High Temperature Expansion for the SU\((n)\) Heisenberg Model in One Dimension

Noboru Fukushima\(^1,2\)* and Yoshio Kuramoto\(^2\)

\(^1\) Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Straße 38, D-01187 Dresden, Germany
\(^2\) Department of Physics, Tohoku University, Sendai 980-8578, Japan

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Thermodynamic properties of the SU\((n)\) Heisenberg model in one dimension is studied by means of high-temperature expansion for arbitrary \(n\). The specific heat up to \(O(\beta J)^2\) and the correlation function up to \(O(\beta J)^3\) are derived with \(\beta J\) being the antiferromagnetic exchange in units of temperature. It is found for \(n > 2\) that the specific heat shows a shoulder in the high-temperature side of a peak. The origin of this structure is clarified by deriving the temperature dependence of the correlation function. With decreasing temperature, the short-range correlation with two-site periodicity develops first, and then another correlation with \(n\)-site periodicity at lower temperature. This behavior is in contrast to that of the inverse square interaction model, where the specific heat shows a single peak according to the exact solution. Our algorithm has an advantage that neither computational time nor memory depends on the multiplicity \(n\) per site; the series coefficients are obtained as explicit functions of \(n\).

KEYWORDS: high temperature series expansion, orbital degeneracy, Heisenberg model, SU\((n)\) symmetry, multipolar interaction, fluctuation, exchange interaction model

Recently, orbitally degenerate systems attract much attention as strongly-correlated electron systems. The orbital degeneracy is regarded as an internal degrees of freedom in addition to the spin degeneracy. The total number \(n\) of internal degrees of freedom thus varies depending on the system. If the number \(n^2 - 1\) of competing fluctuations is large, the transition temperature of the orbital ordering is significantly suppressed from the mean-field value even in three dimensions.\(^1\) Thus reliable theoretical scheme beyond the mean-field theory should be necessary to investigate orbitally degenerate systems.

As the simplest model to describe the orbitally degenerate systems, the SU\((n)\) Heisenberg model has been investigated. In one dimension, it can be solved exactly by the Bethe ansatz.\(^2\) However, some interesting quantities like the correlation function are difficult to be derived by the Bethe ansatz. Some critical exponents have been calculated with use of the non-abelian bosonization\(^3\) and the conformal field theory.\(^4\) Numerical methods have also been used to study the system. For \(n = 4\), the spin-spin correlation function has been calculated using the density matrix renormalization group\(^5\) and the quantum Monte Carlo method.\(^6\) The latter has also derived temperature dependence of the correlation lengths and the entropy. Although these numerical approaches are powerful, they are not always convenient to investigate systems with large \(n\), or in higher dimensions.

As an alternative approach which is applicable to any dimension, the high-temperature expansion has provided significant information on variety of models.\(^7\) We have recently developed an efficient algorithm to carry out the high-temperature expansion for systems in which the Hamiltonian is written in terms of exchange operators. With use of this new algorithm, we report in this paper a peculiar temperature dependence of the spatial correlation, which becomes conspicuous as the number \(n\) of internal degrees of freedom increases. Namely, with decreasing temperature, the short-range correlation with two-site periodicity develops first, and then another correlation with \(n\)-site periodicity at lower temperature. This leads to a corresponding structure in the specific heat.

In our algorithm, neither computational time nor memory depends on the multiplicity \(n\) per site; \(n\) is just a parameter — the series coefficients are obtained as explicit functions of \(n\). Details of the algorithm as well as application to higher dimensional models will be reported separately.

We consider a one-dimensional lattice of \(N\) sites with a periodic boundary condition. Let each site take one of the \(n\) colors, and denote them as \(|\alpha\rangle\) with \(\alpha = 1, 2, \ldots, n\). We define \(X^{\alpha\beta} := |\alpha\rangle\langle\beta|\) and an exchange (or permutation) operator

\[
P_{i,j} := \sum_{\alpha=1}^{n} \sum_{\beta=1}^{n} X^{\alpha\beta}_i X^{\beta\alpha}_j.
\]

(1)

Colors of sites \(i\) and \(j\) are exchanged when \(P_{i,j}\) is applied. The Hamiltonian is given by

\[
\mathcal{H} := J \sum_{i=1}^{N-1} P_{i,i+1} + JP_{1,N}.
\]

(2)

Then, the Hamiltonian has the SU\((n)\) symmetry. We investigate the antiferro-interaction model with \(J > 0\). When \(n = 2\), this model is equivalent to the ordinary

\[\text{e-mail address: fuku@mpipks-dresden.mpg.de}\]
Heisenberg model. The SU(4) Heisenberg model is related to orbital- and spin-degenerate systems. The local four states are denoted as \(|\pm |+\rangle, |+|\pm \rangle, |\pm |\pm \rangle, |\pm |\pm \rangle\), where \(|\pm \rangle\) and \(|\pm \rangle\) stand for a orbital state and a spin state respectively. The pseudo-spin operators are defined as \(t^z|\pm \rangle = \pm \frac{1}{2}|\pm \rangle\), \(t^x|\pm \rangle = |\pm \rangle\), \(s^z|\pm \rangle = \pm \frac{1}{2}|\pm \rangle\), \(s^x|\pm \rangle = |\pm \rangle\), and then the exchange operator for \(n = 4\) is rewritten as

\[
P_{1,i,j} = t_i \cdot t_j + s_i \cdot s_j + 4(t_i \cdot t_j)(s_i \cdot s_j) + \frac{1}{4},
\]

or,

\[
4P_{1,i,j} = \tau_i \cdot \tau_j + \sigma_i \cdot \sigma_j + (\tau_i \cdot \tau_j)(\sigma_i \cdot \sigma_j) + 1
\]

using the Pauli matrices \(\tau = 2t\) and \(\sigma = 2s\).

The high temperature expansion is performed by expanding the Boltzmann factor \(e^{-\beta H}\) in \(\beta\). To investigate the specific heat, we calculate the series \(\langle P_{i,i+1} \rangle\) because the internal energy is obtained by \(\langle H \rangle = NJ\langle P_{i,i+1} \rangle\). We also investigate correlation functions. For \(n = 4\), fifteen components in eq.(4) contribute equally, and thus \(\langle \tau_i^\alpha \tau_j^\alpha \rangle = (\sigma_i^\alpha \sigma_j^\alpha) = (\tau_i^\alpha \tau_j^\alpha + \tau_j^\alpha \tau_i^\alpha) = (4P_{1,i,j} - 1)/15\). For general \(n\), there is a relation,

\[
\langle X_i^{\alpha} X_j^{\beta} \rangle = \frac{1}{n^2 - 1} \left( \langle P_{i,j} \rangle - \frac{1}{n} \right),
\]

for \(i \neq j\) or \(\alpha \neq \beta\).

Although the concept of the high temperature expansion is quite simple, it needs various devices to calculate terms of high orders. We mainly use the finite cluster method.\(^7,8\) In this method, series coefficients in the thermodynamic limit are obtained exactly by weighted-summation of those calculated in finite-size clusters. The cluster of size \(\ell\) is defined by

\[
\mathcal{H}_\ell := J \sum_{i=1}^{\ell-1} P_{i,i+1}.
\]

To obtain the series expansion of \(\langle P_{i,j} \rangle\) up to \(O([\beta J]^M)\), we need to calculate \(\text{Tr}[\mathcal{H}_\ell^m]\) and \(\text{Tr}[P_{i,j}(\mathcal{H}_\ell)^m]\) for \(0 \leq m \leq M\). In calculating the trace, we adopt a method to use combinatorics.\(^9,10\) Then, coefficients are obtained as explicit functions of \(n\). Recently a related expansion for the specific heat and the uniform susceptibility was reported for the Heisenberg model \((n = 2)\).\(^11\) We have checked that the series obtained by our method reproduces the previous result.

In using our method, we have a trick to store data and reduce computational time and memory. Further, we use another trick to reduce the required maximum system size \(\ell_{max}\). If only the finite cluster method is used, the series for \(\langle P_{i,i+1} \rangle\) up to \(O([\beta J]^M)\) requires \(\ell_{max} = M/2 + 1\) (\(M\): even) or \(\ell_{max} = (M + 1)/2 + 1\) (\(M\): odd), and the Fourier transform of \(\langle P_{i,j} \rangle\) requires \(\ell_{max} = M + 1\). However, we reduce \(\ell_{max}\) by formulating a method complementary to the finite cluster method. Namely, we can calculate \(\langle P_{i,i+1} \rangle\) up to \(O([\beta J]^{22})\) with \(\ell_{max} = 11\). The Fourier transform of the correlation function \(\langle P_{i,j} \rangle\) up to \(O([\beta J]^{28})\) is calculated with \(\ell_{max} = 12\). As for the specific-heat in the \(n \to \infty\) limit, coefficients of \(\beta J^m\) with odd \(m\) are equal to zero, and non-zero coefficients are calculated up to \(O([\beta J]^{28})\).

We perform the Padé approximation (PA) and the first-order inhomogeneous differential approximation\(^12\)(FOIDA) to extrapolate the series. In general, the FOIDA shows better convergence than the PA. However, changing the expansion variable can improve the convergence of the PA. We change the variable from \(\beta J\) to \(\tan(c\beta J)\), where \(c\) is an adjustable parameter to improve convergence.\(^13\) For small \(c\), the results do not differ much from those in \(\beta J\). For large \(c\), the convergence becomes better. However the tanh variable saturates for \(\beta J\) much larger than \(1/c\), and the approximant tends to saturate accordingly. Therefore, we take the smallest possible \(c\) as long as the convergence remains good. We refer to this extrapolation as the PAT hereafter.

To investigate the specific heat \(C(T)\), we first analyze the series for the entropy \(S(T)\) and then calculate \(C = T dS/dT\) to use the known fact \(S(T \to \infty) = \log n\). For the PAT, we extrapolate \(S/T\) rather than \(S\) because the exact solution for the ground state\(^2\) behaves as \(S \propto T\) at \(T \to 0\). When \(n = 4\), our result for the entropy shows a good agreement to that of the quantum Monte Carlo method.\(^9\) Although the behavior of the entropy seems simple at a sight, the specific heat clearly shows a structure composed of a peak at low temperature and a shoulder at higher temperature. Figure 1 shows the results of the specific heat for various values of \(n\) using the PAT. At \(T \gtrsim 0.4J\), the results of the PAT and the FOIDA coincide within the width of the line, and thus the estimated error is smaller than the width. The high temperature limit is given by \(C = (1 - n^{-2})\beta^2 J^2\). Note that the existence of the shoulder structure is clearly seen, which accompanies changes of the sign of the curvature. In this range the expansion converges well. The position of the shoulder seems to be independent of \(n\), and the structure remains in the limit \(n \to \infty\). We shall discuss the origin of this structure later in this paper.

As \(n\) increases, the peak in the specific heat becomes sharper and shifts to lower temperature. Such a rapid change of a function at very low temperature is difficult to extrapolate. Hence the error becomes larger with increasing \(n\). Particularly, the FOIDA becomes unstable at \(T \lesssim 0.4J\); the results of the FOIDA are scattered, whereas some results agree with that of the PAT. This is because we do not use any information at \(T \to 0\) for the FOIDA. As for the PAT, we estimate that the error at \(T \simeq 0.2J\) is about 5% when \(n = 6\), and smaller than it when \(n < 6\). The specific heat at \(T \to 0\) using the PAT is by 5% ~ 15% larger than the exact value \(\frac{1}{3} n(n-1)T\), which is derived from the exact solution.\(^2\)

We remark that the behavior of the specific heat is different from that of the \(1/r^2\)-model\(^14\) defined by

\[
\mathcal{H}_{1/r^2} := J \sum_{i<j} \frac{[N/(n\pi) \sin\{\pi(i-j)/N\}]}{-2} P_{i,j}.
\]

The inset of Fig.1 shows the exact result\(^15,16\) for the \(1/r^2\)-model, which does not show the peak-shoulder structure in contrast with the nearest-neighbor model. Furthermore the \(T \to 0\) limit of the specific heat is given by \(\frac{1}{3} n(n-1)T\), which is \(2/n\) of the nearest-neighbor case. We interpret this difference as coming from the differ-
The spinon velocity is related to the Fermi velocity in the non-interacting counterpart and reflects its spectrum. The $1/r^2$-model has a cusps in the bottom of the band, which leads to the finite velocity even for vanishing Fermi energy. While the cosine band $n$-dependence of the nearest-neighbor model gives $1/n$-dependence for the Fermi velocity.

In order to see the temperature-dependent nature of the spatial correlation, we show in Fig.2 the next-nearest-neighbor correlation $\langle \sigma_i^z \sigma_{i+2}^z \rangle$ for $n = 2, 4$. Here we have introduced $J' := J/n$ so as to match the correlation function in the high-temperature limit. We compare systems with $n = 2$

\[ J' \sum \sigma_i \cdot \sigma_j, \]

and $n = 4$

\[ J' \sum \{ \tau_i \cdot \tau_j + \sigma_i \cdot \sigma_j + (\tau_i \cdot \tau_j)(\sigma_i \cdot \sigma_j) \}. \]

The lowest order of the series of $\langle \sigma_i^z \sigma_{i+2}^z \rangle$ is $O(\beta J)^2$ and its sign is given by $(-1)^s$. Then we have $\langle \sigma_i^z \sigma_{i+2}^z \rangle > 0$ at high temperature. As temperature decreases, $\langle \sigma_i^z \sigma_{i+2}^z \rangle$ first grows larger, then starts to decrease and turn to negative when $n = 4$. The reason is the following: Each of 15 components tries to align itself antiparallel. However, this cannot be attained simultaneously — e.g. the Néel states of both $\tau^z$ and $\sigma^z$ makes ferromagnetically aligned $\tau^z\sigma^z$. Therefore, as each antiferromagnetic correlation becomes larger, each short-range order disturbs each other, and thus the correlation turns to a longer period at low temperature.

Such a change of correlation at low temperature also appears in the Fourier transform of the correlation function for $n > 2$. We define $S(q)_n := \sum_x (X_j^{n\beta} X_j^{n\alpha}) e^{-i q x} (\alpha \neq \beta)$, which does not depend on $\alpha$ or $\beta$ because of the SU($n$) symmetry. Thus it is reduced to $S(q) = \sum_x (X_j^{2\beta} X_j^{2\alpha}) e^{-i q x}$ when $n = 4$. A naive extrapolation of the series for $S(q)$ shows bad convergence at several values of $q$. This is because information at distance $x$ is lacking when $\cos(xq) \simeq 0$. To avoid this difficulty we extrapolate the series of a complex function $2\sum_{x>0} (X_j^{2\beta} X_j^{2\alpha}) e^{-i q x}$, and take the real part of the extrapolated function. This method makes use of its imaginary part as well. As a result the convergence becomes better than the naive extrapolation. Figure 3 shows the result at several different temperatures for $n = 4, 20$. The results of the PAT and the FOIDA coincide within the width of the line. In the high temperature limit, only the on-site contribution $\langle X_j^{n\beta} X_j^{n\alpha} \rangle$ remains and $S(q)$ becomes a constant $1/n$. As temperature decreases, $S(\pi)$ increases first, and reaches the maximum at $T_{\text{max}} \simeq 0.8J$. With further decrease of temperature, $S(\pi)$ starts decreasing. Finally the maximum of $S(q)$ starts moving from $q = \pi$ at $T_{\text{mv}} \simeq 0.5J$. Comparing the different $n$ results at the same temperature, the peak of $S(q)$ around $q = \pi$ becomes broader as $n$ increases, especially at lower temperature. However, $T_{\text{max}}$ and $T_{\text{mv}}$ seem to be independent of $n$, even in the $n \to \infty$ limit.

Other numerical studies\(^5,6\) for $n = 4$ show that $S(q)$ at zero temperature has cusps at $q = 0, \pi/2, \pi$ and has the maximum at $q = \pi/2$. For general $n$, the dominant correlation in the ground state\(^2-4\) is that of $q = 2\pi/n$, and the maximum of $S(q)$ is expected to reach $q = 2\pi/n$ in the $T \to 0$ limit. The Fourier transform leading to the cusp type behavior requires data of spatial correlations for large distance. In Fig.3 the temperatures are still too high to observe this behavior.

A plausible characteristic temperature of the long-range correlation is given by the mean-field approximation. Note that the transition temperature in this approximation is given by $T_{\text{MF}}^N = 2J/n$, which decreases with increasing $n$. Therefore, if we scale energies by $T_{\text{MF}}^N$, $S(q)$ starts to shift toward the ground-state cor-
relation at higher temperature as $n$ increases. Namely $T_{\text{nv}}/T_{N}^{\text{MF}}$ increases.

Fig. 3. Fourier Transform $S(q)$ of the correlation function for (a) $n = 4$ and (b) $n = 20$ at temperature $T = \infty$ (dotted line), $T = 2J$ (dash-dotted line), $T = 0.8J$ (dashed line) and $T = 0.4J$ (solid line). The estimated error is within the width of the line. At $T = 0.4J$, the maximum is located at $q \neq \pi$ in both (a) and (b).

From the results of the specific heat and the correlation function, we consider the reason why the structure appears in the specific heat. Let us imagine cooling down the system gradually from the high temperature limit. In the case of the nearest-neighbor interaction, short-range correlation with two-site periodicity develops first at high temperature. It makes energy gain and the specific heat grows as temperature decreases. However, since the dominant correlation in the ground state is not the $q = \pi$ component but for the $q = \pi/n$ component, its energy gain saturates. This saturation should cause the shoulder of the specific heat. Then, there is another energy gain when the system begins to achieve the long-range correlation with $q = 2\pi/n$. It should cause the peak at the temperature.

One may expect that the shift of the peak position of the specific heat is mainly due to the shift of $T_{N}^{\text{MF}} = 2J/n$ to lower temperature with increasing $n$. However, the peak position decreases more rapidly than the $1/n$ behavior. One of the reasons should be that $T_{N}^{\text{MF}}$ is not for the $q = 2\pi/n$ component but for the $q = \pi$ component. Strong quantum effects are required to realize the $q = 2\pi/n$ correlation. Accordingly a temperature lower than $T_{N}^{\text{MF}}$ gives a peak in the specific heat.

For comparison, let us consider the $1/r^2$-model. There are interactions even in the intra-sublattice of the Néel state. These make the short-range two-site periodic correlation less favorable even at high temperature. Further, interactions making different colors attractive, and the same colors repulsive are long-ranged. Then the $n$-site periodic ($q = 2\pi/n$) correlation is favorable at low temperature. As a result, the same correlation as that of the ground state should develop gradually from high temperature. The specific heat therefore shows a single peak.

In conclusion, we find by large orders of high-temperature expansion a peak-shoulder structure in the specific heat which results from different behaviors of spatial correlations at high and low temperatures. Namely the short-range correlation at high temperature has a two-site periodicity, while the ground-state correlation has the $n$-site one. We will discuss applications of the high-temperature expansion to higher dimensional systems in the near future.

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1) N. Fukushima and Y. Kuramoto: J. Phys. Soc. Jpn. 67 (1998) 2460; Y. Kuramoto and N. Fukushima: J. Phys. Soc. Jpn. 67 (1998) 583.
2) B. Sutherland: Phys. Rev. B 12 (1975) 3795.
3) I. Affleck: Nucl. Phys. B265 (1986) 409.
4) N. Kawakami: Phys. Rev. B 46 (1992) 3191.
5) Y. Yamashita, N. Shibata, and K. Ueda: Phys. Rev. B 58 (1998) 9114.
6) B. Frischmuth, F. Mila, and M. Troyer: Phys. Rev. Lett. 82 (1999) 835.
7) G. S. Rushbrooke, G. A. Baker, Jr., and P. J. Wood: *Phase Transitions and Critical Phenomena*, edited by C. Domb and M. S. Green (Academic, London, 1974) vol.3, p.245.
8) M. P. Gelfand, R. R. P. Singh, D. A. Huse: J. Stat. Phys. 59 (1990) 1093; M. P. Gelfand, R. R. P. Singh: Adv. Phys. 49 (2000) 93.
9) D. C. Handscomb: Proc. Camb. Philos. Soc. 60 (1964) 115.
10) H. H. Chen and R. K. Joseph: J. Math. Phys. 13 (1972) 725.
11) A. Bühler, N. Elstner, G. S. Uhrig: Eur. Phys. J. B 16 (2000) 475.
12) A. J. Guttmann: *Phase Transitions and Critical Phenomena*, edited by C. Domb and J. L. Lebowitz (Academic, San Diego, 1989) vol.13, p.1.
13) R. R. P. Singh and R. L. Glenister: Phys. Rev. B 46 (1992) 14313.
14) F. D. M. Haldane: Phys. Rev. Lett. 60 (1998) 635; B. S. Shastry: Phys. Rev. Lett. 60 (1998) 639.
15) Y. Kuramoto and Y. Kato: J. Phys. Soc. Jpn. 64 (1995) 4518; Y. Kato and Y. Kuramoto: J. Phys. Soc. Jpn. 65 (1996) 1622.
16) The $n \to \infty$ limit is not uniformly convergent. Namely, although $C(T = 0) = 0$ for any $n$, all the $C(T > 0)$ values converge to the dotted-line shown in the inset of Fig.1.
17) T. Yamamoto, Y. Saiga, M. Arikawa and Y. Kuramoto: Phys. Rev. Lett. 84 (2000) 1308; J. Phys. Soc. Jpn. 69 (2000) 900.
18) Y. Kuramoto and H. Yokoyama: Phys. Rev. Lett. 67 (1991) 1338.
19) In the high temperature limit, the correlation function is $0 \sim \langle x_{\alpha}^{(A)} x_{\beta}^{(B)} \rangle \propto r^{-2}$ and its Fourier transform $S(q)$ has the maximum at $q = \pi$. However, the peak around $q = \pi$ is much broader than that of the nearest-neighbor model.