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確率論的手法に基づいた摂動論における打ち切りの影響に関する研究

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Truncation effects in perturbation based stochastic methods

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Abstract

The MSQMC[1] (Model Space Quantum Monte Carlo) method has successfully been applied for obtaining solutions of the Schrödinger equation for strongly correlated systems in the FCI accuracy. Our new perturbation based MSQMC(PT-MSQMC) algorithm proceeds in a similar fashion as the original MSQMC, with an extra sampling step. In order to overcome the prohibitive scaling problem, it is possible to impose restrictions on the sampled space, so only determinants up to a predefined excitation level are sampled. Size-extensivity is maintained by limiting the transcription step. The truncation effects and the size-extensivity property are investigated in the current work. We are comparing PT-MSQMC(D) energies in infinite perturbation order with CEPA(0) energies.

Introduction and Method

Quantum Monte Carlo (QMC) methods are a vital tool in the study of many-body systems, regularly providing the most accurate and reliable results for correlated fermionic systems of interest. The Model Space Quantum Monte Carlo (MSQMC) technique is a stochastic method for solving the electronic Schrödinger equation in extremely large Hilbert spaces.

The imaginary time evolution of the nth order component in the perturbation series, obtained by substituting the power series expansion of the wave function and equating the coefficients of the same power of the perturbation is the following:

$$\frac{d}{d\tau}|\psi^{(n)}\rangle = -(\hat{H}_0 - E^{(0)})\psi^{(n)} - \hat{Q}\hat{H}_x\psi^{(n-1)} - (\hat{H_D} - \hat{H}_0 - E^{(1)})\psi^{(n-1)} + \sum_{i=2}^{n-1} E^{(i)}\psi^{(n-i)} \quad (1)$$

The linked diagram theorem states, that the energy and the wave function can be expressed, in each order, as a sum of linked diagrams only:

$$E^{(n)} = \langle 0|\hat{W}(\hat{R}_0\hat{W})^{n-1}|0\rangle_L \tag{2}$$

In the limit of infinite number of walkers PT-MSQMC distributes the walker population on the FCI solution, obeys the linked-diagram theorem, therefore it is extensive in every perturbative order. This is fulfilled by introducing a new transcription step in the walker dynamics that is responsible for sampling the renormalization term to cancel the unlinked diagrams, leaving only the linked diagrams in the expressions, which are always extensive.

The fourth order energy is the first case in which there is a renormalization term:

$$E^{(4)} = \langle 0|\hat{W}\hat{R}_0\hat{W}\hat{R}_0\hat{W}\hat{R}_0\hat{W}|0\rangle - E^{(2)}\langle\psi^{(1)}|\psi^{(1)}\rangle \tag{3}$$

Therefore, size-extensivity error in a truncated space arises from the fourth order energy, as shown in the results section.

Results

PT-MSQMC(D) results for Be are shown in Table 1. The size-extensivity error caused by the truncation grows as the order of perturbation increases when including the transcription step. The algorithm without transcription within the space of at most doubly excited determinants provides a consistent result even beyond third order. The results are calculated by subtracting twice of the monomer energy from the dimer energy at infinite distance.

	trans.	no trans.
E(2)	0.180	0.006
E(3)	0.252	0.020
E(4)	1.028	0.077
E(5)	2.873	0.106
E(6)	4.351	0.106

Table 1: Size-extensivity errors in mEh with and without transcription

References

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