

Exercise sheet 10  
Theoretical Physics 3 : QM SS2018  
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**Exercise 0.**

How much time did it take to complete the task?

**Exercise 1. (50 points)**

Consider a quantum system with just three linearly independent states. Suppose the Hamiltonian, in matrix form, is

$$H = V_0 \begin{pmatrix} 1 - \epsilon & 0 & 0 \\ 0 & 1 & \epsilon \\ 0 & \epsilon & 2 \end{pmatrix},$$

where  $V_0$  is a constant, and  $\epsilon$  is some small number ( $\epsilon \ll 1$ ).

- a) (5 p.) Write down the eigenvectors and eigenvalues of the unperturbed Hamiltonian ( $\epsilon = 0$ ).
- b) (10 p.) Solve for the exact eigenvalues of  $H$ . Expand each of them as power series in  $\epsilon$ , up to second order.
- c) (20 p.) Use first- and second-order nondegenerate perturbation theory to find the approximate eigenvalue for the state that grows out of the nondegenerate eigenvector of  $H^0$ . Compare with the exact result from b).
- d) (15 p.) Use degenerate perturbation theory to find the first-order correction to the two initially degenerate eigenvalues. Compare with the exact results.

**Exercise 2. The Helium Atom (50 points)**

In this exercise we will compute the energy of the ground state of the Helium atom using the perturbation theory, step by step. The Helium atom can be considered as a system with two electrons orbiting around a nucleus of charge  $+2e$  ( $e$  the absolute value of the charge of the electron). The wave function which describes the state of the system in coordinate space is, thus, a function which depends on both coordinates of the two electrons  $\vec{r}_1$  and  $\vec{r}_2$ :  $\Psi(\vec{r}_1, \vec{r}_2)$ .

- a) (10 p.) Considering the Coulomb interaction between the electrons and the nucleus, as well as between the electrons (a repulsion term), write down the Hamiltonian for the system.
- b) (10 p.) If we neglect the repulsion term, the problem decomposes into independent Hydrogen atom problems with a nuclear charge of  $+2e$  instead of  $+e$ . Find the ground state wave function for the Helium atom in that approximation and show that the corresponding energy is  $E_{\text{He}}^{\text{g.s.}} \approx -109$  eV.

- c) (30 p.) The result for the energy in that approximation is quite off the experimental measurement of  $-79$  eV. To improve our computation we can apply the perturbation theory technique. Compute the first-order correction to the energy of the ground state

$$E_{ee} = \langle \Psi_{\text{He}}^{\text{g.s.}} | H' | \Psi_{\text{He}}^{\text{g.s.}} \rangle$$

with the repulsion term  $H' = \frac{1}{4\pi\epsilon_0} \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$ . Compare the corrected result to the experimental value.

*Hints for c):*

- 1) Write down the integral in spherical coordinates and reduce it to

$$E_{ee} = \frac{64}{a^6} \frac{8e^2}{4\pi\epsilon_0} \int dr_1 r_1 e^{-4r_1/a} \int dr_2 r_2 e^{-4r_2/a} ((r_1 + r_2) - |r_1 - r_2|),$$

where  $a$  is the Bohr radius.

- 2) Solve the integral by taking care of the cases  $r_1 > r_2$  and  $r_2 > r_1$ , to finally obtain the result of

$$E_{ee} = \frac{e^2}{4\pi\epsilon_0} \frac{5}{4a}.$$

- 3) Substitute the numerical values and write down the corrected ground state energy in eV.