QIF2023: *Constrained minimisation of the Hohenberg-Kohn energy functional as a basis for multi-scale simulations: challenge for theory and opportunities for applications*

Tomasz A. WESOLOWSKI

Université de Genève, Dept. Physical Chemistry, GENEVA, Switzerland

Tomasz.Wesolowski@unige.ch https://www.unige.ch/sciences/chifi/wesolowski/

The densities considered usually in the Hohenberg-Kohn energy functional $E_v^{HK}[\rho]$ are the optimal ones for a given external potential $v(\mathbf{r})$. Frozen-Density Embedding Theory (FDET) concerns the functional $E_v^{HK}[\rho]$ for other densities. They are obtained from the constrained optimisation of $E_v^{HK}[\rho]$. The constraint ($\forall_{\mathbf{r}}\rho(\mathbf{r}) \geq \rho_B(\mathbf{r})$) is expressed by means of an observable (ρ_B is the electron density such that $\int \rho_B = N_B < \int \rho$). FDET provides the exact relations between the optimal embedded wavefunction, the embedding potential, and the energy, for given ρ_B. Various FDET based multi-scale/multi-level simulation methods are possible differing in:
a) The method to solve the N_A-electron problem (with $N_A < \int \rho$). FDET encompasses Kohn-Sham like non-interacting reference electrons [1] and both variational [2] and non-variational [3].
b) The approach to generate the constraint (from conventional atomistic representation of ρ_B, through experimental ρ_B [4] till continuum representation of ρ_B (see Ref. [5] and the references there).
c) The approximation used for certain components of the FDET energy functional.
In any of such variants, the embedded wavefunction (Ψ_A) is obtained from an eigenvalue equation featuring Ψ_A-dependent external potential.

In the first - introductory - part, the basic FDET relations will be presented. In the second part, we review our recent work on development of approximations to the kinetic-energy component of the FDET embedding potential (see Ref. [6] and the references there). In the third part, we present the recently derived exact FDET relation for excitation energy in case of state-dependent ρ_B [7].

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