Numerical Linked-Cluster Approach to Quantum Lattice Models

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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 (NLC) approach provides a systematic framework to assess finite-size effects and is valid for any quantum lattice model. Unlike high temperature expansions (HTE), 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, $\beta$ \[4\]. These expansions, carried out to order $\beta^N$ (where $N$ is typically around 10), provide accurate numerical results for $\beta < \beta_c$, where $\beta_c$ 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 \[6, 7\]. 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 $T < < J$, 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 $L$, is the relation \[4, 7\]

$$P(L)/N = \sum_c L(c) \times W_P(c),$$

(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 \[4, 5\],

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

(2)

Here $P(c)$ 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, $P$ and equivalently its weight $W_P$ is expanded in powers of $\beta$ and only a finite order of terms are retained. In NLC an exact diagonalization of the cluster is used to calculate $P$ 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 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, 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 \[ S = 0 \] that gives a ground state entropy of 0.50136. The next correction to this result comes from a 12-site cluster of 6 triangles, which leads to $S = 0.50182$, that agrees with the exact result \[ S = 0.50183 \] 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

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

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 at all temperatures \[ 10 \]. In Fig. 1, we show results from a transverse field. This model is known to be disordered.

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 non-zero transverse field, the direct sum converges at all temperature.

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 $T = 0$ \[ 11 \]. Its thermodynamic properties have also been of much interest \[ 12 \]. 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 \[ 14 \]. 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 \[ 15 \].

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 Heisenberg model. The HTE converges only for $T > 1$, and inclusion of larger clusters does not improve convergence at lower $T$. Only a Pade 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. Fig. 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 alter-

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 [3]. These results are compared with those obtained by Bernu and Misguich.
(BM)\(^\text{18}\). 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\(^\text{15}\), 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 (spin-spin correlation length about two lattice spacings\(^\text{15}\), 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 order to accelerate the convergence of NLC 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.\(^\text{18}\). To study models of interest at lower temperatures our approach can be extended to include larger cluster by using Lanczos type methods focussing only on low lying states rather than a complete diagonalization\(^\text{1}\). 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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\[ \text{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 Bernu and Misguich (BM)\(\text{18}\). Subindexes in Wynn’s and Brezinski’s (Brez) extrapolation results show the number of cycles applied to accelerate convergence.}\]