parity of $\hat{D}$?

c) Use symmetry and parity arguments to show that this particle-in-a-box system cannot emit a photon when it is in a state that is a superposition of two energy eigenstates with the same parity. Hint: use the x-representation to evaluate all the elements like $\langle\varphi_n|\hat{D}|\varphi_m\rangle$ in an expression for how the dipole moment oscillates as a function of time during the emission of a photon.

d) An electron is in the third excited state of this system (from the four lowest energy eigenstates, the one with the highest energy). It can (and will) relax to lower energy eigenstates by spontaneous emission of a photon during the transition to this lower state. Discuss which relaxation processes are possible, and for each which photon is (or photons are) emitted, and what the final state is. Use only symbols when answering this question.

More in general one can derive the following rules (so-called *selection rules*, for example for optical transitions):

Matrix elements (expressions like $\langle \varphi_n | \hat{A} | \varphi_m \rangle$) of an even operator are zero between states of opposite parity.

Matrix elements (expressions like $\langle \varphi_n | \hat{A} | \varphi_m \rangle$) of an odd operator are zero between states of the same parity.

Problem W4.3

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 nm 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.

Problem W4.4

Suppose an operator $\hat{A}$ has an eigenfunction φ_1 with eigenvalue a_1. It is non-degenerate: there are no other (linearly independent) eigenfunctions having eigenvalue a_1. An operator $\hat{B}$ commutes with $\hat{A}$, which is usually written as $[\hat{A}, \hat{B}] = 0$.

a) Show that φ_1 is also an eigenfunction of $\hat{B}$.
Hint: Show that $\hat{B}\varphi_1$ is an eigenfunction of $\hat{A}$, and use the fact that φ_1 is non-degenerate.

Now suppose there are two linearly independent eigenfunctions of $\hat{A}$: φ_1 and φ_2, each having eigenvalue a. Any linear combination $c_1 \varphi_1 + c_2 \varphi_2$ is an eigenfunction of $\hat{A}$ corresponding to eigenvalue a, so now all we can say is that $\hat{B}\varphi_1$ and $\hat{B}\varphi_2$ are linear combinations of φ_1 and φ_2. Note that φ_1 and φ_2 are not necessarily also eigenfunctions of $\hat{B}$.

However, it can be shown that when an operator $\hat{A}$ has n linearly independent degenerate eigenfunctions, one can form n linear combinations that are also eigenfunctions of $\hat{B}$ (if $\hat{A}$ and $\hat{B}$ commute).

Let's apply this to a free particle in one dimension.
b) Show that the Hamiltonian of a free particle commutes with the momentum operator.

The functions cos(kx) and sin(kx) are eigenfunctions of the Hamiltionian (with energy $\frac{\hbar^2 k^2}{2m}$), but not of momentum.

c) Show that you can indeed create 2 different linear combinations of cos(kx) and sin(kx) that are eigenfunctions of $\hat{p}_x$.