Advanced Quantum Theory
WS 12/13

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Problem Set 6 (due Monday, 26.11.2012 in the lecture)

Questions

(Q1) What is the essential assumption on which Thomas-Fermi theory is based?

(Q2) What is the difference between Hartree-Fock and density functional theory?

(Q3) What are the statements of the Hohenberg-Kohn theorem?

(Q4) What is the essential idea behind the Kohn-Sham scheme?

(6.1) Single-particle density *(2 points)*

Using the notation introduced in the lecture, show that the single-particle density

$$\rho(\boldsymbol{r}) = \sum_{i=1}^{N} \sum_{m_s} |\psi_i(\boldsymbol{r}, m_s)|^2 \tag{1}$$

can be written as

$$\rho(\boldsymbol{r}) = \langle \Psi | \sum_{i=1}^{N} \delta(\boldsymbol{r}\hat{1} - \hat{\boldsymbol{r}}_i) | \Psi \rangle. \tag{2}$$

(6.2) Hartree-Fock for He *(2 points)*

Write down the Hartree-Fock equation for the spatial ground state orbital $\psi_{1s}(r)$ of helium. Does it differ from the corresponding Hartree equation?

(6.3) 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?

(6.4) An example for non-v-representability *(3 points)*

Let $\rho(x)$ be the density of a one-dimensional single-particle problem.

(i) Derive the potential $V(x)$ in which $\rho(x)$ is the ground state density.
Hint: Solve the Schrödinger equation for $V(x)$.

(ii) Show that densities which for $|x| \to 0$ behave like $\rho(x) = (a + b|x|^{\alpha+1/2})^2$ with $a, b > 0$ and $0 \leq \alpha < 1/2$ are not "v-representable" because of a diverging potential energy $\int \mathrm{d}x\, V(x)\rho(x)$.