Generalized local-density approximation

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Résumé

We will report recent progress on the construction of Generalized Local Density Approximations (GLDAs) for use in density-functional theory (DFT) calculations of electronic structure [1-3].
The GLDAs use both the one-electron Wigner-Seitz radius rs and a newly-defined two-electron parameter η (called the hole curvature) at each point in space. The GLDAs reduce to the well-known Local Density Approximation (LDA) when applied to the infinite homogeneous electron gas but, unlike the LDA, it is also exact for finite uniform electron gases (UEGs).

We will present a comprehensive study of these finite UEGs at high, intermediate and low densities using perturbation theory and quantum Monte Carlo (QMC) calculations. We show that the present GLDA functionals yield accurate estimates of the correlation energy for both weakly and strongly correlated systems [3-4].

We will also discuss the accuracy of the new functionals in applications to chemical problems [5], and compare our results with traditional LDA calculations, as well as traditional wavefunction approaches (HF, MP2, MP3, Full CI and QMC).

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Mots-Clés: density, functional theory, quantum Monte Carlo, correlation energy

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