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):

\[
\left(-\frac{1}{2} \nabla^2 + v_{\text{eff}}(r)\right) \psi_i(r) = \varepsilon_i \psi_i(r)
\]  

(1)

where

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

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

\(v_{\text{eff}}\) 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

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

(2)

\(v_{\text{xc}}([\rho(r)] : r)\) 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.

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