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Some notes on real-space technique in density functional theory

The results of the analysis of the application of the real-space mesh technique ([1], [2]) in density-functional calculations will be presented. Kohn and Sham [3] developed the practical tool for realistic electronic structure computation on a vast array of atoms, their starting point being Hohenberg–Kohn [4] theorems of density functional theory.

The Kohn–Sham self-consistent eigenvalue equations for electronic structure can be written as follows (in atomic units):

$$\Big(-\frac{1}{2}\nabla^2 + v_{\text{eff}}(r)\Big)\psi_i(r) = \varepsilon_i\psi_i(r) \tag{1}$$

where

$$v_{\text{eff}}(r) = v_{\text{es}}(r) + v_{\text{xc}}\big([\rho(r)] : r\big)$$

$$\rho(r) = 2\sum_{i=1}^{N_e/2} |\psi_i(r)|^2$$

v_{eff} is the density dependent effective potential; $v_{\text{es}}(r)$ is the classical electrostatic potential, which can be obtained by numerical solution of the Poisson equation

$$\nabla^2 v_{\text{es}}(r) = -4\pi\rho_{\text{tot}}(r) \tag{2}$$

$v_{\text{xc}}\big([\rho(r)] : r\big)$ is the exact exchange-correlation potential and is the total charge density due to electrons and nuclei.

The presentation will focus on the following issues:

- multiscale solvers will be compared with the most efficient available plane-wave techniques in terms of the number of self-consistency steps required to reach the ground state;
- the Poisson–Boltzmann solvers and computation of the free energies will be discussed;
- application to the analysis of the AOP (all optical poling) processes will be presented;
- results of the analysis of the numerical convergence with respect to grid spacing, domain size and order of the representation will be presented.

Literatura

[1] T. L. Beck, Rev. Mod. Phys. 72, 1041.
[2] P. Wesseling, *An Introduction to Multigrid Methods*, Wiley, 2004.
[3] P. Hohenberg and W. Kohn, Phys. Rev. 136, B864.
[4] W. Kohn and L. J. Sham, Phys. Rev. 140, A1133.