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On exchange-correlation energy in DFT scenarios

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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.

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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 wavefucnction $\Psi_{\sigma e}\,(x_i)$, 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.

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