HIGH TEMPERATURE SERIES EXPANSION FOR ORBITALLY DEGENERATE SYSTEMS*

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We have found an efficient algorithm for high temperature expansion of the SU(n) Heisenberg model, using properties of permutation. We also comment on the $n \to \infty$ limit.

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1. Introduction

The high temperature expansion is the Taylor expansion in inverse temperature around the high-temperature limit. It can be used to any interaction in any dimensions, and has provided significant information on variety of models [1]. Recently, we have found an efficient algorithm to carry out the high-temperature expansion for the SU(n) Heisenberg model. In Ref. [2], we have applied the algorithm to the one dimensional (1D) system, and obtained high order coefficients.

2. Model

We consider a generalized Heisenberg model that has SU(n) symmetry. When $n = 2$, the model is equivalent to the ordinary SU(2) Heisenberg model. Let each site take one of the n colors, and denote them as $|\alpha\rangle$ with $\alpha = 1, 2, \cdots, n$. We define $X^{\alpha\beta} := |\alpha\rangle\langle\beta|$ and an exchange operator $P_{i,j} := \sum_{\alpha=1}^{n} \sum_{\beta=1}^{n} X_i^{\alpha\beta} X_j^{\beta\alpha}$, for $i \neq j$. Colors of sites i and j are exchanged by $P_{i,j}$. The Hamiltonian for the SU(n) Heisenberg model in 1D is given by

$$\mathcal{H} := J \sum_{i=1}^{N-1} P_{i,i+1} + J P_{1,N} \,. \tag{1}$$

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In general, when there are n states per site, the maximum number of independent interacting components is n^2-1. The model, isotropic with respect to these components, is the SU(n) Heisenberg model. Hereafter, $Z := \mathrm{Tr}\ \mathrm{e}^{-\beta\mathcal{H}}$ denotes the partition function, and $\langle\cdots\rangle := \mathrm{Tr}\left(\cdots\ \mathrm{e}^{-\beta\mathcal{H}}\right)/Z$ denotes the average in this system. To investigate the specific heat, we calculate $\langle P_{i,i+1}\rangle$ because the internal energy is obtained by $\langle\mathcal{H}\rangle = NJ\langle P_{i,i+1}\rangle$. Furthermore, to investigate a correlation function $\langle X_i^{\alpha\beta}X_j^{\beta\alpha}\rangle$, we calculate $\langle P_{i,j}\rangle$ because there is a relation, $\langle X_i^{\alpha\beta}X_j^{\beta\alpha}\rangle = \frac{1}{n^2-1}(\langle P_{i,j}\rangle - n^{-1})$, for $\alpha\neq\beta, i\neq j$. In addition, for $i\neq j$, $\langle X_i^{\alpha\beta}X_i^{\beta\alpha}\rangle = 1/n$.

3. High temperature expansion

We use the finite cluster method for the high temperature expansion. That is, series coefficients in the thermodynamic limit are exactly obtained by summing up all the non-zero contribution from each finite-size cluster. The cluster of size ℓ is defined by $\mathcal{H}_\ell := J\sum_{i=1}^{\ell-1} P_{i,i+1}$, and $\langle\cdots\rangle_\ell$ denotes the thermal average using $\mathcal{H}_\ell$. In 1D, it is reduced to a simple equation. Namely, the formula $\sum_{i=1}^{\ell-x}\langle P_{i,i+x}\rangle_\ell - \sum_{i=1}^{(\ell-1)-x}\langle P_{i,i+x}\rangle_{\ell-1}$ gives correct coefficients of $\langle P_{i,i+x}\rangle$ up to $O[(\beta J)^{2\ell-x-1}]$.

In order to obtain the series expansion of $\langle P_{i,j}\rangle$ up to $O[(\beta J)^M]$, we need to calculate $\mathrm{Tr}\{(\mathcal{H}_\ell)^m\}$ and $\mathrm{Tr}\{P_{i,j}(\mathcal{H}_\ell)^m\}$ for $0\le m\le M$. The traces are calculated by decomposing a permutation into a product of independent cyclic permutations [3, 4] as explained in the following. Let us consider a trace of $P := P_{i_1,j_1}P_{i_2,j_2}\cdots P_{i_m,j_m}$, with $\mathrm{Tr}^{(\ell)}$ denoting the trace in the ℓ-site system,

$$\begin{aligned}\mathrm{Tr}^{(\ell)}P &:= \sum_{\alpha_1=1}^{n}\cdots\sum_{\alpha_\ell=1}^{n}\langle\overset{1}{\alpha}_1\overset{2}{\alpha}_2\cdots\overset{\ell}{\alpha}_\ell\,|P|\,\overset{1}{\alpha}_1\overset{2}{\alpha}_2\cdots\overset{\ell}{\alpha}_\ell\rangle \\ &= \sum_{\alpha_1=1}^{n}\cdots\sum_{\alpha_\ell=1}^{n}\langle\overset{1}{\alpha}_1\overset{2}{\alpha}_2\cdots\overset{\ell}{\alpha}_\ell\mid\overset{1}{\alpha}_{P1}\overset{2}{\alpha}_{P2}\cdots\overset{\ell}{\alpha}_{P\ell}\rangle, \qquad (2)\end{aligned}$$

where α_{Pi} refers to the color at position i after the permutation P. The summation of α_i makes a contribution only when $\alpha_i=\alpha_{Pi}$ for every i. Consider using this relation successively starting from i. That is, α_i is equal to α_{Pi}, and then α_{Pi} is equal to α_{P^2i}, ..., one can repeat this procedure until coming back to α_i at a certain power of P, namely, $\alpha_i=\alpha_{Pi}=\alpha_{P^2i}=\cdots=\alpha_i$. In other words, all the variables whose subscript belongs to one cyclic permutation in P have to be equal. Since any permutation is decomposed into a product of independent cyclic permutations, the number of the independent variables of the summation is the number $Y(P)$ of cyclic permutations of P. Therefore the trace is given by, $\mathrm{Tr}^{(\ell)}P = n^{Y(P)}$, and accordingly,

$\langle P\rangle_\ell = \mathrm{Tr}^{(\ell)}P/\mathrm{Tr}^{(\ell)}1 = n^{Y(P)-\ell}$. This equation has been used for the Handscomb's Monte Carlo [3]. It was also used for the high temperature expansion [4] for the ferromagnetic SU(n) Heisenberg model in three dimension to calculate the specific heat and the uniform susceptibility up to $O[(\beta J)^8]$. To investigate the antiferro-interaction model [2], we have calculated wave-number $q \neq 0$ components of the correlation function up to high orders. It requires a further refinement of the algorithm.

If we first expand $(\mathcal{H}_\ell)^m$ and apply the relation above, large clusters have too many terms — *e.g.* $m = 22$ and $\ell = 11$ make $(\ell-1)^m = 10^{22}$ terms. The calculation then consumes too much time. The point is to operate the Hamiltonian order by order. Since the Hamiltonian $\mathcal{H}_\ell$ has only permutation operators, after $\mathcal{H}_\ell$ is operated m times to $|\alpha_1\alpha_2\cdots\alpha_\ell\rangle$, the expression is written with proper coefficients $a_{m,\sigma}$ (σ: permutation) as

$$\begin{aligned}(\mathcal{H}_\ell)^m|\alpha_1\alpha_2\alpha_3\cdots\alpha_\ell\rangle \;=\; & a_{m,123\cdots\ell}|\alpha_1\alpha_2\alpha_3\cdots\alpha_\ell\rangle \\ & +a_{m,231\cdots\ell}|\alpha_2\alpha_3\alpha_1\cdots\alpha_\ell\rangle \\ & +a_{m,312\cdots\ell}|\alpha_3\alpha_1\alpha_2\cdots\alpha_\ell\rangle \\ & +\cdots\cdots . \end{aligned} \tag{3}$$

Assuming we know the coefficients $a_{m,\sigma}$ the trace is calculated by counting the number of cycles of permutation of each term in the r.h.s. of Eq. (3), namely,

$$\mathrm{Tr}^{(\ell)}\{(\mathcal{H}_\ell)^m\} = \sum_\sigma a_{m,\sigma}\, n^{Y(\sigma)}\,. \tag{4}$$

This method has an advantage that contribution from $|\alpha_{i_1}\alpha_{i_2}\cdots\alpha_{i_\ell}\rangle$ is calculated only once, instead of $a_{m,i_1 i_2\ldots i_\ell}$ times. Therefore, we carry out the calculation with the following manner. First, in order to regard $a_{m,\sigma}$ as an array, give a specific number to every permutation σ of numbers $1, 2, \ldots, \ell$. For example, one can regard σ as an ℓ-digits number of base ℓ; or, one can use a number whose p-th digit is of base p. In any case, these numbers can be very large in general. In the practical calculation, however, the array is extremely sparse and it can be compressed. We prepare an array to store the pointers in the ascending order and another array for the coefficients. Every time using the array, we use a binary search, which requires $\log_2 N_\mathrm{a}$ steps for an array with length N_a and thus it does not consume too much time. Then, start from $|\alpha_1\alpha_2\cdots\alpha_\ell\rangle$, operate $\mathcal{H}_\ell$, calculate the trace, and go to the next order; repeat this procedure up to the desired order. This method extremely decreases the number of terms in the array — *e.g.* 22-nd power of $\mathcal{H}_{\ell=11}$ requires only 4903704 terms.

Lastly, we comment on the limit of $n \to \infty$. In Ref. [2], we have obtained the specific heat by calculating the free energy. In this limit, the procedure

is simplified because only the identity permutation has contribution. Odd permutations do not contribute, that is, coefficients of J^m with odd m are equal to zero. Suppose we know $a_{m,\sigma}$ in Eq. (3) for all σ for given m. Since $(\mathcal{H}_\ell)^{2m} = (\mathcal{H}_\ell)^m (\mathcal{H}_\ell)^m$, then σ in $(\mathcal{H}_\ell)^m$ has to make a product with σ^{-1} in the other $(\mathcal{H}_\ell)^m$ in order to make an identity permutation. Therefore,

$$\lim_{n\to\infty} \left\langle (\mathcal{H}_\ell)^{2m} \right\rangle = a_{2m,\text{identity}} = \sum_\sigma a_{m,\sigma} a_{m,\sigma^{-1}}. \tag{5}$$

Let us think about $a_{m,\sigma^{-1}}$. Any product P of $P_{i,j}$'s in $(\mathcal{H}_\ell)^m$, any combination of $P_{i,j}$'s, has a one-to-one correspondence with a product made by reversing the order of $P_{i,j}$'s in P, and the reversed product is nothing but P^{-1}. This one-to-one correspondence leads to $a_{m,\sigma} = a_{m,\sigma^{-1}}$. In the end, we obtain,

$$\lim_{n\to\infty} \left\langle (\mathcal{H}_\ell)^{2m} \right\rangle = \sum_\sigma (a_{m,\sigma})^2. \tag{6}$$

Note that the limit $n \to \infty$ corresponds to $\beta J \ll n$, because the limit is taken with fixed β. Therefore, the limit $\beta \to \infty$ ($T \to 0$) after $n \to \infty$ is not necessarily the same as the $n \to \infty$ limit of the ground state. Hence we expect that the $n \to \infty$ limit of a function of β is not uniformly convergent around $T \simeq 0$ just like the specific heat of the $1/r^2$-model commented in Ref. [2].

4. Conclusion

We have formulated the high temperature expansion for the SU(n) Heisenberg model, which is a fundamental model of orbitally degenerate systems with the multiplicity n per site. In our algorithm, neither computational time nor memory depends on n; the series coefficients are explicit functions of n. Furthermore, $n \to \infty$ is related to a simple combinatorial problem counting the identity permutation. Thus, our method is useful to investigate systematically from $n = 2$ to $n \to \infty$. We expect that the explicit n-dependence will help us to extrapolate the series to low temperature.

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