Pis'ma v ZhETF, vol. 120, iss. 3, pp. 217 – 218

On exchange-correlation energy in DFT scenarios

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Submitted 16 June 2024
Resubmitted 9 July 2024
Accepted 9 July 2024

Motivated by the considerable importance of material properties in modern condensed matter physics research, and using techniques of the N_e-electron systems in terms of the electron density $n_{\sigma e}(r)$ needed to obtain the ground-state energy E_{e0} in Density Functional theory scenarios, we approach the exchange-correlation energy $E_{xc}[n_{\sigma e}(r)]$ by considering the interelectronic position corrections $\Delta r_x^{\uparrow\uparrow,\uparrow\downarrow} = \lambda_x \left|\delta r^{\uparrow\uparrow} - \delta r^{\uparrow\downarrow}\right|$ and $\Delta r_c^{e_i e_{j\neq i}} = \lambda_c \left|r - r'\right|^{-(N_e-1)^{-1}}$ corresponding to the spin and the Coulomb correlation effects, respectively, through the electron-electron potential energy. Exploiting such corrections, we get approximate expressions for the exchange $E_x[n_{\sigma e}]$ and the correlation $E_c[n_{\sigma e}]$ functional energies which could be interpreted in terms of magnetic and electric dipole potential energies associated with the charge density $n_{\sigma e}(r)$ described by inverse-square potential behaviors. Based on these arguments, we expect that such obtained exchange-correlation functional energy could be considered in the Local Density Approximation functional as an extension to frame such interelectronic effects.

DOI: 10.31857/S0370274X24080105, EDN: DWPJPJ

In this work, motivated by the considerable importance of material properties in modern condensed matter physics research, and using techniques of the N_e-electron systems in terms of the electron density $n_{\sigma e}(r)$ needed to obtain the ground-state energy E_{e0} in density functional theory scenarios [1–5], we approach the exchange-correlation energy $E_{xc}[n_{\sigma e}(r)]$. For that, we first present the study of the total electronic energy of many-electron N_e systems from the generalized Schrödinger equation of the many-electron wavefucntion $\Psi_{\sigma e}(x_i)$, discuss the early attempts used to overcome the computational problem by means of the introduction of the electron density $n_{\sigma e}(r)$ reducing the dimensionality of the system, and reconsider the Density Functional Theory (DFT) computational scheme of the N_e-electron systems using the electron density $n_{\sigma e}(r)$ for getting the ground state energy E_{e0} [5–8]. Then, by considering the interelectronic position corrections $\Delta r_x^{\uparrow\uparrow,\uparrow\downarrow} = \lambda_x \left|\delta r^{\uparrow\uparrow} - \delta r^{\uparrow\downarrow}\right|$ and $\Delta r_c^{e_i e_{j\neq i}} = \lambda_c \left|r - r'\right|^{-(N_e-1)^{-1}}$ corresponding to the spin and the Coulomb correlation effects, respectively, through the electron-electron potential energy. Employing such corrections, we get approximate expressions for the exchange $E_x[n_{\sigma e}]$ and the correlation $E_c[n_{\sigma e}]$ functional energies. By making contact with some known physical energy behaviour systems, a close inspection shows that these obtained energies could be interpreted in terms of magnetic and electric dipole potential energies associated with the charge density $n_{\sigma e}(r)$ described by inverse-square potential behaviors [9, 10]. Such inverse-square potential have been largely investigated in different physical scales including high energy physics and related topics [11–13]. Based on these arguments, we expect that such obtained exchange-correlation functional energy could be considered in the Local Density Approximation functional as an extension to frame such interelectronic effects [14, 15]. Particularly, we think that these dipole-like potentials should be implemented in the generalized Schrödinger equation in the DFT framework providing interelectronic interaction energy corrections as well as possible new gates to explore other physical features.

Funding. This work was supported by ongoing institutional funding. No additional grants to carry out or direct this particular research were obtained.

Conflict of interest. The authors of this work declare that they have no conflicts of interest.

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