Numerical Linked-Cluster Approach to Quantum Lattice Models

Marcos Rigol, Tyler Bryant, and Rajiv R. P. Singh
Department of Physics, University of California, Davis, California 95616, USA
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We present a novel algorithm that allows one to obtain temperature dependent properties of quantum lattice models in the thermodynamic limit from exact diagonalization of small clusters. Our numerical linked-cluster approach provides a systematic framework to assess finite-size effects and is valid for any quantum lattice model. Unlike high temperature expansions, which have a finite radius of convergence in inverse temperature, these calculations are accurate at all temperatures provided the range of correlations is finite. We illustrate the power of our approach studying spin models on kagomé, triangular, and square lattices.

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Understanding finite temperature thermodynamic properties of quantum lattice models is a fundamental and challenging task [1,2]. Two general approaches that are commonly used are studies of finite systems, by means of exact diagonalizations (ED) or quantum Monte Carlo (QMC) simulations, and series expansions in the thermodynamic limit (TL). ED are usually limited to rather small clusters and at finite temperatures and dimensions higher than one it is very difficult to assess finite-size effects. On the other hand, QMC methods enable one to study much larger system sizes but then the classes of models that can be addressed are severely limited by the (fundamental [3]) sign problem.

In order to obtain results in the TL one can use high temperature expansions (HTE). Within this approach properties of the system are expanded in powers of inverse temperature, β [4]. These expansions, carried out to order β^N (where N is typically around 10), provide accurate numerical results for $\beta < \beta_c$, where β_c is the radius of convergence of the series. Interestingly, HTE can fail to converge even when correlations are still short ranged. Beyond the region of convergence, series extrapolation methods [5] allow one to calculate thermodynamic properties, but their reliability remains uncertain.

We introduce in this Letter a new method, a numerical linked-cluster (NLC) approach, that works in the TL as HTE, yet makes possible to obtain convergence at all temperatures for models with short-ranged correlations. It is also able to deal with multiple microscopic energy scales in the problem, which can differ by several orders of magnitude, something that is very difficult within HTE. When the correlation length grows, larger clusters begin to contribute and NLC, up to a given cluster size, no longer converges. In some cases, one can accelerate the convergence by using sequence extrapolation techniques [5,6]. We will discuss here the advantages of NLC over HTE and ED for three different classes of models with dominant microscopic energy scale J, referred below as (A) models that remain short ranged at all temperatures, (B) models in which correlations remain short ranged down to $T \ll J$, and (C) models where correlations build up at T of order J.

The fundamental basis for a linked-cluster expansion, for some extensive property P of an infinite lattice $\mathcal{L}$, is the relation [4,7]

$$P(\mathcal{L})/N = \sum_c L(c) W_P(c). \tag{1}$$

Here N is number of lattice sites, $L(c)$ is the lattice constant (number of embeddings of the cluster in the lattice per lattice site) of cluster c, and $W_P(c)$ is the weight of the cluster c for the property P. The latter is defined recursively by the principle of inclusion and exclusion [4],

$$W_P(c) = \mathcal{P}(c) - \sum_{s \subset c} W_P(s). \tag{2}$$

Here $\mathcal{P}(c)$ is the property P calculated for the finite cluster c and the sum on s runs over proper subclusters of c. In HTE, for every cluster, $\mathcal{P}$ and, equivalently, its weight W_P, is expanded in powers of β and only a finite order of terms are retained. In NLC, an exact diagonalization of the cluster is used to calculate $\mathcal{P}$ and hence W_P at any temperature.

Note then that NLC builds in more bare information of the system than HTE. We will show that when HTE converges, NLC gives results that are identical to HTE. However, NLC converges down to lower temperatures, in some cases low enough to obtain ground state properties. In addition, unlike HTE, the region of convergence of NLC increases as larger clusters are included in the sum. Hence, NLC helps to separate cases where the failure of HTE is due to its (not understood) analytic structure in the complex plane, from where the correlations truly exceed the largest clusters studied.

There is a second aspect in which the NLC scheme is fundamentally different to HTE, and that can be used to ones advantage. In HTE, the choice of clusters is dictated by the order in which they first contribute in the power series, which is typically related to the number of bonds in a cluster. In NLC, one has substantial freedom to arrange the choice of clusters. They can be ordered by number of sites, number of bonds, etc. The only requirement is that, with increasing order, the cluster weights, when expanded

in inverse temperature, should give the correct HTE coefficients as well. A small subset of the clusters may limit the order to which HTE coefficients are correct. Such expansions may sacrifice efficiency in the exact HTE coefficients, but can lead to NLC which converge better at intermediate and lower temperatures.

We first apply the NLC method to the kagomé lattice Ising model. This model is exactly soluble and known to stay disordered at all temperature with a finite entropy at $T = 0$. Since a kagomé lattice consists of corner sharing triangles, it is advantageous to restrict the sum to a single site plus clusters that only contain complete triangles, which reduces dramatically the number of clusters to be considered. The number of topologically distinct linked clusters on the kagomé lattice with 1 through 8 triangles is 1, 1, 1, 2, 2, 5, 7, and 15, respectively. (The maximum-site cluster with N triangles has $2N + 1$ sites.) For the entropy of the kagomé lattice Ising antiferromagnet, this leads to a rapidly convergent expansion, whose first term is the well-known Pauling result [8] that gives a ground state entropy of 0.501 36. The next correction to this result comes from a 12-site cluster of 6 triangles, which leads to $S = 0.501\,82$, that agrees with the exact result $S = 0.501\,83$ [9] to 4 significant digits. This very simple example shows that, in contrast to HTE, ground state properties of class (A) models can be obtained within NLC without the need for extrapolation.

We now consider the antiferromagnetic Heisenberg-Ising Hamiltonian

$$\mathcal{H} = \sum_{\langle i,j \rangle} S_i^z S_j^z + J_\perp (S_i^x S_j^x + S_i^y S_j^y) + h_x \sum_i S_i^x + h_z \sum_i S_i^z, \tag{3}$$

where we have chosen the Ising coupling to be unity. The transverse field is denoted h_x and the longitudinal field is denoted h_z.

As a first application of NLC to a class (A) quantum model, we study the kagomé lattice Ising model in a transverse field. This model is known to be disordered at all temperatures [10]. In Fig. 1, we show results from the NLC up to 5 and 6 triangle clusters for the entropy (S) and specific heat (C_v) in transverse fields h_x of 0, 0.01, 0.25, 0.5, and 1.0, respectively. Note that the temperature scale goes down to 0.001, a real challenge for any numerical calculation of a thermodynamic system. For $h_x = 0.0$, 0.5, and 1, the results have fully converged and there is no discernible contribution from 6-triangle clusters at any temperature. Such results are beyond the region of convergence of HTE, and in contrast to ED of finite clusters they do not suffer from finite-size effects. For $h_x = 0.25$, there is a double peaked structure in the specific heat and the largest clusters make a small contribution near the lower peak. Only for the smallest magnetic field the larger clusters contribute. For $h_x = 0.01$, the specific heat exhibits two well-separated peaks. At high temperatures the

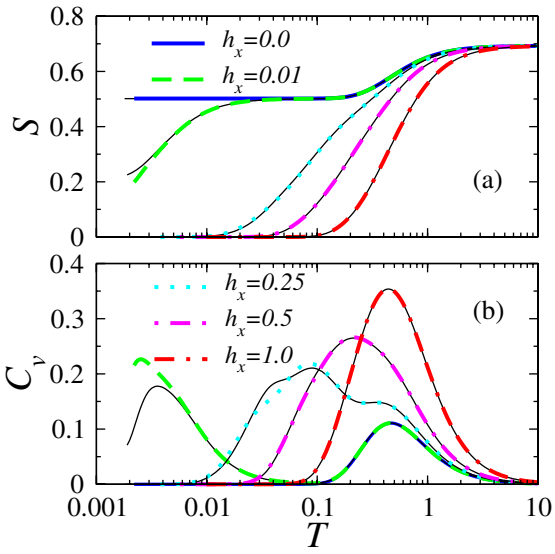

FIG. 1 (color online). NLC results up to 5 (thin lines) and 6 (thick lines) triangles for entropy (a) and specific heat (b) of the transverse Ising model on the kagomé lattice as a function of temperature (T) for five different values of the transverse field (h_x). Except for very low but nonzero transverse field, the direct sum converges at all temperature.

transverse field plays no role and the results are identical to the pure Ising model for the entropy and specific heat. Well below $T = 0.1$, the transverse field causes the entropy to head down towards zero and the second peak arises in the specific heat. At the lowest temperatures the correlations are enhanced by the transverse field [10] causing contribution from clusters larger than those included in our results.

A more challenging, and still open, question is what happens to an Ising-like system when quantum fluctuations are introduced via the XY coupling ($J_\perp$) [class (B) model]. The kagomé-lattice Heisenberg model ($J_\perp = 1$) is one of the most fascinating quantum spin models, where spin-spin correlations likely remain short ranged down to $T = 0$ [11–13]. Its thermodynamic properties have also been of much interest [14–16]. In Fig. 2, we show entropy and specific heat for the XXZ models on kagomé lattice with contributions up to 7 and 8 triangles. For $J_\perp$ up to around 0.25 our calculations converge down to low enough temperatures to see that C_v must have two peaks. As $J_\perp$ is increased even further, the NLC expansion breaks down before a second peak could be resolved [15,16]. The temperature dependence is suggestive that a similar ordering mechanism is operative for the entire range $0 < J_\perp < 1$, and quite likely large unit cells are involved in further ordering at lower temperatures [17].

The high temperature peak in Fig. 2 is associated with short-range order and is perfectly resolved within our approach. However, it is already beyond the radius of convergence of HTE. In Fig. 3 we show a detailed comparison between NLC and HTE [16] for the kagomé lattice

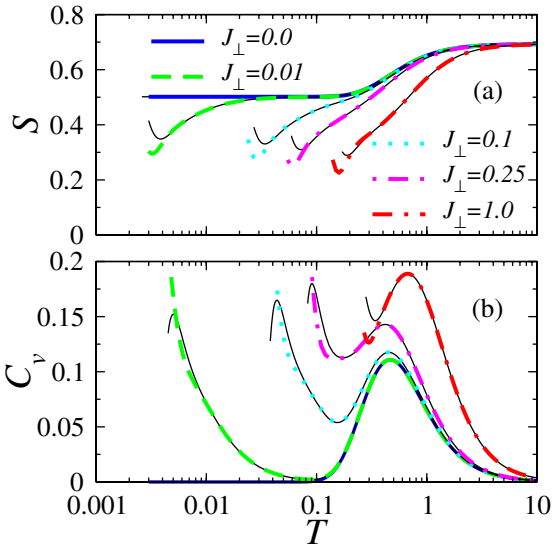

FIG. 2 (color online). NLC results up to 7 (thin lines) and 8 (thick lines) triangles for the entropy (a) and specific heat (b) of the XXZ models on the kagomé lattice.

Heisenberg model. The HTE converges only for $T > 1$, and inclusion of larger clusters does not improve convergence at lower T. Only a Padé extrapolation can help HTE at lower temperatures. Two such extrapolations from Ref. [16] are also shown. They can lead to accurate results but their reliability is, in general, not known. For example, in Fig. 3, one can see that they start to differ from each other right below the peak in C_v. For NLC, on the other hand, we know that our results are converged if the weight of larger graphs is negligible, i.e., it provides a controlled way to approach lower temperatures that is somehow absent in HTE and ED. Figure 3 also shows that, as opposed to HTE, the NLC convergence moves to lower temperatures as larger clusters are included.

Within a NLC approach, one way to accelerate the convergence of the direct sum in (1) is to use sequence extrapolation methods [5,6]. Their power can be seen in Fig. 4, where we plot C_v for the Ising model in a transverse and longitudinal field [10] (the phase diagram is shown in the inset). With a small transverse field, adding a longitudinal field causes a bond-ordered phase to arise. Here we have chosen a small longitudinal field, which enhances the correlations of the system, but does not drive it into the ordered phase. Larger clusters begin to contribute to specific heat below $T = 1$, and the simple sum no longer converges at lower temperature. However, two different extrapolation methods (Euler [6] and Wynn [5]) lead to results that converge at all temperatures. Euler's method is a powerful tool when terms in the sum alternate in sign [6]. On the other hand, Wynn's algorithm is more general and allows several cycles of improvements [5].

As a final test of our method we study the Heisenberg model on the triangular and square lattices [class (C) models], which are known to develop long range order at zero temperature. For the triangular lattice, we use NLC based on triangular clusters (up to 8 triangles), whereas for the square lattice we use a site-based expansion of up to 13 sites. In Fig. 5 we show the entropy of these models obtained by various orders of extrapolations with the Wynn and Berezenski methods [5]. These results are compared with those obtained by Bernu and Misguich (BM) [18]. The agreement is quite good down to $T = 0.3$ for the square-lattice case, where the entropy is <0.05 (spin-spin correlation length about 20 lattice spacings [15], i.e., larger than our cluster sizes), whereas for the triangular-lattice it is good down to $T = 0.2$ where the entropy is about 0.2

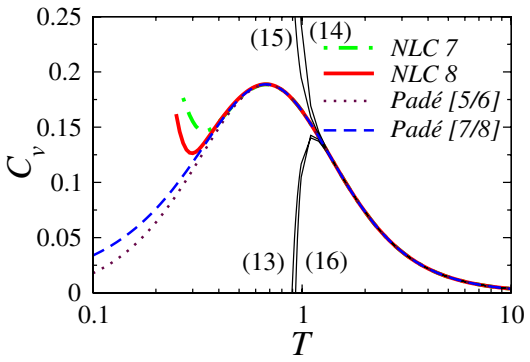

FIG. 3 (color online). Specific heat of kagomé lattice Heisenberg model as a function of temperature T. The direct sum of HTE to order 13–16 is shown to diverge around $T = 1$. NLC up to 7 and 8 triangle clusters converges below $T = 0.4$. Two Padé approximants are also shown (see Ref. [16] for details), one of which is close to NLC result down to $T = 0.3$. The NLC results indicate that there may be a second peak below $T = 0.3$.

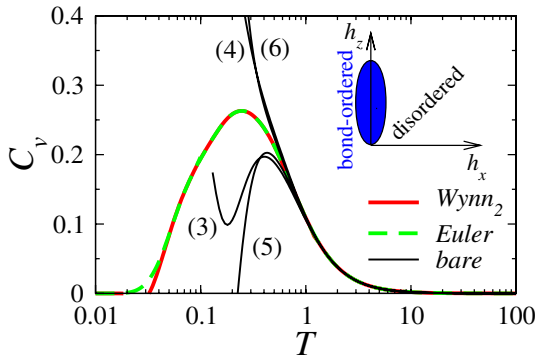

FIG. 4 (color online). Specific heat of kagomé lattice Ising model in a transverse field $h_x = 0.5$ and a longitudinal field $h_z = 0.25$. The $T = 0$ phase diagram of the model is shown in the inset (the line $h_x = 0$ is critical). The parameters correspond to large but finite correlation length, where bare sums up to 3, 4, 5, and 6 triangle clusters diverge below $T = 1$ but the sequence extrapolation methods converge at all temperatures. The subscript "2" in Wynn means that two cycles were applied to accelerate convergence [19].

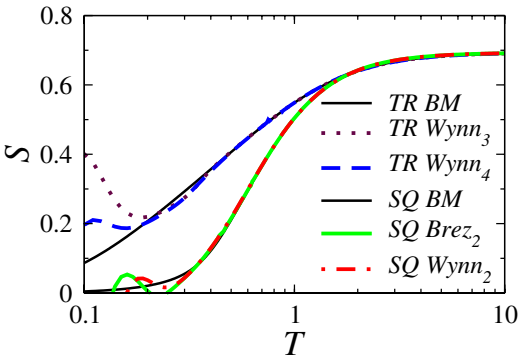

FIG. 5 (color online). The entropy of square (SQ) and triangular (TR) lattice Heisenberg models. Various extrapolations of NLC are compared with results obtained by BM [18]. Subscripts in Wynn's and Brezinski's (Brez) extrapolation results show the number of cycles applied to accelerate convergence [5].

(spin-spin correlation length about two lattice spacings [15], which raises the question, what other correlations are building up leading to a breakdown of NLC convergence?). In general, the extrapolations do not converge well below the peak for the specific heat. Hence, *a priori*, there is no advantage of NLC (with extrapolation) over HTE (with Padé extrapolations) for models of class (C), as both methods require extrapolations, whose convergence is difficult to judge. NLC, however, does provide a scheme that like HTE allows for systematic extrapolations.

In summary, we have introduced a numerical linked-cluster method to calculate properties of quantum lattice models. It provides a framework to study observables in the TL while performing exact diagonalization on finite-size clusters. This approach allows us to go beyond the radius of convergence of HTE, and is better suited to models where correlations remain short ranged down to low temperatures.

We have used NLC to study the thermodynamic properties of frustrated two-dimensional quantum antiferromagnets. We have shown that one can obtain accurate results for short-ranged models (Ising and transverse Ising models on a kagomé lattice) at all temperatures. For models where correlations develop slowly, like XXZ models on the kagomé lattice, there is a large temperature window (which is $0.3 < T < 1.0$ for the Heisenberg case) where NLC converges but HTE diverges. Hence, NLC provides for these [class (B)] models a framework to approach lower temperatures in a controlled way. We have also shown that the region of convergence of NLC increases as larger clusters are included.

In order to accelerate the convergence of the bare NLC sum one can use sequence extrapolation methods, but then uncertainty similar to Padé extrapolations for HTE remains. As examples, we have studied Heisenberg models on triangular and square lattices, where our results compare very well with those in Ref. [18]. To study models of interest at lower temperatures our approach can be extended to include larger clusters by using Lanczos type methods focusing only on low lying states rather than a complete diagonalization [1]. Furthermore, the method can be applied to $t - J$ and other models, and to various susceptibilities and correlation functions. These are left for future work.

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