Introduction to Density Functional Theory (SS 2008)

Dozent: E.K.U. Gross, Freie Universität Berlin

Problem set No. 2

Hand out : Tuesday 22 April 2008
Hand in : Friday 2 May 2008

1. Functional derivative: The Hartree energy and the Hartree potential

Given the density functional (Hartree energy):

$$U[\rho] = \frac{1}{2}\int d^3r \int d^3r' \frac{\rho(\vec{r})\ \rho(\vec{r'})}{|\vec{r}-\vec{r'}|} \tag{1}$$

prove that:

$$\frac{\delta U[\rho]}{\delta\rho(\vec{r})} = \int d^3r' \frac{\rho(\vec{r'})}{|\vec{r}-\vec{r'}|} \tag{2}$$

(Hartree potential). (2 points)

2. Universal functional: A comment

Let $V[\rho](\vec{r})$ be the potential which, by virtue of the Hohenberg-Kohn theorem, uniquely corresponds to a given ground state (GS) density $\rho(\vec{r})$. Consider the functional:

$$E[\rho] = <\psi[\rho]|\ \hat{T} + \hat{W} + \hat{V}[\rho]\ |\psi[\rho]> \tag{3}$$

where $\psi[\rho]$ is the GS wavefunction which uniquely corresponds to $\rho(\vec{r})$ (for potentials leading to non degenerate states). What is the meaning of the functional in Eq. (3)? Does it have a minimum? Write a comment on that issue. (2 points)

3. Bose-Einstein condensate

A Bose-Einstein condensate of N particles is characterized by the fact that all N particles are in the same state $\varphi(\vec{r})$.
(a) Express the total kinetic energy of the system as a functional of the

density for the case that $\varphi(\vec{r})$ is real-valued. (3 points)
(b) Show that for complex-valued $\varphi(\vec{r})$ the total kinetic energy can be expressed as a functional of the density *and* of the current density. The current density, for a system of N particles occupying orbitals $\varphi_j, (j = 1, \ldots, N)$, is defined as:

$$\vec{j}(\vec{r}) = \frac{1}{2i} \sum_{j=1}^{N} \left[\varphi_j^*(\vec{r}) \nabla \varphi_j(\vec{r}) - \varphi_j(\vec{r}) \nabla \varphi_j^*(\vec{r}) \right]. \tag{4}$$

(3 points)