Problem set for Chapters 7 and 8 for werkcollege Kwantumfysica 1

Study year 2010-2011, see also werkcollege schedule with planning per group

During this werkcollege, first work on the problems C7-8.1 - C7-8.6 (below).

Also make these problems from Chapter 7 in the book: 9, 14, 18, 24, 26, 33, 34, 35, 41, 45, 67, 68, 69, and these problems from Chapter 8 in the book: 7, 44, 45.

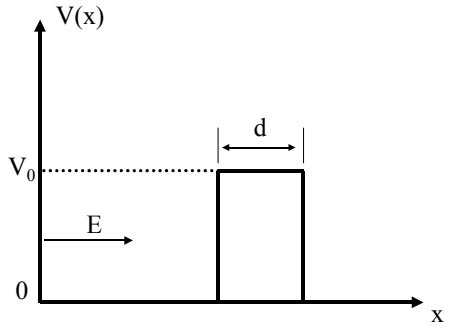
It is probably too much work for this week, so you can also work on it next week.

(Homework was from Chapter 7 problems: 1, 2, 5, 13, 23, 27, 31, 36, 38, 39, 43, 46,
and from Chapter 8 problems: 2, 3, 28, 31, 36, 39, 46, 48.)

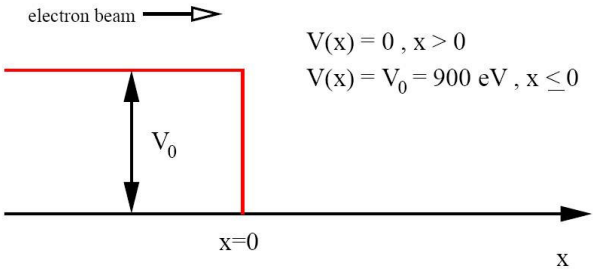
Problem C7-8.1

Particles that are incident on a step in a potential will scatter off this sudden change in the potential. In the book (p. 216 and further) this is described with the time-*independent* Schrödinger equation, while it is also described in terms of an incoming wave that is then (later) reflected or transmitted. This seems a contradiction. The justification for this method is as follows. It is assumed that the incoming wave is a wave packet with central k-value k_0, but with only a very narrow spectrum of k-values around k_0. This allows for treating the incoming and scattered wave packet as plane waves during the scatter event (solutions for the Schrödinger equation on certain sections of the x-axis). While this wave packet is scattering (say, half still coming in, half already scattered), we describe the problem with the time fixed (take a snapshot), and for this moment in time it is analyzed what part is being reflected, what and part is being transmitted. This gives a good description for how much of the wave packet is transmitted or reflected during the entire scatter event. Use this method for this problem here.

a) An electron with energy E = 1 eV is incident upon a rectangular barrier of potential energy V_0 = 2 eV (see fig). About how wide must the barrier be so that the transmission probability is 10^{-3}?



b) An electron beam with a well defined energy of E = 1000 eV is incident from x = -∞ on the potential step shown below:

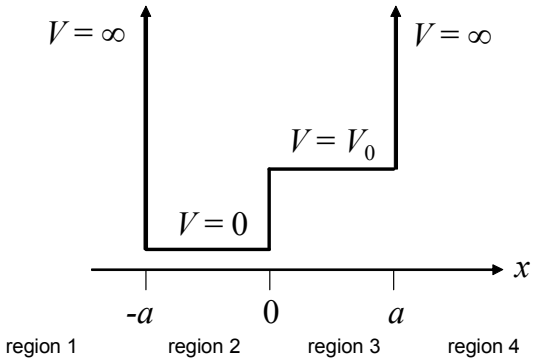


Write down the energy eigenstate (wavefunction) for an electron in this system while it is in the region with the step, and plot the real part of the wavefunction.
Use the continuity conditions on the wavefunction to determine the transmission and reflection coefficients.

c) What is the probability that a human being, running at its maximum speed, will tunnel through a door? Use the (oversimplified!) assumption that the potential for a human being inside the door while tunneling is determined by the potential energy that would be built up while jumping over the door. Calculate a number by using some estimates for the typical dimensions of doors and human beings.

Problem C7-8.2

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).

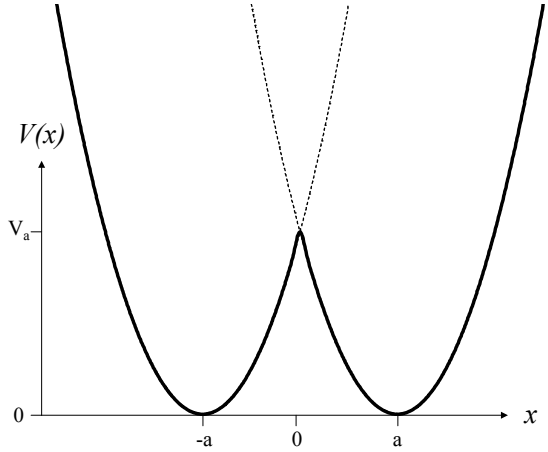
e) Show that working out this problem of **d)** is equivalent to solving the following linear algebra problem: $\mathbf{M}\vec{v} = \vec{s}$, with

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

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 W7-8.3
This problem is meant to clarify the method *Linear Combination of Atomic Orbitals* (LCAO), in section 8.7 of the book. It is an important *variational* method for finding an *approximation* for the energy eigenstates and eigenvalues of a system, for which the Hamiltonian is known, but difficult to solve exactly. The method is used a lot in solid-state physics and molecular physics.

Consider a one-dimensional system, with a single particle with mass $m = 10^{-20}$ kg, that is in the potential *V(x)* as depicted in the figure below. The particle is attracted to the positions $x=-a$ and $x=+a$ with spring-like forces $F=-K(x \pm a)$ that act over a certain range only. The potential can be very well approximated by two intersecting parabolas, symmetric around $x=0$ (harmonic potentials), that dominate the potential energy for the particle when it is either on the left or the right of the point $x=0$.



a) We like to study the low-energy eigenstates of this system. Show that the Hamiltonian of this system is in principle known. That is, find *K*, write down an expression for *V(x)* and use it for writing the Hamiltonian *H* of this system.

b) First assume that the particle is either on the left or on the right of the barrier between the wells. Find the eigenfrequency ω_0 for the harmonic-oscillator behavior that the system then would have.
Use $a=10^{-10}$ m and $V_a=8\cdot10^{-24}$ J.

c) Still assume that the particle is either on the left or on the right of the barrier between the wells . What is then the energy of the ground state? Is this then a degenerate state in the double-well system? Show that the energy of the ground state is lower than the top of the barrier (use section 7.2 in the book). Approximately how many energy eigenstates of the total system have an energy below the top of the barrier?

d) Make a sketch of the wavefunction for the states(s) that have the ground state energy of **c)** (use results from section 7.3 in the book).

e) Now we will assume that the particle *can* tunnel through the barrier, and we like to find what the energy eigenstates of the system are for this case. We will assume that the eigenstates can be approximated very well by forming linear combinations (as in section 8.7) of the harmonic-oscillator eigenstates considered under **a)-d)**. Say that the real (but still unknown to us) ground state energy of the system is now E_0, with a corresponding eigenstate $|\chi_0\rangle$. Can you already say what value E_0 has approximately as compared to your answer for **c)**?

f) Continuation on **e)**: Proof that for some arbitrary ket $|\Psi\rangle$ one always gets $\dfrac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} \geq E_0$.

g) The results of **f)** suggest that equality $\dfrac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle} = E_0$ holds only for the case $|\Psi\rangle=|\chi_0\rangle$. Here $\dfrac{\langle\Psi|\hat{H}|\Psi\rangle}{\langle\Psi|\Psi\rangle}$ has a minimum value, so $|\chi_0\rangle$ and E_0 can be approximated by a procedure that minimizes

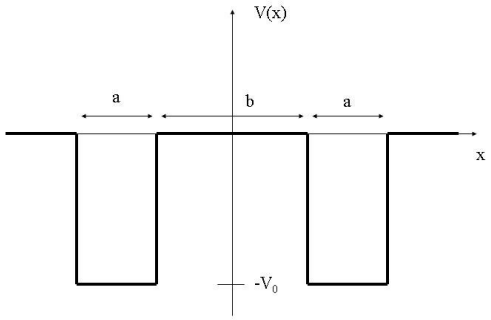
the expression with respect to some trial wavefunction for $|\chi_0\rangle$. Let's assume that $|\chi_0\rangle$ can be written as $|\chi_0\rangle = c_L|\varphi_{0,L}\rangle + c_R|\varphi_{0,L}\rangle$, where $|\varphi_{0,L}\rangle$ and $|\varphi_{0,R}\rangle$ the left and right harmonic-oscillator ground states. The minimum is characterized by $\frac{\partial\langle E\rangle}{\partial c_L} = \frac{\partial\langle E\rangle}{\partial c_R} = 0$, with $\langle E\rangle = \frac{\langle\chi_0|\hat{H}|\chi_0\rangle}{\langle\chi_0|\chi_0\rangle}$. Use this to derive Eq. (8.126) on p. 333, and write it in the matrix notation of Eq. (8.126a) (follow section 8.7 from the book, and assume all *c*'s and φ's etc. real).

h) Derive the steps from Eq. (8.126) to Eq. (8.133) later at home. Now, follow the derivation to understand the result, and sketch the wavefunction of the ground state and first excited state of the system. Does the system still have degenerate states?

i) With other methods, someone estimated for this system, *S<<1*, and $H_{LR}=8\cdot10^{-28}$ J. With what frequency does the position of the particle oscillate when it was prepared in the ground state of the right well alone?

Problem W7-8.4

Consider the potential in the figure. There is one particle in this potential, with a mass that is large enough for having several bound states in this system.



a) Discuss qualitatively and sketch the ground state and first excited state in each of the following cases: i) b=0; ii) b~a; iii) b>>a.
b) How do the energies for the ground state and the first excited state vary as b goes from 0 to infinity? Give only qualitative answer.

Problem W7-8.5

Consider two (identical) electrons confined in a single 1D infinite potential well, with walls at $x = 0$ and $x = L$. There is no Coulomb repulsion between the two electrons, so the Hamiltonian H of the system can be written as $H = H_a + H_b$, where 'a' and 'b' are used to label the electrons.
Each part of the Hamiltonian acts only on the electron a or b separately:
$H_a\,\varphi_a(x) = E_a\,\varphi_a(x)$ and $H_b\,\varphi_b(x) = E_b\,\varphi_b(x)$.
The eigenstates of H can simply be written as a product of the two one-electron functions:
$\psi(x_1, x_2) = \varphi_a(x_1)\varphi_b(x_2)$, where $\varphi_a(x_1)$ and $\varphi_b(x_2)$ are eigenfunctions of H_a and H_b, respectively, and the positions of electrons 'a' and 'b' are taken as x_1 and x_2 respectively.

- **a)** Show that the wavefunction $\psi(x_1, x_2) = \varphi_a(x_1)\varphi_b(x_2)$ is an eigenfunction of the Hamiltonian $H = H_a + H_b$. Find the expectation value for energy for this state.
- **b)** Since both electrons are identical, labeling 'a' and 'b', or positioning 'x_1' and 'x_2' has only illustrative character. Namely, if you will measure the presence of an electron at position x_1 you will not (cannot!) know whether it was electron 'a' or 'b'. In terms of quantum mechanics this means that the observables of a system with two identical particles in the same volume

cannot depend on labeling of the particles. To illustrate this, calculate the probability density (observable for position) $\psi^*(x_1, x_2)\ \psi(x_1, x_2)$. Check whether this probability density depends on the way (order) you have labeled your particles. Keep in mind that the single particle wavefunctions $\varphi_a(x_1)$ and $\varphi_b(x_2)$ in general can be, and usually are different.

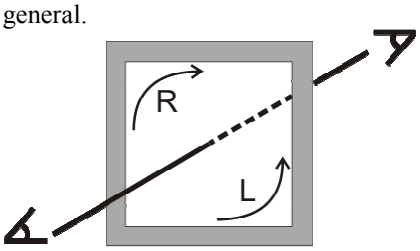
c) If for (b) you have found, that the density $\psi^*(x_1, x_2)\ \psi(x_1, x_2)$ is invariant with respect to the labeling do it again☺. Otherwise proceed with construction following wavefunctions:

$$\psi_S(x_1, x_2) = \frac{1}{\sqrt{2}} [\varphi_a(x_1)\varphi_b(x_2) + \varphi_a(x_2)\varphi_b(x_1)]$$
$$\psi_A(x_1, x_2) = \frac{1}{\sqrt{2}} [\varphi_a(x_1)\varphi_b(x_2) - \varphi_a(x_2)\varphi_b(x_1)]$$

1. Are these states normalized?
2. Find the expectation value for energy for these states. Is it the same as in question (a)?
3. Interchange the particle's labeling for both the 'A' and 'S' state. What happens with the wavefunctions. Does the labeling 'A' (anti-symmetric) and 'S' (symmetric) make sense?
4. Show that the probability densities $\psi^*_A(x_1, x_2)\ \psi_A(x_1, x_2)$ and $\psi^*_S(x_1, x_2)\ \psi_S(x_1, x_2)$ are invariant with respect to the labeling of the particles.

d) Suppose that one electron is in the ground state φ_a and that the other in the first excited state φ_b. We want to get an expression for the expectation value of d^2 in the corresponding states ψ_A and ψ_S, where d is the operator for interparticle separation, $d = x_2 - x_1$. Show that
$\langle\psi_S| d^2 |\psi_S\rangle = \langle \varphi_a| x^2 |\varphi_a\rangle + \langle \varphi_b| x^2 |\varphi_b\rangle - 2 \langle \varphi_a| x |\varphi_a\rangle \langle \varphi_b| x |\varphi_b\rangle$,
where x is the one-particle position operator (derive these results formally, do *not* evaluate any integral with sine functions, etc., only assume that you can use that the φ_n's are real).
Show that in the antisymmetric state ψ_A it is
$\langle\psi_A| d^2 |\psi_A\rangle = \langle\psi_S| d^2 |\psi_S\rangle + 2(\langle \varphi_a| x |\varphi_b \rangle)^2$.
This result implies that the probability density associated with the antisymmetric state is different from that of the symmetric state. In particular, the Pauli principle (valid for the case of the antisymmetric state) tends to separate the two electrons apart. This has nothing to do with Coulomb repulsion: it represents somehow an additional "exchange interaction" between the two electrons which has no classical analogue!

e) It is not only about identical particles and their positions, it is about undistinguishable states in general.



If you have superconducting loop you can have persistent currents which are flowing clockwise (R) or anti-clockwise (L). These are described as quantum states |R> and |L>. Imagine that you can measure the direction of the current, just by looking at this loop – this is will be your observable. Now, you can easily see that direction of the current in the loop will strongly depend whether you are looking from the 'front' or from the 'back' side on the loop (see figure), which is physically not acceptable. Construct states which will be invariant with respect to the side of view of the observable.

Problem W7-8.6
An electron is trapped in a rectangular potential well of width 15 Å and depth 1 eV. What are the possible frequencies of emission of this system? Give the answer in Hertz.
Hint: Solve the expressions (8.27) numerically or graphically to obtain ξ.