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LETTER TO THE EDITOR

High temperature expansion of the emptiness formation probability for the isotropic Heisenberg chain

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Abstract

Recently, Göhmann, Klümper and Seel have derived novel integral formulae for the correlation functions of the spin-1/2 Heisenberg chain at finite temperature. We have found that the high temperature expansion (HTE) technique can be effectively applied to evaluate these integral formulae. Actually, as for the emptiness formation probability $P(n)$ of the isotropic Heisenberg chain, we have found a general formula of the HTE for $P(n)$ with arbitrary $n \in \mathbb{Z}_{\geqslant 2}$ up to $O((J/T)^4)$. If we fix a magnetic field to a certain value, we can calculate the HTE to much higher order. For example, the order up to $O((J/T)^{42})$ has been achieved in the case of $P(3)$ when $h = 0$. We have compared these HTE results with the data by quantum Monte Carlo simulations. They exhibit excellent agreement.

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The spin-1/2 Heisenberg chain has been one of the most fundamental models in the study of low-dimensional magnetism, partially because it can be solved exactly by the Bethe ansatz. In fact, many physical quantities of the model have been evaluated *exactly* even at finite temperature [1]. However, they are usually the bulk properties, which may be derived directly from the free energy of the system. The exact evaluation of the correlation functions at finite temperature, on the other hand, has remained a much more difficult problem. Actually the evaluation of the correlation functions is still not solved fully even in the case of the ground state, although there have been various developments recently [2–5]. Note, however, that it is established that the correlation functions in the ground state are expressed in terms of multiple integrals. More recent researches have tried to evaluate these integrals, thereby to obtain the precise numerical values of the correlation functions [6–10].

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Considering these situations, it was a great surprise that Göhmann, Klümper and Seel [11–13] succeeded in generalizing the multiple integral formulae to finite temperature, by combining the algebraic Bethe ansatz technique and the quantum transfer matrix approach [14–18]. Their results will be a basis for further study of the model at finite temperature. Then, naturally, it is a significant problem to explore these integrals and find a way to extract numerical values of the correlation functions at finite temperature. Unfortunately it is not a straightforward task to generalize those methods developed in the case of the ground state to finite temperature. This is because the latter formula contains an additional auxiliary function $\mathfrak{a}(v)$, which is a solution of a certain nonlinear integral equations (NLIE), and is more complicated. The purpose of this letter is to address this challenging problem with the high temperature expansion (HTE) technique. Surprisingly enough, once we introduce the HTE, we can perform multiple integrals for each term in the HTE series simply by taking a residue at the origin.

The Hamiltonian of the spin-1/2 isotropic Heisenberg chain in a magnetic field h is defined by

$$H = J\sum_{j=1}^{L}\left(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y + \sigma_j^z\sigma_{j+1}^z\right) - \frac{h}{2}\sum_{j=1}^{L}\sigma_j^z, \tag{1}$$

where σ_j^k $(k = x, y, z)$ are the Pauli matrices σ^k acting non-trivially on the jth site of a chain of length L. Here we adopt the periodic boundary condition $\sigma_{j+L}^k = \sigma_j^k$. In this letter, we mainly consider a special correlation function called the emptiness formation probability (EFP) $P(n)$, which is the probability of n adjacent spins being aligned upward:

$$P(n) = \frac{\mathrm{Tr}\left\{\mathrm{e}^{-\frac{H}{T}}\prod_{j=1}^{n}\frac{1+\sigma_j^z}{2}\right\}}{\mathrm{Tr}\,\mathrm{e}^{-\frac{H}{T}}}. \tag{2}$$

At zero temperature, $T = 0$, it was introduced in [3] and studied further, for example, in [6–8]. Recently Göhmann, Klümper and Seel obtained [11, 12] the multiple integral formulae of the EFP at finite temperature as

$$P(n) = \left[\prod_{j=1}^{n}\int_C \frac{\mathrm{d}y_j}{2\pi(1+\mathfrak{a}(y_j))}\right]\det_{1\leqslant j,k\leqslant n}\left(\frac{\partial_\xi^{(k-1)}G(y_j,\xi)|_{\xi=0}}{(k-1)!}\right)\frac{\prod_{j=1}^{n}(y_j-\mathrm{i})^{j-1}y_j^{n-j}}{\prod_{1\leqslant j<k\leqslant n}(y_j-y_k+\mathrm{i})}, \tag{3}$$

where functions $\mathfrak{a}(v)$ and $G(v,\xi)$ are solutions of the NLIE:

$$\log\mathfrak{a}(v) = -\frac{h}{T} + \frac{2J}{v(v+\mathrm{i})T} - \int_C \frac{\mathrm{d}y}{\pi}\frac{\log(1+\mathfrak{a}(y))}{1+(v-y)^2}, \tag{4}$$

$$G(v,\xi) = -\frac{1}{(v-\xi)(v-\xi-\mathrm{i})} + \int_C \frac{\mathrm{d}y}{\pi}\frac{1}{1+(v-y)^2}\frac{G(y,\xi)}{1+\mathfrak{a}(y)}. \tag{5}$$

Here the contour C surrounds the real axis in an anti-clockwise manner.

First, let us calculate the HTE of $\mathfrak{a}(v)$ from the NLIE (4). This is done by a similar procedure in [17], where a certain order of the HTE for the free energy was calculated from a NLIE. We assume the following expansion for small J/T,

$$\mathfrak{a}(v) = \exp\left(\sum_{k=1}^{\infty}a_k(v)\left(\frac{J}{T}\right)^k\right). \tag{6}$$

Substituting (6) into (4), and comparing coefficients of $(J/T)^m$ on both sides, we obtain an integral equation over $\{a_k(v)\}_{k=1}^m$ for each m ($m \in \mathbb{Z}_{\geqslant 1}$). As the resultant integral equation is linear with respect to $a_m(v)$, we can solve it recursively. For example, we obtain

$$\begin{aligned} a_1(v) &= -\frac{h}{J} - \frac{2\mathrm{i}}{v(1+v^2)}, \\ a_2(v) &= \frac{h}{J(1+v^2)} + \frac{2\mathrm{i}v}{(1+v^2)^2}, \\ a_3(v) &= -\frac{h}{J(1+v^2)}. \end{aligned} \tag{7}$$

Note that only $a_1(v)$ has a pole at the origin. Next let us consider the integral equation (5). We assume the following expansion for small J/T,

$$G(v,\xi) = \sum_{k=0}^{\infty} g_k(v,\xi) \left(\frac{J}{T}\right)^k. \tag{8}$$

In a similar way, we can determine the coefficients $g_k(v,\xi)$ successively by using the results on (4). For example, we obtain

$$\begin{aligned} g_0(v,\xi) &= \frac{-\mathrm{i}}{(1+(v-\xi)^2)(v-\xi)}, \\ g_1(v,\xi) &= \frac{\mathrm{i}(2v-\xi)}{(1+v^2)(1+(v-\xi)^2)(1+\xi^2)} + \frac{h}{2J(1+(v-\xi)^2)}, \\ g_2(v,\xi) &= -\frac{\mathrm{i}(2v-\xi)\xi^2}{(1+v^2)(1+(v-\xi)^2)(1+\xi^2)^2} - \frac{h(2+2v^2-2v\xi+\xi^2)}{2J(1+v^2)(1+(v-\xi)^2)(1+\xi^2)}. \end{aligned} \tag{9}$$

Note that only $g_0(v,\xi)$ has a pole at $v = \xi$. Finally, substituting (6) and (8) into (3), we can obtain the HTE of $P(n)$. Unexpectedly we have found that we only have to calculate residues at the origin. In fact, in this way, we could calculate the HTE of the $P(n)$ for small n ($n \in \{2,3,4,5,6\}$). The result up to the order $O((J/T)^4)$ is compactly presented as

$$\begin{aligned} P(n) = {} & \frac{1}{2^n} + \frac{-2J(-1+n)+hn}{2^{1+n}T} + \{4J^2(-4+n)(-1+n) + h^2(-1+n)n \\ & - 4hJ(2+(-1+n)n)\}\frac{1}{2^{3+n}T^2} + \{12hJ^2(-2+n)^2(-1+n) \\ & + h^3(-3+n)n^2 - 8J^3(-24+(-9+n)(-3+n)n) \\ & - 6h^2J(-1+n)(2+(-1+n)n)\}\frac{1}{3\cdot 2^{4+n}T^3} + \{24h^2J^2(-2+n)^2(-1+n)^2 \\ & + 16J^4(-5+n)(-32+n(26+(-17+n)n)) \\ & + h^4n(2+n(3+(-6+n)n)) - 32hJ^3(24+(-9+n)n(6+(-3+n)n)) \\ & - 8h^3J(-4+(-4+n)n(3+n^2))\}\frac{1}{3\cdot 2^{7+n}T^4} + O((J/T)^5). \end{aligned} \tag{10}$$

We observe that $P(n)$ has the following form:

$$P(n) = \frac{1}{2^n}\sum_{m=0}^{\infty}\frac{1}{m!}\left(\sum_{k=0}^{m} p_{m,k}(n)\left(\frac{h}{J}\right)^k\right)\left(\frac{J}{2T}\right)^m,$$

where $p_{0,0}(n) = 1$ and $p_{m,k}(n)$ for $m \in \mathbb{Z}_{\geqslant 1}$ are functions of n, which are independent of J, h and T. If we admit that $p_{m,k}(n)$ is a polynomial of n whose degree is at most m, our formula (10) is also valid for any $n \in \mathbb{Z}_{\geqslant 2}$ as the mth order polynomial is determined by distinct $m+1$ points.

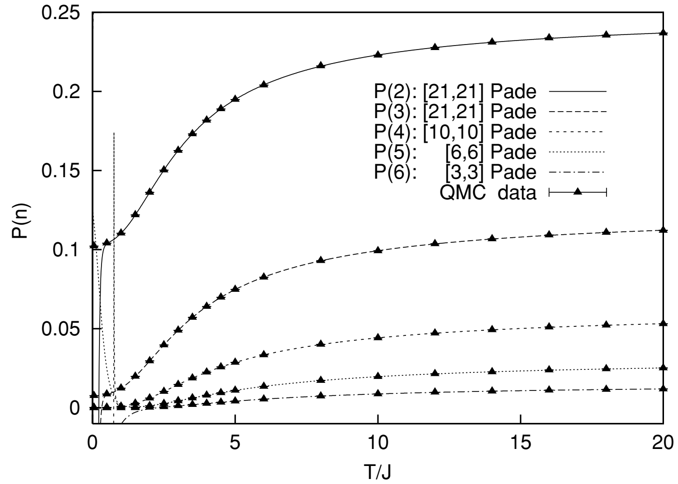

Figure 1. $P(n)$ for $J > 0$ at $h = 0$.

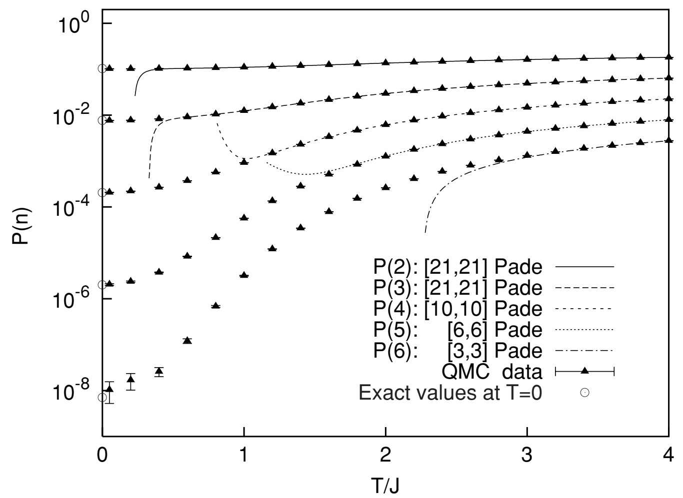

Figure 2. $P(n)$ for $J > 0$ at $h = 0$ in low T. The exact values at $T = 0$ were obtained in [6–8].

Next we fix the magnetic field h to certain values and calculate the HTE to much higher order. Then we have succeeded in obtaining coefficients of $P(3)$ up to the order $O((J/T)^{42})$ in the case of $h = 0$. For a finite h, we can calculate them at least up to the order $O((J/T)^{30})$. It will not be easy to obtain HTE coefficients, in particular under the magnetic field, to such a high order by other methods except for the free models. We list some of our results on the $h = 0$ case in table 1.

Moreover, we have applied the Padé approximation to our HTE and plot the results in figures 1–5. Note that although formula (3) was originally derived for $J > 0$ case, our HTE results can be analytically continued to the $J < 0$ case. For comparison, we have also performed quantum Monte Carlo simulation (QMC) using recent open source software in the ALPS project [20]. In particular we have chosen the SSE algorithm [21] so as to treat finite magnetic field cases. We have performed the simulations with the system size $L = 128$. In figures 1–5, these QMC data are represented by solid triangles, which show excellent agreement with the

Table 1. Series coefficients $p_k(n)$ for the high temperature expansion of $P(n) = \sum_k p_k(n)(\frac{J}{T})^k$ at $h = 0$.

k	$p_k(3)$	21	$-\frac{475\,666\,635\,106\,757}{89\,391\,802\,500}$	k	$p_k(4)$	k	$p_k(5)$
0	$\frac{1}{8}$	22	$\frac{73\,241\,259\,005\,444\,676\,467}{204\,177\,262\,038\,750}$	0	$\frac{1}{16}$	0	$\frac{1}{32}$
1	$-\frac{1}{4}$	23	$\frac{14\,342\,832\,948\,901\,512\,027\,127}{39\,447\,047\,025\,886\,500}$	1	$-\frac{3}{16}$	1	$-\frac{1}{8}$
2	$-\frac{1}{8}$	24	$-\frac{354\,494\,436\,182\,818\,781\,071}{297\,489\,042\,427\,500}$	2	0	2	$\frac{1}{16}$
3	$\frac{1}{2}$	25	$-\frac{39\,877\,735\,294\,663\,490\,409\,548\,941}{14\,792\,642\,634\,707\,437\,500}$	3	$\frac{11}{24}$	3	$\frac{1}{3}$
4	$\frac{5}{6}$	26	$\frac{491\,132\,965\,711\,734\,931\,876\,859\,809}{192\,304\,354\,251\,196\,687\,500}$	4	$\frac{17}{48}$	4	0
5	$-\frac{21}{20}$	27	$\frac{66\,961\,305\,287\,544\,998\,239\,794\,361}{4767\,876\,551\,682\,562\,500}$	5	$-\frac{343}{240}$	5	$-\frac{21}{16}$
6	$-\frac{487}{120}$	28	$\frac{9692\,024\,436\,454\,844\,294\,876\,678\,309}{4038\,391\,439\,275\,130\,437\,500}$	6	$-\frac{937}{360}$	6	$-\frac{301}{288}$
7	$\frac{271}{630}$	29	$-\frac{4098\,815\,896\,973\,029\,894\,033\,624\,285\,217}{70\,268\,011\,043\,387\,269\,612\,500}$	7	$\frac{221}{63}$	7	$\frac{2923}{630}$
8	$\frac{5161}{315}$	30	$-\frac{232\,435\,776\,187\,690\,664\,677\,091\,074\,186\,001}{3513\,400\,552\,169\,363\,480\,625\,000}$	8	$\frac{17\,267}{1260}$	8	$\frac{84\,319}{10\,080}$
9	$\frac{1105}{84}$	31	$\frac{46\,326\,083\,992\,727\,076\,268\,552\,170\,704\,552\,473}{245\,059\,688\,513\,813\,102\,773\,593\,750}$	9	$-\frac{185}{81}$	9	$-\frac{566\,639}{45\,360}$
10	$-\frac{256\,276}{4725}$	32	$\frac{8813\,049\,514\,657\,368\,316\,161\,218\,121\,220\,189}{18\,850\,745\,270\,293\,315\,597\,968\,750}$	10	$-\frac{668\,573}{11\,340}$	10	$-\frac{47\,129}{1008}$
11	$-\frac{21\,532\,949}{207\,900}$	33	$-\frac{23\,560\,005\,035\,480\,782\,300\,479\,589\,437\,217\,351}{63\,427\,213\,497\,692\,803\,070\,812\,500}$	11	$-\frac{456\,671}{10\,395}$	11	$\frac{324\,749}{27\,720}$
12	$\frac{420\,091}{3300}$	34	$-\frac{27\,945\,437\,643\,781\,625\,566\,445\,986\,974\,785\,072}{11\,720\,245\,972\,399\,757\,089\,171\,875}$	12	$\frac{4924\,421}{23\,760}$	12	$\frac{3162\,705\,559}{14\,968\,800}$
13	$\frac{2660\,539\,279}{4864\,860}$	35	$-\frac{926\,901\,382\,890\,398\,878\,135\,256\,848\,861\,535\,464\,573}{1374\,784\,852\,562\,491\,506\,559\,860\,937\,500}$	13	$\frac{12\,185\,848\,483}{32\,432\,400}$	k	$p_k(6)$
14	$-\frac{6793\,954\,613}{340\,540\,200}$	36	$\frac{18\,696\,605\,034\,197\,142\,286\,345\,924\,338\,927\,419\,869\,073}{1924\,698\,793\,587\,488\,109\,183\,805\,312\,500}$	14	$-\frac{180\,113\,062\,933}{340\,540\,200}$	0	$\frac{1}{64}$
15	$-\frac{37\,743\,598\,006}{16\,372\,125}$	37	$\frac{4364\,774\,409\,085\,808\,451\,234\,535\,985\,560\,619\,072\,990\,519}{356\,069\,276\,813\,685\,300\,199\,003\,982\,812\,500}$	15	$-\frac{38\,034\,664\,397}{18\,243\,225}$	1	$-\frac{5}{64}$
16	$-\frac{1327\,276\,364\,741}{638\,512\,875}$	38	$-\frac{71\,422\,507\,032\,359\,703\,142\,873\,531\,724\,137\,016\,664\,174\,319}{2341\,840\,243\,659\,237\,935\,924\,218\,502\,343\,750}$	16	$\frac{29\,988\,604\,741}{98\,232\,750}$	2	$\frac{5}{64}$
17	$\frac{336\,925\,562\,547\,463}{43\,418\,875\,500}$	39	$-\frac{7272\,089\,125\,489\,543\,224\,633\,329\,075\,851\,883\,666\,829\,606\,991}{87\,949\,111\,372\,980\,269\,149\,153\,983\,754\,687\,500}$	17	$\frac{11\,380\,401\,164\,189}{1240\,539\,300}$	3	$\frac{13}{64}$
18	$\frac{26\,889\,108\,889\,501}{1669\,956\,750}$	40	$\frac{634\,149\,726\,978\,610\,912\,172\,163\,815\,072\,882\,174\,172\,080\,282\,077}{11\,873\,130\,035\,352\,336\,335\,135\,787\,806\,882\,812\,500}$	18	$\frac{1902\,555\,753\,434\,863}{260\,513\,253\,000}$	4	$-\frac{17}{96}$
19	$-\frac{43\,793\,345\,212\,356\,097}{2474\,875\,903\,500}$	41	$\frac{66\,831\,923\,892\,050\,783\,799\,016\,502\,839\,247\,559\,821\,880\,338\,345\,693}{162\,266\,110\,483\,148\,596\,580\,189\,100\,027\,398\,437\,500}$	19	$-\frac{481\,157\,848\,754\,889\,239}{14\,849\,255\,421\,000}$	5	$-\frac{19}{20}$
20	$-\frac{3162\,447\,776\,015\,376\,619}{37\,123\,138\,552\,500}$	42	$\frac{556\,085\,532\,621\,818\,295\,062\,304\,191\,328\,067\,921\,669\,214\,230\,014\,169}{3407\,588\,320\,146\,120\,528\,183\,971\,100\,575\,367\,187\,500}$	20	$-\frac{139\,195\,329\,414\,966\,479}{2249\,887\,185\,000}$	6	$\frac{31}{480}$

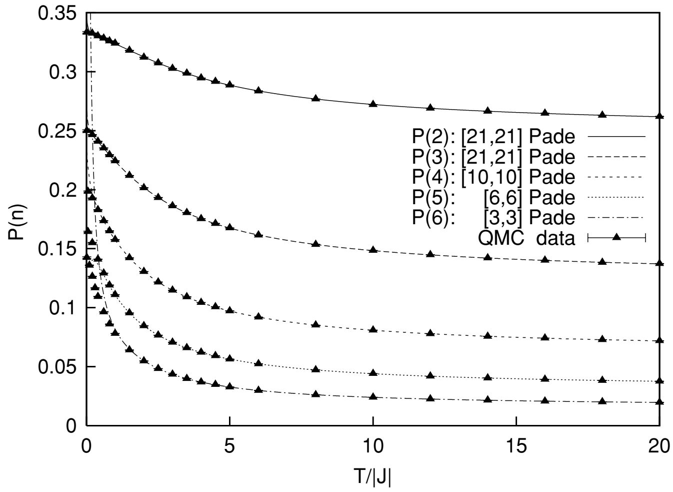

Figure 3. $P(n)$ for $J < 0$ at $h = 0$.

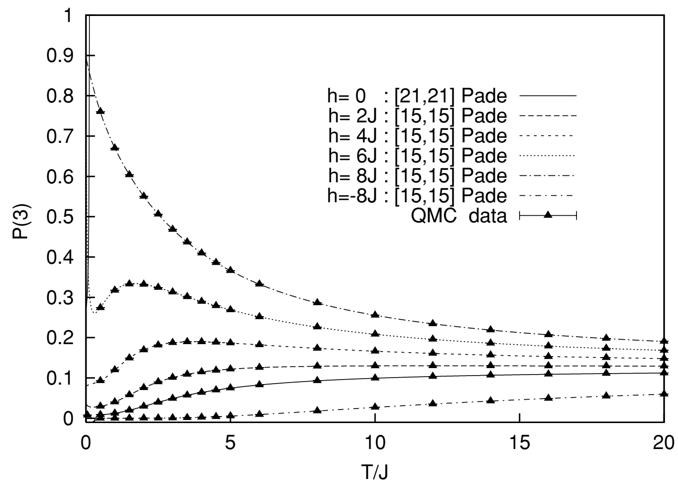

Figure 4. $P(3)$ for $J > 0$ at $h = 0, 2J, 4J, 6J, \pm 8J$.

HTE results. Discrepancies appear only in the very low temperature regions, where even the Padé approximation of the HTE ceases to converge. We omit these apparent deviations of the Padé approximation in figure 2. We remark that we have also tested the validity of our general formula (10) up to $n = 20$.

In the case of $J > 0$ and $h = 0$, we see that $P(n)$ monotonously increases as the temperature increases. On the other hand, it decreases monotonously for $J < 0$. In this case we have found $P(n) \to 1/(n+1)$ as $T \to 0$. Another interesting observation in figure 4 is that, when $J > 0$, a peak appears for positive values of the magnetic field. Its position moves from $T = \infty$ to 0 as h increases. For example, the peak position $T^{\max}$ and the peak $P(3)^{\max}$ are given by $(h/J, T^{\max}/J, P(3)^{\max}) = (2, 12.030, 0.130\,15), (4, 3.7467, 0.189\,73), (6, 1.6904, 0.334\,16)$, respectively. Note that in this case, the critical field is $h_c = 8J$ at $T = 0$, where all the spins are directed upward.

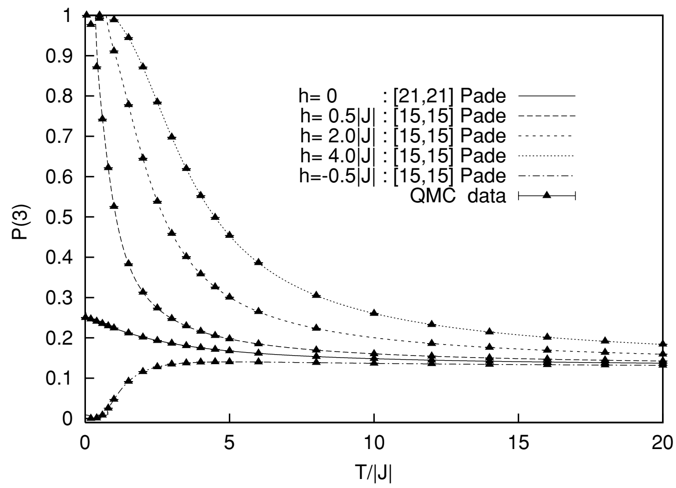

Figure 5. $P(3)$ for $J < 0$ at $h = 0, \pm 0.5|J|, 2|J|, 4|J|$.

In conclusion we have found that our HTE method is very powerful to evaluate the integral formula for $P(n)$ at finite temperature. As an alternative method, it may be possible to solve the NLIEs (4) and (5) numerically and perform numerical integration for the multiple integrals in (3). We have tried this, but found it difficult to get reliable numerical results even for $P(3)$.

It is straightforward to generalize the results in this letter to more general correlation functions. Actually, as for the nearest- and the next-nearest-neighbour correlation functions for $h = 0$, we can immediately calculate their HTEs from our results through the relations $\langle S_j^z S_{j+1}^z \rangle = P(2) - 1/2$, $\langle S_j^z S_{j+2}^z \rangle = 2(P(3) - P(2) + 1/8)$, from which we can obtain the coefficients whose order is higher than the ones by other method [19]. We can evaluate the HTE for other complicated correlation functions based on the multiple integral formula on the density matrix of the XXZ chain at finite temperatures [13]. We will report on the details in a forthcoming paper.

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