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New method of optimizing the Jastrow factor for solids with the transcorrelated method MASAYUKI OCHI, Department of Physics, The University of Tokyo, SHINJI TSUNEYUKI, Department of Physics, The University of Tokyo, ISSP, The University of Tokyo — Transcorrelated (TC) method[1-5] is one of the promising theories for *ab initio* electronic structure calculation of solids. It is one of the wave-function-based approaches which are considered to be advantageous for high-accuracy calculation. In the TC method, the total wave function is approximated as the Jastrow-Slater-type wave function, and the many-body Hamiltonian is similarity-transformed by the Jastrow factor. Then we solve an SCF equation and optimize one-body orbitals in the Slater determinant with relatively low computational cost. On the other hand, optimization of the Jastrow factor has been computationally much more demanding although it is indispensable to high-accuracy calculation. In this study, a new method of optimizing the Jastrow factor is developed by use of variance minimization of the total energy. It is demonstrated that, by truncating the basis-set expansion of the variance, the optimization is realized with low computational cost. [1] S. F. Boys and N. C. Handy, Proc. R. Soc. London Ser. A 309, 209 (1969). [2] S. Ten-no, Chem. Phys. Lett. 330, 169 (2000). [3] N. Umezawa and S. Tsuneyuki, J. Chem. Phys. 119, 10015 (2003). [4] R. Sakuma and S. Tsuneyuki, J. Phys. Soc. Jpn. 75, 103705 (2006). [5] H. Luo, J. Chem. Phys. 133, 154109 (2010).

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