Problem set Chapter 6 for werkcollege Kwantumfysica 1

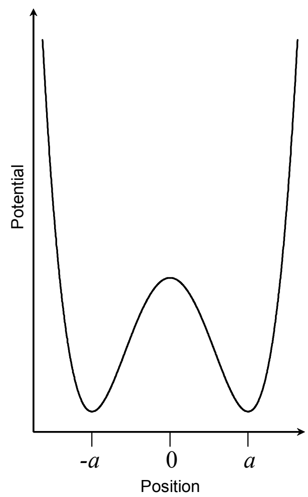
For werkcolleges in study year 2010-2011, see the schedule with detailed planning per group

During this werkcollege, first work on the problems C6.1-C6.3 (below).
Then continue with these problems from Chapter 6 in the book: 7, 11, 13, 20, 21, 23, 25, (4 as bonus)

(Homework was Chapter 6 problems: 2, 5, 8, 9, 10, 14, 15, 16, 17, 19, 22)

Problem C6.1

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 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)

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

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) 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 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 C6.2
This problem is meant to clarify the importance of symmetry and the parity operator (section 6.4 in the book). 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 $x = +a/2$. The book gives the energy eigenvalues and corresponding energy eigenstates $\varphi_n(x)$ in Eq. (6.100) on p. 179 (also section 6.4) for this system.

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.

a) $\hat{P}$ is the parity operator. Evaluate $\hat{P}\,\varphi_n(x)$ (with $\varphi_n(x)$ as in Eq. (6.100) for n = 1,2,3,4,...) 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 C6.3
Say $\varphi(x)$ is an arbitrary function. Define

$$\varphi_e(x) = \frac{\varphi(x) + \varphi(-x)}{2}$$

$$\varphi_o(x) = \frac{\varphi(x) - \varphi(-x)}{2}$$

Prove that $\varphi_e(x)$ is an even function, that $\varphi_o(x)$ is an odd function, and express $\varphi(x)$ in terms of $\varphi_e(x)$ and $\varphi_o(x)$.