Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

The Transcorrelated Method Combined with the Variational Monte Carlo Calculation: Application to Atoms NAOTO UMEZAWA, National Institute for Materials Science, Tsukuba, Japan, SHINJI TSUNEYUKI, Department of Physics, University of Tokyo, Tokyo, Japan, TAKAHISA OHNO, National Institute for Materials Science, Tsukuba, Japan, KENJI SHIRAISHI, Institute of Physics, University fo Tsukuba, Tsukuba, Japan, TOYOHIRO CHIKYOW, National Institute for Materials Science, Tsukuba, Japan — The transcorrelated (TC) method is a useful approach to optimize the Jastrow-Slater-type many-body wave function FD. The basic idea of the TC method [1] is based on the similarity transformation of a many-body Hamiltonian $\mathcal{H}$ with respect to the Jastrow factor F: $\mathcal{H}_{\rm TC} = frac1F\mathcal{H}F$ in order to incorporate the correlation effect into $\mathcal{H}_{\rm TC}$. Both the F and D are optimized by minimizing the variance $\sigma^2 = \int |\mathcal{H}_{rmTC}D - ED|^2 d^{3N}x$. The optimization for F is implemented by the variational Monte Carlo calculation, and D is determined by the TC self-consistent-field equation for the one-body wave functions $\phi_\mu(x)$, which is derived from the functional derivative of σ^2 with respect to $\phi_{mu}(x)$. In this talk, we will present the results given by the transcorrelated variational Monte Carlo (TC-VMC) method for the ground state [2] and the excited states of atoms [3]. [1]S. F. Boys and N. C. Handy, Proc. Roy. Soc. A, **309**, 209; **310**, 43; **310**, 63; **311**, 309 (1969). [2]N. Umezawa and S. Tsuneyuki, J. Chem. Phys. **119**, 10015 (2003). [3]N. Umezawa and S. Tsuneyuki, J. Chem. Phys. **121**, 7070 (2004).

Naoto Umezawa
National Institute for Materials Science

Date submitted: 30 Nov 2004 Electronic form version 1.4