Quantum Chemistry
Seminar 3

Hydrogen atom

Exercise 1 (unassigned)

Derive the form of the classical Hamilton function for the hydrogen atom in the center-of-mass (CMS) system.

(Hint: Find the CMS form of the Lagrange function, $L(\dot{\vec{r}}_\mathrm{p}, \dot{\vec{r}}_\mathrm{e}, \vec{r}_\mathrm{p}, \vec{r}_\mathrm{e}) = \frac{1}{2} m_\mathrm{p} \dot{\vec{r}}_\mathrm{p}^2 + \frac{1}{2} m_\mathrm{e} \dot{\vec{r}}_\mathrm{e}^2 - \left(-\frac{e^2}{4\pi\varepsilon_0} \frac{1}{\|\vec{r}_\mathrm{p} - \vec{r}_\mathrm{e}\|}\right)$, first, and then transform it to the Hamilton function.)

Exercise 2 (unassigned)

Prove the following commutation relations, $[\Delta, \hat{L}^2] = 0$, $[\Delta, \hat{L}_z] = 0$. (Hint: Use the operators expressed in the spherical coordinates; see lesson 2, page 5, and lesson 3, page 8.)

Exercise 3 (unassigned)

Derive the „boundary" condition $\int_0^{+\infty} r^2\, R_{kl}^2(r) \mathrm{d}r < +\infty$ by supposing that $\int_0^{\pi} \int_0^{2\pi} |Y_{lm}(\theta, \phi)|^2 \sin\theta \,\mathrm{d}\theta \mathrm{d}\phi = 1$.

Exercise 4 (Anila)

Derive the equation for $\chi_{kl}(r)$ (lesson 3, page 11) from related equation obtained for $R_{kl}(r)$ (lesson 3, page 10).

Exercise 5 (Shamal)

Write down the formulas (without normalization constants) for $\Psi_{nlm}(r, \theta, \phi)$ for $n = 1, 2$ and 3 (lesson3, page 13).