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Problem Set 7 (due Monday, 02.12.2013 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?

(7.1) the "exponential wall" *(2 points)*

Assume you wrote a code that is able to find the ground state of atomic hydrogen within one second total CPU time. The wavefunction in your code is represented on a cleverly chosen, discrete grid of only $N_\mathrm{H} = 10$ grid points. The run time of your code scales linearly with N_H, that is, on a doubled grid it takes two seconds to find the (perhaps more accurate) ground state.

Estimate lower limits for the CPU times and the required storage capacities an extended code based on the same numerical algorithm would consume to determine the ground state of copper by

(a) solving the full many-electron Schrödinger equation,

(b) solving the corresponding Hartree-Fock equation.

(7.2) thomas-fermi *(5 points)*

(a) Starting from $\int \mathrm{d}^3r\, \rho(\boldsymbol{r}) \stackrel{!}{=} N$, show that

$$Z \int_0^{x_0} [\chi(x)]^{3/2} \sqrt{x}\, \mathrm{d}x = N,$$

where $\chi(x)$ is the Thomas-Fermi function introduced in the lecture, Z is the nuclear charge number, N is the number of electrons, and x_0 is the zero of $\chi(x)$.

(b) 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?

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(7.3) AN EXAMPLE FOR NON-v-REPRESENTABILITY *(3 points)*

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

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

(b) 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 $\int \mathrm{d}x\, V(x)\rho(x)$.