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Effective one-body potential fitted for many-body interactions associated with a Jastrow function: application to the quantum Monte Carlo calculations NAOTO UMEZAWA, National Institute for Materials Science, BRIAN AUSTIN, WILLIAM A. LESTER, JR, University of California, Berkeley — An efficient method of optimizing a Slater determinant, D, in the Jastrow-Slater-type wave function, FD, is suggested. Here, the so-called transcorrelated Hamiltonian, $\frac{1}{F}\mathcal{H}F$, which is a similarity transformation of the usual Hamiltonian of an electronic system with respect to a Jastrow function F, is fitted to an effective Hamiltonian, $\mathcal{H}_{\rm eff} = \sum_i^N \left(-\frac{1}{2}\nabla_i^2 + v(\mathbf{r_i})\right)$, in which all the electron-electron and electron-neucleus interactions are represented by a one-body potential, $v(\mathbf{r})$. A single-particle Schrödinger equation is then solved by using $v(\mathbf{r})$ to determine the orbitals, of which the Slater determinant consists. The obtained orbitals improve the atomic total energies in the variational Monte Carlo calculations compared to those given by the density-functional-based orbitals. Advantages of using the optimized orbitals in the diffusion Monte Carlo calculations are also discussed.

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