Approximation of correction functions in the refined Thomas-Fermi model

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The thermodynamics of substance electrons in the concept of spherical Wigner-Seitz cells in the semi-classical approximation is presented as an expansion in the semi-classical parameter ξ within the framework of the self-consistent field model. The zero approximation by ξ corresponds to the Thomas-Fermi (TF) model, and the following terms are the exchange, quantum (gradient) and shell corrections. Smallness condition ξ is violated near the nucleus under any external conditions. The consequences of this are: 1. overestimated values of integral energy quantities in the TF model; 2. divergence at zero of volume integrals for gradient corrections to these energy quantities; 3. in the regions of ultrahigh compressions or temperatures, the results of the perturbation theory valid there are not reproduced. To eliminate the defects, modifications of the expressions for the gradient correction to free energy of electrons and for the shell correction to number of their states have been proposed [1]. The modification includes the introduction of the rather complex functions $\phi(x)$ and $\Psi_k(y)$, which require additional computational efforts. In this paper, their approximations are proposed: $\phi(x) = \frac{2}{45}x^3e^{-x} + (1-e^{-x})[\frac{x}{3} - \frac{1}{2}\mathrm{arctg}\frac{2x}{3}]$, $\Psi_k(y) = \Psi(y) = \mathrm{tg}[\frac{\pi}{8} - \frac{1}{2}\mathrm{arctg}\left(\mathrm{th}(\frac{\pi y}{4})\right)]$.

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