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Calculation of the electronic structure in the field of a homogeneously charged core of a large radius.

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Abstract. Calculation of the electronic density and potential distribution in the field of a homogeneously charged core of a large radius are reviewed. The Hartree-Fock self-consistent field method and the density-functional method are applied for the problem. These methods are compared with simple model where not interacting electrons are in spherical potential well with infinite border. The applicability of model with infinite potential well is discussed.

1. Introduction

For modeling small gas bubbles with number of electrons up to $N = 10^8$ very simple model of spherical potential well with infinite border is used, where electrons do not interact with each other. The distribution of electron density and potential looks similar to distribution in small metal particles described, for example in [1], where calculations were made using spherical jellium-background model (SJBM). But computations for metal particles were made only for number of electrons up to 6000 [2]. The model of potential well with infinite border is very rough and may not describe behavior of electrons correctly. So these two models should be compared for large number of electrons.

2. Methods

In the case of spherically symmetrical potential we can separate radial part of wavefunction. Core potential has a simple form:

$$V_{core}(r) = -N \begin{cases} \frac{1}{2R}\left(3 - \left(\frac{r}{R}\right)^2\right), & r \le R \\ 1/r, & r > R \end{cases}$$

Equations for the radial part of the wave functions are obtained for closed-shell clusters, so electron distribution also will have spherical symmetry. Three methods were applied for this problem:

1. Hartree-Fock method without exchange-correlation part, in this case equations are homogeneous:

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} + V_{core}(r) + V_{nl}(r) + \frac{l(l+1)}{2r^2}\right) P_{nl}(r) = E_{nl} P_{nl}(r)$$

$$V_{nl}(r) = \int_0^\infty \frac{\left(\sum_{n_i l_i} 2(2l_i+1)P^2_{n_i l_i}(s)\right) - P^2_{nl}(s)}{\max(r,s)} ds$$

2. Density functional theory (DFT:) using Kohn-Sham scheme:

$$\left(-\frac{1}{2}\frac{d^2}{dr^2} + V_{es}(r;\rho(r)) + V_{xc}(r;\rho(r)) + \frac{l(l+1)}{2r^2}\right) P_{nl}(r) = E_{nl}P_{nl}(r)$$

where $\rho(r)$ is electron density, $V_{es}(r;\rho(r))$ is the electrostatic potential and $V_{xc}(r;\rho(r))$ is the exchange-correlation potential taken in local-density approximation (LDA) [3].

$$V_{es}(r;\rho(r)) = \frac{1}{R}\left(\int_0^r 4\pi s^2 \rho(s) ds\right) + \int_r^{+\infty} 4\pi s \rho(s) ds$$

$$V_{xc} = -1.222/r_s(r) - 0.0666\ln\left(11.4/r_s(r)\right), r_s(r) = \left[3/4\pi\rho(r)\right]^{1/3}$$

3. Infinite spherical potential well model, which has analytical automodel solution depending on radius of potential well R:

$$P_{nl}(r) = R^{-3/2} C_{nl} r j_{l+1/2}(x_{nl} r/R)$$

where x_{nl} is a nth zero of spherical Bessel functions of 1st kind $j_{l+1/2}(x)$. In this case radius R should be a little different from core radius, because electron density is zero on the infinite border and in the other methods is not. So we should choose R value more than core radius for better accordance with other methods.

3. Results

Calculations were made for metal particles with radius $R = r_s N^{1/3}$, where the r_s is the Wigner-Seitz radius. There was used value of $r_s = 4.0 a.u.$ for Na. Results for $N = 198$, $N = 890$ and $N = 5006$ electrons are shown in figure 1, figure 2 and figure 3.

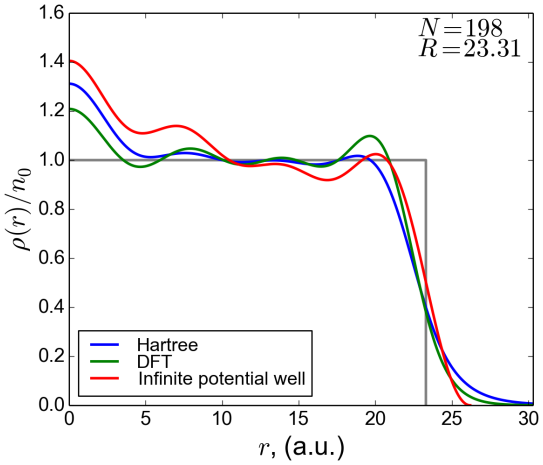

Figure 1. Electron density for $N = 198$ divided by constant density of positive ions $n_0 = 3/(4\pi r_s^3)$

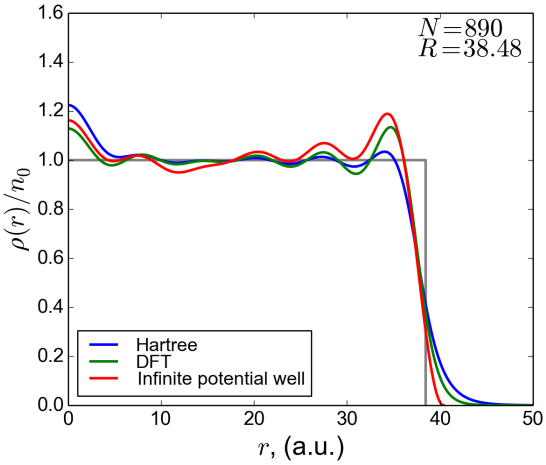

Figure 2. The same for $N = 890$ electrons

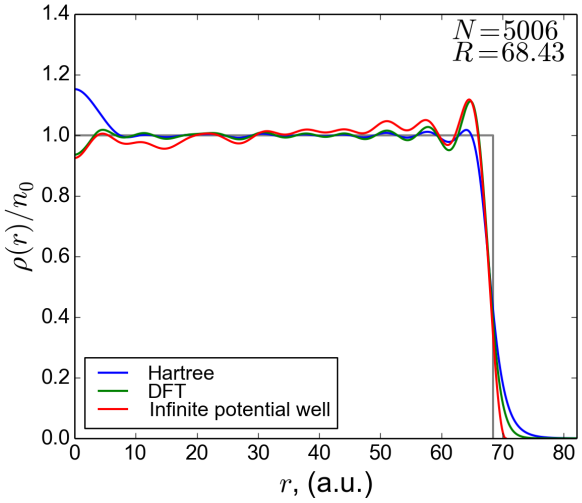

Figure 3. Electron density for 5006 electrons divided by constant density of positive ions $n_0 = 3/(4\pi r_s^3)$

As we can see a behavior of electron density looks not very similar for small number of electrons, but for more electrons such different models like DFT and infinite potential well show good agreement with each other. Electron density has the same oscillations in different methods. Also level structures given by method which uses density functional theory and given by infinite potential well model are almost the same.

4. Conclusion

The infinite potential well model can be very good approximation for structures with a large number of electrons, a comparison with more precise methods like Hartree-Fock with exchange interaction and for bigger number of electrons up to $N = 10^6$ is needed. But computations with complicated methods could be very difficult for these values.

5. Acknowledgments

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