Exercise sheet 10
Theoretical Physics 3 : QM WS2020/2021
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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 ϵ 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 ϵ, 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 $H' = \frac{1}{4\pi\varepsilon_0} \frac{e^2}{|\vec{r}_1 - \vec{r}_2|}$. Compare the corrected result to the experimental value.

Hints for c):

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

$$E_{ee} = \frac{64}{a^6}\frac{8e^2}{4\pi\varepsilon_0}\int \mathrm{d}r_1 r_1 e^{-4r_1/a}\int \mathrm{d}r_2 r_2 e^{-4r_2/a}\left((r_1+r_2)-|r_1-r_2|\right),$$

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

$$E_{ee} = \frac{e^2}{4\pi\varepsilon_0}\frac{5}{4a}.$$

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