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Calculation of specific heat and susceptibilities with the use of the Trotter approximation

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The Trotter approximation has been used extensively in quantum Monte Carlo simulations. We consider here different ways of calculating the general zero-field susceptibility χ and the specific heat C when a Trotter approximation is used, deriving analytically the error dependence on the imaginary-time increment $\Delta\tau$ as well as the low-temperature behavior. We find that certain definitions of χ and C exhibit spurious divergences at low temperatures, and suggest the most appropriate ways to extract these quantities. We test our general predictions on two models, and discuss the implications of our results for numerical simulations.

I. INTRODUCTION

Quantum Monte Carlo techniques have come into increasing use in the past few years as a very powerful tool for studying nonperturbative properties of model Hamiltonians.[1-3] Many of these techniques rely on the so-called "Trotter approximation,"[4] which consists of replacing the operator $e^{-\beta H}$ with a form more amenable to numerical simulation,

$$e^{-\beta H}=(e^{-\Delta\tau H})^L \tag{1.1}$$

$$=\lim_{L\to\infty}\left(\prod_{m=1}^{M} e^{-\Delta\tau H_m}\right)^L \tag{1.2}$$

$$\approx\left(\prod_{m=1}^{M} e^{-\Delta\tau H_m}\right)^L \tag{1.3}$$

for L finite, where

$$\Delta\tau=\beta/L \ , \tag{1.4}$$

$$H=\sum_{m=1}^{M} H_m \ , \tag{1.5}$$

and

$$\prod_{m=1}^{M} e^{-\Delta\tau H_m}=e^{-\Delta\tau H}+o((\Delta\tau)^2) \ . \tag{1.6}$$

Here and in the remainder of the paper we will denote any quantity Q calculated using the above Trotter approximation as Q_{tr}. Quantities calculated with no approximation will be denoted Q_{ex}. We will also denote the error made when a Trotter approximation is used by $\Delta Q=Q_{\text{ex}}-Q_{\text{tr}}$.

Trotter-like approximations which are correct to a higher order in $\Delta\tau$ than Eq. (1.6) have also been proposed and used.[5-7] In this paper, we will specifically treat only the first-order approximant given by Eq. (1.6), but we note that our general techniques for the β dependence are easily applied to such higher-order approximants, with the results unchanged. We will also assume that each of the H_m in Eq. (1.2) is a Hermitian operator; i.e., the "Trotter breakup" is Hermitian. Again, results for the β dependence are easily generalized if certain of the H_m are not Hermitian. However, to derive the $\Delta\tau$ dependence in the case of a higher-order approximation or a non-Hermitian breakup, it may be necessary to use the techniques of Ref. 8, rather than those which we use here.

Many of the properties of Trotter-like approximations have already been elucidated.[8,9] However, the dependence of the approximate general zero-field susceptibility χ_{tr} on $\Delta\tau$ for $\Delta\tau$ small has not been rigorously derived, and various anomalies seen in the approximate heat capacity C_{tr} have remained unexplained. For this reason, we explore in detail in this paper the errors in χ_{tr} and C_{tr} which arise due to a Trotter approximation.

After introducing the approximate Hamiltonian $\mathcal{H}$ equivalent to a Trotter breakup, we consider a simple definition of $\chi_{\text{tr}}^{\mathcal{O}}$, the approximate zero-field susceptibility corresponding to an operator $\mathcal{O}$, and show that for constant β the first-order correction in $\Delta\tau$ vanishes, so that

$$\Delta\chi^{\mathcal{O}}=\chi_{\text{ex}}^{\mathcal{O}}-\chi_{\text{tr}}^{\mathcal{O}}=o((\Delta\tau)^2) \ . \tag{1.7}$$

Then, for $\Delta\tau$ held constant, we show how a naive definition of $\chi_{\text{tr}}^{\mathcal{O}}$ may lead to an artificial divergence of $\Delta\chi^{\mathcal{O}}$ linear in β at low temperatures, and show how this divergence can be corrected.

We then focus on different expressions for the approximate heat capacity C_{tr}. We first show that, for constant β, ΔC is of order $(\Delta\tau)^2$ for each of our definitions. Then, for $\Delta\tau$ held constant and β varied, we find two definitions of C_{tr} which lead to no divergence in ΔC at low temperatures; two definitions of C_{tr} which may lead to a divergence in ΔC linear in β at low temperatures; and one definition which may lead to a divergence in ΔC proportional to β^2. We then consider the β dependence of C_{tr} when L rather than $\Delta\tau$ is held constant, and, in particular, explain the "anomalous peak" seen in C_{tr} in such calculations.[10-12]

Not all of our results are new. In particular, the results of Eqs. (3.23) and (4.9) were either derived or noted in Ref. 8. However, we include them here for completeness.

We test our predictions numerically for two systems, the simple spin-$\frac{1}{2}$ model first used by De Raedt and De Raedt[6]

$$H=-a\sigma_x-h\sigma_z\ , \tag{1.8}$$

where σ_x and σ_z are the Pauli spin matrices, and the one-dimensional periodic fermion Hamiltonian

$$H=-t\sum_{i=1}^{N}(c_i^\dagger c_{i+1}+c_{i+1}^\dagger c_i)\ . \tag{1.9}$$

This latter model is of particular interest, both because of its equivalence to the one-dimensional XY model through a Jordan-Wigner transformation and because it frequently appears as the noninteracting limit of the Hamiltonian in the Monte Carlo simulation of interacting fermion systems. By exploring these examples in some detail, we hope clearly to illustrate our general predictions.

We conclude with a summary and a discussion of the implications of our results for numerical simulations.

II. APPROXIMATE HAMILTONIAN

We begin by defining the "approximate Hamiltonian" $\mathcal{H}$ by

$$e^{-\Delta\tau\mathcal{H}}=\prod_{m=1}^{M}e^{-\Delta\tau H_m} \tag{2.1}$$

or, equivalently,

$$\mathcal{H}=-\frac{1}{\Delta\tau}\ln\left[\prod_{m=1}^{M}e^{-\Delta\tau H_m}\right]\ , \tag{2.2}$$

so that

$$e^{-\beta\mathcal{H}}=\left[\prod_{m=1}^{M}e^{-\Delta\tau H_m}\right]^L \tag{2.3}$$

is the unnormalized approximate "density-matrix" operator. Because β and L only enter into Eq. (2.1) in the form $\Delta\tau=\beta/L$, we have

$$\mathcal{H}(\beta,L)=\mathcal{H}\left[\frac{\beta}{L}\right]=\mathcal{H}(\Delta\tau)\ . \tag{2.4}$$

We will assume that $\mathcal{H}$ is diagonalizable; i.e., we assume that the matrix $\mathcal{M}$ of right eigenvectors of $\mathcal{H}$ with respect to any basis is invertible. (This property is, of course, independent of basis.) Because $\mathcal{H}$ is not necessarily Hermitian, right and left eigenvectors of $\mathcal{H}$ corresponding to the same nondegenerate eigenvalue may not be the same. However, under the above assumption, $\mathcal{M}^{-1}$ will be the properly normalized matrix of left eigenvectors of $\mathcal{H}$, so that

$$(\mathcal{M}^{-1}e^{-\beta\mathcal{H}}\mathcal{M})_{ij}=e^{-\beta\varepsilon_i}\delta_{ij}\ , \tag{2.5}$$

where here and in the remainder of the paper we will use ε_i to denote the ith eigenvalue of the approximate Hamiltonian $\mathcal{H}$.

We note that certain of our results may be extended to the case where $\mathcal{H}$ is not diagonalizable. However, as that case has not occurred, to our knowledge, in numerical simulations, we do not treat it here.

Now it has been shown that the operator expansion of $\mathcal{H}(\Delta\tau)$ in powers of $\Delta\tau$, given by the Baker-Campbell-Hausdorff formula,[13] converges for nonzero $\Delta\tau$ sufficiently small.[14] However, little is known about the large-$\Delta\tau$ limit of $\mathcal{H}(\Delta\tau)$, which is the appropriate one in simulations where L is held constant while $\beta\to\infty$. In particular, to our knowledge, it is not known whether the radius of convergence of the $\Delta\tau$ power series for $\mathcal{H}(\Delta\tau)$ is finite or infinite, or even whether $\lim_{\Delta\tau\to\infty}\mathcal{H}(\Delta\tau)$ is well defined.

As we have been unable to analyze the large-$\Delta\tau$ limit of $\mathcal{H}(\Delta\tau)$ in the general case, we consider rather the solvable model of Eq. (1.8). Since the behavior of this admittedly simple model has always reflected that of the general case when a Trotter approximation is used,[8] we hope by studying it to gain some insight into the general large-$\Delta\tau$ behavior of $\mathcal{H}(\Delta\tau)$.

We set

$$e^{-\Delta\tau\mathcal{H}}=e^{-\Delta\tau H_1}e^{-\Delta\tau H_2}\ , \tag{2.6}$$

where $H_1=-a\sigma_x$ and $H_2=-h\sigma_z$. We then use the fact that for an arbitrary diagonalizable operator $\mathcal{P}$,

$$[f(\mathcal{P})]_{ij}=\sum_k\langle i\mid k\rangle_r f(\lambda_k)_l\langle k\mid j\rangle\ , \tag{2.7}$$

where f is some function, the λ_k are the eigenvalues of $\mathcal{P}$, and $\rangle k\mid_r$ and $_l\langle k\mid$ are the normalized right and left eigenvectors of $\mathcal{P}$, respectively. We obtain, choosing $h=a$ for simplicity,

$$\mathcal{H}^{11}(\Delta\tau)=-\mathcal{H}^{22}(\Delta\tau)=\left[-\frac{d}{2\Delta\tau}\right]\left[\frac{c}{b}\right]\ , \tag{2.8}$$

$$\mathcal{H}^{12}(\Delta\tau)=\left[-\frac{d}{2\Delta\tau}\right]\left[\frac{e_-}{b}\right]\ , \tag{2.9}$$

and

$$\mathcal{H}^{21}(\Delta\tau)=\left[-\frac{d}{2\Delta\tau}\right]\left[\frac{e_+}{b}\right]\ , \tag{2.10}$$

where

$$c=\cosh(a\Delta\tau)\ , \tag{2.11}$$

$$s=\sinh(a\Delta\tau)\ , \tag{2.12}$$

$$b=(c^2+1)^{1/2}\ , \tag{2.13}$$

$$e\pm=e^{\pm a\Delta\tau}\ , \tag{2.14}$$

and

$$d=\ln\left[\frac{c^2+sb}{c^2-sb}\right]\ . \tag{2.15}$$

Assuming $a>0$ and taking the limit of $\Delta\tau$ large, we then find that, through $o((e_-)^2)$,

$$\mathcal{H}^{11}(\Delta\tau)=-\mathcal{H}^{22}(\Delta\tau)\approx -2a+\frac{1}{\Delta\tau}[\ln 2-2(1+\ln 2)e_{-}^{2}] , \tag{2.16}$$

$$\mathcal{H}^{12}(\Delta\tau)\approx \frac{1}{\Delta\tau}2(\ln 2)e_{-}^{2} , \tag{2.17}$$

and

$$\mathcal{H}^{21}(\Delta\tau)\approx -4a+\frac{1}{\Delta\tau}[2\ln 2-(4+6\ln 2)e_{-}^{2}] . \tag{2.18}$$

Thus, for this Hamiltonian and Trotter decomposition, we see that $\lim_{\Delta\tau\to\infty}\mathcal{H}(\Delta\tau)$ is well defined, that the leading correction is of $o((\Delta\tau)^{-1})$ (though in this case, at least, the lowest-order effect is simply to change the $\mathcal{H}$ matrix prefactor), and that the radius of convergence of the power series in $\Delta\tau$ for $\mathcal{H}(\Delta\tau)$ is finite. This general behavior is consistent with further numerical and analytic calculations of $\mathcal{H}(\Delta\tau)$ for the case $a\neq h$ and for a different Trotter breakup of the Hamiltonian.

It may be possible, however, that in some cases $\lim_{\Delta\tau\to\infty}\mathcal{H}(\Delta\tau)$ is not a constant operator. For example, if the series for $\mathcal{H}(\Delta\tau)$ is a finite one of order n, then

$$\lim_{\Delta\tau\to\infty}\mathcal{H}(\Delta\tau)=(\Delta\tau)^{n}\mathcal{F} , \tag{2.19}$$

where $\mathcal{F}$ is some constant operator. A similar situation may occur for higher order Trotter-like approximations.[6] However, we conjecture, where noted, that $\lim_{\Delta\tau\to\infty}\mathcal{H}(\Delta\tau)$ is well defined in that it may be written in the general form

$$\lim_{\Delta\tau\to\infty}\mathcal{H}(\Delta\tau)=f(\Delta\tau)\mathcal{F} , \tag{2.20}$$

where $f(\Delta\tau)$ is some function of $\Delta\tau$ and $\mathcal{F}$ is a constant operator.

III. APPROXIMATE SUSCEPTIBILITY

We now consider the error, when a Trotter approximation is used, in the zero-field susceptibility corresponding to a Hermitian operator $\mathcal{O}$,

$$\chi_{\rm ex}^{\mathcal{O}}=\int_0^{\beta}d\tau\langle\mathcal{O}(\tau)\mathcal{O}(0)\rangle_{\rm ex}-\beta\langle\mathcal{O}\rangle_{\rm ex}^{2} , \tag{3.1}$$

where

$$Z_{\rm ex}={\rm Tr}(e^{-\beta H}) , \tag{3.2}$$

$$\langle\mathcal{O}\rangle_{\rm ex}=Z_{\rm ex}^{-1}{\rm Tr}(\mathcal{O}e^{-\beta H}) , \tag{3.3}$$

and

$$\mathcal{O}(\tau)=e^{\tau H}\mathcal{O}e^{-\tau H} . \tag{3.4}$$

For an infinite system, we will assume implicitly that the susceptibility is properly normalized.

We will compare this to the approximation

$$\chi_{\rm tr}^{\mathcal{O}}=\Delta\tau\sum_{l=0}^{L-1}\langle\mathcal{O}(\tau_l)\mathcal{O}(0)\rangle_{\rm tr}-\beta\langle\mathcal{O}\rangle_{\rm tr}^{2} , \tag{3.5}$$

where

$$\tau_l=l\Delta\tau , \tag{3.6}$$

$$Z_{\rm tr}={\rm Tr}(e^{-\beta\mathcal{H}}) , \tag{3.7}$$

$$\langle\mathcal{O}\rangle_{\rm tr}=Z_{\rm tr}^{-1}{\rm Tr}(\mathcal{O}e^{-\beta\mathcal{H}}) , \tag{3.8}$$

and

$$\langle\mathcal{O}(\tau_l)\mathcal{O}(0)\rangle_{\rm tr}=Z_{\rm tr}^{-1}{\rm Tr}[e^{-\beta\mathcal{H}}(e^{\tau_l\mathcal{H}}\mathcal{O}e^{-\tau_l\mathcal{H}})\mathcal{O}] , \tag{3.9}$$

with $\mathcal{H}$ given by Eq. (2.1). We will consider first the case where β is held constant while $\Delta\tau$ small is varied, and then the case where $\Delta\tau$ is held constant while β large is varied.

In the spirit of Ref. 9, we explore the $\Delta\tau$ dependence of $\chi_{\rm tr}(\beta,\Delta\tau)$ for fixed β by considering the evenness of $\chi_{\rm tr}^{\mathcal{O}}$ as a function of $\Delta\tau$. Since $\langle\mathcal{O}\rangle_{\rm tr}$ is already an even function of $\Delta\tau$ under the conditions assumed in this paper, we will need to consider only the first term on the right-hand side of Eq. (3.5).

We begin by noting that the sign of the $\Delta\tau$ prefactor of this first term under the replacement $\Delta\tau\to-\Delta\tau$ with β held constant will not change. The prefactor does not arise directly from the Trotter approximation; rather, it arises from the replacement of the integral $\int_0^{\beta}d\tau$ by the discrete sum $\Delta\tau\sum_{l=0}^{L-1}$. Thus, it is tied to the sign of β.

Then, since $Z_{\rm tr}$ is already an even function of $\Delta\tau$ under our assumed conditions, we need only consider the evenness of the quantities

$$J_l(\beta,\Delta\tau)={\rm Tr}[e^{-\beta\mathcal{H}}(e^{\tau_l\mathcal{H}}\mathcal{O}e^{-\tau_l\mathcal{H}})\mathcal{O}]$$
$$={\rm Tr}\left[\left[\prod_{m=1}^{M}e^{-\Delta\tau H_m}\right]^{(\beta-\tau_l)/\Delta\tau}\mathcal{O}\times\left[\prod_{m=1}^{M}e^{-\Delta\tau H_m}\right]^{\tau_l/\Delta_\tau}\mathcal{O}\right] . \tag{3.10}$$

Again, since $0<\tau_l<\beta$, the sign of τ_l will be unchanged under $\Delta\tau\to-\Delta\tau$.

Now,

$$J_l(\beta,-\Delta\tau)={\rm Tr}\left[\left[\prod_{m=M}^{1}e^{-\Delta\tau H_m}\right]^{(\beta-\tau_l)/\Delta\tau}\mathcal{O}\times\left[\prod_{m=M}^{1}e^{-\Delta\tau H_m}\right]^{\tau_l/\Delta\tau}\mathcal{O}\right] , \tag{3.11}$$

where

$$\prod_{m=M}^{1}e^{-\Delta\tau H_m}=e^{-\Delta\tau H_M}e^{-\Delta\tau H_{M-1}}\cdots e^{-\Delta\tau H_1}$$
$$=\left[\prod_{m=1}^{M}e^{-\Delta\tau H_m}\right]^{\dagger} , \tag{3.12}$$

since each H_m is assumed Hermitian. Thus,

$$J_l(\beta,-\Delta\tau)={\rm Tr}[e^{-\beta\mathcal{H}^{\dagger}}(e^{\tau_l\mathcal{H}^{\dagger}})\mathcal{O}e^{-\tau_l\mathcal{H}^{\dagger}})\mathcal{O}] . \tag{3.13}$$

However, if $J_l(\beta,\Delta\tau)$ is assumed real, as is generally the case in numerical simulations, we also have

$$J_l(\beta,\Delta\tau)=[J_l(\beta,\Delta\tau)]^{*}$$
$$={\rm Tr}[e^{-\beta\mathcal{H}^{\dagger}}(e^{\tau_l\mathcal{H}^{\dagger}}\mathcal{O}e^{-\tau_l\mathcal{H}^{\dagger}})\mathcal{O}] . \tag{3.14}$$

Thus,

$$J_l(\beta,\Delta\tau)=J_l(\beta,-\Delta\tau)\ , \tag{3.15}$$

and, hence, $\chi_{\rm tr}^{\mathcal{O}}(\beta,\Delta\tau)$ is an even function of $\Delta\tau$. Since $\chi_{\rm tr}^{\mathcal{O}}$ and $\chi_{\rm ex}^{\mathcal{O}}$ agree in zeroth order, we then have

$$\Delta\chi^{\mathcal{O}}=o((\Delta\tau)^2) \tag{3.16}$$

for $\Delta\tau$ small.

Two other papers, to our knowledge, have considered the $\Delta\tau$ dependence of $\chi_{\rm tr}^{\mathcal{O}}$. In Ref. 15 it is noted that the authors' definition of the approximate in plane susceptibility is good to order $(\Delta\tau)^2$, and in Ref. 16 it is shown that the given definition of the approximate canonical correlation function, of which the zero-field susceptibility is a special case, is an even function of $\Delta\tau$. However, our definition of $\chi_{\rm tr}^{\mathcal{O}}$ is simpler than that of either reference, particularly for $M>2$; our results are more general than that of Ref. 15; and we do not rely upon an assumed asymptotic expansion, as was done in Ref. 16.

We also note, without proof, that our techniques and results can be extended to the double susceptibility

$$\chi_{\rm ex}^{\mathcal{O}_1\mathcal{O}_2}=\int_0^\beta d\tau\langle\mathcal{O}_1(\tau)\mathcal{O}_2(0)\rangle_{\rm ex}-\beta\langle\mathcal{O}_1\rangle_{\rm ex}\langle\mathcal{O}_2\rangle_{\rm ex} \tag{3.17}$$

with the following definition:

$$\chi_{\rm tr}^{\mathcal{O}_1\mathcal{O}_2}=\Delta\tau\left[\tfrac{1}{2}[\langle\langle\mathcal{O}_1\mathcal{O}_2\rangle_{\rm tr}+\langle\mathcal{O}_2\mathcal{O}_1\rangle_{\rm tr}]+\sum_{l=1}^{L-1}\langle\mathcal{O}_1(\tau_l)\mathcal{O}_2\rangle_{\rm tr}\right]-\beta\langle\mathcal{O}_1\rangle_{\rm tr}\langle\mathcal{O}_2\rangle_{\rm tr}\ , \tag{3.18}$$

where $\mathcal{O}_1$ and $\mathcal{O}_2$ are both Hermitian. If $[\mathcal{O}_1,\mathcal{O}_2]=0$, $[\mathcal{O}_1,\mathcal{H}]=0$, or $[\mathcal{O}_2,\mathcal{H}]=0$, the simpler form

$$\chi_{\rm tr}^{\mathcal{O}_1\mathcal{O}_2}=\Delta\tau\sum_{l=0}^{L-1}\langle\mathcal{O}_1(\tau_1)\mathcal{O}_2(0)\rangle_{\rm tr}-\beta\langle\mathcal{O}_1\rangle_{\rm tr}\langle\mathcal{O}_2\rangle_{\rm tr} \tag{3.19}$$

can be used. Of course, $[\mathcal{O},\mathcal{H}]=0$ if $[\mathcal{O},H_m]=0$ for each H_m.

We now consider the dependence of $\Delta\chi^{\mathcal{O}}$ on β when $\Delta\tau$ is held constant. We first note that, if $[\mathcal{O},H]=0$, the expression for $\chi_{\rm ex}^{\mathcal{O}}$ given by Eq. (3.1) reduces to

$$\chi_{\rm ex}^{\mathcal{O}}=\beta(\langle\mathcal{O}^2\rangle_{\rm ex}-\langle\mathcal{O}\rangle_{\rm ex}^2)\ , \tag{3.20}$$

which might suggest the correspondingly simple form

$$\chi_{{\rm tr}(1)}^{\mathcal{O}}=\beta(\langle\mathcal{O}^2\rangle_{\rm tr}-\langle\mathcal{O}\rangle_{\rm tr}^2)\ . \tag{3.21}$$

However, as mentioned in Ref. 8, if the "ground state" of $\mathcal{H}(\Delta\tau)$ is not an eigenstate of $\mathcal{O}$, then

$$\lim_{\beta\to\infty}(\langle\mathcal{O}^2\rangle_{\rm tr}-\langle\mathcal{O}\rangle_{\rm tr}^2)=f(\Delta\tau)\neq 0 \tag{3.22}$$

in general, so that

$$\lim_{\beta\to\infty}\Delta\chi_{(1)}^{\mathcal{O}}=(\beta)f(\Delta\tau)\ , \tag{3.23}$$

where $f(\Delta\tau)$ is some function of $\Delta\tau$. Thus, using the definition for $\chi_{\rm tr}^{\mathcal{O}}$ given by Eq. (3.21) may lead to an artificial divergence in $\Delta\chi^{\mathcal{O}}$ at low temperatures for constant $\Delta\tau$. If this divergence occurs, it will be corrected by using the definition for $\chi_{\rm tr}^{\mathcal{O}}$ given by Eq. (3.5), except in the unlikely case where the ground state of $\mathcal{H}$ is degenerate and $\mathcal{O}$ has different expectation values within that degenerate subspace. The oppositive situation can of course also occur, with a true divergence being suppressed, if the Trotter approximation breaks the appropriate symmetry of H.

IV. $C_{\rm tr}(\beta,\Delta\tau)$

We now explore the behavior of different definitions of $C_{\rm tr}$. We define five different ways of calculating $C_{\rm tr}$, denoting the different definitions by a right superscript. In the Appendix we show that each of these definitions is an even function of $\Delta\tau$ for constant β, so that

$$\Delta C^{(i)}=o((\Delta\tau)^2) \tag{4.1}$$

in each instance for $\Delta\tau$ sufficiently small. In this section, we consider the behavior of each definition when $\Delta\tau$ is held constant and β large is varied.

We assume that the system we are studying has a discrete spectrum, with a bounded ground state. However, we note without proof that, as long as the density of energy states does not increase faster than exponentially immediately above the ground state, all of our results concerning the β dependence apply to systems with a continuous spectrum as well. For an infinite system, of course, the specific heat rather than the heat capacity must be used.

We begin with $C_{\rm tr}^{(1)}$, which we write as

$$C_{\rm tr}^{(1)}(\beta,\Delta\tau)=\beta^2\frac{\partial^2}{\partial\beta^2}\left[\ln\left\{{\rm Tr}\left[\left[\prod_{m=1}^{M}e^{-\Delta\tau H_m}\right]^{\beta/\Delta\tau}\right]\right\}\right]_{\Delta\tau={\rm const}} \tag{4.2}$$

$$=\beta^2\frac{\partial^2}{\partial\beta^2}\{\ln[{\rm Tr}(e^{-\beta\mathcal{H}(\Delta\tau)})]\}_{\Delta\tau={\rm const}}\ . \tag{4.3}$$

Thus, we see that $C_{\rm tr}^{(1)}$ is the thermodynamic heat capacity determined by the temperature-independent approximate Hamiltonian $\mathcal{H}(\Delta\tau)$. With $\mathcal{H}(\Delta\tau)$ assumed diagonalizable, we then have

$$\lim_{\beta\to\infty} C_{\rm tr}^{(1)}(\beta,\Delta\tau)=0 \ , \tag{4.4}$$

in analogy with the exact case. Unfortunately, this definition is difficult to implement in quantum Monte Carlo simulations, as it involves either calculation of the expectation values of logarithms of operators or calculation of $Z_{\rm tr}(\beta,\Delta\tau)$ at different temperatures.

However, $C_{\rm tr}^{(2)}$, which we write[8,17–19] as

$$C_{\rm tr}^{(2)}(\beta,\Delta\tau)=\frac{\partial}{\partial T}\langle H\rangle_{\rm tr}\Bigg|_{\Delta\tau=\rm const} \ , \tag{4.5}$$

is an alternative definition which is also divergence free. This definition may be implemented by graphing $\langle H\rangle_{\rm tr}$ versus T for $\Delta\tau$ constant and then numerically differentiating.

As in the preceding definition, $\mathcal{H}(\Delta\tau)$ will be temperature independent, so that

$$C_{\rm tr}^{(2)}(\beta,\Delta\tau)=-\beta^2\frac{\partial}{\partial\beta}\left[\frac{{\rm Tr}(He^{-\beta\mathcal{H}(\Delta\tau)})}{{\rm Tr}(e^{-\beta\mathcal{H}(\Delta\tau)})}\right]_{\Delta\tau=\rm const} \tag{4.6}$$

$$=\beta^2(\langle H\mathcal{H}\rangle_{\rm tr}-\langle H\rangle_{\rm tr}\langle\mathcal{H}\rangle_{\rm tr}) \ . \tag{4.7}$$

Working in the right- and left-hand bases in which $\mathcal{H}$ is diagonal, and denoting the eigenvalues of $\mathcal{H}$ by ε_i as before, we obtain

$$\lim_{\beta\to\infty} C_{\rm tr}^{(2)}(\beta,\Delta\tau)=\lim_{\beta\to\infty}\beta^2\left[\frac{\sum_i H_{ii}\varepsilon_i e^{-\beta\varepsilon_i}}{\sum_i e^{-\beta\varepsilon_i}}-\frac{\left[\sum_i H_{ii}e^{-\beta\varepsilon_i}\right]\left[\sum_i \varepsilon_i e^{-\beta\varepsilon_i}\right]}{\left[\sum_i e^{-\beta\varepsilon_i}\right]^2}\right] \tag{4.8}$$

$$=\lim_{\beta\to\infty}\beta^2[(\overline{H}_{00}\varepsilon_0-\overline{H}_{00}\varepsilon_0)+o(e^{-\beta\Delta\varepsilon})]=0 \ . \tag{4.9}$$

Here, $\overline{H}_{00}$ is the expectation value of the operator H in the possibly degenerate ground state of $\mathcal{H}$ and $\Delta\varepsilon>0$ is an "approximate energy" splitting. Thus, there is again no divergence in ΔC.

We now consider a third definition[6,20,21] of $C_{\rm tr}$,

$$C_{\rm tr}^{(3)}(\beta,\Delta\tau)=\beta^2\frac{\partial^2}{\partial\beta^2}\left[\ln\left\{{\rm Tr}\left[\left[\prod_{m=1}^{M}e^{-(\beta/L)H_m}\right]^L\right]\right\}\right]_{L=\rm const} \tag{4.10}$$

$$=\beta^2\frac{\partial^2}{\partial\beta^2}\{\ln[{\rm Tr}(e^{-\beta\mathcal{H}(\beta/L)})]\}_{L=\rm const} \ . \tag{4.11}$$

Because L rather than $\Delta\tau$ is held constant when the β derivatives are taken, $\mathcal{H}$ is now temperature dependent.

We write $\partial/\partial\beta=(1/L)(\partial/\partial\Delta\tau)$ and let primes denote differentiation with respect to $\Delta\tau$. Then, using Eq. (2.1) of Ref. 13 and the cyclic property of the trace, we obtain

$$C_{\rm tr}^{(3)}(\beta,\Delta\tau)=-\beta\langle(\Delta\tau)\mathcal{R}\rangle_{\rm tr}+\beta\chi_{{\rm tr}(2)}^{\mathcal{S}}(\beta,\Delta\tau) \ , \tag{4.12}$$

where

$$\mathcal{R}=2\mathcal{H}'(\Delta\tau)+\Delta\tau\mathcal{H}''(\Delta\tau) \ , \tag{4.13}$$

$$\mathcal{S}=\mathcal{H}(\Delta\tau)+\Delta\tau\mathcal{H}'(\Delta\tau) \ , \tag{4.14}$$

and

$$\chi_{{\rm tr}(2)}^{\mathcal{S}}=\int_0^\beta d\tau\langle\mathcal{S}(\tau)\mathcal{S}(0)\rangle_{\rm tr}-\beta\langle\mathcal{S}\rangle_{\rm tr}^2 \ . \tag{4.15}$$

Now, for $\Delta\tau$ held constant,

$$\lim_{\beta\to\infty}\langle(\Delta\tau)\mathcal{R}\rangle_{\rm tr}=f_1(\Delta\tau) \tag{4.16}$$

and

$$\lim_{\beta\to\infty}\chi_{{\rm tr}(2)}^{\mathcal{S}}(\beta,\Delta\tau)=f_2(\Delta\tau) \ , \tag{4.17}$$

where f_1 and f_2 are some functions of $\Delta\tau$, unless, as mentioned in Sec. III, the ground state of $\mathcal{H}$ is degenerate and $\mathcal{S}$ has different expectation values in that degenerate subspace. Thus, we find, in general, that

$$\lim_{\beta\to\infty} C_{\rm tr}^{(3)}(\beta,\Delta\tau)=(\beta)f(\Delta\tau) \ . \tag{4.18}$$

Next we consider $C_{\rm tr}^{(4)}$, given by

$$C_{\rm tr}^{(4)}(\beta,\Delta\tau)=\beta\left[\Delta\tau\sum_{l=0}^{L-1}\langle H(\tau_l)H(0)\rangle_{\rm tr}-\beta\langle H\rangle_{\rm tr}^2\right] \ . \tag{4.19}$$

This can be written in the form $C_{\rm tr}^{(4)}=\beta\chi_{\rm tr}^H$, where $\chi_{\rm tr}^H$ is the approximate "zero-field" susceptibility corresponding to H given by Eq. (3.5). Because this approximate susceptibility will approach a constant dependent on $\Delta\tau$ as $\beta \to \infty$, except in the unlikely case similar to that mentioned previously for $C_{\rm tr}^{(3)}$, we have

$$\lim_{\beta\to\infty} C_{\rm tr}^{(4)} = (\beta) g(\Delta\tau) , \tag{4.20}$$

where g is some function of $\Delta\tau$, so that $C_{\rm tr}^{(4)}$ has the same type of low-temperature divergence as $C_{\rm tr}^{(3)}$. However, for $M > 2$, the definition of $C_{\rm tr}^{(4)}$ is easier to implement algorithmically than that of $C_{\rm tr}^{(3)}$, since the imaginary time correlations involved are less complicated. This definition might be useful if there were insufficient data or too much statistical scatter to determine $C_{\rm tr}^{(2)}$ accurately, as we discuss in the Conclusion.

Lastly, we consider $C_{\rm tr}^{(5)}$, where[6,17,18]

$$C_{\rm tr}^{(5)}(\beta,\Delta\tau) = \beta^2(\langle H^2\rangle_{\rm tr} - \langle H\rangle_{\rm tr}^2) . \tag{4.21}$$

As noted in Ref. 8, unless the ground state of $\mathcal{H}$ is an eigenstate of H, $C_{\rm tr}^{(5)}$ will diverge as β^2 at low temperature for fixed $\Delta\tau$.

V. $C_{\rm tr}(\beta,L)$

We now discuss the case in which L rather than $\Delta\tau$ is held fixed when $C_{\rm tr}$ is determined for different β. We note that then the effective expansion parameter $\Delta\tau = \beta/L$ becomes infinite in the $\beta \to \infty$ limit, so that the approximation is in that sense uncontrolled. For this reason we consider only $C_{\rm tr}^{(3)}(\beta,L)$, as it is the $C_{\rm tr}$ definition which has been commonly used in the literature[10–12] for fixed L.

We begin by defining an approximate thermodynamic expectation value of the Hamiltonian

$$G(\beta,L) = -\frac{\partial}{\partial\beta}\left[\ln\left\{\mathrm{Tr}\left[\left[\prod_{m=1}^{M} e^{-(\beta/L)H_m}\right]^L\right]\right\}\right]_{L=\rm const} . \tag{5.1}$$

Working on an arbitrary basis, we can always write

$$(e^{-(\beta/L)H_m})_{ij} = \sum_{n=1}^{N_s} a_{ij}^{(n)} e^{-(\beta/L)E_m^n} , \tag{5.2}$$

where a discrete energy spectrum is assumed, with N_s possible states of the system; E_m^n denotes the nth eigenvalue of H_m; and the $a_{ij}^{(n)}$ are independent of β and L. Then, retaining only lowest order terms and assuming that none of the ground states of the H_m are orthogonal to each other, we find for β large

$$G(\beta,L) \approx -\frac{\partial}{\partial\beta}\left[\ln\left\{\kappa_1 \exp\left[-\beta\left[\sum_{m=1}^{M} E_m^0\right]\right][1+L(\kappa_2)e^{-\beta(\Delta E)/L}]\right\}\right] \tag{5.3}$$

$$\approx \sum_{m=1}^{M} E_m^0 + \kappa_2(\Delta E) e^{-\beta\Delta E/L} . \tag{5.4}$$

Here, the right superscript 0 refers to the lowest eigenvalues of the operators H_m, $\Delta E > 0$ is some smallest energy difference, and κ_1 and κ_2 are constants.

A similar argument holds if certain of the ground states of the H_m are orthogonal to each other—one simply picks out the eigenvalues E_m^n of the H_m corresponding to the nonorthogonal set(s) of states which minimize(s) the quantity $\sum_{m=1}^{M} E_m^n$. Thus, this approximate ground-state energy can be written as

$$\lim_{\beta\to\infty} G(\beta,L) = G_0 , \tag{5.5}$$

where G_0 is independent of L.

Then, from Eq. (5.4), we have for β large

$$C_{\rm tr}^{(3)} \approx \kappa_2 \frac{(\beta\Delta E)^2}{L} e^{-\beta\Delta E/L} , \tag{5.6}$$

so that

$$\lim_{\beta\to\infty} C_{\rm tr}^{(3)}(\beta,L) = 0 . \tag{5.7}$$

Thus, $C_{\rm tr}^{(3)}(\beta,L)$ must always return to 0 at sufficiently low temperatures. However, low-temperature "anomalous peaks" have been seen in $C_{\rm tr}^{(3)}(\beta,L)$. We explain these as follows.

The approximate Hamiltonian $\mathcal{H}$ equivalent to a Trotter approximation depends on the effective expansion parameter $\Delta\tau = \beta/L$ only. Thus, when $G(\beta,L)$ is graphed versus T, the resulting curve will follow closely the curve of $\langle H\rangle_{\rm ex}$ until β/L reaches a value of $\Delta\tau$ at which the Trotter approximation is no longer valid. At this point, $G(\beta,L)$ will begin to "crossover" from behavior governed by $\mathcal{H}(0)=H$ to behavior approaching the low-temperature limit G_0. We denote this "crossover" value of $\Delta\tau$ by $(\Delta\tau)_c$.

As L becomes larger and larger, the temperature at which this crossover occurs, given by

$$T_c = \frac{1}{L(\Delta\tau)_c} , \tag{5.8}$$

will become smaller and smaller. However, as $T \to 0$, the graph of $G(\beta,L)$ must always jump to the limiting L-independent ground-state value G_0. Since by making L sufficiently large we can make $\Delta\tau$ very small at all but the lowest temperatures, this will lead to a very steep slope in the graph of $G(\beta,L)$ versus T at low temperatures for large L. This, in turn, will lead to the "anomalous peak" in $C_{\rm tr}^{(3)}$ seen in previous publications, with a height very roughly given for large L by

$$(C_{\rm tr}^{(3)})_{\rm max} \approx L(\Delta\tau)_c(E_0-G_0) \ . \tag{5.9}$$

Thus, for a given system, we predict the "anomalous peak" to occur at temperatures inversely proportional to L and to have a maximum height proportional to L, for L sufficiently large.

We note that we expect behavior qualitatively similar to this for $G(\beta,L)$ to occur for $\langle \mathcal{O} \rangle_{\rm tr}(\beta,L)$, where $\mathcal{O}$ is an arbitrary operator. Assuming $\mathcal{H}(\infty)$ of the form of Eq. (2.20), we will have

$$\lim_{\beta\to\infty} \langle \mathcal{O} \rangle_{\rm tr} = \lim_{\beta\to\infty} \frac{{\rm Tr}(\mathcal{O}e^{-\beta\mathcal{H}(\beta/L)})}{{\rm Tr}(e^{-\beta\mathcal{H}(\beta/L)})} = \overline{\mathcal{O}}_{00} \ , \tag{5.10}$$

where $\overline{\mathcal{O}}_{00}$ is the expectation value of $\mathcal{O}$ in the possibly degenerate ground state of $\mathcal{H}(\infty)$. Thus, there will again be a crossover, from high-temperature behavior governed by $\mathcal{H}(0)=H$ to low-temperature behavior governed by $\mathcal{H}(\infty)$.

This prediction is consistent with most published numerical results. It does appear to be in disagreement with certain graphs of Refs. 11 and 12; however, we conjecture that the lowest temperature in the references ($T=0.05$) was not low enough to obtain the true $\beta\to\infty$ limit in those cases.

Finally, if E_0 and G_0 are the same, there will be no crossover behavior for $G(\beta,L)$ and, hence, no "anomalous peak" in $C_{\rm tr}^{(3)}(\beta,L)$. This will occur, for example, if H and each of the H_m have common ground states. This prediction is consistent with numerical results for the spin-$\frac{1}{2}$ ferromagnetic Heisenberg model.[10,12,22]

VI. NUMERICAL RESULTS

To illustrate these general remarks, we considered two test Hamiltonians. The first is the model used in Ref. 6,

$$H=-a\sigma_x - h\sigma_z \ , \tag{6.1}$$

where σ_x and σ_z are Pauli spin matrices, with the Trotter breakup

$$e^{-\Delta\tau H} \approx e^{a\,\Delta\tau\sigma_x} e^{h\,\Delta\tau\sigma_z} \ . \tag{6.2}$$

The approximate Hamiltonian $\mathcal{H}(\Delta\tau)$ can be calculated exactly for this case [see Eqs. (2.8)–(2.15)], as well as the approximate partition function.[6] Thus, all five definitions of $C_{\rm tr}$ are easily implementable. All numerical results for $C_{\rm tr}$ were in agreement with predictions. As the graphs obtained are qualitatively similar to those of the second, less trivial, model which we consider, we only present and discuss graphs for the second model.

The second model is given by the Hamiltonian

$$H=(-t)\sum_{i=1}^{N}(c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}) \ , \tag{6.3}$$

with the periodic boundary conditions $c_{N+1}=c_1$. $c_i^\dagger$ and c_i are the creation and annihilation operators, respectively, of a fermion at site i, and N is the number of spatial lattice sites. It is interesting to consider this Hamiltonian for several reasons. The first is that it is the noninteracting limit of many numerical simulations reported in the literature.[1–3] Secondly, as mentioned previously, it is equivalent to the XY model through a Jordan-Wigner transformation. Third, in the continuum limit, there is no gap in the energy spectrum for this model, so that $C_{\rm ex}$ goes to zero linearly in T as T approaches zero. This is quite different from the exponential behavior of the spin model of Eq. (6.1), which has a finite gap. Of course, for any finite N there is a Schottky-like effect due to the opening of a finite-size gap.

The exact partition function, energy, and specific heat are given by

$$Z_{\rm ex}=\prod_k (1+e^{-\beta\varepsilon_k}) \ , \tag{6.4}$$

$$\langle H \rangle_{\rm ex}=\sum_k \frac{\varepsilon_k}{1+e^{-\beta\varepsilon k}} \ , \tag{6.5}$$

and

$$C_{ex}=\beta^2\sum_k \frac{\varepsilon_k^2 e^{-\beta\varepsilon_k}}{(1+e^{-\beta\varepsilon_k})^2} \ , \tag{6.6}$$

where

$$\varepsilon_k=-2t\cos k \tag{6.7}$$

and the discrete allowed k values are

$$k=\frac{2\pi}{N}\left\{-\frac{N}{2},-\frac{N}{2}+1,\ldots,\frac{N}{2}-1\right\}$$

for finite N. In the $N\to\infty$ limit, k ranges continuously over $(-\pi,\pi)$ and the sums are replaced by integrals. In this continuum limit, the low-temperature behavior is, setting $t=1$ here for simplicity,

$$\frac{1}{N}\langle H \rangle_{\rm ex}=\frac{-2}{\pi}+\frac{\pi}{12}T^2+o(T^3) \tag{6.8}$$

and

$$\frac{1}{N}C_{\rm ex}=\frac{\pi}{6}T+o(T^2) \ . \tag{6.9}$$

For finite N, Eqs. (6.7) hold only for $T>2\pi/N$. For $T<2\pi/N$, $C_{\rm ex}$ goes exponentially to zero.

To consider the Trotter case, we divide the Hamiltonian via the "checkerboard breakup"[23,24]

$$e^{-\Delta\tau H}\approx e^{-\Delta\tau H_1}e^{-\Delta\tau H_2} \ , \tag{6.10}$$

where

$$H_1=(-t)\sum_{i\ {\rm odd}}(c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}) \tag{6.11}$$

and

$$H_2=(-t)\sum_{i\ {\rm even}}(c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}) \ . \tag{6.12}$$

We then find the analytic form

$$Z_{\rm tr}=\prod_k (1+\lambda_{k+}^L)(1+\lambda_{k-}^L) \ , \tag{6.13}$$

where

$$\lambda_{k\pm}=1+2x^2\pm 2x(1+x^2)^{1/2} \tag{6.14}$$

and

$$x=\sinh(t\,\Delta\tau)\cos k \ . \tag{6.15}$$

The momentum k now runs over the reduced zone $(-\pi/2, \pi/2)$. For finite N,

$$k=\frac{2\pi}{N}\left[-\frac{N}{4}, \frac{N}{4}+1, \ldots, \frac{N}{4}-1\right] .$$

With this expression, we can calculate $C_{\rm tr}^{(1)}$, $C_{\rm tr}^{(3)}$, and also $C_{\rm tr}^{(2)}$, since

$$\langle H\rangle_{\rm tr}=-\frac{\partial}{\partial\beta}[\ln(Z_{\rm tr})]_{L=\rm const} \tag{6.16}$$

with $M=2$ [see Eq. (1.2)]. Comparing Eqs. (5.1) and (6.16), we also see that, for $M=2$,

$$\langle H\rangle_{\rm tr}(\beta,L)=G(\beta,L) \ . \tag{6.17}$$

Choosing $C_{\rm tr}^{(3)}$ as an illustration, and denoting $\lambda'=d\lambda/d\,\Delta\tau$ and $\lambda''=d^2\lambda/(d\,\Delta\tau)^2$, we have

$$\langle H\rangle_{\rm tr}=-\sum_{k,\mu=\pm}\frac{\lambda_{k\mu}^{(L-1)}\lambda'_{k\mu}}{(1+\lambda_{k\mu}^L)} \tag{6.18}$$

and

$$C_{\rm tr}^{(3)}=L(\Delta\tau)^2\sum_{k,\mu=\pm}\left[\frac{\lambda_{k\mu}^{(L-2)}}{(1+\lambda_{k\mu}^L)}\right]\times\left[(L-1)(\lambda'_{k\mu})^2+\lambda_{k\mu}\lambda''_{k\mu}-\frac{L\lambda_{k\mu}^L}{(1+\lambda_{k\mu}^L)}(\lambda'_{k\mu})^2\right] . \tag{6.19}$$

For small $\Delta\tau$, we find

$$\langle H\rangle_{\rm tr}\approx -2t\sum_k \cos k-4t^3(\Delta\tau)^2\sum_k(\cos k-\cos^3 k) \tag{6.20}$$

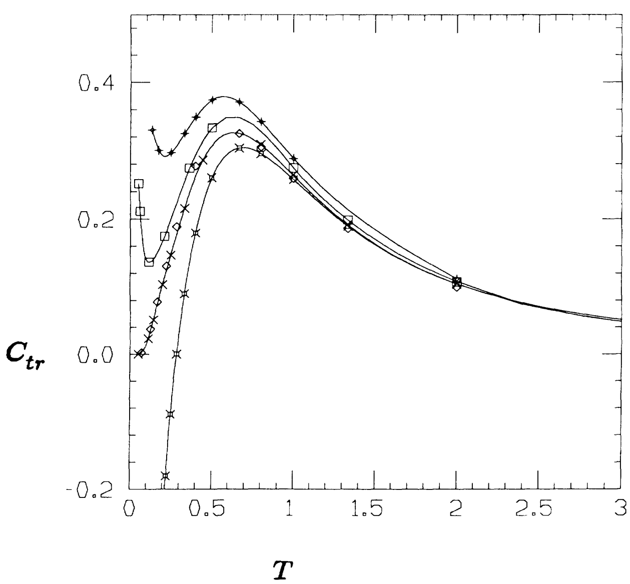

FIG. 1. Results for the five definitions $C_{\rm tr}^{(1)}$ (diamond), $C_{\rm tr}^{(2)}$ (cross), $C_{\rm tr}^{(3)}$ (square), $C_{\rm tr}^{(4)}$ (open-centered plus), and $C_{\rm tr}^{(5)}$ (open-centered cross) are shown as a function of temperature for $t=1$ and fixed $\Delta\tau=\frac{1}{4}$. Lines are drawn as a guide to the eye. $C_{\rm tr}^{(1)}$ and $C_{\rm tr}^{(2)}$ follow the exact heat capacity for all temperatures. $C_{\rm tr}^{(3)}$ and $C_{\rm tr}^{(4)}$ diverge to $+\infty$ as $T\to 0$, while $C_{\rm tr}^{(5)}$ diverges to $-\infty$ as $T\to 0$. Note: In this and the other figures, all graphed energies and heat capacities are normalized to per-site values.

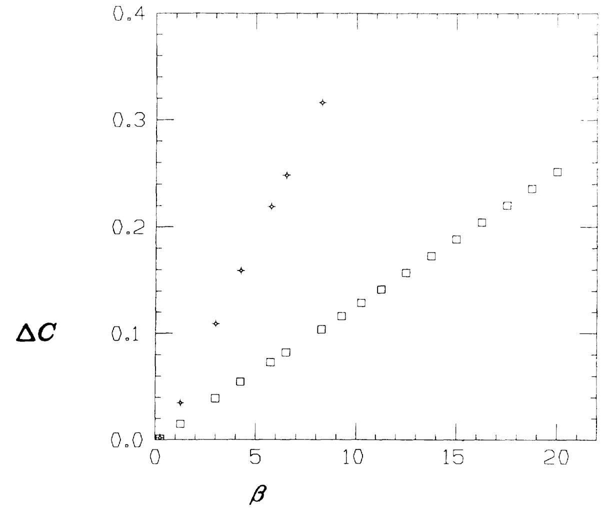

FIG. 2. Results for $C_{\rm tr}^{(3)}$ (square) and $C_{\rm tr}^{(4)}$ (open-centered plus) are shown for fixed $\Delta\tau$ as a function of β. It is seen that these two definitions diverge linearly in β as $\beta\to\infty$.

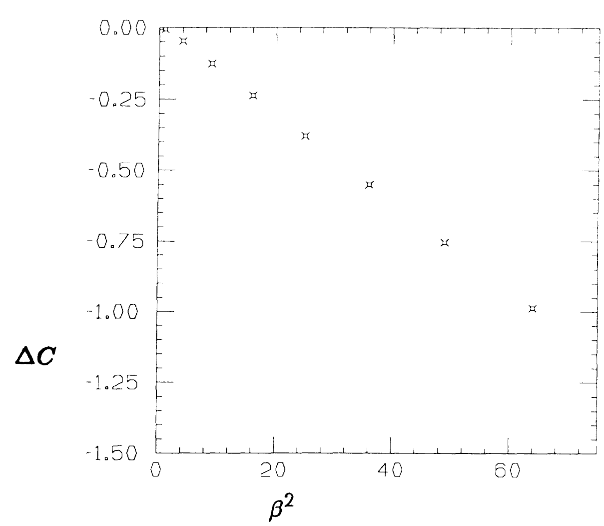

FIG. 3. Results for $C_{\rm tr}^{(5)}$ are shown for fixed $\Delta\tau$ as a function of β^2. It is seen that this definition diverges linearly in β^2 as $\beta\to\infty$.

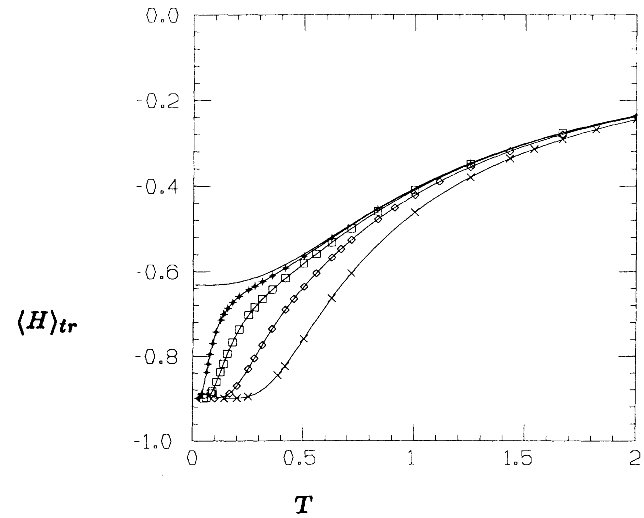

FIG. 4. The exact energy $\langle H\rangle_{ex}$ as a function of temperature T is shown as the curve without data points. Data for $\langle H\rangle_{tr}$ are shown for different fixed $L=1$ (cross), 2 (diamond), 4 (square), and 8 (open-centered plus). Lines are drawn as a guide to the eye. As L increases, $\langle H\rangle_{tr}$ follows $\langle H\rangle_{ex}$ to lower temperatures, but then must make the crossover to the $\Delta\tau=\infty$ value in an increasingly small temperature interval.

and

$$C_{tr}^{(3)} \approx 2\beta t (t\Delta\tau)^2 \sum_k (\cos k - \cos^3 k) . \tag{6.21}$$

In the continuum limit, we convert the sum into an integral and obtain

$$\frac{1}{N} C_{tr}^{(3)} \approx \frac{2}{3\pi} \beta t^3 (\Delta\tau)^2 . \tag{6.22}$$

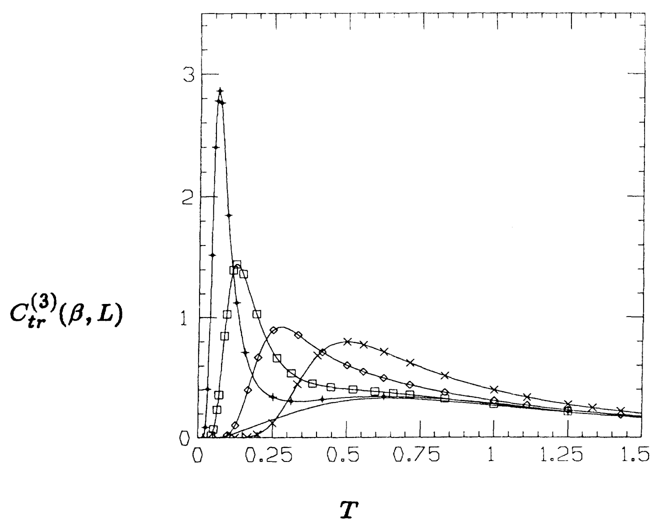

FIG. 5. The exact heat capacity as a function of temperature T is shown as the curve without data points. Data for $C_{tr}^{(3)}$ are shown for different fixed $L=1$ (cross), 2 (diamond), 4 (square), and 8 (open-centered plus). Lines are drawn through the values for $C_{tr}^{(3)}$ as a guide to the eye. There is an anomalous peak in $C_{tr}^{(3)}$ associated with the crossover of Fig. 4 which becomes higher and shifts to lower temperatures as L increases.

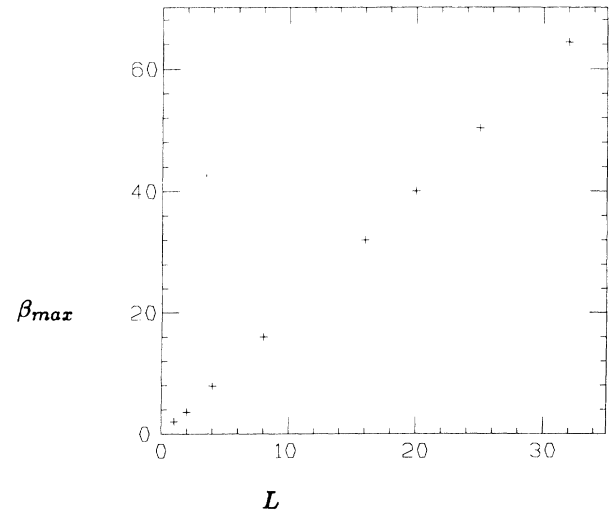

FIG. 6. The position β_{max} of the anomalous peak in $C_{tr}^{(3)}$ is shown for different L.

Thus, $C_{tr}^{(3)}$, properly normalized, diverges linearly with β at low temperatures for small fixed $\Delta\tau$ regardless of whether N is finite or infinite, as predicted.

To compute $C_{tr}^{(4)}$, we use the relation, valid for $M=2$,

$$C_{tr}^{(4)} = C_{tr}^{(3)} + \beta\Delta\tau \langle [H_1, H_2] \rangle_{tr} , \tag{6.23}$$

and compute $\langle [H_1,H_2]\rangle_{tr}$ by the determinantal method.[25] Similarly, for $C_{tr}^{(5)}$, we also compute $\langle H^2\rangle_{tr}$ by the determinantal method.

We consider first the behavior of the heat capacity for fixed $\Delta\tau$. The hopping parameter $t=1$, $\Delta\tau=0.25$, and there are 20 spatial lattice sites. In Fig. 1 we show the five

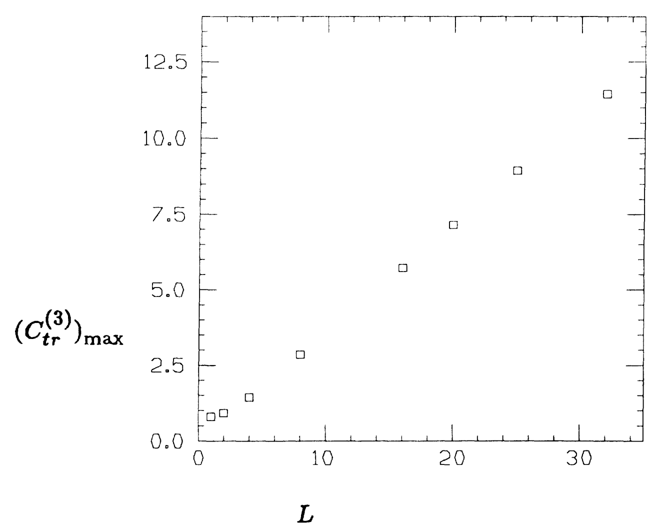

FIG. 7. The maximum peak height of $C_{tr}^{(3)}$ is shown for different L.

definitions $C_{\rm tr}^{(i)}$ for $i=1,2,\ldots,5$ as a function of temperature. At low temperatures $C_{\rm tr}^{(3)}$, $C_{\rm tr}^{(4)}$, and $C_{\rm tr}^{(5)}$ diverge. In Fig. 2 we plot $\Delta C_{\rm tr}^{(3)}$ and $\Delta C_{\rm tr}^{(4)}$ versus β and see that the deviation is linear in β, in agreement with Eqs. (4.18) and (4.20). We note that the slope of $\Delta C_{\rm tr}^{(3)}$ in this graph is in reasonable agreement with the continuum value of Eq. (6.21). In Fig. 3 we show $\Delta C_{\rm tr}^{(5)}$ versus β^2.

Next we turn to the study of the behavior of the energy and heat capacity at fixed L. In Fig. 4 we plot the approximate energy $\langle H\rangle_{\rm tr}$ [see Eq. (6.17)] versus temperature T for different L. This illustrates our picture of the origin of the anomalous peak in the specific heat, also seen graphically in other publications,[10–12] since we clearly see the crossover behavior described in Sec. V. Figure 5 gives $C_{\rm tr}^{(3)}$ versus temperature T for fixed L. Data for $L=1$, 2, 4, and 8 are shown. As expected from Fig. 4, $C_{\rm tr}^{(3)}$ exhibits an anomalous peak whose position shifts to lower temperature, and whose height increases, as L in made larger. Finally, in Figs. 6 and 7, respectively, we show the position of the peak, $\beta_{\rm max}$, and the maximum peak value, $(C_{\rm tr}^{(3)})_{\rm max}$, versus L, giving results in accordance with Eqs. (5.8) and (5.9).

VII. CONCLUSION

When a Trotter approximation is used, we have considered various approximate forms for the susceptibility χ and heat capacity C, each of which differ from their exact counterparts only by terms of second order in the expansion parameter $\Delta\tau$. However, certain of these forms may diverge as $\beta=1/T\to\infty$ for fixed $\Delta\tau$. Thus, at low temperature, one must either make $\Delta\tau$ smaller or use a definition which avoids these divergences. The definition[27]

$$\chi_{\rm tr}^{\mathcal{O}}=\Delta\tau\sum_{l=0}^{L-1}\langle\mathcal{O}(\tau_l)\mathcal{O}(0)\rangle_{\rm tr}-\beta\langle\mathcal{O}\rangle_{\rm tr}^2 \tag{7.1}$$

for χ and the definition

$$C_{\rm tr}^{(2)}=\frac{\partial}{\partial T}(\langle H\rangle_{\rm tr})_{\Delta\tau={\rm const}} \tag{7.2}$$

for C are algorithmically implementable and in general have no divergence at low temperatures if $\Delta\tau$ is held constant.

However, $C_{\rm tr}^{(2)}$ may be difficult to implement in practice in certain quantum Monte Carlo simulations. With discrete data points for $\langle H\rangle_{\rm tr}$, one will approximate, to lowest order,

$$C_{\rm tr}^{(2)}\left[T+\frac{\Delta T}{2},\,\Delta\tau\right]=\frac{1}{\Delta T}[\langle H\rangle_{\rm tr}(T+\Delta T,\Delta\tau)-\langle H\rangle_{\rm tr}(T,\Delta\tau)]+o((\Delta T)^2)\ . \tag{7.3}$$

Assuming a statistical error of $\delta\langle H\rangle_{\rm tr}$ for each data point, we then have for the statistical error of $C_{\rm tr}^{(2)}$,

$$\delta C_{\rm tr}^{(2)}=\frac{\sqrt{(2)}\delta\langle H\rangle_{\rm tr}}{\Delta T}\ . \tag{7.4}$$

Thus, a compromise must be struck between taking ΔT small, which will increase $\delta C_{\rm tr}^{(2)}$, and taking ΔT large, which will increase the error in replacing a derivative by a discrete difference. (Of course, $\delta\langle H\rangle_{\rm tr}=0$ if exact transfer matrix methods[3,11,12,26] are used.)

The error due to finite ΔT may be reduced by using a higher-order approximation than that of Eq. (7.3). For example, to next-highest even order,

$$C_{\rm tr}^{(2)}\left[T+\frac{\Delta T}{2},\,\Delta\tau\right]=\frac{1}{\Delta T}\{\tfrac{9}{8}[\langle H\rangle_{\rm tr}(T+\Delta T,\,\Delta\tau)-\langle H\rangle_{\rm tr}(T,\,\Delta\tau)]-\tfrac{1}{24}[\langle H\rangle_{\rm tr}(T+2\Delta T,\,\Delta\tau)-\langle H\rangle_{\rm tr}(T-\Delta T,\,\Delta\tau)]\}+o((\Delta T)^4)\ , \tag{7.5}$$

with

$$\delta C_{\rm tr}^{(2)}\approx\frac{9}{8}\frac{\sqrt{2}\delta\langle H\rangle_{\rm tr}}{\Delta T}\ . \tag{7.6}$$

Thus, if finite-ΔT error dominates, higher-order approximations can be used without appreciably increasing $\delta C_{\rm tr}^{(2)}$. Alternatively, if $\delta\langle H\rangle_{\rm tr}$ error dominates, higher-order approximations can be used for different values of larger ΔT and the results extrapolated to the $\Delta T\to 0$ limit.

If, however, $C_{\rm tr}^{(2)}$ is still difficult to implement, we suggest using the definition[27]

$$C_{\rm tr}^{(4)}=\beta\left[\Delta\tau\sum_{l=0}^{L-1}\langle H(\tau_l)H(0)\rangle_{\rm tr}-\beta(\langle H\rangle_{\rm tr}^2)\right]\ , \tag{7.7}$$

or, possibly, $C_{\rm tr}^{(3)}$. These definitions will diverge linearly in β as $\beta\to\infty$, but may be extrapolated linearly in $(\Delta\tau)^2$. Of course, the extrapolated result may again be washed out by statistical error in these cases.

When the number of imaginary time slices L is held constant instead of $\Delta\tau$, we have determined the general origin of the anomalous peak in the heat capacity seen previously be certain authors. We also explained qualitatively the behavior of peak height and position as a function of β and L.

Finally, we have considered two simple examples. In addition to illustrating our general remarks, this has allowed us to underscore some of the problems which may arise for certain definitions of $\chi_{\rm tr}$ and $C_{\rm tr}$ within the context of a specific model. We hope that this, in particular, may serve as a guide to future numerical simulation.

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APPENDIX

As in Ref. 9, we have

$$Z_{\rm tr}(\beta,\Delta\tau)=Z_{\rm tr}(\beta,-\Delta\tau) \tag{A1}$$

or, equivalently,

$$Z_{\rm tr}(\beta,L)=Z_{\rm tr}(\beta,-L)\ , \tag{A2}$$

since $\Delta\tau=\beta/L$. Similarly,

$$\langle H\rangle_{\rm tr}(\beta,\Delta\tau)=\langle H\rangle_{\rm tr}(\beta,-\Delta\tau) \tag{A3}$$

and

$$\langle H^2\rangle_{\rm tr}(\beta,\Delta\tau)=\langle H^2\rangle_{\rm tr}(\beta,-\Delta\tau)\ , \tag{A4}$$

since H^2 is Hermitian. Then,

$$\begin{aligned}C_{\rm tr}^{(1)}(\beta,\Delta\tau)&=\beta^2\frac{\partial^2}{\partial\beta^2}\{\ln[Z_{\rm tr}(\beta,\Delta\tau)]\}\\&=\beta^2\frac{\partial^2}{\partial\beta^2}\{\ln[Z_{\rm tr}(\beta,-\Delta\tau)]\}\\&=C_{\rm tr}^{(1)}(\beta,-\Delta\tau)\ .\end{aligned} \tag{A5}$$

Similarly,

$$\begin{aligned}C_{\rm tr}^{(2)}(\beta,\Delta\tau)&=-\beta^2\frac{\partial}{\partial\beta}\langle H\rangle_{\rm tr}(\beta,\Delta\tau)\\&=-\beta^2\frac{\partial}{\partial\beta}\langle H\rangle_{\rm tr}(\beta,-\Delta\tau)\\&=C_{\rm tr}^{(2)}(\beta,-\Delta\tau)\ ,\end{aligned} \tag{A6}$$

$$\begin{aligned}C_{\rm tr}^{(3)}(\beta,\Delta\tau)&=\beta^2\frac{\partial^2}{\partial\beta^2}\{\ln[Z_{\rm tr}(\beta,L)]\}\\&=\beta^2\frac{\partial^2}{\partial\beta^2}\{\ln[Z_{\rm tr}(\beta,-L)]\}\\&=C_{\rm tr}^{(3)}(\beta,-\Delta\tau)\ ,\end{aligned} \tag{A7}$$

and

$$\begin{aligned}C_{\rm tr}^{(5)}(\beta,\Delta\tau)&=\beta^2\{\langle H^2\rangle_{\rm tr}(\beta,\Delta\tau)-[\langle H\rangle_{\rm tr}(\beta,\Delta\tau)]^2\}\\&=\beta^2\{\langle H^2\rangle_{\rm tr}(\beta,-\Delta\tau)-[\langle H\rangle_{\rm tr}(\beta,-\Delta\tau)]^2\}\\&=C_{\rm tr}^{(5)}(\beta,-\Delta\tau)\ .\end{aligned} \tag{A8}$$

Now,

$$C_{\rm tr}^{(4)}(\beta,\Delta\tau)=\beta\chi_{\rm tr}^{H}(\beta,\Delta\tau)\ , \tag{A9}$$

where $\chi_{\rm tr}^{\mathcal{O}}(\beta,\Delta\tau)$ is defined by Eq. (3.5). Since it was shown that

$$\chi_{\rm tr}^{\mathcal{O}}(\beta,\Delta\tau)=\chi_{\rm tr}^{\mathcal{O}}(\beta,-\Delta\tau) \tag{A10}$$

for any Hermitian $\mathcal{O}$, one has then

$$C_{\rm tr}^{(4)}(\beta,\Delta\tau)=C_{\rm tr}^{(4)}(\beta,-\Delta\tau)\ . \tag{A11}$$

Since all five of our definitions reduce to $C_{\rm ex}$ for fixed β in the $\Delta\tau\to 0$ limit, we conclude that

$$\Delta C=o((\Delta\tau)^2) \tag{A12}$$

for sufficiently small $\Delta\tau$ for each definition of $C_{\rm tr}$.

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[27] Using Simpson's rule rather than the trapezoidal rule implicit in Eqs. (7.1) and (7.7) also leads to definitions of $\chi_{\rm tr}$ and $C_{\rm tr}$ even in $\Delta\tau$, and may significantly reduce the error prefactor in some cases.