February 16, 2015

PHY 752 – Problem Set #14

Read Chapter 10 in **Marder**

1. This problem involves finding the functional form of an exchange potential by evaluating the functional derivative of the exchange energy expression with respect to the density. In class we noted that for

$$E_{xc} = \int d^3r f(n(\mathbf{r}, |\nabla n(\mathbf{r})|),$$

the corresponding potential is given by

$$V_{xc}(r) = \frac{\partial f(n(\mathbf{r}, |\nabla n(\mathbf{r})|)}{\partial n} - \nabla \cdot \left(\frac{\partial f(n(\mathbf{r}), |\nabla n(\mathbf{r})|)}{\partial |\nabla n|} \frac{\nabla n}{|\nabla n|} \right).$$

Suppose

$$f(n(\mathbf{r}, |\nabla n(\mathbf{r})|) = -\frac{3e^2}{4\pi} \left(3\pi^2\right)^{1/3} (n(\mathbf{r}))^{4/3} \left(1 + \beta |\nabla n(\mathbf{r})|^2\right).$$

Here β represents a given constant. Also suppose that the system is spherically symmetric so that $n(\mathbf{r}) = n(r)$. Find the expression for $V_{xc}(r)$ in terms of $n(r)$ and its radial derivatives.

Note that the PBE-GGA form of the exchange contribution (*Phys. Rev. Lett.* **77** 3865-3868 (1996)) is somewhat more complicated than in this homework.