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イニシエーター近似の摂動補正に関する研究

[1]神戸大学院計算科学インテンシブコース
[2]神戸大学科学技術イノベーション研究科
0 Ladoczki Bence[1]、天能 精一郎[2]

Perturbative corrections to the initiator approximation

O Ladoczki Bence[1]、Seiichiro L. Ten-no[2]
[1] *Graduate School of System Informatics, Kobe University*
[2] *Graduate School of Science, Technology, and Innovation, Kobe University*

[ABSTRACT]
The Model Space Quantum Monte Carlo (MSQMC)[1] method based on the stochastic sampling in Slater determinant space can be applied to solve the Schrödinger equation of a many-body system. Parallel to Full Configuration Interaction QMC (FCIQMC) the initiator approximation has been introduced to bridle exponential walker growth that would result in large number of determinants with little occupation. The spawning restrictions of non-initiator determinants lead to a truncated wave function that is similar to that of calculated by Adaptive CI (ACI) methods. The variational energy is usually improved upon using second order Epstein-Nesbet perturbation theory. Our research sheds light on a similar correction that improves the i-MSQMC energy significantly. Namely, that whenever a walker is discarded due to the initiator criteria a contribution to the second order correction[2] is accumulated. The third order correction can be sampled in an analogous fashion and we report on these calculation details as well.

[METHOD]
In the initiator adaptation, the truncated i-MSQMC wave function can be regarded as a similar object to those sampled by ACI methods. Usually these results are improved upon using perturbation theory. The second order Epstein-Nesbet energy correction can be expressed using the following formula:

$$E^{(2)}(\tau) = \sum_{a \notin \nu} \frac{(\sum_{i \in \nu} H_{ia} c_i(\tau))^2}{E_{var}(\tau) - H_{aa}}$$

In MSQMC, the walker population on a given determinant is proportional to the following quantity:

$$S_a = -\Delta\tau \sum_{i \in \nu} H_{ia} N_i(\tau)$$

The walkers that don't satisfy the initiator criteria are removed and the second order correction to the initiator error can be sampled (after appropriate normalization) using these walkers:

$$E^{(2)}(\tau) = \frac{1}{(\Delta\tau)^2} \sum_{a \notin \nu} \frac{S_a^{(1)}(\tau) S_a^{(2)}(\tau)}{E_{var}(\tau) - H_{aa}}$$

Simply squaring the contribution introduces bias to the results and in order to avoid this we use the previously introduced replica trick[3] to overcome this problem.

[RESULTS· EXPLANATION]
The second order Epstein-Nesbet correction (EN2) seem to compare well with other corrections (Meisner, Pople, Davidson) as it is apparent from FIG. 1. We found that in many cases it provides more accurate (relative to FCI) results than other *a posteriori* corrections and also our studies show that it is less sensitive to calculation parameters such as the number of walkers (Booster weights).

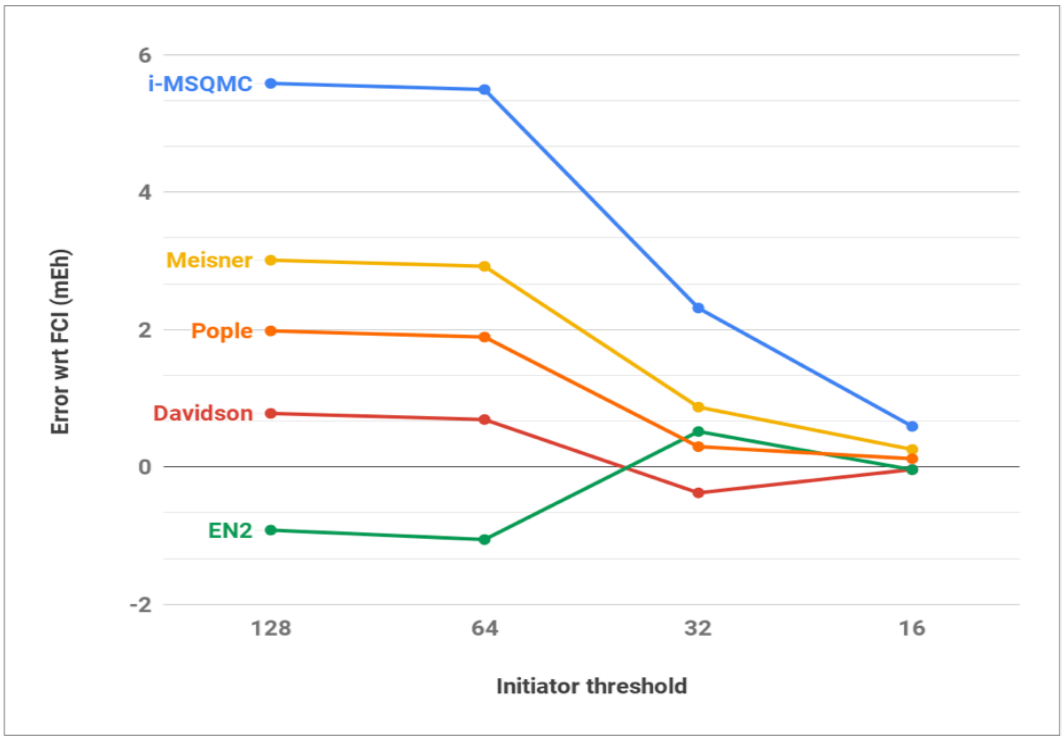

FIG. 1. Calculation results for a Ne atom in cc-pVDZ basis (8,13) using 1000 Booster weights

Initiator approximation is necessary to reduce calculation costs for larger systems and the error it introduces should be corrected. The proposed method can be applied for calculations that are impossible to carry out without a truncation in the Hilbert space. As a rule of thumb, such calculations can be run with the initiator threshold set to <16 and use the energy value corrected by EN2. In the limit of infinite initiator threshold and in the single reference limit, the i-MSQMC wave function consists of the reference determinant and its connected subspace. The time-average of such a wave function is equal to the CISD wave function and the corresponding energy is not size-consistent. Details regarding this issue of size-consistency at finite initiator threshold with(out) *a posteriori* corrections will be discussed in the talk. Calculation results on larger systems will be presented during the session and further explanation will also be given.

[REFERENCES]
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