

TFY4205 Quantum Mechanics II

NTNU

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Problem 1 (time independent perturbation theory)

The nuclei of for instance hydrogen and deuterium are not point charges, but have a finite extent. We are interested in an estimate of the effect of this finite extent of the nuclei on the electronic states. Let us assume that the nucleus can be modelled as an evenly charged sphere with radius R that ultimately gives rise to the following potential for the electron:

$$V(r) = \begin{cases} -\frac{Ze^2}{4\pi\epsilon_0 r} & \text{for } r \geq R \\ -\frac{Ze^2}{4\pi\epsilon_0 R} \left(\frac{3}{2} - \frac{r^2}{2R^2} \right) & \text{for } r \leq R \end{cases}$$

Within the radius R , this potential differs from the electrostatic potential from a point charge. Consider this difference as a perturbation and compute the first order correction to the ground state energy.

To solve this, you may use that the ground state in the Coulomb potential is $\psi(r) = (\pi a^3)^{-1/2} e^{-r/a}$, but for $r \leq R$ it is sufficient to use the approximation $\psi \simeq (\pi a^3)^{-1/2}$ since $R \ll a$. The unperturbed ground state energy is $E_1^0 = -\frac{Ze^2}{8\pi\epsilon_0 a} = -13.6Z^2 \text{ eV}$.

Express the first order correction in terms of E_1^0 , a , and R . Comment on the sign of the correction and how the correction varies with nuclear charge Z . For hydrogen, we have $R \simeq 10^{-15} \text{ m}$ and $a = a_0 = 0.53 \times 10^{-10} \text{ m}$. What is the order of magnitude of the correction measured in eV?

Problem 2 (variational method)

Use the variational method with two different trial functions:

- $f(x) = e^{-\lambda x^2}$
- $f(x) = e^{-\lambda|x|}$

to compute the approximate ground state energy for a particle with mass m in the delta-function potential $V(x) = -\alpha\delta(x)$.

Problem 3 (variational method)

Use the variational method with the trial function $f(z) = ze^{-\frac{1}{2}\alpha z^2}$ when $z \geq 0$ and $f(z) = 0$ when $z < 0$ to find an approximate expression for the ground state energy E_0 in a triangular potential. This potential has the form $V(z) = Fz$ when $z \geq 0$ and $V(z) \rightarrow \infty$ when $z < 0$.

In order to avoid too many mathematical manipulations, you may make use of this integral:

$$I_n = \int_0^\infty z^n e^{-\alpha z^2} dz = c_n \alpha^{-(n+1)/2} \quad (1)$$

where the number c_n is:

- $c_0 = \frac{1}{2}\sqrt{\pi}$
- $c_1 = \frac{1}{2}$
- $c_2 = \frac{1}{4}\sqrt{\pi}$
- $c_3 = \frac{1}{2}$
- $c_4 = \frac{3}{8}\sqrt{\pi}$
- $c_5 = 1$
- $c_6 = \frac{15}{16}\sqrt{\pi}$
- $c_7 = 3$