HOMEWORK SET 01

ÚFV/ACMM/20 – Atomistic Computer Modeling of Materials
lecture by Martin Gmitra
Summer Semester 2020/2021

1. [*1 point*] Show that kinetic energy is of order of the Hartree energy $E_{\mathrm{Hartree}} = e^2/4\pi\varepsilon_0 a_0$. Hint: use Bohr's model of atom (semi-classical argument) and that electron trajectories are quantized as $m_e e a_0 = \hbar$.

2. [*1 point*] Show that time independent Schrödinger equation for the He atom (two electrons and $Z = 2$) in clamped nuclei approximation is given by
$$\left[-\frac{1}{2}\left(\nabla_1^2 + \nabla_2^2\right) - 2\left(\frac{1}{|\mathbf{r}_1|} + \frac{1}{|\mathbf{r}_2|}\right) + \frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|}\right]\Psi(\mathbf{r}_1, \mathbf{r}_2) = E\Psi(\mathbf{r}_1, \mathbf{r}_2).$$

3. [*1 point*] Investigate electronic ground state of the He atom using Schrödinger equation in task 2 neglecting Coulomb interaction between the electrons and consider approximation of independent electrons, where the wavefunction is given in the product form $\Psi(\mathbf{r}_1, \mathbf{r}_2) = \phi_{1s}(\mathbf{r}_1)\phi_{1s}(\mathbf{r}_2)$. Using the fact that for the hydrogenic atom $\phi_{1s}(\mathbf{r}) = \dfrac{Z^{3/2}}{\sqrt{\pi}} \exp(-Z|\mathbf{r}|)$ and $E_{1s} = -Z^2/2$ show that the total energy of the He atom is $E = -4\,\mathrm{Ha}$.

4. [*1 point*] Show by using $\psi(\mathbf{r}_1, \mathbf{r}_2) = \dfrac{1}{\sqrt{2}}[\phi_1(\mathbf{r}_1)\phi_2(\mathbf{r}_2) - \phi_1(\mathbf{r}_2)\phi_2(\mathbf{r}_1)]$ that if the two solutions of the single-particle Schrödinger equation are such $\int \phi_1^*(\mathbf{r})\phi_2(\mathbf{r})\mathrm{d}\mathbf{r} = 0$ then the electron charge density $n(\mathbf{r}) = |\phi_1(\mathbf{r})|^2 + |\phi_2(\mathbf{r})|^2$.

5. [*1 point*] Show that ground state electron density $n(\mathbf{r})$ of the He atom is given by $n(\mathbf{r}) = (16/\pi)\exp(-4|\mathbf{r}|)$. Hint: *Use approximations as in the task 3.*

6. [*1 point*] Refine the ground state of the Helium atom by including the Coulomb repulsion interaction between the electrons within the mean-field approximation. Show that the Hartree potential is equal to $V_{\mathrm{H}} = (2/r)[1 - (1 + 2r)\exp(-4r)]$. Hint: *Use for the radial part of the Laplace operator* $\nabla^2 = \dfrac{1}{r^2}\dfrac{\partial}{\partial r}\left[r^2 \dfrac{\partial}{\partial r}\right]$, *and for density* $n(\mathbf{r}) = (16/\pi)\exp(-4|\mathbf{r}|)$.