Problem set for the 7th week of the course Quantum Physics 1
For the tutorials sessions of 15 and 17 October 2014

Homework, to be made before the werkcollege:
From the book (Griffiths 2nd Ed.) Appendix chapter -   A.25.
From the book (Griffiths 2nd Ed.) Chapter 5 -   5.4, 5.8, 5.9, 5.10.

Problems to work on during werkcollege:
Problem W7.1, W7.2   (this hand out),
and from the book Chapter 5 - 5.2 (just use the results of 5.1 as listed in the problem, making 5.1 is optional), 5.5, 5.12 (W7.1 replaces 5.6). 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 5 - 5.1.

Problem W7.1
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 $H = H_1 + H_2$, where '1' and '2' are used to label the electrons.
Each part of the Hamiltonian acts only on the electron 1 or 2 separately. Since the electrons identical, and since they are confined in the same potential well, H_1 and H_2 have the same eigenvalues and eigenfunctions. For this problem consider two eigenfunctions (labeled with 'a' and 'b') that are eigenfunctions of both H_1 and H_2:
$H_i \varphi_a(x_i) = E_a \varphi_a(x_i)$ and $H_i \varphi_b(x_i) = E_b \varphi_b(x_i)$ (with $i = 1,2$).
As a starting point for describing the eigenfunctions of H, first assume that they can simply be written as a product of the two one-electron functions. For example, $\psi(x_1, x_2) = \varphi_a(x_1)\varphi_b(x_2)$ appears to be an eigenfunctions of H (it is mathematically consistent with the eigenvalue problem for H, we will later see that for identical particles we must apply an additional symmetrizing step). In this description $\varphi_a(x_1)$ and $\varphi_b(x_2)$ are eigenfunctions of H_1 and H_2, respectively. Note the label '1' in the factor $\varphi_a(x_1)$ indicates that this factor is for electron 1, while the label 'a' indicates that it is for electron 1 in eigenfunction a. Also note that x_1 and x_2 describe positions that are in fact the same space (same x-axis).

   a) Show that the wavefunction $\psi(x_1, x_2) = \varphi_a(x_1)\varphi_b(x_2)$ is an eigenfunction of the Hamiltonian $H = H_1 + H_2$ (again, note that it is only an eigenfunction if the two particles are not identical, for identical particles the eigenfunction must be made (anti-)symmetric). Find the expectation value for energy for this state.

   b) Since both electrons are identical, the labeling 'x_1' and 'x_2' has some arbitrary character. You could also use the label 2 for the electron in state a, and 1 for the electron in state b. Namely, if you will measure the presence of an electron at position x_1 you will not (cannot!) know whether it was electron '1' or '2'. 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 $\psi^*(x_1, x_2) \psi(x_1, x_2)$ (note that this should predict something that you can check by measurement in an experiment). 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 constructing the 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 (let's call it φ_a) and that the other in the first excited state (let's call it 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, $d = x_2 - x_1$.

[*Note: You may now wonder why the symmetric state ψ_S plays a role for electrons, since electrons are fermions for which you should always only consider anti-symmetric states. This is because we neglect the spin of the electrons in this problem. We only consider the* orbital *part of the quantum state of the electrons in this problem, while the full quantum state of an electron should also describe the spin. In real atoms and molecules, two electrons can be in an orbital state that is symmetric when the spins of the two electrons are in a state that is anti-symmetric. The full quantum state is then anti-symmetric, as it should be.*]
Show that

$$\langle\psi_S| d^2 |\psi_S\rangle = \langle\varphi_a| x^2 |\varphi_a\rangle + \langle\varphi_b| x^2 |\varphi_b\rangle - 2\langle\varphi_a| x |\varphi_a\rangle\langle\varphi_b| x |\varphi_b\rangle - 2 |\langle\varphi_a| x |\varphi_b\rangle|^2,$$

where x is the one-particle position operator. **Hint:** derive these results formally. Switch to x-representation when useful, but do *not* evaluate any integral with sine functions etc. Only assume that you can use that φ_a and φ_b are real.
Also show that in the antisymmetric state ψ_A it is

$$\langle\psi_A| d^2 |\psi_A\rangle = \langle\psi_S| d^2 |\psi_S\rangle + 4 |\langle\varphi_a| x |\varphi_b\rangle|^2 .$$

This result implies that the probability density associated with the antisymmetric state is different from that of the symmetric state. In particular, in the antisymmetric state the two electrons are (on average, in the sense of expectation value) a bit further apart. This has nothing to do with Coulomb repulsion or any other real force: it purely results from the fact that the actual quantum states in nature for 2 or more identical particles must be anti-symmetric for fermions and symmetric for bosons. Still, it seems to act as an additional "exchange interaction": if two electrons (fermions) are in the same spin state the orbital state must anti-symmetric, while if two bosons are in the same spin state the orbital state must symmetric. So, in this case the symmetry requirements act as if they are pushing the fermions a bit away from each other, while for bosons they act as if the bosons attracting each other a bit. This occurs even when there are no real forces between the particles. This effect has no classical analogue!

Problem W7.2

Consider again the type of system that you considered in **Problem W4.1** of week **4**. Now, however, consider that you have two identical versions of it at two different locations (two double-well potentials, each with one particle in it). One of the systems is at place P1, and the other at place P2, and the distance between these two places is much larger than the size of the double-well potential.

a) At both places, you will do a measurement with observable $\hat{A}$ (observable for position in the double-well system). What is the probability that you will get the outcome -a (particle is in the left well) for both systems, if the states of the systems at the moment just before the measurement are as follows?

  a-i) the system at P1 is in the state $|\varphi_g\rangle$ and the system at P2 is in the state $|\varphi_e\rangle$.

  a-ii) the system at P1 is in the state $|\varphi_e\rangle$ and the system at P2 is in the state $|\varphi_g\rangle$.

b) Now consider that you have again only a single double-well potential (exactly the same as before), but that this double-well potential contains two identical particles (the same type of particle as before). To describe this system, we need to label the particles from now on. We will use the indices 1 and 2 to label the particles, and the index T refers to the total system (see also this week's handout *Extra note on two-level systems, and exchange degeneracy for identical particles*).

These two particles do not interact. This means that the Hamiltonian of the total system is now

$$\hat{H}_T = \hat{H}_1 + \hat{H}_2 \ ,$$

where $\hat{H}_1$ and $\hat{H}_2$ the operators $\hat{H}$ for each particle (now in the Hilbert space with states of the two-particle system).

Assume that this total system (combined system with two particles) is prepared in a state with total energy $E_T = E_g + E_e$. Show that the following three states are all an eigenstate of $\hat{H}_T$ with energy $E_T = E_g + E_e$.

  b-i) $\left|\Psi_T\right\rangle_{C\alpha} = \left|\varphi_{g1}\right\rangle\left|\varphi_{e2}\right\rangle$

  b-ii) $\left|\Psi_T\right\rangle_{C\beta} = \left|\varphi_{e1}\right\rangle\left|\varphi_{g2}\right\rangle$

  b-iii) $\left|\Psi_T\right\rangle_{\alpha\beta} = \alpha\left|\Psi_T\right\rangle_{C\alpha} + \beta\left|\Psi_T\right\rangle_{C\beta}$ (see definitions in b-i) and b-ii))

c) It can be shown that in the case of identical particles, the only states $\left|\Psi_T\right\rangle_{\alpha\beta}$ (see definition in **b)**) that occur in nature are for $\alpha = +\frac{1}{\sqrt{2}}$ and $\beta = \pm\frac{1}{\sqrt{2}}$,

$$\left|\Psi_T\right\rangle_S = \tfrac{1}{\sqrt{2}}\left|\varphi_{g1}\right\rangle\left|\varphi_{e2}\right\rangle + \tfrac{1}{\sqrt{2}}\left|\varphi_{e1}\right\rangle\left|\varphi_{g2}\right\rangle$$
$$\left|\Psi_T\right\rangle_{AS} = \tfrac{1}{\sqrt{2}}\left|\varphi_{g1}\right\rangle\left|\varphi_{e2}\right\rangle - \tfrac{1}{\sqrt{2}}\left|\varphi_{e1}\right\rangle\left|\varphi_{g2}\right\rangle$$

Show that $\left|\Psi_T\right\rangle_S$ is symmetric and that $\left|\Psi_T\right\rangle_{AS}$ is anti-symmetric with respect to exchanging the two particles in the system.

d) We do a measurement to determine for both particles whether they are in the right well or in the left well (measurement in the sense of observable $\hat{A}$). Calculate for the following two states the probability that you will get the outcome -a for both particles.

  d-i) $\left|\Psi_T\right\rangle_S$ (see definition in **c)**).

  d-ii) $\left|\Psi_T\right\rangle_{AS}$ (see definition in **c)**).