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A short introduction to numerical linked-cluster expansions

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ABSTRACT

We provide a pedagogical introduction to numerical linked-cluster expansions (NLCEs). We sketch the algorithm for generic Hamiltonians that only connect nearest-neighbor sites in a finite cluster with open boundary conditions. We then compare results for a specific model, the Heisenberg model, in each order of the NLCE with the ones for the finite cluster calculated directly by means of full exact diagonalization. We discuss how to reduce the computational cost of the NLCE calculations by taking into account symmetries and topologies of the linked clusters. Finally, we generalize the algorithm to the thermodynamic limit, and discuss several numerical resummation techniques that can be used to accelerate the convergence of the series.

1. Introduction

1.1. High-temperature expansions

Calculating exact finite-temperature properties of quantum lattice models can be very challenging. One general approach to achieve that goal is to devise series expansions for the lattice model in question in the thermodynamic limit [1,2]. Common examples of these series expansions are high-temperature expansions (HTEs), in which extensive properties of the system are expanded in powers of the inverse temperature $\beta = (k_B T)^{-1}$ (in what follows we set the Boltzmann constant k_B to unity). For example, consider the Ising Hamiltonian with nearest-neighbor interactions:

$$\hat{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j, \tag{1}$$

where J is the strength of the interaction, $\langle \cdots \rangle$ denotes nearest neighbors, and σ_i ($= \pm 1$) is the Ising spin on site i. The partition function can be written as

$$\mathcal{Z} = \sum_{\{\sigma\}} e^{-\beta \hat{H}} = \sum_{\{\sigma\}} e^{\beta J \sum_{\langle i,j \rangle} \sigma_i \sigma_j}, \tag{2}$$

where the sum runs over all possible configurations of the spins. We define $K = \beta J$, which serves as a small parameter in the expansion:

$$\mathcal{Z} = \sum_{\{\sigma\}} \prod_{\langle i,j \rangle} e^{K \sigma_i \sigma_j} = \sum_{\{\sigma\}} \prod_{\langle i,j \rangle} \sum_{l=0}^{\infty} \frac{K^l}{l!} (\sigma_i \sigma_j)^l. \tag{3}$$

If we associate $(\sigma_i \sigma_j)^l$ to an l-fold bond between sites i and j, a typical term in the above expansion can be represented graphically as the lattice with various numbers of lines (including no line) connecting every two nearest-neighbor sites. Therefore, one can write the partition function in terms of contributions from all possible graphs that can be embedded on the lattice. (In the Ising model, the fact that $\sigma = \pm 1$ makes the calculations much easier than in quantum models such as the Heisenberg model.) The order in K that each graph contributes to is equal to the number of bonds it has (see Ref. [2] for more details on this derivation). Eq. (3) implies that the series with finite number of terms converges only at high temperatures, above or of the order of J. In what follows, we will see how this type of expansion is related to linked-cluster expansions.

1.2. Low-temperature expansions

Similar to HTEs, low-temperature expansions (LTEs) can be devised to describe properties of a system with discrete excited states close to its ground state, i.e., for $\beta \to \infty$. In this approach, the partition function is written as

$$\mathcal{Z} = e^{-\beta E_0} \left[1 + \sum_{n \neq 0} e^{-\beta (E_n - E_0)} \right], \tag{4}$$

where E_0 (E_n) is the ground state (nth excited state). If there is an energy increment, ϵ, satisfying $E_n - E_0 = m_n \epsilon$ with m_n being integer for all n, any thermodynamic property can be expressed as an expansion in powers of $e^{-\beta \epsilon}$. Then, cluster expansions similar to the ones discussed above for HTEs follow [2].

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1.3. Linked-cluster expansions

The idea behind linked-cluster expansions (LCEs) [2,3] is that for any extensive property P of a lattice model (such as the logarithm of the partition function or the internal energy) one can compute its value per lattice site $P(\mathcal{L})/N$ in the thermodynamic limit in terms of a sum over contributions from all clusters c that can be embedded on the lattice:

$$P(\mathcal{L})/N = \sum_c L(c) \times W_P(c), \tag{5}$$

where $L(c)$ is the multiplicity of c, namely, the number of ways per site in which cluster c can be embedded on the lattice, and $W_P(c)$ is the weight of that cluster for the property P. $W_P(c)$ is defined according to the inclusion–exclusion principle:

$$W_P(c) = P(c) - \sum_{s \subset c} W_P(s), \tag{6}$$

where

$$P(c) = \frac{\mathrm{Tr}\left[\hat{P}(c)e^{-\beta \hat{H}_c}\right]}{\mathrm{Tr}\left[e^{-\beta \hat{H}_c}\right]} \tag{7}$$

is the property calculated for the finite cluster c and the sum on s runs over all subclusters of c. In Eq. (7), $\hat{H}_c$ is the Hamiltonian of cluster c. One can check that the weight of a disconnected cluster vanishes because $P(c)$ can be written as the sum of its parts (see Section 2.2), hence, the name linked-cluster expansions.

The convergence of the series in Eq. (5), when all the terms are considered, is guaranteed by the definition of weights in Eq. (6). In fact, by swapping the place of $P(c)$ and $W_P(c)$ in Eq. (6), one can write the property of a *finite* cluster c as the sum of its weight and the weights of its subclusters. Taking the thermodynamic limit $c \to \mathcal{L}$ brings one back to Eq. (5). However, in that limit, only a finite number of terms can be accounted for, and the series has to be truncated.

Because of the inclusion–exclusion principle (Eq. (6)), the weight of every cluster contains only the contribution to the property that results from correlations that involve all the sites in the cluster, and in a unique fashion in accord with its specific geometry. At low temperature, when correlations grow beyond the size of the largest clusters considered in the series, the results show a divergent behavior (due to the missing contributions of clusters in higher orders of the expansion). In most of the two-dimensional quantum models of interest, this occurs near or at zero temperature, e.g., for the nearest-neighbor antiferromagnetic (AF) Heisenberg model on a bipartite lattice.

The clusters in the sum (5) are usually grouped together based on common characteristics to represent different orders [4,5]. For instance, in the *site expansion*, where sites are used as building blocks to generate the clusters, the order of the expansion is determined by the number of sites of the largest clusters. All the clusters with n sites are said to belong to the nth order. In LCEs, one has the freedom to devise an expansion (with a certain building block for generating the clusters in different orders) that best suits the particular model of interest. Some of these include the site, bond, or square expansions on the square lattice, and site, bond, or triangle expansions on the triangular and Kagomé lattices, and so on [5].

Despite the simple form of the LCE equations above, its computational implementation can be challenging, as one has to (i) generate all the linked clusters that can be embedded on the lattice, (ii) identify their symmetries and topologies to compute multiplicities (this step dramatically reduces the computational effort as, for any given model, many different clusters have identical values of $P(c)$), (iii) identify the subclusters of each cluster to calculate weights, and (iv) calculate the property of each cluster and perform the sums. LCEs are computationally very demanding as the number of embedded clusters, and their subclusters, grows exponentially with increasing the order of the expansion. Below, we explain all those steps in the context of an example (the site expansion on a finite square lattice). We should stress that the HTE explained above for the Ising model can be seen as a LCE in which the property for each cluster is calculated using a perturbative expansion of Eq. (7) in terms of K.

1.4. Numerical linked-cluster expansions

In this work, we present a pedagogical overview of the *numerical* linked-cluster expansions (NLCEs) introduced in Ref. [4]. NLCEs use the basis of LCEs, but employ exact diagonalization (ED), instead of perturbation theory as done in HTEs, to calculate the properties of finite clusters in the series. This means that the properties of each cluster are calculated to all orders in β. The main advantage of NLCEs over HTEs is that, for models with short-range correlations, it is possible to access arbitrarily low temperatures because of the lack of a small parameter in the series. Furthermore, for models in which correlations grow slowly as the temperature is lowered, NLCEs can converge well below the temperature at which HTEs diverge. In NLCEs, as opposed to HTEs, the convergence temperature is controlled by the correlations in the model, and by the highest order in the series that can be calculated.

The basics of NLCEs, and results for various spin and itinerant models in the square, triangular and Kagomé lattices, were presented in Refs. [4–6]. Recent applications of this method exploring properties of frustrated magnetic systems can be found in Refs. [7–9]. NLCE studies of the Hubbard model in the square and honeycomb lattices were reported in Refs. [10–12]. How to deal with Hamiltonians and observables that break some of the symmetries of the underlying lattice was discussed in Refs. [13,14]. Finally, how to generalize NLCEs to calculate ground-state as well as low-temperature properties of lattice Hamiltonians with dimerized ground states was the subject of Ref. [15], while direct ground state calculations in the thermodynamic limit were done in Ref. [16] and dynamics were explored in Ref. [17].

Here, we introduce NLCEs for finite clusters, in order to show how they converge to the exact result with increasing the order in the expansion, and, later, discuss NLCEs in the thermodynamic limit. The exposition is organized as follows. In Section 2, we present the algorithmic details and the numerical implementation of NLCE in two dimensions for a finite 4×4 lattice. In Section 2.7, we report results of the expansion for the AF Heisenberg model on this cluster and compare them, in each order, to exact results that can be obtained by means of full exact diagonalization of the 4×4 lattice. In Section 3, we discuss how to extend NLCEs to the thermodynamic limit, and compare NLCE results for the Heisenberg model to those from large-scale quantum Monte Carlo (QMC) simulations. In Section 4, we describe two resummation techniques that have been found to be widely applicable to accelerate the convergence of the NLCEs for thermodynamic properties of the lattice models of interest.

2. Implementation of NLCEs for finite systems

In this section, we sketch the NLCE algorithm for an arbitrary Hamiltonian that only connects nearest-neighbor sites on a $N = 16$ site square lattice with open boundary conditions, which is shown in Fig. 1. We have chosen this small lattice because it allows us to carry out the NLCE to all orders in the site expansion. It also allows us to compare the properties in each order of the expansion to exact results calculated directly by ED of the entire 16-site system.