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Correlation Energy of 3D Spin-Polarized Electron Gas: A Single Interpolation Between High- and Low-Density Limits JIANWEI SUN, JOHN PERDEW, Department of Physics and Quantum Theory Group, Tulane University, MICHAEL SEIDL, Department of Physics, University of Regensburg —
We present an analytic model for the correlation energy per electron $e_c(r_s, \zeta)$ in the three-dimensional (3D) uniform electron gas, covering the full range $0 \leq r_s < \infty$ and $0 \leq \zeta \leq 1$ of the density parameter r_s and the relative spin polarization ζ. An interpolation is made between the exactly known high-density ($r_s \to 0$) and low-density ($r_s \to \infty$) limits, using a formula which (unlike previous ones) has the right analytic structures in both limits. We find that there is almost enough information available from these limits to determine the correlation energy over the full range. By minimal fitting to numerical quantum Monte Carlo data, we predict the value of $b_1(\zeta)$ at ζ=0 close to the theoretical value [1], where $b_1(\zeta)$ is the coefficient of the $r_s$term in the high-density expansion. The model finds correlation energies for the unpolarized (ζ=0) and fully polarized (ζ=1) cases in excellent agreement with Monte Carlo data.
[1] T. Endo, M. Horiuchi, Y. Takada and H. Yasuhara, Phys. Rev. B 59, 7367 (1999)

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