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Study of Trotter-like Approximations

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Many quantum Monte Carlo techniques require a Trotter-like approximation before they can be implemented. In an effort to understand better the performance of these techniques, we explore the errors when Trotter-like approximations are used for calculating free energies and operator expectation values.

We consider first the original form of the Trotter formula[1,2]

$$e^{-\beta H} = \lim_{L \to \infty} \left[\left(\prod_{m=1}^{M} e^{-(\Delta\tau) H_m} \right)^L \right] \tag{1.1}$$

where

$$\Delta\tau = \beta/L \tag{1.2}$$

$$H = \sum_{m=1}^{M} H_m \tag{1.3}$$

and

$$\prod_{m=1}^{M} e^{-(\Delta\tau) H_m} = e^{-(\Delta\tau) H} + \text{order}(\Delta\tau)^2 \tag{1.4}$$

as well as the generalizations of Suzuki[2] and of De Raedt and De Raedt.[3] These generalizations can all be written in the form

$$e^{-\beta H} = \lim_{L \to \infty} [f^{(n)}]^L \tag{1.5}$$

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where

$$f^{(n)} = e^{-(\Delta\tau)H} + \text{order}(\Delta\tau)^{n+1} \tag{1.6}$$

and where we define n as the order of the Trotter approximant. We also consider an expansion of $e^{-(\Delta\tau)H}$ in powers of $(\Delta\tau)H$ so that[2]

$$f(n) = \sum_{k=0}^{n} \frac{1}{(k!)} [-(\Delta\tau)H]^k \tag{1.7}$$

We define

$$\Delta F = F_{\text{exact}} - \frac{1}{\beta} \ln\{\text{tr}[(f^{(n)})^L]\} \tag{1.8}$$

and

$$\Delta\langle\mathcal{O}\rangle = \langle\mathcal{O}\rangle_{\text{exact}} - \{\text{tr}[\mathcal{O}(f^{(n)})^L]\}/\{\text{tr}[(f^{(n)})^L]\} \tag{1.9}$$

We investigate finite lattice systems specifically, letting N denote the number of sites in the lattice. We consider the dependence of ΔF and $\Delta\langle\mathcal{O}\rangle$ on $\Delta\tau$ for $\Delta\tau$ small, on N for N large, and on β for β large, and obtain analytically the following main results.

Suppose that a first-order Trotter approximation of the form of (1.1) is used. Then, if all of the H_m are Hermitian, with N and β constant, the correction term linear in $\Delta\tau$ for the free energy and for the expectation values of Hermitian operators vanishes; i.e., for a Hermitian breakup, the error due to using a first-order Trotter approximation has a $(\Delta\tau)^2$ dependence rather than the $\Delta\tau$ dependence that might be expected.[2] This dependence is in general not improved by using a second-order approximant $f^{(2)}$. Next, for any Trotter approximation, we find for constant $\Delta\tau$ and β that the errors in the free energy per site and in the expectation values of local operators are independent of N if the lattice is sufficiently large and all interactions are of finite range. This means that, for a certain desired accuracy, $\Delta\tau$ may be chosen independently of lattice size. Last, we find for $\Delta\tau$ and N constant that ΔF and $\Delta\langle\mathcal{O}\rangle$ approach constants as $\beta \to \infty$.

We then consider the behavior when an approximate expansion of $e^{-(\Delta\tau)H}$ in powers of $(\Delta\tau)H$ is used. For $\Delta\tau$ sufficiently small and N constant, we show that the error in the approximate expectation value of an

[2] Upon reading this result at the Frontiers of Quantum Monte Carlo Conference, M. Suzuki subsequently derived an elegant theorem concerning the coefficients of all odd powers of $\Delta\tau$ in the series for ΔF and $\Delta\langle\mathcal{O}\rangle$. However, as we are interested in the small $\Delta\tau$ limit, we concern ourselves with the lowest order $\Delta\tau$ correction term only. Regarding that term, Suzuki's assumptions are a special case of the more generalized conditions which we assume.[4]

operator vanishes as $\beta \to \infty$, so that one approaches the exact ground state value. However, to retain a given accuracy in the expectation values of local operators at finite β, we find that $\Delta\tau$ must be chosen smaller for larger lattices. Also, the value of β at which operator expectation value corrections become small can be quite large. Thus, this approximation seems in general less useful for exploring the properties of larger systems.

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