Accelerated convergence in exact-diagonalization studies

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A simple method is proposed and tested for obtaining accelerated convergence of quantum systems on small lattices with N sites. The main idea is to perform exact diagonalizations with some added irrelevant parameter, and use this parameter to accelerate the convergence to the infinite-lattice limit. In this paper different boundary conditions are used to improve the convergence for the Heisenberg model. In particular, we find that the application of the method to the $d=1$ antiferromagnetic Heisenberg model changes the rate of convergence of the ground-state energy per site, $|E_0(N) - E_0(\infty)| \sim N^{-x}$, to $x \approx 4$ from the value $x = 2$, which is found using only periodic boundary conditions.

I. INTRODUCTION

Whenever a model is studied numerically using a digital computer, the model system is restricted to a small number N of discrete lattice points. This paper proposes and tests a method of obtaining better results for the desired bulk ($N \rightarrow \infty$) quantities based on a careful analysis of finite N systems.

Two of the most widely used methods of studying quantum spin systems numerically are quantum Monte Carlo¹ and exact-diagonalization² methods. Both of these techniques have their own strengths and weaknesses. The quantum Monte Carlo method in general has the "minus-sign problem",¹ and always has statistical errors associated with measured quantities. On the other hand, the exact-diagonalization method does not have a "minus-sign problem," but it is restricted to small system sizes. Consequently, it is important to be able to extract the largest amount of information available from exact-diagonalization studies carried out on system sizes which are amenable to the method. It is this topic which this paper addresses.

As N increases, the finite-size estimates for a given desired quantity, f_N , may approach the infinite-size result as $|f_N - f_\infty| \sim N^{-x}$ if low-energy modes are present in the system (gapless excitations). If one is limited to small values of N , then it would be convenient to make the convergence exponent $x > 0$ as large as possible. In certain instances, if a large number of lattice sizes are available, convergence may be accelerated using a filtering procedure.³ In some cases, such as p_c in percolation⁴ or T_c for Ising-type models,⁵ it is also possible to find

estimators which converge faster with N than normal estimators for these quantities. Here a method is described which in principle should work for any desired quantity, and which does not require the availability of too many lattice sizes. This method is tested numerically for the ground-state energy per site of the antiferromagnetic spin- $\frac{1}{2}$ Heisenberg model.

II. CONVERGENCE ACCELERATION METHOD

The idea to improve the convergence with N is to perform a Taylor expansion for the thermodynamic quantity of interest, f . f is a function of the system size N , and some parameter g (to be defined below) which is expected to be irrelevant in the thermodynamic limit. For example, f may be the ground-state energy per site of the system. Although the parameter g can be any suitable irrelevant parameter, in this paper we will choose g to be the strength of the bond(s) at the boundary of the finite lattice. The idea of tuning boundary conditions to improve finite-size convergence is not new, but the scheme we use is different from other methods.⁶⁻⁸ Let us assume that for large systems at fixed g the value of f approaches the thermodynamic limit as a power law, $|f_N - f_\infty| \sim N^{-s}$.⁹ Explicitly,

$$f(N^{-s}, g + \delta g) = f(0, g) + \left[\frac{1}{N^s} \frac{\partial}{\partial x} + \delta g \frac{\partial}{\partial y} \right] f(x, y) \Big|_{x=0, y=g} + \dots \quad (1)$$

Here we have assumed that it is possible to take derivatives with respect to the system size, and that such derivatives are fairly well defined. However, the existence or lack thereof of the derivatives in the thermodynamic limit should be immaterial to the method described below, since we will replace the derivatives by finite differences.

The quantity which can be calculated through exact diagonalization is $f(N^{-s}, g + \delta g)$, while the quantity desired in the thermodynamic limit ($N \rightarrow \infty$) is $f(0, g)$. The central idea is to choose δg such that the term in square brackets of the Taylor expansion in Eq. (1) vanishes. To make this term vanish, the derivatives with respect to y and N should be calculated. However, in practice, finite-size estimates for these derivatives will be used. The derivative with respect to the irrelevant parameter y , i.e.,

$$\left. \frac{\partial f(x, y)}{\partial y} \right|_{x=0, y=g} \approx \left. \frac{\partial f(x, y)}{\partial y} \right|_{x=\frac{1}{N^s}, y=g}, \quad (2)$$

can be estimated easily at a fixed value of N using numerical differentiation. This is possible since the exact diagonalization can be performed easily for any value of δg . (In practice, some of the symmetries of the exact diagonalization for $\delta g = 0$ may be lost for finite δg , which can change the size of the Hilbert space required by exact diagonalization studies.)

The derivative with respect to N is more problematic, since one is restricted to integer values of N . However, it is still possible to take a finite difference for finite N as an approximation to the derivative. Using a two-point difference approximation to this derivative can be done in several different ways which are not equivalent for finite N if $s \neq 1$. For two system sizes with $N_1 < N_2$ two difference equations are

$$N^{-s} \left. \frac{\partial f(x, y)}{\partial x} \right|_{x=0, y=g} \approx N_2^{-s} \frac{f(N_2^{-s}, g) - f(N_1^{-s}, g)}{N_2^{-s} - N_1^{-s}}, \quad (3)$$

and using the chain rule

$$N^{-s} \left. \frac{\partial f(x, y)}{\partial x} \right|_{x=0, y=g} \approx -\frac{N_2}{s} \frac{f(N_2^{-s}, g) - f(N_1^{-s}, g)}{N_2 - N_1}. \quad (4)$$

We will use both approximations to try to accelerate the convergence.

III. MODEL AND CALCULATIONAL METHOD

To test this method, we have applied it to the anti-ferromagnetic spin- $\frac{1}{2}$ Heisenberg model in one and two dimensions. The Hamiltonian is

$$\mathcal{H} = \sum_{\langle i, j \rangle} J_{i, j} \mathbf{S}_i \cdot \mathbf{S}_j, \quad (5)$$

where the interaction is only between nearest-neighbor spins on the lattice. The interaction strength is taken to be $J = 1$ for interior bonds, and $J = g$ for bonds on the

boundary. Consequently, $g = 1$ gives periodic boundary conditions, while $g = 0$ gives free boundary conditions. For $g \neq 1$ the translational symmetry of the lattice is broken, and consequently translational symmetry is not used to block diagonalize the Hamiltonian. For the $d = 1$ model there is only one bond of strength g . For the $d = 2$ square lattice we studied, the number of boundary bonds on the tilted squares¹⁰ depends on the tilted square.

We used a Lanczos¹¹ procedure to obtain the ground-state energy per site of the Heisenberg model. Smaller systems were run on a CRAY Y-MP/432 using a program similar to one used for the $d=2$ t - J (Ref. 12) and Hubbard¹³ models. For the largest system sizes, we used a massively parallel Thinking Machines Corporation CM-2 with 2¹⁶ processors, 2 Gbytes of main memory, and a 10 Gbyte disk-storage device. The program for the CM-2 was written in the C and PARIS programming languages, and is similar to the program described in Ref. 14 and recently used in Ref. 15 for exact diagonalizations of the $d=2$ Hubbard model.

IV. RESULTS

For the $d = 1$ Heisenberg model, the ground-state energy per site, E_0 , as a function of the strength of the boundary interaction g is shown in Fig. 1. Also shown in Fig. 1 is the exact infinite-lattice value $E_0(\infty) = \frac{1}{4} - \ln(2)$.¹⁶ The method described in Sec. II attempts to find the value of g for finite N which is a better approximation to $E_0(\infty)$ than is the quantity $E_0(N, g = 1)$.

In Fig. 2 we show the differences between the finite-size estimates and the exact $E_0(\infty)$ obtained from several different methods to select g . One way to try to select the optimal value of g would be to search for the crossing value of g where two system sizes satisfy $E_0(N_1, g) = E_0(N_2, g)$. As seen in Fig. 1 this is near $g \approx 0.7$ where the finite-size effects for the lattice sizes

FIG. 1. The ground-state energy per site of the $d=1$ anti-ferromagnetic Heisenberg model is shown as a function of the strength of the bond at the boundary, g , for different lattice sizes. Periodic boundary conditions correspond to $g = 1$, and free boundary conditions to $g = 0$. The dashed horizontal line is the exact infinite-lattice result.

studied appear to be the smallest. Figure 2(a) illustrates that the use of the crossing criteria to pick g converges to the difference for periodic boundary conditions extremely quickly. Consequently, there is no accelerated convergence when crossing is used to select g . In other words, the convergence toward the exact value, $|E_0(N) - E_0(\infty)| \sim N^{-x}$, has $x \approx 2$, the same value as found for periodic boundary conditions. Also note that,

FIG. 2. The difference between the exact ground-state energy and the finite-size estimates is shown as a function of N for the $d=1$ antiferromagnetic Heisenberg model. (a) shows estimates using periodic boundary conditions ($\circ$), the crossing of two system sizes (roman cross), and the procedure outlined in the text with the exponent $s = 1$ ($\times$). Since two lattice sizes are required for the last two estimates, each estimate has two symbols associated with it. The solid line has a slope of -2 drawn from the periodic boundary condition value for $N = 24$. (b) shows the periodic boundary condition points ($\circ$) and line with slope -2 from (a). Also shown are estimates using the procedure described in the text with exponent $s = 2$ using the procedures for numerical differences with respect to N from Eq. (3) ($\diamond$) and from Eq. (4) ($\square$). The lines are drawn through the points for $N = 24$ and have slopes of -2 , -3 , and -4 . Note that for the largest system studied ($N = 24$) the estimates described in the text obtain results 1–2 orders of magnitude closer to infinite-lattice results than do the periodic boundary condition results.

in Fig. 2(a), since crossing requires two values of N to attempt accelerated convergence, each value is plotted at both N_1 and N_2 . If the “wrong” exponent, $s = 1$, is used with Eq. (3) [or equivalently here with Eq. (4)], one also sees from Fig. 2(a) that the convergence is not accelerated noticeably.

However, it is expected that the convergence with system size is $|E_0(N) - E_0(\infty)| \sim N^{-2}$,¹⁷ as can be seen in Fig. 2(a). Consequently, one expects that $s = 2$ should be used to attempt accelerated convergence. The use of $s = 2$ indeed *does* accelerate the convergence, as seen in Fig. 2(b). Both the amplitude and exponent of convergence are changed when $s = 2$ is used in combination with either Eq. (3) or Eq. (4). Consequently, this acceleration method *works very well* for this model. In particular, Fig. 2(b) shows that the effective convergence exponents have changed from the value $x = 2$ for periodic boundary conditions to about $x = 3$ using Eq. (3) [or Eq. (4) with the smaller system size used in the approximation of the derivative of Eq. (2)]. If the best estimate for the approximation of the derivative of Eq. (2) and Eq. (4) is used, the effective convergence exponent has a value of approximately $x = 4$. Consequently, as Fig. 2(b) demonstrates, the accelerated convergence method works extremely well in this case.

It is also possible to use three-point differentiation formulas to estimate the derivative with respect to N in Eq. (2). With $s = 2$ and using either Eq. (3) or Eq. (4) we also found accelerated convergence with effective convergence exponents between $x = 3$ and $x = 4$.

It is natural to ask how the value of g which is needed for the various estimators changes as a function of system size (Fig. 3). As expected, as N increases the values of g used in the estimators approach $g = 1$, since this is the value of g around which the Taylor expansion is performed.

There are other known acceleration schemes, such as the Aitken δ -squared method or the Levin u transform, for sequences of values versus N .¹⁸ We point out that such techniques can also be used on the sequence of num-

FIG. 3. The value of the boundary condition g used to estimate the infinite-lattice ground-state energy is shown as a function of N . The symbols have the same meaning as in Fig. 2.

FIG. 4. The ground-state energy per site of the $d=2$ antiferromagnetic Heisenberg model is shown as a function of g , the strength of the bond at the boundary. For $N=26$ the only data shown are for periodic boundary conditions. The solid horizontal line is the “consensus” of recent quantum Monte Carlo estimates, $E_0 = -0.6692 \pm 0.001$, from Ref. 20.

bers obtained with our convergence acceleration technique. However, small errors introduced in approximating the numerical derivatives in our procedure can be magnified by the other acceleration schemes.

Figure 4 shows results for the ground-state energy per site, E_0 , as a function of N for the square lattice $d = 2$ antiferromagnetic Heisenberg model. This model is currently of interest in the context of high-temperature superconductivity.^{19,20} Although the plot looks very similar to Fig. 1, we were not able to find any accelerated convergence with the system sizes which could be studied. This is most likely due to the lack of an adequate number of tilted squares to construct a fixed sequence (for example, all squares tilted at the same angle with respect to a lattice axis). The lack of such a sequence leads to severe difficulties in estimating the derivatives with respect to N .

V. DISCUSSION AND CONCLUSIONS

We have proposed a general method for accelerating the convergence of finite-size estimates of physical quantities to the thermodynamic limit in computer studies. This method should also make possible accelerated convergence to a continuum limit. We have demonstrated our proposed technique by successfully applying it to accelerate the convergence of the ground-state energy per site, E_0 , of the $d=1$ antiferromagnetic Heisenberg model. We found that the application of our method to this model changes the rate of convergence, $|E_0(N) - E_0(\infty)| \sim N^{-x}$, to $x \approx 4$ from the value $x = 2$ which is found using only periodic boundary conditions.

The remaining problem is to determine the criteria by which g must be chosen to accelerate convergence. In principle any parameter g should work. However, in order to cancel the first term in the Taylor expansion in

Eq. (1) for any system size N , it must be possible to have a *small* value of δg which changes the value of the desired quantity for finite N to its value for infinite N . That the boundary condition strength for the $d=1$ and $d=2$ antiferromagnetic Heisenberg model has this property can be seen in Figs. 1 and 4. We also attempted to perform accelerated convergence for the t - J model, but we found that a small change in the boundary strength of t and/or J is not sufficient to change the ground-state energy per spin to the infinite N value for the finite values of N we can diagonalize exactly.

Another requirement for our method of accelerated convergence to work is that it must be possible to accurately estimate derivatives with respect to N . As Fig. 2 shows, different finite-difference approximations to the derivatives with respect to N can produce different convergence rates. Also, to obtain an efficient cancellation of the first term of the Taylor expansion in Eq. (1) the finite-size behavior of the desired quantity should be known and used (in our case for $d=1$ the best results were obtained with $s=2$). These restrictions require first of all that the sizes studied belong to the same sequence. For example, for antiferromagnets in $d=2$ sequences of regular $N=L \times L$ lattices can be used ($N = 4, 16, 36, \dots$), or tilted squares belonging to sequences such as $N = 2L^2$ ($N = 8, 18, 32, 50, \dots$) or $N = 1 + M^2$ ($N = 10, 26, 50, \dots$) can be used. Since supercomputers with large memories are starting to become available, it will soon be possible to perform exact-diagonalization studies on the squares with $N = 26, 32$, and 36 with arbitrary boundary conditions, since periodic boundary conditions for $N=36$ have been recently accomplished.²¹ In principle, the accelerated convergence technique used here can also be applied to Monte Carlo studies. However, in that case one might expect severe difficulties in calculating the derivatives (particularly derivatives with respect to N) due to the statistical errors inherent in the method.

It should also be possible to improve the convergence further by using a parameter g to cancel higher-order terms in the Taylor expansion of Eq. (1). For example, to cancel the first two terms in the expansion would require that the value of g used be obtained from a quadratic equation. In this case, the second derivative with respect to N as well as a mixed derivative with respect to N and g must be approximated. It is expected that the error in estimating these higher derivatives limits the applicability of this method to cases where extremely large systems are available.

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