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A numerically tractable method for a non-uniform electron gas system with an atomic center KOICHI KUSAKABE, MASANORI TAKAHASHI, NAOSHI SUZUKI, Graduate School of Engineering Science, Osaka University — To perform the first-principles calculation of a non-uniform electron system with both localized and delocalized electrons, we have developed a tractable algorithm using the transcorrelated method and Pahl-Handy's mixed basis. Both two-body and three body potentials are expanded in terms of spherical harmonics or in the Fourier series. Radial integrals are analytically evaluated, which makes the numerical simulation as simple as series of matrix multiplication and the fast Fourier transformation. Possible application for a Kondo system is addressed. Our numerical simulation could provide a first-principles evaluation of the U-term and residual exchange-correlation energy functional for an effective many-body system of the density functional theory.

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