Optimization of finite-size errors in finite-temperature calculations of unordered phases

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(Received 14 May 2015; published 29 June 2015)

It is common knowledge that the microcanonical, canonical, and grand-canonical ensembles are equivalent in thermodynamically large systems. Here, we study finite-size effects in the latter two ensembles. We show that contrary to naive expectations, finite-size errors are exponentially small in grand canonical ensemble calculations of translationally invariant systems in unordered phases at finite temperature. Open boundary conditions and canonical ensemble calculations suffer from finite-size errors that are only polynomially small in the system size. We further show that finite-size effects are generally smallest in numerical linked cluster expansions. Our conclusions are supported by analytical and numerical analyses of classical and quantum systems.

DOI: 10.1103/PhysRevE.91.062142 PACS number(s): 05.20.−y, 05.30.−d

I. INTRODUCTION

The use of identically prepared systems, or ensembles, has been essential to our understanding of equilibrium and far-from-equilibrium properties of classical and quantum systems. Traditionally, three types of ensembles are used: (a) the microcanonical ensemble, which involves systems with fixed energy and particle number; (b) the canonical ensemble (CE), which involves systems with fixed particle number in contact with a large reservoir (at temperature T) with which they can exchange energy; and (c) the grand canonical ensemble (GE), which involves systems in contact with a reservoir with which they can exchange energy and particles (in equilibrium, the average particle number is determined by the chemical potential μ). Whereas these three ensembles pose fundamentally different physical constraints, it can be shown that they are equivalent in the thermodynamic limit (provided, of course, that temperatures and chemical potentials are selected appropriately). Being technically easier to deal with, the canonical and grand canonical ensembles are the most commonly used ensembles in the literature. Several texts on statistical mechanics cover these topics in detail; see, e.g., Ref. [1].

In finite systems, differences appear between calculations carried out using the three ensembles. These differences, dubbed finite-size effects, have to do with the effect of energy and particle number fluctuations, and with boundary effects. For example, to describe an isolated system with mean energy E, it is most appropriate to use the microcanonical ensemble with that energy. However, one can also use a canonical ensemble at a temperature T for which the mean energy is E. Since the systems used to construct the canonical ensemble have different energies from the ones used to construct the microcanonical ensemble, one finds differences in the predictions of each ensemble. Remarkably, one can show that energy fluctuations in the canonical ensemble typically scale as the square root of the volume of the system, whereas the average energy scales as the volume of the system. Hence, the ratio between the energy fluctuations and the average energy scales as the inverse of the square root of the volume, and vanishes in the thermodynamic limit. One then finds that differences between the predictions of each ensemble decrease polynomially with increasing volume (at fixed density). The same applies if one considers the grand canonical ensemble, where particle number fluctuations typically scale with the square root of the volume of the system. Indeed, explicit calculations in one-dimensional (1D) lattices have shown that the differences between the predictions of the canonical and grand-canonical ensembles for various observables decrease with the inverse of the number of particles (or lattice sites) in the system [2,3].

Experiments usually deal with thermodynamically large systems, whereas numerical analyses of many-body interacting systems can generally be done for only (relatively) much smaller system sizes. Hence, when trying to theoretically predict or reproduce the outcome of an experimental measurement, a question of much relevance is: *Which ensemble should one use to minimize finite-size effects and obtain the "thermodynamic limit" or experimental result?* From the previous discussion about the differences between ensembles, one might naively conclude that finite-size effects always scale polynomially with system size and that, therefore, the best one can do theoretically is to optimize exponents and prefactors.

In this article we show that this is not the case. There is a preferred ensemble (the grand-canonical ensemble) and preferred boundary conditions (periodic boundary conditions, so that the system is translationally invariant) for which finite-size effects are exponentially small in the system size. This holds if the system of interest is in an unordered (i.e., without long- or quasilong-range order) phase at finite temperature. We also consider a different approach to calculating finite-temperature properties of many-particle systems, namely, numerical linked cluster expansions (NLCEs) [4–6]. We show that NLCEs not only exhibit exponential convergence with increasing system size but generally outperform grand canonical ensemble calculations in systems with periodic boundary conditions.

The paper is organized as follows. In Sec. II we argue, based on a high-temperature expansion of the partition function, that grand-canonical ensemble calculations in translationally invariant systems have exponentially small finite-size errors. In Sec. III, we discuss analytically solvable examples, the 1D and 2D Ising models, that substantiate the arguments in Sec. II. In Sec. IV, we present a proof that finite-size errors are indeed exponentially small in the grand-canonical ensemble for translationally invariant noninteracting systems and that, within perturbation theory, the same scaling applies

to interacting systems. We then study numerically, in Sec. V, three examples where we systematically compare results from canonical and grand-canonical ensemble calculations, each for open boundary conditions (OBC) and periodic boundary conditions (PBC), and NLCEs. We summarize our results and conclude in Sec. VI.

II. GENERAL CONSIDERATIONS

In this section, we argue that the GE for a translationally invariant system [we abbreviate the CE (GE) with open and periodic boundary conditions as CE-O (GE-O) and CE-P (GE-P), respectively] has exponentially small finite-size corrections. For that, we make use of a β expansion of the free energy, where $\beta = (k_B T)^{-1}$ is the inverse temperature and k_B is the Boltzmann constant. This kind of expansion has been used extensively in the literature to compute partition functions for various models [7–9].

Consider the Taylor expansion of the grand partition function $Z \equiv \mathrm{Tr}\, e^{-\beta \hat{H}}$ (we set $\mu = 0$ for brevity; all the arguments below are valid for nonzero μ, which will be required for bosons to prevent Bose-Einstein condensation):

$$Z(\beta) = \mathrm{Tr}(1) - \beta\, \mathrm{Tr}(\hat{H}) + \frac{\beta^2}{2!}\, \mathrm{Tr}(\hat{H}^2) + \dots \tag{1}$$

We are interested in $\ln Z$, from which thermodynamic quantities can be obtained by taking suitable β or μ derivatives,

$$\ln Z(\beta) = \ln \mathrm{Tr}(1) - \beta \frac{\mathrm{Tr}(\hat{H})}{\mathrm{Tr}(1)} + \frac{\beta^2}{2}\left[\frac{\mathrm{Tr}(\hat{H}^2)}{\mathrm{Tr}(1)} - \frac{\mathrm{Tr}(\hat{H})^2}{\mathrm{Tr}(1)^2}\right] + \cdots \tag{2}$$

We note that

$$\frac{\mathrm{Tr}(\hat{H}^n)}{\mathrm{Tr}(1)} = \frac{\mathrm{Tr}(\hat{H}^n e^{-0\cdot\hat{H}})}{\mathrm{Tr}(e^{-0\cdot\hat{H}})} \tag{3}$$

is an infinite temperature expectation value. At infinite temperature all unconnected parts of the system, however close to each other, are uncorrelated. Therefore, the expansion in Eq. (2) reduces to a sum over only the connected graphs that can be embedded in the finite system [1,7,10]. In the CE, the particle number constraint, i.e., that the total particle number is fixed, implicitly correlates unconnected pieces of a graph, and therefore this simplification does not occur.

For a system that has no ordered phase at finite temperature, the above expansion must converge beyond a certain order (because the correlation length is finite). Since this must occur for any inverse temperature $\beta < \infty$, the convergence must come from the coefficients of the β expansion, i.e., from the traces in Eq. (2). In other words, for the expansion $(\ln Z)/N = a_0 + a_1\beta + a_2\beta^2 + \cdots$, the coefficient a_n must fall faster than e^{-n} for the series to converge for any β. The convergence cannot come from cancellation of terms of opposite sign, since any such cancellation can work only at some fine-tuned value of β.

For a system that has a phase transition between an unordered high-temperature phase and an ordered low-temperature phase at a finite critical inverse temperature β_c, the coefficients do not exhibit this behavior—at criticality the correlation length is infinite and all orders of this expansion are relevant. The convergence of the series for $\beta < \beta_c$ instead comes from the fact that $\beta/\beta_c < 1$. We verify these arguments in the 1D and 2D Ising models.

From here on, we assume that we are in a phase where the β expansion converges. We will now show that with PBC (when the system is translationally invariant), all orders of the expansion Eq. (2) up to the system size (to be properly defined below) are identical to those in the thermodynamic limit. We will further show that this is not the case with open boundary conditions.

A. Periodic boundary conditions

Consider a system with N sites and periodic boundary conditions (a system that is translationally invariant). The β expansion of $\ln Z$ is shown in Eq. (2), in which each term can be represented by a graph embedded on the finite system. We will call these graphs clusters [1]. First note that each cluster has N equivalent positions on the lattice since the system is translationally invariant. That gives a factor of N that we move to the left-hand side in Eq. (2) to get $(\ln Z)/N$, i.e., an intensive quantity. Let us now consider a cluster with c sites. First, since we have a cumulant expansion, as discussed above, only connected clusters enter (see, e.g., Refs. [1,7,9] for details). If the extent of our cluster in each direction is less than the system size in that direction (say L), then the cluster has open boundary conditions. Furthermore, even if the system size is increased in any direction, this cluster is present. Hence, this cluster is present in the thermodynamic limit. In general, *every cluster with c sites that, in the finite lattice with N sites, does not wrap around any boundary appears in the infinite system, and vice versa*. Therefore, the contribution of this cluster in a finite system is exactly the same as its contribution in the thermodynamic limit. On the other hand, a cluster with L sites in any given direction wraps around a boundary, i.e., it does not appear in the thermodynamic limit. As a result, clusters that wrap around boundaries give contributions that are not present in the thermodynamic limit [2]. Hence, the difference between results in the thermodynamic limit and in finite-size periodic systems is $O(\beta^{L-p})$, p being determined by the Hamiltonian. We note that p is $O(1)$ for local Hamiltonians, which are the ones of interest here. Further, based on the earlier argument, we must have that the coefficient at this order falls faster than $e^{-(L-p)}$ or that the expansion parameter (β/β_c) is smaller than one. Therefore, finite-size errors in a GE calculation of a translationally invariant system at any temperature in the unordered phase are smaller than $O(e^{-L})$, for systems with linear dimension L.

B. Open boundary conditions

For a system with OBC, one immediately realizes that clusters do not have N equivalent positions on the lattice. As a result, even if a given cluster in the finite system appears in the thermodynamic limit, its contribution in the finite system will differ from the thermodynamic limit. For example, for a lattice model in which the Hamiltonian is a sum of terms involving only nearest-neighbor sites, the term linear in β in Eq. (2) for a system with OBC has a correction $O(A/2N)$ relative to the

result for PBC, where A is the number of sites in the boundary. This correction vanishes as $1/L$ with increasing system size. Complicated geometric and combinatorial factors appear at higher orders, all of which approach the thermodynamic limit result with increasing system size. Hence, none of the coefficients of a β expansion for a finite system with OBC match the result in the thermodynamic limit, and finite size errors in $(\ln Z)/N$ are $O(1/L)$.

C. Numerical-linked cluster expansions

Rather than making calculations of finite systems with periodic or open boundary conditions, and then extrapolating the results to the thermodynamic limit, another way to calculate finite-temperature properties of lattice systems in the thermodynamic limit is to use NLCEs [4–6,11]. The idea in this case is to directly use the linked cluster expansion of the infinite (translationally invariant) system, for which any extensive quantity $\mathcal{O}$ per site can be computed as the sum

$$\frac{\mathcal{O}}{N} = \sum_c M(c) \times W_{\mathcal{O}}(c), \tag{4}$$

over all connected clusters c that can be embedded in the infinite lattice. In Eq. (4), $M(c)$ is the *multiplicity* of cluster c, namely, the number of ways per site in which cluster c can be embedded on the lattice, and $W_{\mathcal{O}}(c)$ is the *weight* of the cluster c for observable $\mathcal{O}$. $W_{\mathcal{O}}(c)$ is calculated by an inclusion-exclusion principle, one systematically subtracts contributions from the connected subclusters of c [10],

$$W_{\mathcal{O}}(c) = \mathcal{O}(c) - \sum_{s \subset c} W_{\mathcal{O}}(s). \tag{5}$$

$\mathcal{O}(c)$ is the value of the observable evaluated on the cluster c. In NLCEs, $\mathcal{O}(c)$ is obtained using a full exact diagonalization of the Hamiltonian for cluster c.

Due to computational limitations, only a finite number of clusters can ultimately be calculated in Eq. (4). Nevertheless, as shown in Refs. [4–6], NLCEs can converge at lower temperatures than high-temperature expansions, and sometimes all the way to the ground state for systems with unordered ground states. Also, NLCEs can provide very accurate results for temperatures at which exact diagonalization results for systems with periodic boundary conditions suffer from very large finite-size effects. A pedagogical introduction to implementing NLCEs can be found in Ref. [11].

In what follows, we compare NLCE results with those obtained in calculations in finite systems with different boundary conditions. Our goal is to find how each of them converges to the thermodynamic limit result and which converges the fastest. For NLCEs, the accuracy of the results is determined by the size of the largest clusters considered in the sum in Eq. (4) and the model under consideration.

III. VERIFICATION IN ISING MODELS

In this section, we verify the arguments given in Sec. II in the 1D and 2D Ising models, both of which can be solved analytically.

A. 1D Ising model

In the thermodynamic limit, the log of the partition function per site, Ω, can be obtained using the transfer matrix method [1], and is given by (we set $J = 1$)

$$\Omega(\beta) = \ln(e^{\beta} + e^{-\beta}). \tag{6}$$

The expansion in powers of β of this result is

$$\Omega(\beta) = \ln 2 + \frac{\beta^2}{2} - \frac{\beta^4}{12} + \frac{\beta^6}{45} - \frac{17\beta^8}{2520} + \frac{31\beta^{10}}{14175} + \cdots \tag{7}$$

The result for finite systems with periodic boundary conditions is given by

$$\begin{aligned}\Omega_L(\beta) &= \frac{1}{L}\ln[(e^{\beta} + e^{-\beta})^L + (e^{\beta} - e^{-\beta})^L] \\ &= \Omega(\beta) + \frac{\tanh^L \beta}{L} + \cdots\end{aligned} \tag{8}$$

Since $0 \leqslant \tanh\beta < 1$ for $0 \leqslant \beta < \infty$, the finite-size error is indeed faster than exponential. Quantities like the energy, which are derivatives of the free energy, converge exponentially fast with L.

Expanding Eq. (8) in powers of β for different values of L, we get

$$\begin{aligned}\Omega_2(\beta) &= \ln 2 + \beta^2 + \ldots, \\ \Omega_3(\beta) &= \ln 2 + \frac{\beta^2}{2} + \frac{\beta^3}{3} + \ldots, \\ \Omega_4(\beta) &= \ln 2 + \frac{\beta^2}{2} + \frac{\beta^4}{6} + \ldots, \\ \Omega_5(\beta) &= \ln 2 + \frac{\beta^2}{2} - \frac{\beta^4}{12} + \frac{\beta^5}{5} + \ldots, \\ \Omega_6(\beta) &= \ln 2 + \frac{\beta^2}{2} - \frac{\beta^4}{12} + \frac{17\beta^6}{90} + \ldots.\end{aligned} \tag{9}$$

As one can see, the results are exact to $O(\beta^{L-1})$. Naturally, as one goes to lower temperatures, the correlation length increases and larger systems are required to capture the relevant powers of β. It is easy to verify that, with open boundary conditions, the corrections are always $O(1/L)$.

As discussed in Sec. II, although the coefficients in Eq. (9) are exact up to $O(\beta^{L-1})$, the convergence for *all* temperatures comes from the fact that they fall off rapidly (faster than exponential) with increasing expansion order. Figure 1 shows a plot of the coefficients of expansion in Eq. (7) along with a fit to ab^{-L}/L that demonstrates the faster-than-exponential behavior.

To conclude our discussion of the 1D Ising model, we evaluate the first few orders of the NLCE for this model (instead of numerical exact diagonalization of the clusters, we obtain these results analytically). First, we evaluate the partition function $[\ln Z_L(\beta)]$ on finite clusters with OBC

$$\begin{aligned}\ln Z_1(\beta) &= \ln 2, \\ \ln Z_2(\beta) &= \ln 2 + \ln(e^{\beta} + e^{-\beta}), \\ \ln Z_3(\beta) &= \ln 2 + \ln(e^{2\beta} + e^{-2\beta} + 2),\end{aligned} \tag{10}$$

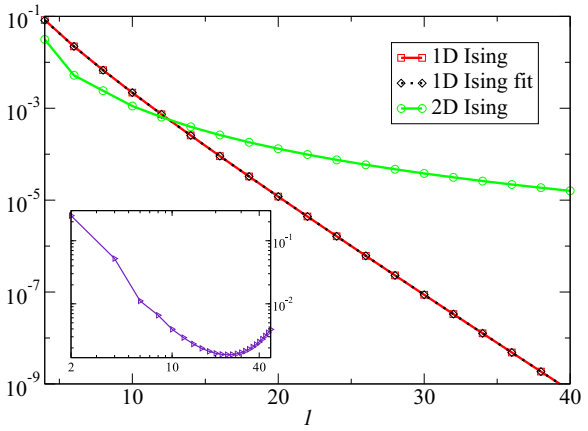

FIG. 1. (Color online) Coefficients (absolute value) of the β expansion of the free energy vs. the expansion order l. We show the coefficients in Eq. (7) for the 1D Ising model, and a fit to the function ab^{-l}/l with $a = 2.0000$ and $b = 1.5708$ (the difference between the exact result and $2(\pi/2)^{-l}/l$ vanishes exponentially fast with l), and from Eq. (15) for the 2D Ising model. The coefficients in the latter case do not fall off exponentially fast. Because of this, the β expansion only converges for $\beta < \beta_c$. It is only in this regime that finite-size errors in grand-canonical ensemble calculations of translationally invariant systems are exponentially small in system size. Inset: Shows the rational part of the coefficients in Eq. (15). They decrease at first but increase after $O(\eta^{24})$. See text for further discussion.

and then carry out the subtractions. The weights are given by [see Eq. (5)]

$$\begin{aligned} W_1 &= \ln Z_1(\beta) = \ln 2, \\ W_2 &= \ln Z_2(\beta) - 2W_1 = \ln(e^{\beta} + e^{-\beta}) - \ln 2, \\ W_3 &= \ln Z_3(\beta) - 2W_2 - 3W_1 = 0. \end{aligned} \tag{11}$$

Hence, the result for Ω obtained in calculations including up to n sites, $(\Omega)_n$, is given by [see Eq. (4)]

$$\begin{aligned} &(\Omega)_1 = W_1 = \ln 2, \quad (\Omega)_2 = W_1 + W_2 = \ln(e^{\beta} + e^{-\beta}), \\ &(\Omega)_3 = W_1 + W_2 + W_3 = \ln(e^{\beta} + e^{-\beta}). \end{aligned} \tag{12}$$

It can be verified that the last result is valid at all higher orders in the "NLCE." The thermodynamic limit result is therefore obtained by just considering clusters with one and two sites. This is an infinite improvement over the use of the grand-canonical ensemble with periodic boundary conditions. Whereas this infinite gain is specific to the 1D Ising model—the model can, after all, be solved using a 2D transfer matrix—we show in what follows that the fact that NLCEs outperform exact calculations in finite systems appears to be generic.

B. 2D Ising model

For the 2D Ising model, Ω is given by [1,12]

$$\Omega(\beta) = \ln[2\cosh(2\beta)] + \int_0^{\pi} \frac{d\phi}{2\pi} \ln\left[\frac{1 + \sqrt{1 - \frac{4\sin^2\phi}{\cosh^2(2\beta)\coth^2(2\beta)}}}{2}\right]. \tag{13}$$

The β expansion of this result is given by

$$\Omega(\beta) = \ln 2 + \beta^2 + \frac{5\beta^4}{6} + \frac{32\beta^6}{45} + \frac{425\beta^8}{252} + \ldots \tag{14}$$

One can see that the coefficients become larger than 1 for higher orders. The correct expansion parameter for models with a finite-temperature transition is β/β_c. For the classical 2D Ising model on a square lattice, $\beta_c = \ln(1+\sqrt{2})/2$. This gives (with $\eta \equiv \beta/\beta_c$),

$$\Omega(\beta) = \ln 2 + \frac{a^2\eta^2}{4} + \frac{5a^4\eta^4}{96} + \frac{a^6\eta^6}{90} + \frac{425a^8\eta^8}{64512} + \ldots, \tag{15}$$

where $a \equiv \ln(1+\sqrt{2}) < 1$. The coefficients of the η expansion are plotted versus the order of the expansion in Fig. 1. They do not fall off faster than exponential, or exponentially. We note that the rational part of the coefficients of the first few orders of the η expansion reported in Eq. (15) is deceiving. They decrease with increasing order of expansion. This, together with the fact that $a < 1$, suggests that the coefficients of the η expansion should fall off faster than exponentially. However, as shown in the inset in Fig. 1, the aforementioned rational part *increases* with increasing order of expansion after $O(\eta^{24})$. Because of this, convergence in the η expansion is only expected for $\eta < 1$ and does not come from the coefficients.

We also calculate $\ln Z_{L\times L}$ for small systems with $N = L \times L$ sites in the GE for both periodic and open boundary conditions. With PBCs

$$\begin{aligned} \ln Z^{\mathrm{2D-P}}_{1\times1} &= \ln 2, \\ \ln Z^{\mathrm{2D-P}}_{2\times2} &= \ln 2 + \ln(e^{4\beta} + e^{-4\beta} + 2), \\ \ln Z^{\mathrm{2D-P}}_{3\times3} &= \ln 2 + \ln(e^{-18\beta} + 9e^{-10\beta} + 24e^{-6\beta} \\ &\quad + 99e^{-2\beta} + 72e^{2\beta} + 51e^{6\beta}), \end{aligned} \tag{16}$$

whereas, with OBCs,

$$\begin{aligned} \ln Z^{\mathrm{2D-O}}_{1\times1} &= \ln 2 \\ \ln Z^{\mathrm{2D-O}}_{2\times2} &= \ln 2 + \ln(e^{4\beta} + e^{-4\beta} + 2) \\ \ln Z^{\mathrm{2D-O}}_{3\times3} &= \ln 2 + \ln(e^{-12\beta} + 4e^{-8\beta} + 16e^{-6\beta} \\ &\quad + 23e^{-4\beta} + 48e^{-2\beta} + 48e^{2\beta} + 23e^{4\beta} \\ &\quad + 16e^{6\beta} + 4e^{8\beta} + e^{12\beta} + 72). \end{aligned} \tag{17}$$

For the β expansion of the 3×3 systems, up to the first term that differs from Eq. (14), we obtain

$$\begin{aligned} \Omega^{\mathrm{2D-O}}_{3\times3} &= \ln 2 + \frac{2\beta^2}{3} + \ldots, \\ \Omega^{\mathrm{2D-P}}_{3\times3} &= \ln 2 + \beta^2 + \frac{2\beta^3}{3} + \ldots. \end{aligned} \tag{18}$$

We see that whereas for OBC the coefficient of the second-order term is incorrect, for PBC it is correct, i.e., once again GE-P gives results that are correct to $O(\beta^{L-1})$, with $L = 3$ in this case.

For the NLCE calculation with clusters with up to four sites, we obtain

$$\begin{aligned} (\Omega)_4 &= 20\ln(e^{-\beta} + e^{\beta}) + 54\ln(e^{-\beta}e^{2\beta} + 1) \\ &\quad - 38\ln(e^{-2\beta} + e^{2\beta} + 2) + \ln(e^{-4\beta} + e^{4\beta} + 6). \end{aligned} \tag{19}$$

Expanding in powers of β, and reporting terms up to the first one that differs from Eq. (14), we get

$$(\Omega)_4 = \ln 2 + \beta^2 + \frac{5\beta^4}{6} - \frac{58\beta^6}{45} + \ldots. \tag{20}$$

The above result is correct to $O(\beta^5)$. We must stress that Eq. (20) was obtained in an expansion in which the largest cluster has $N = 4$, while Eq. (18) are for systems with $N = 9$. The gain is evident.

IV. FINITE-TEMPERATURE PERTURBATION THEORY TO ALL ORDERS

In the case of bosons or fermions on a lattice that can be treated by finite-temperature perturbation theory (with a noninteracting theory as the unperturbed starting point), a proof that finite-size errors are exponentially small to all orders in perturbation theory can be made based on the momentum-space representation of the Hamiltonian. The proof is essentially identical for bosons and fermions, so we focus on the former.

We consider a generic massive scalar field theory in a 1D lattice, with unit lattice spacing, L sites, and PBC:

$$\hat{H}_s = \frac{1}{2}\sum_{j=1}^{L}\left[\hat{\pi}_j^2 + (\hat{\varphi}_{j+1} - \hat{\varphi}_j)^2 + m^2\hat{\varphi}_j^2\right], \tag{21}$$

where $[\hat{\varphi}_j, \hat{\pi}_{j'}] = i\delta_{jj'}$ and $\hat{\varphi}_{j+L} \equiv \hat{\varphi}_j$, $\hat{\pi}_{j+L} \equiv \hat{\pi}_j$. This Hamiltonian is diagonalized via

$$\begin{aligned}\hat{\varphi}_j &= \frac{1}{\sqrt{2L}}\sum_{n=0}^{L-1}\omega_n^{1/2}\left[e^{\frac{2\pi i n j}{L}}\hat{a}_n + e^{-\frac{2\pi i n j}{L}}\hat{a}_n^\dagger\right],\\ \hat{\pi}_j &= -\frac{i}{\sqrt{2L}}\sum_{n=0}^{L-1}\omega_n^{-1/2}\left[e^{\frac{2\pi i n j}{L}}\hat{a}_n - e^{-\frac{2\pi i n j}{L}}\hat{a}_n^\dagger\right],\end{aligned} \tag{22}$$

so that

$$\hat{H}_s = \sum_{n=0}^{L-1}\omega_n\hat{a}_n^\dagger\hat{a}_n + \text{constant}, \tag{23}$$

where $[\hat{a}_n, \hat{a}_{n'}^\dagger] = \delta_{nn'}$, $\omega_n = \omega(k_n)$, $k_n = 2\pi n/L$, $n \in [0, L-1]$, and

$$\omega(k) = \sqrt{2(1-\cos k) + m^2} = \sqrt{4\sin^2(k/2) + m^2}. \tag{24}$$

We now want to compute the grand canonical partition function

$$Z(\beta,\mu) \equiv \mathrm{Tr}\, e^{-\beta(\hat{H}-\mu\hat{N})}, \tag{25}$$

where $\hat{N} = \sum_n \hat{a}_n^\dagger\hat{a}_n$ is the total number operator. We take the trace in the Fock basis of eigenstates of each $\hat{a}_n^\dagger a_n$,

$$Z_L(\beta,\mu) = \prod_{n=0}^{L-1}\sum_{N_n=0}^{\infty} e^{-\beta(\omega_n-\mu)N_n} = \prod_{n=0}^{L-1}\frac{1}{1-e^{-\beta(\omega_n-\mu)}}. \tag{26}$$

Equivalently,

$$\Omega_L(\beta,\mu) = \frac{1}{L}\ln Z_L(\beta,\mu) = \frac{1}{L}\sum_{n=0}^{L-1}F(k_n), \tag{27}$$

where we have defined

$$F(k) \equiv -\ln[1 - e^{-\beta(\omega(k)-\mu)}]. \tag{28}$$

In the thermodynamic limit, the sum over n becomes an integral,

$$\Omega(\beta,\mu) \equiv \lim_{L\to\infty}\Omega_L(\beta,\mu) = \frac{1}{2\pi}\int_0^{2\pi} dk\, F(k). \tag{29}$$

We now wish to show that $|\Omega_L(\beta,\mu) - \Omega(\beta,\mu)|$ is exponentially small in L.

We first note that $F(k)$ is periodic in k with period 2π. Therefore, its Fourier expansion takes the form

$$F(k) = \sum_{j=-\infty}^{+\infty}\tilde{F}_j\, e^{ijk}, \tag{30}$$

where the Fourier coefficients are given by

$$\tilde{F}_j = \frac{1}{2\pi}\int_0^{2\pi} dk\, e^{-ijk}F(k). \tag{31}$$

Using Eqs. (29) and (31), we get

$$\Omega(\beta,\mu) = \tilde{F}_0. \tag{32}$$

Using Eqs. (27) and (30), we get

$$\begin{aligned}\Omega_L(\beta,\mu) &= \frac{1}{L}\sum_{n=0}^{L-1}F(2\pi n/L) = \frac{1}{L}\sum_{n=0}^{L-1}\sum_{j=-\infty}^{+\infty}\tilde{F}_j\, e^{2\pi i j n/L}\\ &= \sum_{j=-\infty}^{+\infty}\tilde{F}_j\left[\frac{1}{L}\sum_{n=0}^{L-1}e^{2\pi i j n/L}\right]\\ &= \sum_{j=-\infty}^{+\infty}\tilde{F}_j\delta_{j \bmod L,\,0} = \sum_{j'=-\infty}^{+\infty}\tilde{F}_{j'L}.\end{aligned} \tag{33}$$

Subtracting Eq. (32) from Eq. (33), we get

$$O_L(\beta,\mu) - \Omega(\beta,\mu) = \sum_{j\neq 0}\tilde{F}_{jL}. \tag{34}$$

Examining Eqs. (24) and (28), we see that if $m > 0$ and $\mu < m$ (necessary to avoid Bose condensation), then $F(k)$ is continuous and infinitely differentiable for all real k. It then follows from a general theorem of Fourier series [13] that $\tilde{F}_{jL}$ goes to zero faster than any power of $|j|L$ as $L \to \infty$. The sum over j in Eq. (34) will then be dominated by the $j = \pm 1$ terms. We conclude that $|O_L(\beta,\mu) - \Omega(\beta,\mu)|$ is exponentially small in L if $m > 0$ and $\mu < m$.

We can verify this explicitly. Again examining Eqs. (24) and (28), we see that $F(k)$ is changing most rapidly near $k = 0$. For $m > 0$ and small enough k, $F(k)$ can be approximated

via

$$F(k) \simeq -\ln[1 - e^{-\beta(m-\mu)}e^{-\beta k^2/2m}]. \quad (35)$$

Assuming $\mu < m$, we have

$$F(k) \simeq \sum_{n=1}^{\infty} \frac{1}{n} e^{-n\beta(m-\mu)}e^{-n\beta k^2/2m}. \quad (36)$$

In this approximation, we get

$$\tilde{F}_{jL} \simeq \sqrt{\frac{m}{2\pi\beta}} \sum_{n=1}^{\infty} \frac{1}{n^{3/2}} e^{-n\beta(m-\mu)}e^{-j^2L^2m/2\beta n}. \quad (37)$$

The sum over n can be approximated by steepest descent. For $j^2L^2 \gg 1/m(m-\mu)$, we find

$$\tilde{F}_{jL} \simeq \frac{1}{|j|L} \exp[-[2m(m-\mu)]^{1/2}|j|L]. \quad (38)$$

This is exponentially small in L, as expected from the general theorem. The sum over j in Eq. (34) is then dominated by $j = \pm 1$, and we have

$$|\Omega_L(\beta,\mu) - \Omega(\beta,\mu)| \simeq \frac{2}{L} \exp\{-[2m(m-\mu)]^{1/2}L\}, \quad (39)$$

which is the behavior observed for the 1D Ising model in Fig. 1.

This proof extends straightforwardly to higher dimensions, assuming periodic boundary conditions in each dimension.

Now consider adding an interaction term to $\hat{H}_s$, such as $g\sum_j \varphi_j^4$. We can compute $\Omega_L(\beta,\mu)$ order by order in finite-temperature perturbation theory. Each term is represented by a connected Feynman diagram [14]. The expression for a diagram with p propagators and v vertices takes the form

$$\frac{1}{L}\sum_{n_1=0}^{L-1} \cdots \frac{1}{L}\sum_{n_{p-v+1}=0}^{L-1} g^v F\left(k_{n_1},\ldots,k_{n_{p-v+1}}\right). \quad (40)$$

For $m > 0$ and $\mu < m$, F is infinitely differentiable in each k_{n_i}. Hence, one can once again apply the general theorem that says that the difference between Eq. (40) and the $L \to \infty$ limit must be exponentially small in L.

Other models of bosons and/or fermions can be analyzed in exactly the same way, with only the form of $F(k)$ changing. As long as $F(k)$ is infinitely differentiable, the argument holds.

V. NUMERICAL TESTS

In this section, we discuss numerical results that support the generality of the conclusions reached so far. The results are obtained using full exact diagonalization calculations for fermionic systems in one dimension. We study spinless fermions with nearest-neighbor hoppings that are either noninteracting or that have nearest and next-nearest-neighbor interactions. They are described by the following generic Hamiltonian

$$\hat{H}_{\rm f} = \sum_i \Big[-t(\hat{c}_i^\dagger \hat{c}_{i+1} + \text{H.c.}) + V\left(\hat{n}_i - \frac{1}{2}\right)\left(\hat{n}_{i+1} - \frac{1}{2}\right) + V'\left(\hat{n}_i - \frac{1}{2}\right)\left(\hat{n}_{i+2} - \frac{1}{2}\right)\Big], \quad (41)$$

where $\hat{n}_i = \hat{c}_i^\dagger \hat{c}_i$ is the number operator. We present results for different values of the parameters V and V', and using both the canonical and grand canonical ensembles with open and periodic boundary conditions. We also report NLCE results.

In all cases, we calculate the energy per site E_l. For noninteracting fermions, we also compute the occupation of the momentum $k = 0$ mode, $n^l_{k=0} \equiv \sum_{i,j}\langle \hat{c}_i^\dagger \hat{c}_j\rangle$. For the interacting models, we compute the the nearest-neighbor single-particle correlation function $K_l = \sum_i \langle \hat{c}_i^\dagger \hat{c}_{i+1} + \text{H.c.}\rangle$. For the results reported, by l we mean the number of sites of the finite system or the number of sites of the largest cluster in the NLCE. We plot the finite size errors δE_l, $\delta n^l_{k=0}$, and δK_l, with $\delta O_l \equiv (O_l - O)/O$ where O (E, $n_{k=0}$, K) is either the exact analytic result in the thermodynamic limit, when known, or the highest-order result from a numerical-linked cluster expansion.

Figure 2 reports results for δE_l and $\delta n^l_{k=0}$ for noninteracting fermions [Eq. (41) with $t = 1$ and $V = V' = 0$]. Figures 2(a) and 2(b) show the finite-size errors of the energy at two temperatures, and Fig. 2(c) shows the finite-size errors of the zero-mode occupation (the sum of all one-particle correlations). The results for the grand-canonical energy in finite

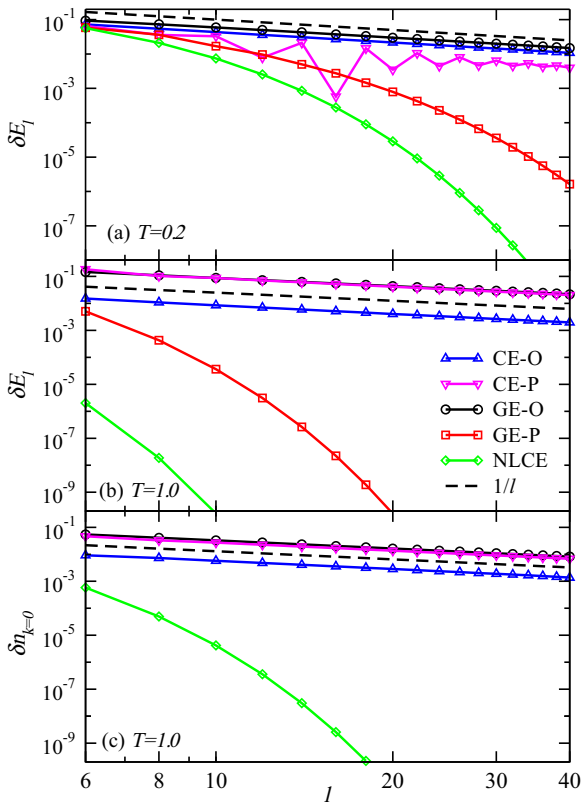

FIG. 2. (Color online) Comparison of results of canonical and grand-canonical ensembles with open and periodic boundary conditions, and NLCEs, for noninteracting fermions hopping on a one-dimensional lattice [corresponds to Eq. (41) with $t = 1, V = V' = 0$]. The energy difference δE_l (see text) is plotted for two different temperatures in panels (a) and (b). Panel (c) shows the occupation of the $k = 0$ mode, or, equivalently, the correlation $L^{-1}\sum_{ij}\langle c_i^\dagger c_j\rangle$. $\delta n_{k=0}$ is zero for the grand-canonical ensemble with PBCs; see text.

systems can be obtained analytically,

$$E_l = \sum_{n=0}^{l-1} \frac{\epsilon_n e^{-\beta\epsilon_n}}{1+e^{-\beta\epsilon_n}}, \tag{42}$$

where ϵ_n are the single-particle eigenenergies. The momentum distribution function with periodic boundary conditions is given by the Fermi-Dirac distribution

$$n_k = \frac{1}{1+e^{-\beta\epsilon_k}}. \tag{43}$$

We note that n_k for finite systems (for the values of k allowed) is exactly the same as in the thermodynamic limit. Hence, $\delta n^l_{k=0} = 0$ for the grand-canonical ensemble with PBC. Therefore, no error is reported for the GE-P in Fig. 2(c). The results in the canonical ensemble are obtained as described in Ref. [3].

For the two temperatures and two quantities reported in Fig. 2, one can see that the errors of the GE-O, CE-P, and CE-O results decrease as $1/l$. This is expected and is made apparent in the plots by comparing those results to the $1/l$ plots (dashed lines) depicted for reference. On the other hand, the GE-P (for the energy) and NLCE errors can be seen to decrease exponentially with increasing l. For the energy, the NLCE errors are much smaller than the GE-P ones, showing once again that NLCEs generally (n_k for noninteracting fermions being a counterexample) outperform grand-canonical calculations in finite translationally invariant systems.

Figures 3 and 4 show the results for: (a) δE_l and (b) δK_l for interacting fermions [Eq. (41)] with $(t,V,V') = (1,1,0)$ and $(1,1,1)$, respectively. In all cases, it is apparent that only the GE-P and NLCE errors decrease exponentially fast with l, while the GE-O and CE errors decrease as $1/l$. Once again, these results (now for interacting systems) show that the NLCE errors are significantly smaller than those of the GE-P. Here, we have used the highest order of the NLCE ($l = 18$) as the estimate for the thermodynamic limit [17]. All results for the interacting models were obtained using full exact diagonalization of the Hamiltonian.

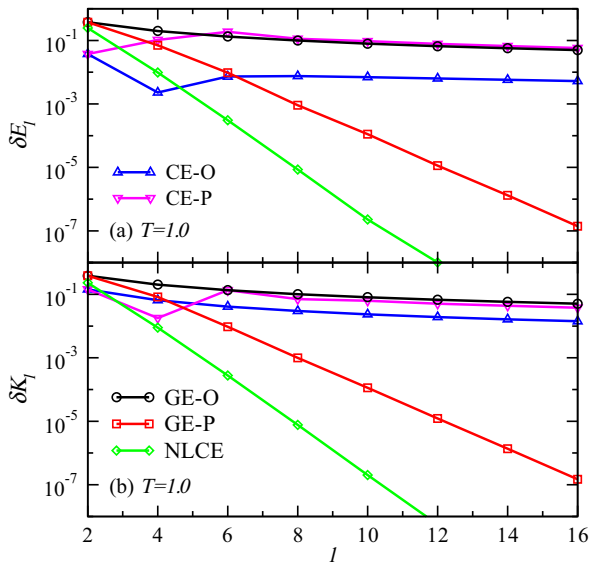

FIG. 3. (Color online) (a) δE_l and (b) δK_l for interacting fermions [Eq. (41)] with $t = 1$ (unit of energy), $V = 1.0$, $V' = 0$, and $T = 1.0$.

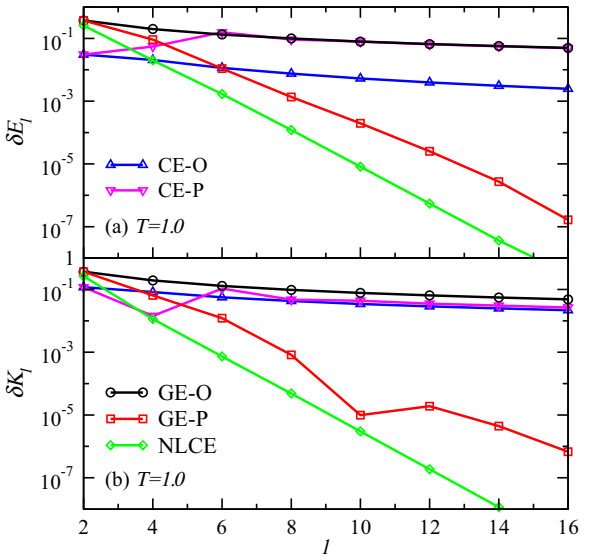

FIG. 4. (Color online) (a) δE_l and (b) δK_l for interacting fermions [Eq. (41)] with $t = 1$ (unit of energy), $V = 1.0$, $V' = 1.0$, and $T = 1.0$.

Finally, although we cannot make an analysis in 2D equivalent to that presented for interacting models in 1D (because of the exponential scaling of the computational cost combined with the fast increase of N), we can still verify that NLCE calculations have exponentially small errors. In Fig. 5, we show results for δE_l for the 2D Heisenberg model in four different lattice geometries—square [11], honeycomb [15,16], kagome, and triangular [5]. In all cases, the error is once again seen to decrease exponentially fast with increasing the number of sites in the clusters considered.

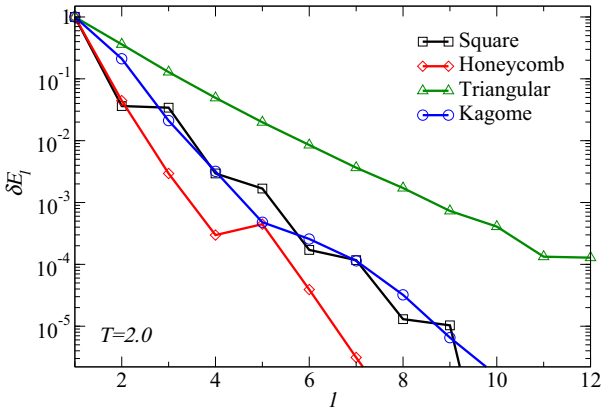

FIG. 5. (Color online) δE_l in NLCE calculations of the Heisenberg model in four different two-dimensional lattices, as indicated. The approach to the thermodynamic limit result is again exponentially fast as one increases the order of the expansion. The results presented here were taken from Refs. [5,11,15,16]. $J = 1$ is taken to be the unit of energy.

VI. CONCLUSIONS

We have shown that grand-canonical ensemble calculations in translationally invariant systems that are in unordered phases at finite temperatures have exponentially small finite-size errors, whereas canonical ensemble calculations have errors that are power law in system size. Hence, while full exact diagonalization calculations in the canonical ensemble are computationally less demanding than grand-canonical ones, if one is interested in accurately computing quantities in an unordered finite-temperature phase, using the grand-canonical ensemble is preferable. The additional computational cost incurred by diagonalizing all particle sectors (around a factor two for spinless fermions at half filling) for the GE is far less than the speed up gained by having to study smaller systems (exponential). Furthermore, we have shown that numerical linked cluster expansions generally have even smaller errors than grand canonical ensemble calculations in translationally invariant systems. The additional cost incurred in the diagonalization of many clusters with a given size is far less than the speed up gained by having to study clusters that are much smaller than finite systems with periodic boundary conditions. The benefit of using NLCEs is most striking in two-dimensional lattices.

The specific system sizes (cluster sizes) required to observe exponential convergence in grand-canonical calculations of systems with periodic boundary conditions (in numerical-linked cluster expansions) depend on details such as the model under consideration and the temperatures of interest, which set the relevant correlation length. Otherwise, our conclusions are completely general.

ACKNOWLEDGMENTS

We thank Anders Sandvik and Cristian Batista for stimulating discussions. This work was supported by the Office of Naval Research (D.I. and M.R.), and by NSF Grant No. PHY13-16748 (M.S.).

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