Problem set for the 8th week of the course Quantum Physics 1

(version 2015-2016, still valid in later years if handed out as a print or provided on the course website)

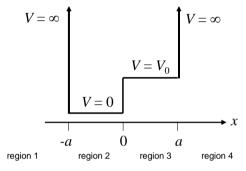
Homework, to be made before the werkcollege: From the book (Griffiths 2^{nd} Ed.) Chapter 5 - 5.15, 5.16, 5.27, 5.28, 5.31.

Problems to work on during werkcollege:

Problems W8.1 – W8.4 (this hand out, W8.4 extends 2.10 from the book), and from the book Chapter 2 - 2.33, and from Chapter 5 - (5.7 + 5.22), 5.29, 5.31, 5.32. This is the minimal set you need to do. Other good problems that we selected: from the book Chapter 5 - 5.17, 5.18, 5.19, 5.21.

Problem W8.1

In a molecule, an electron is tightly bound to the other particles in the system. In one direction, however, it is free to move a little bit from one atom to a neighboring atom. Along this direction, the electron experiences a one-dimensional potential V(x) as a function of position x. The potential V(x) can be approximated very well by the potential landscape as in the following sketch.



a) Give the Hamiltonian for this system, with the potential V(x) written out for each region along x.

b) It turns out that the energy for the ground state of this system $E_g > V_0$. Consequently, a general form for the part of the wavefunctions of the energy eigenstates in region 2 will be $\varphi_2(x) = Ae^{ik_2x} + Be^{-ik_2x}$, while for region 3 it will be $\varphi_3(x) = Ce^{ik_3x} + De^{-ik_3x}$. In regions 1 and 4 the wavefunctions will be zero. Explain why this can be assumed for regions 1, 2, 3 and 4 (see also question **c**).

c) Give expressions for k_2 and k_3 . Show how these expressions can be derived from the time-independent Schrödinger equation.

d) To find the energy eigenvalues and eigenfunctions of this system, one needs to write down equations that can be used to solve for *A*, *B*, *C* and *D*. Explain how one can define the set of equations needed to solve this problem, and give these equations (do not worry about normalization of the eigenstates yet).

e) Show that working out this problem of d) is equivalent to solving the following linear algebra problem: $\mathbf{M}\vec{v} = \vec{s}$, with

$$\mathbf{M} = \begin{pmatrix} 1 & 1 & -1 & -1 \\ ik_2 & -ik_2 & -ik_3 & ik_3 \\ e^{-ik_2a} & e^{ik_2a} & 0 & 0 \\ 0 & 0 & e^{ik_3a} & e^{-ik_3a} \end{pmatrix}, \qquad \vec{v} = \begin{pmatrix} A \\ B \\ C \\ D \end{pmatrix}, \qquad \vec{s} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

f) Use qualitative reasoning to find out what the shape is of the wavefunction for ground state and the first excited state as a function of x. Draw a sketch for these two wavefunctions, and explain your answer. Hint: consider this system as the result of two coupled particle-in-a-box systems, where the width of the tunnel barrier between the two boxes is reduced to zero, and the degeneracy of the two boxes is lifted. Also use the answer on **c**) if needed.

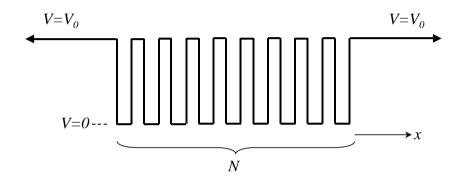
Problem W8.2

An electron is trapped in a rectangular potential well of width 1.5 nm and depth 1 eV (you can assume a one-dimensional description is valid). What are the possible frequencies of emission of this system? You can assume that none of the transitions between the energy levels is "forbidden" due to symmetry. Give the answer in Hertz.

Hint: Estimate the solutions to equation [2.156] (in Griffiths 2^{nd} Ed.) numerically, after first sketching the solution graphically (see Griffiths 2^{nd} Ed. Fig. 2.18 for an example for the *odd n* solutions).

Problem W8.3

This problem is meant to clarify the link between the *particle-in-a-box* system, and the description of electrons in solid state material as treated in a course on solid state physics. Consider a one-dimensional array of N potential wells, formed by the potential V(x) as in the following figure. The width of the wells is a, the width of the barriers between the wells is b.



a) Consider the case N = 1, with the width of that well a = 0.2 nm, and $V_0 = 3$ eV. This well contains a single particle with mass *m*. Show that for values of *m* in the range $2.86 \cdot 10^{-30}$ kg to $1.14 \cdot 10^{-29}$ kg this system has exactly 2 (and not more) bound energy eigenstates.

b) READ QUESTION c) FIRST. Consider the case N = 2. Assume that the system contains a particle with mass $m = 1.00 \cdot 10^{-29}$ (giving 2 bound energy eigenstates). For a = 0.2 nm, b = 0.1 nm and $V_0 = 3$ eV, the tunnel coupling T_0 between the ground states of the left and the right well is $T_0 = 0.1$ eV. (Note that we mean here the ground states for the case that each well is not yet coupled to another well.) Make a rough sketch of the spectrum (as a function of b) of the bound energy eigenstates for a particle in this double well system, for the range b = 0 nm to b = 10 nm. *Hint:* As a reminder, use what you found problem W4.1 (the energy eigenstates of the system with tunnel coupling show an energy splitting of $2|T_0|$), and consider how the strength of the tunnel coupling depends on b.

c) Add to the sketch of the spectrum of question b), several of the unbound energy eigenstates. Sketch only the ones with the lowest energy eigenvalues. Put labels in the sketch to point out which energy eigenvalues are bound states, and which energy eigenvalues are unbound states.

d) What is the level spacing between the unbound energy eigenvalues of question c)?

e) Now consider the case where N is a very large number. Repeat question b) for this case.

f) Give an example of a real physical situation where the model system considered in **e**) is relevant. Explain your answer.

Problem W8.4

Do exercise 2.10 form the book, and continue with:

d) Calculate explicitly the **number operator** $\hat{N} = a_{+}a_{-}$.

e) Apply \hat{N} on ψ_n and check if ψ_n is an eigenfunction of \hat{N} and what is its eigenvalue. *Hint: Don't*

use the explicit expressions for the operators \hat{a}_+ , but work with their eigenvalue equations.