

Stochastic and Deterministic Methods for Selected Coupled-cluster

Seiichiro L. Ten-no

Graduate School of Science, Technology, and Innovation

Kobe University, Japan

Email: tenno@garnet.kobe-u.ac.jp

Abstract:

The model space quantum Monte Carlo (MSQMC) [1] is an extension of full configuration interaction QMC (FCIQMC), allowing us to calculate quasi-degenerate and excited electronic states by sampling the effective Hamiltonian in the model space. The initiator adaptation (i-MSQMC) to restrict the sampling space causes size-inconsistency errors. Several ways to mitigate this problem are discussed based on the many-body perturbation and coupled-cluster frameworks [2]. We shall also propose a deterministic full coupled-cluster reduction (FCCR) [3] that is capable of providing very accurate solutions of the many-body Schrodinger equation exploiting the sparsity of the exponential ansatz of FCC. We introduce two screening schemes to the projection manifold and commutator operations. Numerical results will be presented for systems including polyacenes and the chromium dimer.

[1] S. Ten-no, J. Chem. Phys., **138** 164126 (2013).

[2] S. L. Ten-no, J. Chem. Phys., **147** 244107 (2017).

[3] E. Xu, M. Uejima, and S. L. Ten-no, Phys. Rev. Lett., **121** 113001 (2018).