Theoretical Concepts and Simulations for Materials Scientists Summer term 2009

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Exercises 4

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1. Calculate the Laplacian of the scalar isotropic field $\varphi(\mathbf{r}) = \varphi(|\mathbf{r}|)$, i.e. calculate

$$\nabla^2 \varphi(|\mathbf{r}|) \,.$$

2. Thomas-Fermi screening

   Consider the homogeneous electron gas, where the ionic charge density is smeared out to give a positive background neutralizing the electronic charge density and where, by construction, Thomas-Fermi theory is exact. In this case, the total potential seen by the electrons like the electron density itself is a constant

$$v_{eff}(\mathbf{r}) = v_{ext}(\mathbf{r}) + v_H(\mathbf{r}) \stackrel{!}{=} v_{eff} \quad .$$

   Note that the ionic and the Hartree potential themselves are not constant, since they must obey the respective Poisson equation and thus have a constant Laplacian derivative. Write down the Thomas-Fermi equation for this system.

   Next place into this ensemble a small test charge δZ at $\mathbf{r} = \mathbf{0}$. It will generate an external potential

$$\delta v_{ext}(\mathbf{r}) = -\delta \frac{Z}{|\mathbf{r}|} \quad ,$$

   which adds to the ionic potential. Formulate the Thomas-Fermi equation for the combined system and derive an effective equation for the additional potential for $\mathbf{r}$ being far away from the test charge, where this potential is small. Solve this equation and relate the screening parameter entering the additional potential to the Bohr radius.