New results on Trotter-like approximations

R. M. Fye
Department of Physics, University of California, San Diego, La Jolla, California 92093
(Received 9 December 1985)

We explore the errors in the free energy and in operator expectation values when the quantum operator $e^{-\beta H}=\prod_{l=1}^{L}e^{-(\Delta\tau)H}$ is approximated by $\prod_{l=1}^{L}f$, where $\Delta\tau=\beta/L$ and f is an approximant to $e^{-(\Delta\tau)H}$. We determine analytically the dependence of the resulting errors on $\Delta\tau$ for $\Delta\tau$ small, on β for β large, and on the size of the system in the limit of a large system. We focus on Trotter approximations, as well as on the expansion of $e^{-(\Delta\tau)H}$ in powers of $(\Delta\tau)H$. Our results are particularly relevant to Monte Carlo studies of quantum systems, and can be used effectively to eliminate the error due to Trotter-like approximations and to provide a guide for choosing a particular type of approximation.

I. INTRODUCTION

The Trotter formula,[1] first proven rigorously by Suzuki,[2] can be written as the identity

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

where

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

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

and

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

Systematic higher-order approximants to $e^{-(\Delta\tau)H}$ have been proposed by Suzuki[2-4] and by De Raedt and De Raedt[5] to improve the convergence of the approximate, finite L formula as a function of $\Delta\tau$. These generalized Trotter formulas may be written in the form

$$e^{-\beta H}=\lim_{L\to\infty}\prod_{l=1}^{L}f^{(n)}\ , \tag{1.5}$$

where

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

and the dependence of $f^{(n)}$ on $\Delta\tau$ is taken to be implicit. In this paper, the right superscript n of $f^{(n)}$ will be defined as the order of the approximant. Also, the denotation "Trotter approximation" or "Trotter formula" will include the above generalizations of the original formula in the remainder of the paper.

Another possible approximant to $e^{-(\Delta\tau)H}$ is an expansion in powers of $(\Delta\tau)H$.[2,6] Such a Trotter-like expansion may also be written in the form of Eq. (1.6), with

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

For finite $\Delta\tau$, these approximations have been used to calculate approximate expectation values of operators for various quantum Hamiltonians, as well as, in some cases, free energies. For the partition function, we have

$$Z_{\text{exact}}=\mathrm{Tr}(e^{-\beta H}) \tag{1.8}$$

and

$$Z_{\text{approx}}=\mathrm{Tr}\left[\prod_{l=1}^{L}f^{(n)}\right], \tag{1.9}$$

so that for the free energy

$$F_{\text{exact}}=-\frac{1}{\beta}\ln(Z_{\text{exact}}) \tag{1.10}$$

and

$$F_{\text{approx}}=-\frac{1}{\beta}\ln(Z_{\text{approx}})\ . \tag{1.11}$$

For an operator $\mathcal{O}$, we have

$$\langle\mathcal{O}\rangle_{\text{exact}}=\frac{\mathrm{Tr}(\mathcal{O}e^{-\beta H})}{\mathrm{Tr}(e^{-\beta H})} \tag{1.12}$$

and

$$\langle\mathcal{O}\rangle_{\text{approx}}=\frac{\mathrm{Tr}\left[\mathcal{O}\prod_{l=1}^{L}f^{(n)}\right]}{\mathrm{Tr}\left[\prod_{l=1}^{L}f^{(n)}\right]}\ . \tag{1.13}$$

We will also define

$$\Delta F=F_{\text{exact}}-F_{\text{approx}} \tag{1.14}$$

and

$$\Delta\langle\mathcal{O}\rangle=\langle\mathcal{O}\rangle_{\text{exact}}-\langle\mathcal{O}\rangle_{\text{approx}}\ . \tag{1.15}$$

We now note that approximations to certain quantities may be calculated either by using Eq. (1.13) or by taking derivatives of $\ln(Z_{\text{approx}})$. For example, one may calculate an approximate energy either by substituting the Hamiltonian H for $\mathcal{O}$ in Eq. (1.13) or by taking the negative of

the first derivative of $\ln(Z_{\text{approx}})$ with respect to β. To denote this distinction, we will let unprimed quantities be those computed using Eq. (1.13) and primed quantities be those computed from derivatives of $\ln(Z_{\text{approx}})$. Thus, for example, we have

$$\langle H' \rangle_{\text{approx}} = -\frac{\partial}{\partial \beta}[\ln(Z_{\text{approx}})] \tag{1.16}$$

and

$$C'_{\text{approx}} = \beta^2 \frac{\partial^2}{\partial \beta^2}[\ln(Z_{\text{approx}})] , \tag{1.17}$$

while, for comparison,

$$\langle H \rangle_{\text{approx}} = \frac{\text{Tr}\left[H \prod_{l=1}^{L} f^{(n)}\right]}{\text{Tr}\left[\prod_{l=1}^{L} f^{(n)}\right]} \tag{1.18}$$

and

$$C_{\text{approx}} = \beta^2[\langle H^2 \rangle_{\text{approx}} - (\langle H \rangle_{\text{approx}})^2] . \tag{1.19}$$

Also, in analogy to Eqs. (1.14) and (1.15), we will define

$$\Delta Q' = Q_{\text{exact}} - Q'_{\text{approx}} , \tag{1.20}$$

where Q'_{approx} is any quantity calculated by taking derivatives of $\ln(Z_{\text{approx}})$.

Our calculations and general results will be equally valid whether $\Delta\tau$ is held constant or whether L is held constant [see Eqs. (1.1) and (1.2)] when derivatives of $\ln(Z_{\text{approx}})$ are taken to compute a Q'_{approx}. Thus, unless explicitly stated otherwise, either of the two conditions may be assumed in the remainder of the paper.

In certain cases, either for a test Hamiltonian or for an $L=1$ Trotter approximation, the traces of Eqs. (1.9) and (1.13) have been computed exactly;[5-11] in others, the trace is approximated by using a quantum Monte Carlo technique.[12,13] Trotter-like approximations have proven particularly useful in conjunction with such techniques, as many of them require such an approximation before they can be implemented.

Use of these Trotter-like approximations will thus add a systematic error to certain of the quantum Monte Carlo methods, in addition to the statistical sampling error. In an effort mainly to improve the efficiency of these methods, we explore here the convergence of the free energy and of operator expectation values, when a Trotter-like approximation is used, as a function of $\Delta\tau$, β, and the size of the system. Although certain results can be extended, we confine ourselves to the study of finite lattice systems, letting N denote the number of lattice sites of the system under consideration in the remainder of the paper. To our knowledge, this general problem has not been systematically addressed in the literature.

In Secs. II, III, and IV, we consider the dependence of the error on $\Delta\tau$ for $\Delta\tau$ small, on β for β large, and on N for N large, respectively. This is followed by a section on numerical results and a discussion section. Our main results may be summarized as follows.

Suppose that a first-order Trotter approximation of the form of Eq. (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. In contradiction to what has generally been assumed in the literature, this dependence is, in general, not improved by using a second-order approximant $f^{(2)}$ [see Eq. (1.6)]. Next, for any Trotter approximation, we find for $\Delta\tau$ and N constant that ΔF and $\Delta\langle \mathcal{O} \rangle$ approach constants as $\beta \to \infty$. Lastly, again 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. We note that all of the above results can be shown to hold for primed as well as unprimed quantities.

Suppose, alternatively, that an approximate expansion of $e^{-(\Delta\tau)H}$ in powers of $(\Delta\tau)H$ is used. For sufficiently small $\Delta\tau$, and N constant, we show that the error in the approximate expectation value of an (unprimed) 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, $\Delta\tau$ must be chosen smaller as N increases. Thus, this approximation is in general less useful for exploring the properties of larger systems.

II. $\Delta\tau$ DEPENDENCE

In this section we will consider the case only of $f^{(1)}$, where the lowest-order correction to $e^{-(\Delta\tau)H}$ is of order $(\Delta\tau)^2$. The generalization to the case of $f^{(n)}$ is straightforward. We will also drop the right superscript (1) in this and all following equations whenever $e^{-(\Delta\tau)H}$ is approximated by $f^{(1)}$. Then, retaining correction terms through second order,

$$f = e^{-(\Delta\tau)H} + \mathcal{C}_1(\Delta\tau)^2 + C_2(\Delta\tau)^3 + O((\Delta\tau)^4) \tag{2.1}$$

$$= e^{-(\Delta\tau)[H - (\Delta\tau)\mathcal{C}_1 - (\Delta\tau)^2\mathcal{C}_2]} + O((\Delta\tau)^4) , \tag{2.2}$$

where

$$\mathcal{C}_2 = C_2 - \tfrac{1}{2}\{\mathcal{C}_1, H\} , \tag{2.3}$$

so that

$$\prod_{l=1}^{L} f = \prod_{l=1}^{L} e^{-(\Delta\tau)[H - (\Delta\tau)\mathcal{C}_1 - (\Delta\tau)^2\mathcal{C}_2]} + O((\Delta\tau)^3) \tag{2.4}$$

$$= e^{-\beta[H - (\Delta\tau)\mathcal{C}_1 - (\Delta\tau)^2\mathcal{C}_2]} + O((\Delta\tau)^3) . \tag{2.5}$$

Defining

$$\mathcal{C}_1(\tau) = e^{\tau H}\mathcal{C}_1 e^{-\tau H} \tag{2.6}$$

and

$$\mathcal{C}_2(\tau) = e^{\tau H}\mathcal{C}_2 e^{-\tau H} , \tag{2.7}$$

and using the ordering label technique of Feynman,[14] we find

$$e^{-\beta[H-(\Delta\tau)\mathscr{C}_1-(\Delta\tau)^2\mathscr{C}_2]}$$
$$=e^{-\beta H}\left[I+(\Delta\tau)\int_0^\beta d\tau\mathscr{C}_1(\tau)+(\Delta\tau)^2\left[\int_0^\beta d\tau\mathscr{C}_2(\tau)+\int_0^\beta d\tau\int_0^\tau d\tau\mathscr{C}_1(\tau)\mathscr{C}_1(\tau)\right]\right]+O((\Delta\tau)^3)\,. \quad (2.8)$$

The procedure may be extended to any order in $\Delta\tau$.

We now define

$$\mathscr{D}_1(\beta)=\int_0^\beta d\tau\mathscr{C}_1(\tau) \quad (2.9)$$

and omit in all subsequent equations the right subscript "exact" if a quantity is calculated with no approximation. Then, using Eqs. (1.9), (1.11), (1.13), and (2.8),

$$Z_{\text{approx}}=Z[1+(\Delta\tau)\langle\mathscr{D}_1(\beta)\rangle+O((\Delta\tau)^2)]\,, \quad (2.10)$$

$$F_{\text{approx}}=F-\left[\frac{\Delta\tau}{\beta}\right]\langle\mathscr{D}_1(\beta)\rangle+O((\Delta\tau)^2)\,, \quad (2.11)$$

and

$$\langle\mathscr{O}\rangle_{\text{approx}}=\frac{\langle\mathscr{O}\rangle+(\Delta\tau)\langle\mathscr{D}_1(\beta)\mathscr{O}\rangle}{1+(\Delta\tau)\langle\mathscr{D}_1(\beta)\rangle}+O((\Delta\tau)^2)$$
$$=\langle\mathscr{O}\rangle+(\Delta\tau)[\langle\mathscr{D}_1(\beta)\mathscr{O}\rangle \quad (2.12)$$
$$-\langle\mathscr{D}_1(\beta)\rangle\langle\mathscr{O}\rangle]+O((\Delta\tau)^2)\,. \quad (2.13)$$

Further defining

$$\mathscr{D}_2(\beta)=\int_0^\beta d\tau\mathscr{C}_2(\tau)+\int_0^\beta d\tau\int_0^\tau d\tau'\mathscr{C}_1(\tau)\mathscr{C}_1(\tau')\,, \quad (2.14)$$

we find, if $\langle\mathscr{D}_1(\beta)\rangle$ vanishes,

$$Z_{\text{approx}}=Z[1+(\Delta\tau)^2\langle\mathscr{D}_2(\beta)\rangle+O((\Delta\tau)^3)] \quad (2.15)$$

and

$$F_{\text{approx}}=F-\frac{(\Delta\tau)^2}{\beta}\langle\mathscr{D}_2(\beta)\rangle+O((\Delta\tau)^3)\,. \quad (2.16)$$

If, in addition, $\langle\mathscr{D}_1(\beta)\mathscr{O}\rangle$ vanishes, we obtain

$$\langle\mathscr{O}\rangle_{\text{approx}}=\langle\mathscr{O}\rangle+(\Delta\tau)^2[\langle\mathscr{D}_2(\beta)\mathscr{O}\rangle-\langle\mathscr{D}_2(\beta)\rangle\langle\mathscr{O}\rangle]+O((\Delta\tau)^3)\,. \quad (2.17)$$

We now assume all relevant operators are simultaneously real representable. This is not unduly restrictive in practice, as most Monte Carlo algorithms require real representation. We will show that if $\mathscr{C}_1$ is anti-Hermitian and if $\mathscr{O}$ is Hermitian, then the correction terms linear in $\Delta\tau$ vanish for Z_{approx} and $\langle\mathscr{O}\rangle_{\text{approx}}$.[15] If the correction term linear in $\Delta\tau$ vanishes for Z_{approx}, we note that it will also then vanish for F_{approx} and any Q'_{approx} [see Eqs. (1.16)–(1.20)].

This result for $\mathscr{C}_1$ anti-Hermitian may be applied in particular to a first-order Trotter approximation of the form of Eq. (1.1) with a Hermitian break-up. In that case,

$$\mathscr{C}_1=\tfrac{1}{2}\sum_{m=1}^{M}\sum_{k<m}[H_k,H_m]\,, \quad (2.18)$$

which is anti-Hermitian, as desired, since all of the H_m are Hermitian.

If a non-Hermitian break-up is used, $\mathscr{C}_1$ can still be made anti-Hermitian.[16] Let H_i be the Hermitian piece of the Hamiltonian in Eq. (1.3) which is to be further broken down into the non-Hermitian pieces $H_i^{(1)}$ and $H_i^{(2)}$, for example. Making the substitution

$$e^{-(\Delta\tau)H_i}=e^{-(\Delta\tau/2)H_i^{(1)}}e^{-(\Delta\tau)H_i^{(2)}}\times e^{-(\Delta\tau/2)H_i^{(1)}}+O((\Delta\tau)^3) \quad (2.19)$$

instead of the substitution

$$e^{-(\Delta\tau)H_i}=e^{-(\Delta\tau)H_i^{(1)}}e^{-(\Delta\tau)H_i^{(2)}}+O((\Delta\tau)^2) \quad (2.20)$$

in Eq. (1.4) will guarantee that $\mathscr{C}_1$ is anti-Hermitian. This procedure also holds if there is more than one H_i which must be broken up into non-Hermitian pieces.

For the special case of an $M=2$ [see Eq. (1.4)] Trotter break-up, an analogous result for the vanishing of the lowest-order $\Delta\tau$ term is already known for Z_{approx} (Refs. 5 and 6) and, hence, F_{approx} and Q'_{approx}, though not for $\langle\mathscr{O}\rangle_{\text{approx}}$. In that case,

$$Z_{\text{approx}}=\mathrm{Tr}\left[\prod_{l=1}^{L}e^{-(\Delta\tau)H_1}e^{-(\Delta\tau)H_2}\right] \quad (2.21)$$
$$=\mathrm{Tr}\left[\prod_{l=1}^{L}e^{-(\Delta\tau/2)H_1}e^{-(\Delta\tau)H_2}e^{-(\Delta\tau/2)H_1}\right]\,, \quad (2.22)$$

using the cyclic property of the trace. Then, since

$$e^{-(\Delta\tau/2)H_1}e^{-(\Delta\tau)H_2}e^{-(\Delta\tau/2)H_1}=e^{-(\Delta\tau)H}+O((\Delta\tau)^3)\,, \quad (2.23)$$

one has that

$$Z_{\text{approx}}=Z[1+O((\Delta\tau)^2)]\,. \quad (2.24)$$

Again using the cyclic property of the trace, we can extend this $M=2$ result to the expectation value of any operator which is a sum of operators each of which commutes with either H_1 or H_2. For example, considering the Hamiltonian H,

$$\langle H\rangle_{\text{approx}}=\frac{\mathrm{Tr}\left[H\prod_{l=1}^{L}(e^{-(\Delta\tau)H_1}e^{-(\Delta\tau)H_2})\right]}{\mathrm{Tr}\left[\prod_{l=1}^{L}e^{-(\Delta\tau)H_1}e^{-(\Delta\tau)H_2}\right]} \quad (2.25)$$
$$=\frac{\mathrm{Tr}\left[H_1\prod_{l=1}^{L}(e^{-(\Delta\tau/2)H_1}e^{-(\Delta\tau)H_2}e^{-(\Delta\tau/2)H_1})\right]}{\mathrm{Tr}\left[\prod_{l=1}^{L}e^{-(\Delta\tau/2)H_1}e^{-(\Delta\tau)H_2}e^{-(\Delta\tau/2)H_1}\right]}$$

$$+\frac{\mathrm{Tr}\left[H_2\prod_{l=1}^{L}(e^{-(\Delta\tau/2)H_2}e^{-(\Delta\tau)H_1}e^{-(\Delta\tau/2)H_2})\right]}{\mathrm{Tr}\left[\prod_{l=1}^{L}e^{-(\Delta\tau/2)H_2}e^{-(\Delta\tau)H_1}e^{-(\Delta\tau/2)H_2}\right]} \tag{2.26}$$

$$=\langle H\rangle+O((\Delta\tau)^2)\ . \tag{2.27}$$

However, the cyclic property of the trace by itself cannot be used to show that the correction terms linear in $\Delta\tau$ vanish for $\langle\mathcal{O}\rangle_{\text{approx}}$ in general, or that they vanish for Z_{approx} if $M>2$.

To show this vanishing of the first-order correction term when $\mathcal{C}_1$ is anti-Hermitian, we begin by considering the Hermitian conjugate

$$[e^{-\beta H}\mathcal{D}_1(\beta)]^\dagger=\left[\int_0^\beta d\tau e^{-(\beta-\tau)H}\mathcal{C}_1 e^{-\tau H}\right]^\dagger \tag{2.28}$$

$$=\int_0^\beta d\tau\, e^{-\tau H}\mathcal{C}_1^\dagger e^{-(\beta-\tau)H} \tag{2.29}$$

$$=\int_0^\beta d\tau e^{-(\beta-\tau)H}\mathcal{C}_1^\dagger e^{-\tau H}\ , \tag{2.30}$$

through a change in variables. We thus find that the product $e^{-\beta H}\mathcal{D}_1(\beta)$ has the same Hermiticity as $\mathcal{C}_1$; i.e., if $\mathcal{C}_1$ is Hermitian, then $e^{-\beta H}\mathcal{D}_1(\beta)$ is Hermitian, and if $\mathcal{C}_1$ is anti-Hermitian, then $e^{-\beta H}\mathcal{D}_1(\beta)$ is anti-Hermitian. The trace of an anti-Hermitian operator with real representation vanishes. Therefore, if $\mathcal{C}_1$ is anti-Hermitian,

$$\langle\mathcal{D}_1(\beta)\rangle=\frac{\mathrm{Tr}(e^{-\beta H}\mathcal{D}_1(\beta))}{\mathrm{Tr}(e^{-\beta H})}=0\ , \tag{2.31}$$

and, from Eqs. (2.10) and (2.11), the corrections linear in $\Delta\tau$ vanish for Z_{approx} and, thus, F_{approx} and Q'_{approx}.

Suppose, in addition, that $\mathcal{O}$ is a Hermitian operator. Then, since $\langle\mathcal{D}_1(\beta)\mathcal{O}\rangle$ is the trace of the real-representable product of a Hermitian and an anti-Hermitian operator, one has

$$\langle\mathcal{D}_1(\beta)\mathcal{O}\rangle=0\ , \tag{2.32}$$

so that the correction to $\langle\mathcal{O}\rangle_{\text{approx}}$ linear in $\Delta\tau$ also vanishes.

If $\mathcal{O}$ is not Hermitian (for example, if $\mathcal{O}$ is a Green's function), one can combine $\mathcal{O}$ with its Hermitian conjugate to obtain

$$\langle\tfrac{1}{2}(\mathcal{O}+\mathcal{O}^\dagger)\rangle_{\text{approx}}=\langle\mathcal{O}^{(H)}\rangle_{\text{approx}}$$

$$=\langle\mathcal{O}\rangle+O((\Delta\tau)^2)\ , \tag{2.33}$$

with the correction term linear in $\Delta\tau$ again vanishing. Here, $\mathcal{O}^{(H)}$ is the Hermitian part of $\mathcal{O}$, defined by

$$\mathcal{O}^{(H)}=\tfrac{1}{2}(\mathcal{O}+\mathcal{O}^\dagger)\ . \tag{2.34}$$

For an $M=2$ first-order Hermitian break-up, one notes that using either the second-order Suzuki approximant[2]

$$f_S^{(2)}=e^{-(\Delta\tau)H_1}e^{-(\Delta\tau)H_2}e^{-[(\Delta\tau)^2/2][H_1,H_2]} \tag{2.35}$$

$$=e^{-(\Delta\tau)H}+\mathcal{C}_{1,S}^{(2)}(\Delta\tau)^3+O((\Delta\tau)^4)\ , \tag{2.36}$$

or the second-order Hermitian approximant[5,6]

$$f_H^{(2)}=e^{-(\Delta\tau/2)H_1}e^{-(\Delta\tau)H_2}e^{-(\Delta\tau/2)H_1} \tag{2.37}$$

$$=e^{-(\Delta\tau)H}+\mathcal{C}_{1,H}^{(2)}(\Delta\tau)^3+O((\Delta\tau)^4) \tag{2.38}$$

will not improve the convergence of $\langle\mathcal{O}^{(H)}\rangle_{\text{approx}}$ with respect to $\Delta\tau$, as both $\mathcal{C}_{1,S}^{(2)}$ and $\mathcal{C}_{1,H}^{(2)}$ have nonvanishing Hermitian parts, in general. Both approximants can be straightforwardly extended to $M>2$, with this result then remaining the same for both Z_{approx} and $\langle\mathcal{O}^{(H)}\rangle_{\text{approx}}$.

We also note at this point that if a first-order non-Hermitian break-up is used, the correction terms linear in $\Delta\tau$ for Z_{approx} and $\langle\mathcal{O}\rangle_{\text{approx}}$ may vanish due to symmetry properties besides Hermiticity. This will depend, in general, upon the particular Hamiltonian and operators under consideration.

III. DEPENDENCE ON β

We now discuss the β dependence, for a given $\Delta\tau$ and N, of ΔF and $\Delta\langle\mathcal{O}\rangle$. We are interested in the limit of sufficiently large β so that the system approaches its ground state; i.e.,

$$\beta(E_2-E_1)\gg 1\ , \tag{3.1}$$

where E_1 and E_2 are the ground state and first excited state energies of the system, respectively. Since general results are the same if degeneracies exist, we will assume for notational purposes that all eigenstates of H are non-degenerate. We also note that in taking the large-β limit, β will actually be allowed only certain discrete values in our formulation, since $L=\beta/\Delta\tau$ is assumed to be always integral.

Holding the N dependence implicit in the remainder of this section, we will first show that, with a sufficiently small constant $\Delta\tau$,

$$\lim_{\beta\to\infty}\Delta F=\text{function}(\Delta\tau) \tag{3.2}$$

and

$$\lim_{\beta\to\infty}\Delta\langle\mathcal{O}\rangle=\text{function}(\Delta\tau) \tag{3.3}$$

for a Trotter approximation. For an expansion of $e^{-(\Delta\tau)H}$ in powers of $(\Delta\tau)H$, we will show that

$$\lim_{\beta\to\infty}\Delta F=\text{function}(\Delta\tau) \tag{3.4}$$

and, for sufficiently small $\Delta\tau$,

$$\lim_{\beta\to\infty}\Delta\langle\mathcal{O}\rangle=0\ . \tag{3.5}$$

The functions of $\Delta\tau$ in Eqs. (3.2)–(3.4) all vanish as $\Delta\tau\to 0$, and we will note without explicit demonstration that the general behavior of $\Delta\langle\mathcal{O}'\rangle$ follows the behavior of ΔF in both of the above cases.

We begin by treating Trotter approximations, assuming initially that all relevant operators are represented by real matrices in an arbitrary representation. In this representation, we consider the eigenvalues and eigenvectors of $f^{(n)}$, denoting the eigenvalues of $f^{(n)}$ by $\lambda_i^{(n)}$. We remind the reader that $f^{(n)}$ is an approximation to $e^{-(\Delta\tau)H}$. As

before for the operator H, we assume that the eigenvectors of $f^{(n)}$ are nondegenerate, as results are the same in the case of degeneracies.

Now, $f^{(n)}$ will be real representable; however, it will not, in general, be Hermitian. Thus, the eigenvalues $\lambda_i^{(n)}$ will not necessarily be real, though complex eigenvalues must come in complex conjugate pairs. We denote the eigenvalue of $f^{(n)}$ with greatest magnitude as $\lambda_{i\max}^{(n)}$, and we assume that there is only one such eigenvalue. We further assume that $\lambda_{i\max}^{(n)}$ is real and positive. In some situations, both of these assumptions will hold automatically. However, if the eigenvalues of $f^{(n)}$ with greatest magnitude are complex, the imaginary parts can always be made negligibly small by choosing sufficiently small $\Delta\tau$, and the double degeneracy will not change our results.

Since $f^{(n)}$ is not Hermitian, right and left eigenvectors belonging to the same eigenvalue are not necessarily the same. However, eigenvectors can be normalized so that, if $\mathscr{M}$ is the matrix of right eigenvectors, then $\mathscr{M}^{-1}$ is the matrix of left eigenvectors. Thus, we find that

$$\lim_{\beta\to\infty} F_{\text{approx}} = \lim_{\beta\to\infty}\left[-\frac{1}{\beta}\right]\ln(\mathrm{Tr}\{(\mathscr{M}^{-1})[(f^{(n)})^{\beta/\Delta\tau}](\mathscr{M})\}) \tag{3.6}$$

$$= \lim_{\beta\to\infty}\left[-\frac{1}{\beta}\right]\ln\left[\sum_{i=1}^{N_S}(\lambda_i^{(n)})^{\beta/\Delta\tau}\right] \tag{3.7}$$

$$= -\frac{\ln(\lambda_{i\max}^{(n)})}{\Delta\tau}\,, \tag{3.8}$$

where N_S is the number of independent states of the system characterized by H. Similarly,

$$\lim_{\beta\to\infty}\langle\mathscr{O}\rangle_{\text{approx}} = \lim_{\beta\to\infty}\frac{\mathrm{Tr}\{[(\mathscr{M}^{-1})\mathscr{O}(\mathscr{M})][(\mathscr{M}^{-1})(f^{(n)})^{\beta/\Delta\tau}(\mathscr{M})]\}}{\mathrm{Tr}\{(\mathscr{M}^{-1})[(f^{(n)})^{\beta/\Delta\tau}](\mathscr{M})\}} \tag{3.9}$$

$$= \lim_{\beta\to\infty}\frac{\sum_{i=1}^{N_S}\mathscr{O}_{ii}(\lambda_i^{(n)})^{\beta/\Delta\tau}}{\sum_{i=1}^{N_S}(\lambda_i^{(n)})^{\beta/\Delta\tau}} \tag{3.10}$$

$$= \mathscr{O}_{i\max,i\max}\,, \tag{3.11}$$

where the matrix elements $\mathscr{O}_{ij}$ here are those of $\mathscr{O}$ taken in the left- and right-hand representation in which $f^{(n)}$ is diagonal. Since $f^{(n)}$ and $\mathscr{O}$ are simultaneously real representable, $\lim_{\beta\to\infty}\langle\mathscr{O}\rangle_{\text{approx}}$ will always be real, as expected.

Thus, as we approach the ground state,

$$\Delta F \to \text{function}(\Delta\tau) \tag{3.12}$$

and

$$\Delta\langle\mathscr{O}\rangle \to \text{function}(\Delta\tau) \tag{3.13}$$

for a Trotter approximation. The $\Delta\tau$ dependence of the errors is due to the implicit $\Delta\tau$ dependence of $f^{(n)}$ and hence, $\lambda_{i\max}^{(n)}$ and the right and left eigenstates corresponding to it.

We now note, since

$$C_{\text{approx}} = \beta^2[\langle H^2\rangle_{\text{approx}} - (\langle H\rangle_{\text{approx}})^2] \tag{3.14}$$

that, unless the eigenstate of $f^{(n)}$ corresponding to $\lambda_{i\max}^{(n)}$ is also an eigenstate of H, we expect as $\beta\to\infty$

$$\Delta C = C - C_{\text{approx}} \to \beta^2\text{function}(\Delta\tau)\,. \tag{3.15}$$

Similarly, since

$$\chi_{M,\text{approx}} = \beta[\langle(\mathbf{M})^2\rangle_{\text{approx}} - (\langle\mathbf{M}\rangle_{\text{approx}})^2]\,, \tag{3.16}$$

assuming $\mathbf{M}$ commutes with H, we expect, unless the eigenstate of $f^{(n)}$ corresponding to $\lambda_{i\max}^{(n)}$ is also an eigenstate of $\mathbf{M}$, that as $\beta\to\infty$

$$\Delta\chi_M = \chi_M - \chi_{M,\text{approx}} \to \beta\text{function}(\Delta\tau)\,. \tag{3.17}$$

In other words, ΔC and $\Delta\chi_M$ may diverge as we approach the ground state.

The divergence in the approximate heat capacity, however, will not occur if the approximate heat capacity is computed from the slope of $\langle H\rangle_{\text{approx}}$ versus $k_BT = 1/\beta$, assuming here that $\Delta\tau$ is held constant. Denoting the heat capacity so computed by C''_{approx}, one has then that

$$\lim_{\beta\to\infty} C''_{\text{approx}} = \lim_{\beta\to\infty}\beta^2\frac{\partial}{\partial\beta}(\langle H\rangle_{\text{approx}}) \tag{3.18}$$

$$= 0\,, \tag{3.19}$$

so that

$$\lim_{\beta\to\infty}\Delta C'' = \lim_{\beta\to\infty}(C - C''_{\text{approx}}) = 0\,. \tag{3.20}$$

The divergence also will not occur if C'_{approx} is used instead of C_{approx}. In analogy to the limit for C''_{approx}, one has that

$$\lim_{\beta\to\infty}\Delta C'=0\ . \tag{3.21}$$

However, if one regraphs $\Delta C'$ versus β for constant $\Delta\tau$, the data from Figs. 12 and 15 of Ref. 17 indicate that, even in this case, a large peak in $\Delta C'$ may occur at low but finite temperatures for a given $\Delta\tau$.

Suppose alternatively that we now expand $e^{-(\Delta\tau)H}$ in powers of $(\Delta\tau)H$. In this case, from Eq. (1.7),

$$\lambda_i^{(n)}=\sum_{k=0}^{n}\frac{1}{(k!)}[-(\Delta\tau)E_i]^k\ , \tag{3.22}$$

where the E_i's are the eigenvalues of H and the eigenstate of $f^{(n)}$ corresponding to $\lambda_i^{(n)}$ is the same as the eigenstate of H corresponding to E_i. We note that, here, the $\lambda_n^{(i)}$'s will always be real. As before, we define $\lambda_{i\max}^{(n)}$ to be the eigenvalue of $f^{(n)}$ with greatest magnitude, and we assume that there is only one such eigenvalue and that it is positive. Then, we obtain in analogy to Eqs. (3.6)—(3.11)

$$\lim_{\beta\to\infty}F_{\text{approx}}=-\frac{\ln(\lambda_{i\max}^{(n)})}{\Delta\tau} \tag{3.23}$$

and

$$\lim_{\beta\to\infty}\langle\mathcal{O}\rangle_{\text{approx}}=\mathcal{O}_{i\max,i\max}\ , \tag{3.24}$$

where the matrix elements $\mathcal{O}_{ij}$ are now taken in a representation in which H is diagonal.

Thus, the ground-state value of $\langle\mathcal{O}\rangle_{\text{approx}}$ will be the value of $\langle\mathcal{O}\rangle$ in whatever energy eigenstate corresponds to $\lambda_{i\max}^{(n)}$. For $\Delta\tau$ sufficiently small, this will be the true ground state; alternatively, one can always add a sufficiently large negative constant to H so that the true ground state is again selected.

IV. DEPENDENCE ON SIZE

We reemphasize now that we are dealing with a finite lattice, where operators are defined only at lattice sites. We define a local operator $\mathcal{B}_i$ as

$$\mathcal{B}_i=\sum_{\{j\}}a_jb_{ij}\ , \tag{4.1}$$

where the a_j's are constants, b_{ij} is a sum of operators which are only defined at sites i and j, and $\{j\}$ is a finite set independent of lattice size. We define an order-N operator $\mathcal{O}$ as

$$\mathcal{O}=\sum_{i=1}^{N}\mathcal{B}_i\ , \tag{4.2}$$

where N is the number of lattice sites. We assume periodic boundary conditions for simplicity, though our results can be shown to be independent of the specific boundary conditions chosen. We also assume that we are not near a phase transition, though, again, results can be made more general. Lastly, we assume that the Hamiltonian H is an order-N operator; i.e., all interactions are of finite range. Then, average energy per site, correlation functions, etc., are expectation values of local operators; total energy, total spin, etc., are expectation values of order-N operators.

We hold $\Delta\tau$ and β fixed. We will show then that, if a Trotter approximation is used, the error in the free energy per site and in the expectation values of local operators is independent of lattice size in the large-N limit. We will next observe that if an expansion of $e^{-(\Delta\tau)H}$ in powers of $(\Delta\tau)H$ is used, $\Delta\tau$ must be chosen smaller for larger lattices. Thus, we find that a Trotter approximation is better suited to exploring larger systems than an expansion of $e^{-(\Delta\tau)H}$ in powers of $(\Delta\tau)H$.

We begin by considering an order-N operator $\mathcal{O}$ defined on a block of $2N$ sites, so that

$$\mathcal{O}=\sum_{i=1}^{2N}\mathcal{B}_i\ . \tag{4.3}$$

We decompose this operator into the sum of two operators

$$\mathcal{O}=\mathcal{O}^{(1)}+\mathcal{O}^{(2)}\ , \tag{4.4}$$

where

$$\mathcal{O}^{(1)}=\sum_{i=1}^{N}\mathcal{B}_i \tag{4.5}$$

and

$$\mathcal{O}^{(2)}=\sum_{i=N+1}^{2N}\mathcal{B}_i\ . \tag{4.6}$$

We then look at the commutator $[\mathcal{O}^{(1)},\mathcal{O}^{(2)}]$.

For sufficiently large N, the number of terms contributing to this commutator will be proportional to the interface "area" of the two blocks of size N, and we see that $[\mathcal{O}^{(1)},\mathcal{O}^{(2)}]$ is of order $N^{(D-1)/D}$, where D is the dimensionality of the blocks. Thus, as $N\to\infty$, we can effectively write

$$\frac{1}{N}[\mathcal{O}^{(1)},\mathcal{O}^{(2)}]\to 0\ . \tag{4.7}$$

This means that commutators of order-N operators from different blocks may be neglected in comparison with the order-N block operators themselves for large N and is, of course, simply in the spirit of neglecting boundary effects in the thermodynamic limit.

We then apply this result to the calculation of approximate partition functions and operator expectation values. To do so, we decompose a Hamiltonian H defined on a lattice of size $2N$ into two Hamiltonians $H^{(1)}$ and $H^{(2)}$ which correspond, within boundary effects, to two independent lattice blocks of size N. In analogy to Eq. (4.4), we have

$$H=H^{(1)}+H^{(2)}\ . \tag{4.8}$$

We now use a first-order Trotter approximation [see Eq. (1.4)]. Neglecting commutators of order-N operators from the two blocks and making the approximation of tracing over the two blocks independently, we obtain

$$Z_{\text{approx}}=\mathrm{Tr}\left[\prod_{l=1}^{L}\left[\prod_{m=1}^{M}e^{-(\Delta\tau)H_m}\right]\right] \tag{4.9}$$

$$=\mathrm{Tr}\left[\prod_{l=1}^{L}\left[\prod_{m=1}^{M}e^{-(\Delta\tau)(H_m^{(1)}+H_m^{(2)})}\right]\right] \tag{4.10}$$

$$\approx\left\{\mathrm{Tr}\left[\prod_{l=1}^{L}\left[\prod_{m=1}^{M}e^{-(\Delta\tau)H_m^{(1)}}\right]\right]\right\}\left\{\mathrm{Tr}\left[\prod_{l=1}^{L}\left[\prod_{m=1}^{M}e^{-(\Delta\tau)H_m^{(2)}}\right]\right]\right\} \tag{4.11}$$

$$=Z^{(1)}_{\text{approx}}Z^{(2)}_{\text{approx}}\ . \tag{4.12}$$

We note that this result is analogous to the case in which no Trotter approximation is used, where

$$Z=\mathrm{Tr}(e^{-\beta(H^{(1)}+H^{(2)})}) \tag{4.13}$$

$$=\mathrm{Tr}\left[\prod_{l=1}^{L}e^{-(\Delta\tau)(H^{(1)}+H^{(2)})}\right] \tag{4.14}$$

$$\approx\left[\mathrm{Tr}\left[\prod_{l=1}^{L}e^{-(\Delta\tau)H^{(1)}}\right]\right]\left[\mathrm{Tr}\left[\prod_{l=1}^{L}e^{-(\Delta\tau)H^{(2)}}\right]\right] \tag{4.15}$$

$$=Z^{(1)}Z^{(2)}\ . \tag{4.16}$$

Therefore, for a first-order Trotter approximation,

$$F_{\text{approx}}\approx F^{(1)}_{\text{approx}}+F^{(2)}_{\text{approx}}\ . \tag{4.17}$$

Similarly, one finds that

$$\langle\mathcal{O}\rangle_{\text{approx}}\approx\langle\mathcal{O}\rangle^{(1)}_{\text{approx}}+\langle\mathcal{O}\rangle^{(2)}_{\text{approx}} \tag{4.18}$$

and

$$\langle\mathcal{O}'\rangle_{\text{approx}}\approx\langle\mathcal{O}'\rangle^{(1)}_{\text{approx}}+\langle\mathcal{O}'\rangle^{(2)}_{\text{approx}}\ . \tag{4.19}$$

Thus, the approximate free energy and the approximate expectation values of order-N operators scale linearly with lattice size when a first-order Trotter approximation is used.

We now note that in a system of N sites, a local operator from one site i will commute with all but a finite number of local operators from other sites, where that number becomes independent of N for N large if we are not near the system boundary. As we are concerned with the large-N limit, we ignore boundary effects, as usual. Thus, we see that the commutator of two order-N operators each defined in the same system of N sites is itself an order-N operator in the large-N limit.

We can use this fact to extend the above size scaling result for a first-order Trotter approximation to the higher-order $M=2$ approximants formulated by Suzuki[2]

$$f^{(n)}=e^{-(\Delta\tau)H_1}e^{-(\Delta\tau)H_2}\prod_{k=1}^{n-1}e^{-[(\Delta\tau)^{k+1}\mathcal{D}_k]} \tag{4.20}$$

$$=e^{-\Delta\tau(H_1+H_2)}+O((\Delta\tau)^{n+1})\ . \tag{4.21}$$

These are approximations to the infinite-product Zassenhaus formula,[18] which we write as

$$e^{-(\Delta\tau)(H_1+H_2)}=e^{-(\Delta\tau)H_1}e^{-(\Delta\tau)H_2}\times\prod_{k=1}^{\infty}e^{-[(\Delta\tau)^{k+1}\mathcal{D}_k]}\ . \tag{4.22}$$

Since each $\mathcal{D}_k$ in the Zassenhaus formula is an order-N operator, being a commutator of order-N operators, we see that these Suzuki approximants can all be written in a form analogous to that of a first-order Trotter approximation,

$$f^{(n)}=\prod_{m=1}^{M'}e^{-(\Delta\tau)H_m}+O(\Delta\tau)^{n+1}\ . \tag{4.23}$$

The H_m here, though not necessarily Hermitian, will all be order N. The generalization of Eq. (4.20) to $M>2$ is straightforward, and we find that similar results hold for the Hermitian approximants of De Raedt and De Raedt.[5]

Thus, if any Trotter approximation is used, F_{approx}, $\langle\mathcal{O}\rangle_{\text{approx}}$, and $\langle\mathcal{O}'\rangle_{\text{approx}}$ scale with the size of the lattice, and, in the large-N limit, the error in the free energy per site

$$\Delta f_i=\left[\frac{1}{N}\right](\Delta F) \tag{4.24}$$

and in the expectation values of local operators

$$\Delta\langle\mathcal{B}_i\rangle=\left[\frac{1}{N}\right](\Delta\langle\mathcal{O}\rangle) \tag{4.25}$$

or

$$\Delta\langle\mathcal{B}_i'\rangle=\left[\frac{1}{N}\right](\Delta\langle\mathcal{O}'\rangle) \tag{4.26}$$

will be independent of the lattice size for a given β and $\Delta\tau$. This will be true individually for each term in an expansion of the error in powers of $\Delta\tau$; it can be shown, for example, to hold for the approximation through order $(\Delta\tau)^2$ given in Eq. (2.8). Thus, $\Delta\tau$ may be chosen independently of lattice size for large lattices.

We note that this result is in disagreement with a conclusion of Ref. 19, which was based numerically on one-dimensional quantum spin chains which were apparently not long enough to exhibit the limiting large-N behavior. It answers the question posed in the more recent Ref. 13, however, as to why the accuracy of results in systems studied in that reference did not seem to deteriorate when the same $\Delta\tau$ was used for lattices of larger size.

Since the approximation

$$[1+(\Delta\tau)\langle\mathscr{D}_1(\beta)\rangle]^{-1}=1-(\Delta\tau)\langle\mathscr{D}_1(\beta)\rangle+O((\Delta\tau)^2) \tag{4.27}$$

was used in Eq. (2.13) and since $\mathscr{D}_1(\beta)$ scales like an order-N operator, it might seem, nevertheless, that $\Delta\tau$ would have to be chosen inversely proportional to lattice size on that basis. However, by the previous argument,

$$\langle\mathscr{O}\rangle_{\text{approx}}\approx\sum_k\langle\mathscr{O}\rangle_{\text{approx},k} \tag{4.28}$$

$$=\sum_k\frac{\langle\mathscr{O}_k\rangle+(\Delta\tau)\langle[\mathscr{D}_1(\beta)]_k\mathscr{O}_k\rangle}{1+(\Delta\tau)\langle[\mathscr{D}_1(\beta)]_k\rangle}\ , \tag{4.29}$$

where the k's refer to sufficiently large blocks. Thus, in order to use an approximation like that of Eq. (4.27), it is only necessary that

$$(\Delta\tau)\langle[\mathscr{D}_1(\beta)]_k\rangle\ll 1 \tag{4.30}$$

for a large enough block that boundary effects with other blocks do not dominate. Similar results hold for higher-order $\Delta\tau$ correction terms.

For comparison, we also consider the approximate expansion

$$f^{(n)}=\sum_{k=0}^{n}\frac{1}{k!}[-(\Delta\tau)H]^k\ . \tag{4.31}$$

In the large-N limit, we note that this expansion will not decouple into a product of operators corresponding to different blocks in the same way that the Trotter approximations did. Since the expansion is in powers of $(\Delta\tau)H$ and since $\langle H\rangle$ scales linearly with N, we conjecture that $\Delta\tau$ should be chosen at least inversely proportional to lattice size if one wishes to keep the error in a local operator constant. In any case, it is clear that a smaller $\Delta\tau$ must be chosen for larger lattices when this approximation is used.

V. NUMERICAL RESULTS

The predicted $(\Delta\tau)^2$ error dependence of F_{approx}, Q'_{approx}, and $\langle H\rangle_{\text{approx}}$ for an $M=2$ Trotter break-up due to the cyclic property of the trace has been supported numerically for a variety of Hamiltonians.[5,7,13,19–21] On the basis of our results for an $M>2$ break-up, we do suggest that, in order to more accurately extrapolate to the $\Delta\tau=0$ limit, the graphs of approximate $\langle H\rangle$ and C versus $\Delta\tau/\beta$ for β constant in Ref. 22 should be replaced by graphs of approximate $\langle H\rangle$ and C versus $[(\Delta\tau)/\beta]^2$. The Hamiltonian studied is the two-dimensional spin-$\frac{1}{2}$ XY Hamiltonian. Although the numerical difference is small in this case, we find that this new extrapolation brings the low-temperature estimate for $\langle H\rangle$ into even closer agreement with the ground-state prediction of Pearson which is cited in that reference.

To our knowledge, only two papers have been published with tabulated numerical results relevant to the $(\Delta\tau)^2$ dependence of $\Delta\langle\mathscr{O}^{(H)}\rangle$ when a first-order Trotter approximation is used with a Hermitian break-up and the cyclic property of the trace is not applicable.[19,23] In Ref. 19, approximate spin correlation functions are calculated and compared with exact values for finite chains of the spin-$\frac{1}{2}$ Heisenberg anti-ferromagnet. In Ref. 23, approximate energy densities and static structure functions are computed for a finite spin-$\frac{1}{2}$ XXZ chain and are then graphed versus $[(\Delta\tau)/\beta]^2$, with β held constant. In both cases, results are consistent with our predictions.

Similarly, there is only one paper of which we are aware with numerical data relevant to the β dependence of ΔC at constant $\Delta\tau$.[24] In this paper, C_{approx} and C are graphed versus β with $\Delta\tau$ constant for the one-dimensional spinless fermion Hamiltonian

$$H=(-t)\sum_i(c_i^+c_{i+1}+c_{i+1}^+c_i)+U\sum_i n_in_{i+1} \tag{5.1}$$

with periodic boundary conditions, with a Monte Carlo technique used to compute C_{approx}. We see no evidence of the low-temperature divergence of ΔC. However, the highest β for which data are taken is $\beta=4$, while the error in C_{approx} is at most of order $(\Delta\tau)^2=0.01$. Thus, we conjecture that the lowest temperature taken may not be low enough for ΔC to be distinguishable in the figure shown.

To further test the predictions for β dependence, non-Hermitian Trotter break-ups, expansions in powers of $(\Delta\tau)H$, and non-Hermitian operators, we used the spin-$\frac{1}{2}$ quantum Hamiltonian first utilized by De Raedt and De Raedt[5]

$$H=-bI-a\delta_x-h\delta_z\ . \tag{5.2}$$

We investigated the Hermitian break-up

$$f=e^{b(\Delta\tau)}e^{a(\Delta\tau)\delta_x}e^{h(\Delta\tau)\delta_z}$$

$$=e^{-(\Delta\tau)H}+O((\Delta\tau)^2)\ , \tag{5.3}$$

the non-Hermitian break-up

$$f=e^{b(\Delta\tau)}e^{[a(\Delta\tau)/2]\delta_+}e^{[a(\Delta\tau)/2]\delta_-}e^{h(\Delta\tau)\delta_z}$$

$$=e^{-(\Delta\tau)H}+O((\Delta\tau)^2)\ , \tag{5.4}$$

and the first-order expansion in $(\Delta\tau)H$

$$f=I+(\Delta\tau)(bI+a\delta_x+h\delta_z)$$

$$=e^{-(\Delta\tau)H}+O((\Delta\tau)^2)\ . \tag{5.5}$$

We computed exact and approximate partition functions and free energies; exact and approximate expectation values of the operators H, δ_z, δ_x, δ_+, and δ_-; and C and C_{approx}.

All predictions concerning $\Delta\tau$ and β dependence were verified for this Hamiltonian if a Trotter approximation was used. In particular, we found that ΔC diverged as β^2 for large β when $\Delta\tau$ was held constant for either of the Trotter approximations.

For an expansion of $e^{-(\Delta\tau)H}$ in powers of $(\Delta\tau)H$, we noted that, for all parameters tested, approximate operator expectation values approached their exact ground state values for β large and $\Delta\tau$ sufficiently small. We did find, however, that very low temperatures were often required to observe the expected large-β dependence.

To test the size scaling predictions of Sec. III for a

Trotter approximation, we studied the one-dimensional periodic spinless fermion Hamiltonian

$$H=-t\sum_{i=1}^{N}(c_i^+c_{i+1}+c_{i+1}^+c_i)\ , \tag{5.6}$$

$$c_{N+1}=c_1\ , \tag{5.7}$$

which is equivalent to the XY model through a Jordan-Wigner transformation, in the grand canonical ensemble. We used a checkerboard break-up[6,25] and compared $\Delta\langle H\rangle$ per site, for a variety of β's, for 6–16 sites in multiples of 2 sites. Predicted results were observed. We have not investigated numerically the size scaling for an expansion of $e^{-(\Delta\tau)H}$ in powers of $(\Delta\tau)H$.

VI. DISCUSSION

We have shown that if we use the simplest first-order Trotter approximant

$$f=\prod_{m=1}^{M}e^{-(\Delta\tau)H_m} \tag{6.1}$$

$$=e^{-(\Delta\tau)H}+O((\Delta\tau)^2)\ , \tag{6.2}$$

where

$$H=\sum_{m=1}^{M}H_m\ , \tag{6.3}$$

and all the H_m are Hermitian (a Hermitian break-up), then the error in the free energy and in the expectation values of Hermitian operators is proportional to $(\Delta\tau)^2$ instead of the expected $\Delta\tau$. We have also shown how this result can be achieved if a non-Hermitian break-up is used. If $\mathcal{O}$ itself is not Hermitian, then $\frac{1}{2}(\mathcal{O}+\mathcal{O}^\dagger)$ can be substituted for $\mathcal{O}$, giving an approximate expectation value of $\mathcal{O}$ which again has an error proportional to $(\Delta\tau)^2$. More complicated Trotter approximants of the form

$$f^{(2)}=e^{-(\Delta\tau)H}+O((\Delta\tau)^3) \tag{6.4}$$

will in general not improve upon this $(\Delta\tau)^2$ error dependence.

We next showed that, if $\Delta\tau$ is held constant and $\beta\to\infty$, then

$$\Delta F\to\text{function}(\Delta\tau) \tag{6.5}$$

and

$$\Delta\langle\mathcal{O}\rangle\to\text{function}(\Delta\tau) \tag{6.6}$$

for a Trotter approximation, where the functions of $\Delta\tau$ vanish as $\Delta\tau\to0$. This means that there should be no intrinsic difficulty in calculating low-temperature expectation values.

Finally, we showed that the error in a local operator is independent of the lattice size for constant $\Delta\tau$ and β if all interactions are of finite range, so that $\Delta\tau$ can be chosen independently of the lattice size. This means that a Trotter approximation is well suited for exploring properties of larger systems.

If a Trotter approximation is used, one can sample a system at fixed β for smaller and smaller values of $\Delta\tau$ until the known dependence on $\Delta\tau$ as $\Delta\tau\to0$ is observed. Of course, larger $\Delta\tau$ can be used in general if the error dependence is $(\Delta\tau)^2$ rather than $\Delta\tau$. One can then extrapolate with confidence to the $\Delta\tau=0$ limit, effectively removing all error due to a Trotter approximation. The references cited indicate that it is not in general necessary to reach prohibitively small values of $\Delta\tau$ before the small-$\Delta\tau$ behavior is observed. Thus, this procedure should be useful when Monte Carlo techniques are combined with the Trotter approximation, as the run time for such algorithms is generally at least proportional to $L=\beta/(\Delta\tau)$.

The main difficulty in this procedure is in computing the low-temperature heat capacity, as mentioned in Secs. IV and V. For constant $\Delta\tau$, we showed that for β large

$$\Delta C(\beta)\to\beta^2\text{function}(\Delta\tau) \tag{6.7}$$

so that

$$C(\beta)_{\text{approx}}\to C(\beta)+\beta^2\text{function}(\Delta\tau)\ , \tag{6.8}$$

where $C(\beta)$ becomes small as β becomes large. Thus, for fixed $\Delta\tau$, the correction to $C(\beta)$ will begin to dominate for a sufficiently large β, unless the terms giving rise to the correction vanish identically.

We suggest that a similar difficulty may also arise in computing susceptibilities. However, to our knowledge, this has not yet been observed.

As mentioned above, errors due to $\Delta\tau$ can be removed with confidence by extrapolation. However, for large β, it may be difficult in practice to isolate the small $C(\beta)$ term in Eq. (6.8). In particular, if Monte Carlo simulations are used, $C(\beta)$ may be buried in statistical noise. Accuracy may be improved by plotting $\langle H\rangle_{\text{approx}}$ versus $k_BT=1/\beta$ for $\Delta\tau$ constant and determining the approximate heat capacity from the slope. Then, as was shown in Sec. III, the approximate heat capacity vanishes as $\beta\to\infty$. However, a small slope may be difficult to see amid the statistical errors of the $\langle H\rangle_{\text{approx}}$ data points.

Two other possibilities for alleviating the heat capacity problem are, first, to use C'_{approx} [see Eq. (1.17)], or, second, to use an expansion of $e^{-(\Delta\tau)H}$ in powers of $(\Delta\tau)H$. In both of these cases, the approximate heat capacity again approaches zero as $\beta\to\infty$ when $\Delta\tau$ is held constant. However, if the $(\Delta\tau)H$ expansion is used, one is limited by the fact that one must choose $\Delta\tau$ smaller for larger lattices, as opposed to a Trotter approximation. In addition, numerical results given in Figs. 12 and 15 of Ref. 17 and in Table I of Ref. 6 suggest that, at least unless β is extremely large, neither method is to be expected to always give significant improvement in the approximate heat capacity.

When one approximates $e^{-(\Delta\tau)H}$ by a power series in $(\Delta\tau)H$, we have shown that, for $\Delta\tau$ sufficiently small, the errors in operator expectation values vanish as one approaches the ground state. However, the size scaling drawbacks of the $(\Delta\tau)H$ expansion approximation make it in general less useful than a Trotter approximation.

ACKNOWLEDGMENTS

The author would like to express his appreciation to J. E. Hirsch for very helpful discussions and comments. He would also like to thank D. L. Cox for referring him to the paper by Wilcox (Ref. 18), and W. D. Toussaint for sharing unpublished data. This work was supported by the National Science Foundation under Grant No. DMR82-07881 and by a grant from the Committee on Research at the University of California at San Diego.

[1]H. F. Trotter, Proc. Am. Math. Soc. **10**, 545 (1959).
[2]M. Suzuki, Commun. Math. Phys. **51**, 183 (1976).
[3]M. Suzuki, Phys. Rev. B **31**, 2957 (1985).
[4]M. Suzuki, J. Math. Phys. **26**, 601 (1985).
[5]H. De Raedt and B. De Raedt, Phys. Rev. A **28**, 3575 (1983).
[6]J. E. Hirsch, R. L. Sugar, D. J. Scalapino, and R. Blankenbecler, Phys. Rev. B **26**, 5033 (1982).
[7]H. Betsuyaku, Phys. Rev. Lett. **53**, 629 (1984).
[8]M. Takahashi and M. Imada, J. Phys. Soc. Jpn. **53**, 3765 (1984).
[9]M. Suzuki, J. Phys. Soc. Jpn. **21**, 2274 (1966).
[10]A. Lagendijk and B. De Raedt, Phys. Rev. Lett. **49**, 602 (1982).
[11]T. Onogi, S. Miyashita, and M. Suzuki, Prog. Theor. Phys. **73**, 833 (1985).
[12]*Monte Carlo Methods in Quantum Problems,* edited by M. Kalos (Reidel, Dordrecht, Holland, 1982), and references therein.
[13]H. De Raedt and A. Lagendijk, Phys. Rep. **127**, 233 (1985), and references therein.
[14]R. P. Feynman, Phys. Rev. **84**, 108 (1951).
[15]This result for Z_{approx} and $\langle \mathcal{O} \rangle_{\text{approx}}$ was presented in an earlier draft of this paper at the Conference on Frontiers of Quantum Monte Carlo at Los Alamos, 1985. Upon learning of it there, M. Suzuki subsequently derived an elegant theorem concerning the evenness of ΔZ and $\Delta\langle \mathcal{O} \rangle$ considered as functions of $\Delta\tau$ under certain conditions. This work was published in Phys. Lett. **113A**, 299 (1985). However, in the case of a first-order Trotter approximation, Suzuki's conditions are a special case of those which we assume when applied to the vanishing of the lowest-order $\Delta\tau$ correction terms of Z_{approx} and $\langle \mathcal{O} \rangle_{\text{approx}}$.
[16]The author is indebted to J. E. Hirsch for bringing this to his attention.
[17]J. J. Cullen and D. P. Landau, Phys. Rev. B **27**, 297 (1983).
[18]R. M. Wilcox, J. Math. Phys. **8**, 962 (1967).
[19]H. De Raedt, A. Lagendijk, and J. Fivez, Z. Phys. B **46**, 261 (1982).
[20]H. De Raedt and A. Lagendijk, J. Stat. Phys. **27**, 731 (1982).
[21]J. E. Hirsch, Phys. Rev. B **28**, 4059 (1983).
[22]H. De Raedt, B. De Raedt, J. Fivez, and A. Lagendijk, Phys. Lett. **104**, 430 (1984).
[23]M. Marcu and A. Wiesler, J. Phys. A **18**, 2479 (1985).
[24]J. E. Hirsch, in *Monte Carlo Methods in Quantum Problems,* edited by M. Kalos (Reidel, Dordrecht, Holland, 1982).
[25]M. Barma and B. S. Shastry, Phys. Rev. B **18**, 3351 (1978).