Advanced Quantum Theory
WS 11/12

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Problem Set 7 (due 29.11.2011)

Questions

(Q1) What are the differences between the Hartree-Fock method and the Kohn-Sham approach?

(Q2) Which element has the highest, which one has the lowest ionization potential, and why?

(Q3) Why are M_L and M_S *no* good quantum numbers anymore when spin-orbit coupling is taken into account, while L and S *are*?

(7.1) Thomas-Fermi *(3 points)*

Show that for $x \to \infty$ the Thomas-Fermi function becomes $\chi(x) = 144/x^3$. Use this result to prove that the asymptotic behavior of the Thomas-Fermi density $\rho(r)$ is $\sim r^{-6}$. *Instead, how should the correct asymptotic behavior be?

(7.2) An inverse problem à la DFT *(1 point)*

Let $\rho(x)$ be the density of a one-dimensional single-particle problem. Derive a potential $V(x)$ such that $\rho(x)$ is the ground state density in this potential.

(7.3) Variational calculus to determine a Kohn-Sham potential *(1 point)*

Given the functional of the density $\rho(\boldsymbol{r})$,

$$E_{\mathrm{x}}[\rho(\boldsymbol{r})] = A_{\mathrm{x}} \int \rho(\boldsymbol{r})^{4/3}\,\mathrm{d}^3 r, \tag{1}$$

with A_{x} a constant, calculate the functional derivative $V_{\mathrm{x}}[\rho(\boldsymbol{r})] = \frac{\delta E_{\mathrm{x}}}{\delta \rho}$.

(7.4) Hellmann-Feynman and the Virial Theorem *(5 points)*

(i) Let a Hamiltonian $\hat{H}_\lambda$ and the corresponding normalized eigenfunctions ψ_λ depend on a parameter λ. Prove the *Hellmann-Feynman* theorem

$$\frac{\mathrm{d}E_\lambda}{\mathrm{d}\lambda} = \langle \psi_\lambda | \frac{\partial \hat{H}_\lambda}{\partial \lambda} | \psi_\lambda \rangle \tag{2}$$

where $E_\lambda = \langle \psi_\lambda | \hat{H}_\lambda | \psi_\lambda \rangle$.

(ii) Let $\psi(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N)$ be a normalized eigenfunction of a Hamiltonian $\hat{H} = \hat{T} + \hat{V}$. Let $\hat{V}$ be *homogeneous of degree* n, that is,

$$V(\gamma \boldsymbol{r}_1, \ldots, \gamma \boldsymbol{r}_N) = \gamma^n V(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_N). \tag{3}$$

Show that

$$2\langle \psi | \hat{T} | \psi \rangle - n \langle \psi | \hat{V} | \psi \rangle = 0 \tag{4}$$

(*Virial Theorem*).