Quantum Mechanics II — Problem Sheet 4

Problem 9: Variational Principle (8 points)

a) Consider a Hamilton operator $\hat{H}$ with an orthonormal basis $|n\rangle$ fulfilling the eigenvalue problem

$$\hat{H}|n\rangle = E_n|n\rangle \, . \tag{1}$$

Let $|\psi\rangle$ be a general state. Show that one can then find an upper bound for the ground-state energy in the form of the inequality

$$E_0 \leq \frac{\langle\psi|\hat{H}|\psi\rangle}{\langle\psi|\psi\rangle} \, . \tag{2}$$

b) Assume now that the state $|\psi(\alpha)\rangle$ is a function of some parameter α. Then the inequality

$$E_0(\alpha) \leq \frac{\langle\psi(\alpha)|\hat{H}|\psi(\alpha)\rangle}{\langle\psi(\alpha)|\psi(\alpha)\rangle} \tag{3}$$

defines according to **a)** for any α an upper bound for the ground-state energy. How could you determine the optimal upper bound?

c) Use this variational method to evaluate approximately the ground-state energy of a quartic oscillator, i.e. a particle of mass M subject to the potential $V(x) = gx^4$ with $g > 0$. Use for this purpose a Gaussian trial function $\psi(x) = e^{-\alpha x^2}$. Due to dimensional reasons the ground-state energy must be of the form

$$E_0 = c \left(\frac{g\hbar^4}{M^2}\right)^{1/3} \, . \tag{4}$$

Which value do you get for c? Which error do you have in comparison with the exact result $c = 0.667986\ldots$?

Problem 10: Ground State of Helium (16 points)

The Helium atom consists of $Z = 2$ electrons moving around a nucleus, which consists of two protons and two neutrons. The Hamilton operator for the eletrons of the Helium atom $\hat{H} = \hat{H}_0 + \hat{V}$ decomposes into a contribution of two free electrons

$$\hat{H}_0 = -\frac{\hbar^2}{2M}\left(\Delta_1 + \Delta_2\right) - \frac{Ze^2}{4\pi\varepsilon_0|\mathbf{r}_1|} - \frac{Ze^2}{4\pi\varepsilon_0|\mathbf{r}_2|} \tag{5}$$

and a repulsive Coulomb interaction

$$\hat{V} = \frac{e^2}{4\pi\varepsilon_0|\mathbf{r}_{12}|} \, , \tag{6}$$

where $\mathbf{r}_{12} = \mathbf{r}_1 - \mathbf{r}_2$ denotes the relative position of both electrons.

a) The ground-state wave function of $\hat{H}_0$ of the hydrogen-like Helium atom is given by

$$\psi(\mathbf{r}_1, \mathbf{r}_2) = \frac{Z^3}{\pi a_\mathrm{B}^3} \exp\left[-\frac{Z\left(|\mathbf{r}_1| + |\mathbf{r}_2|\right)}{a_\mathrm{B}}\right] . \tag{7}$$

Determine the value of the corresponding ground-state energy E_0.

b) Calculate within first-order perturbation theory how the repulsive Coulomb interaction (6) changes the ground-state energy.

c) An even better approximation is obtained by applying the variational method from **problem 9**. Use as trial functions again (7), however consider now Z as a paramter to be determined by minimizing the function

$$E(Z) = \int d^3r_1 \int d^3r_2 \, \psi(\mathbf{r}_1, \mathbf{r}_2) \hat{H} \psi(\mathbf{r}_1, \mathbf{r}_2) \, . \tag{8}$$

Compare your variational result with **a)**, **b)**, and the experimental value $-78.98\,\text{eV}$.

d) Interpret physically the optimal value for the variational parameter $Z_{\text{opt.}}$ by comparing it with the value $Z = 2$ for the Helium atom.

Drop the solutions in the post box on the 5th floor of building 46 or, in case of illness/quarantine, send them via email to jkrauss@rhrk.uni-kl.de until November 21 at 12.00.