Exercise sheet 11
Theoretical Physics 3: QM WS2023/2024

24.01.2024

Exercise 0.

How much time did you take to complete this homework sheet?

Exercise 1. Degenerate Perturbation Theory (50 points)

Consider a quantum system with just three linearly independent states. Assume 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 non-degenerate perturbation theory to find the approximate eigenvalue for the state that grows out of the non-degenerate 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 (35 points + 20 Bonus)

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) *(15 p. + 20 Bonus)* 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:

1) *(15 p.)* 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) *(15 p.) (Bonus)* 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) *(5 p.) (Bonus)* Substitute the numerical values and write down the corrected ground state energy in eV.

Spherically symmetric Hamiltonian (15 points)

Assume a spherically symmetric non-relativistic Hamiltonian given as $H = \frac{p^2}{2m} + V(r)$.

a) *(10 p.)* Show that $[H, L_z] = 0$.

b) *(5 p.)* Show that $[H, L^2] = 0$.

Hint: Use the differential form of the operators and express the kinetic energy in terms of r and L^2.