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Elementary excitations for the integrable spin-*S* Heisenberg chain with an impurity spin

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Abstract. Elementary excitations for the integrable spin-S antiferromagnetic Heisenberg chain with an impurity spin S' are investigated by using the Bethe *ansatz* solution. Dressed holes are introduced in order to describe the elementary excitation. The characteristic energy dependence of the spectral density for the elementary excitation at zero temperature is discussed in connection with behaviour patterns of physical quantities. We extend our calculation for the elementary excitation to the case of finite temperatures, applying the method developed by Yang and Yang for one-dimensional interacting boson systems. At finite temperatures, in the case where $S < S'$, the spectral density shows a divergence property at zero excitation energy irrespective of the temperature, whereas in the case where $S > S'$, the peak structure develops in the low-energy region as the temperature is decreased.

1. Introduction

The one-dimensional Heisenberg model has attracted much interest for many years. The model has been diagonalized by the Bethe *ansatz* method [1, 2]. Integrable generalization of the model for an arbitrary spin S was achieved by Takhtajan [3] and Babujian [4]. In the case of antiferromagnetic couplings, it was shown that the ground state is a singlet [3, 4], and that the dispersion curve for the elementary excitation shows the form $\epsilon(k) = (\pi J/2)\sin k$ (for $0 \leqslant k \leqslant \pi$), irrespective of S [3]. This is identified as a kink mode, since the total spin changes to $1/2$ in the elementary excitation. Thermodynamic properties have been investigated both analytically [4] and numerically [5].

The integrable spin-S Heisenberg chain with an impurity spin S' interacting with neighbouring host spins has been studied intensively by several authors [6–11]. This model was first diagonalized by Andrei and Johannesson [6] for the case where $S = 1/2$ and for arbitrary S'. They investigated the thermodynamic properties of the model. In this model, the interaction between the impurity spin and its neighbouring host spins has to be of a special form in order to preserve the integrability. For arbitrary S and S', the model was solved by Schlottmann [8]. The properties of this model can be divided into three cases: (i) $S = S'$; (ii) $S < S'$; and (iii) $S > S'$. In the case where $S = S'$, an impurity spin is just one more site in the host spin chain. If $S < S'$, host spins are not able to compensate the impurity spin into a singlet, and so there remains a spin degeneracy corresponding to an effective spin $(S' - S)$. Due to this effective spin, the specific heat shows a Schottky anomaly, and the zero-field susceptibility diverges as described by a Curie law. If $S > S'$, a peculiar spin degeneracy exists in the ground state, yielding unusual physical properties.

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The entropy takes the form [8]

$$S(T=0, H=0) = \ln\left\{\frac{\sin[\pi(2S'+1)/(2S+2)]}{\sin[\pi/(2S+2)]}\right\} \tag{1}$$

$$S(T=0, H\neq 0) = 0. \tag{2}$$

At zero temperature, the susceptibility caused by an impurity spin shows a power-law behaviour in a low magnetic field. At zero magnetic field, the susceptibility and the specific heat diverge over the temperature range following a power law, as the temperature tends to zero. It is noted that these exponents depend only on the magnitude of the host spin. Based on these findings, it was concluded that properties of this model are closely related to those of the multichannel Kondo model [8].

In this paper, we investigate the elementary excitation of the integrable spin-S Heisenberg chain with an impurity spin S' in the cases where $S < S'$ and $S > S'$ with the use of the Bethe *ansatz* solution. We turn our attention to the contribution from an impurity spin. We treat only the case of antiferromagnetic couplings and take the coupling constant to be 1. In section 2, we investigate the elementary excitation for the model at zero temperature, introducing a *dressed hole* which is a local analogue of the kink mode. We discuss characteristic properties of the excitation spectra in connection with patterns of behaviour of physical quantities. In section 3, we extend the calculation of the elementary excitation to the case of finite temperatures, following the method developed by Yang and Yang for one-dimensional interacting boson systems [12–15]. Section 4 is devoted to a brief summary.

2. Elementary excitations at zero temperature

We consider the elementary excitation of the integrable spin-S Heisenberg chain with an impurity spin S' at zero temperature. As mentioned in section 1, the model was solved exactly by the Bethe *ansatz* method and the basic equation was obtained for the rapidity $\{\Lambda_j\}$ [8]:

$$\left(\frac{\Lambda_j + \mathrm{i}S}{\Lambda_j - \mathrm{i}S}\right)^N \left(\frac{\Lambda_j + \mathrm{i}S'}{\Lambda_j - \mathrm{i}S'}\right) = -\prod_{i=1}^{M} \frac{\Lambda_j - \Lambda_i + \mathrm{i}}{\Lambda_j - \Lambda_i - \mathrm{i}} \qquad (j = 1, 2, \ldots, M) \tag{3}$$

where N is the number of host spins and M is related to the magnetization via

$$S^z = NS + S' - M.$$

The expression for the energy is written in terms of the rapidity as [8]

$$E = -\sum_{j=1}^{M} \frac{S}{{\Lambda_j}^2 + S^2}. \tag{4}$$

It was shown that the ground state of the model is determined by $2S$-string solutions which are distributed densely [8]. In the thermodynamic limit, the density function for the $2S$-string solution is obtained as [8]

$$\sigma_0(\Lambda) = \frac{1}{2}\,\mathrm{sech}(\pi\Lambda) + \frac{1}{N}\int_{-\infty}^{+\infty} f(\Lambda - \Lambda')\frac{1}{2}\,\mathrm{sech}(\pi\Lambda')\;\mathrm{d}\Lambda' \tag{5}$$

where

$$f(\Lambda) = \begin{cases} \dfrac{1}{2S} \dfrac{\sin(S'\pi/S)}{\cosh(\pi\Lambda/S) + \cos(S'\pi/S)} & (S > S') \\ \delta(\Lambda) & (S = S') \\ \dfrac{1}{\pi} \dfrac{S' - S}{\Lambda^2 + (S' - S)^2}. & (S < S') \end{cases} \tag{6}$$

The first term in (5) is the contribution from the host spin and the second one is that from an impurity spin.

The elementary excitation from the ground state is obtained by introducing a *hole* into the $2S$-string solution, the real part of which is denoted by q. We refer to this as a *dressed-hole* excitation. By introducing a dressed hole, the backflow effect which is attributed to the interaction rearranges the distribution of the $2S$-string solution, and the density function $\sigma(\Lambda)$ is modified from that of the ground state:

$$\sigma(\Lambda) = \sigma_0(\Lambda) + \frac{1}{N}\,\Delta\sigma(\Lambda). \tag{7}$$

The change of the density function $\Delta\sigma(\Lambda)$ is characterized by q and is determined by the following equation:

$$\Delta\sigma(\Lambda) + \int_{-\infty}^{+\infty} g(\Lambda - \Lambda')\,\Delta\sigma(\Lambda')\,\mathrm{d}\Lambda' = -\delta(\Lambda - q) \tag{8}$$

where $g(\Lambda)$ is defined by

$$g(\Lambda) = \frac{1}{\pi}\frac{2S}{\Lambda^2 + (2S)^2} + \frac{2}{\pi}\frac{2S - 1}{\Lambda^2 + (2S - 1)^2} + \cdots + \frac{2}{\pi}\frac{1}{\Lambda^2 + 1}. \tag{9}$$

The above integral equation is solved by Fourier transformation:

$$\Delta\sigma(\Lambda) = -\frac{1}{2\pi}\int_{-\infty}^{+\infty} \frac{1 - \mathrm{e}^{-|\omega|}}{(1 - \mathrm{e}^{-2S|\omega|})(1 + \mathrm{e}^{-|\omega|})}\,\mathrm{e}^{-\mathrm{i}\omega(\Lambda - q)}\,\mathrm{d}\omega. \tag{10}$$

Using (10), the change of the magnetization is calculated as

$$-2S\int_{-\infty}^{+\infty} \Delta\sigma(\Lambda)\,\mathrm{d}\Lambda = 1/2.$$

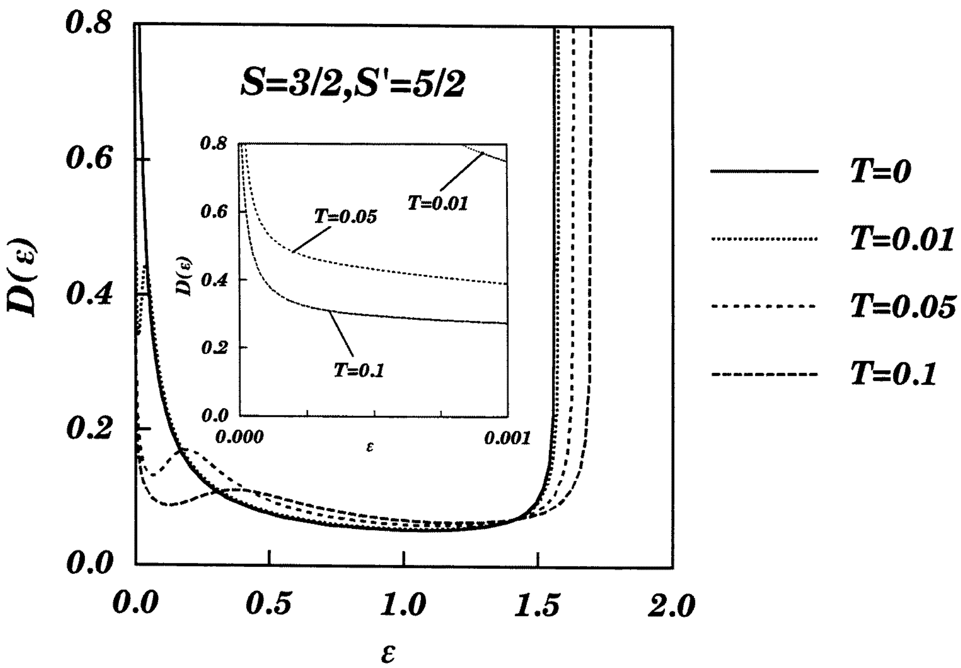
Accordingly, the dressed-hole excitation can be regarded as a local analogue of the kink mode. From (4) and (10), we obtain the excitation energy as

$$\epsilon(q) = \frac{\pi}{2}\,\mathrm{sech}(\pi q). \tag{11}$$

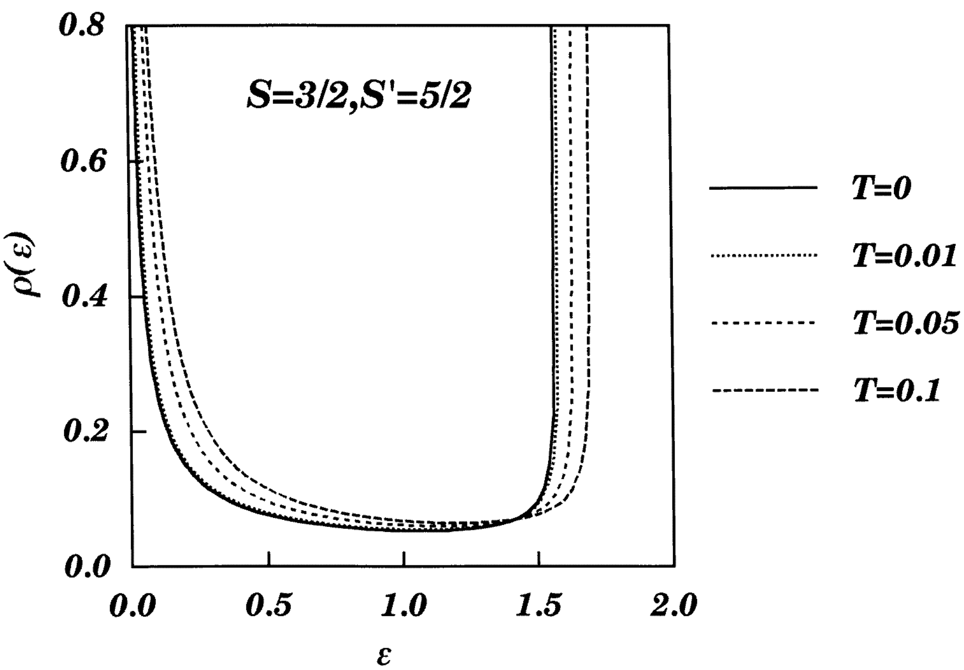
Here, we introduce the spectral density for the dressed-hole excitation as a function of the excitation energy, $\epsilon = \epsilon(q)$. This is given by the number of states in a given range of the excitation energy $[\epsilon, \epsilon + \mathrm{d}\epsilon]$. The contribution from the impurity spin to the spectral density is written as

$$D_0(\epsilon) = \frac{\sigma_{0I}(q)}{|\mathrm{d}\epsilon/\mathrm{d}q|} \tag{12}$$

where $\sigma_{0I}(q)$ denotes the impurity part of the density function. Using expressions (5) and (11), we calculate the spectral density for the elementary excitation at zero temperature.



(*a*)



(*b*)

Figure 1. (*a*) Plots of the spectral density for the dressed-hole excitation for several temperatures in the cases where $S = 3/2$ and $S' = 5/2$. (*b*) Plots of the whole excitation spectrum for several temperatures in the cases where $S = 3/2$ and $S' = 5/2$.

When $S = S'$, the model reduces to the integrable spin-S Heisenberg chain which consists of $(N + 1)$ spins. In this case, the ground state is a singlet due to the antiferromagnetic coupling [3, 4, 8], and the spectral density takes the form

$$D_0(\epsilon) = \frac{1}{2\pi} \frac{1}{\sqrt{(\pi/2)^2 - \epsilon^2}} \tag{13}$$

which is independent of S. This is the same form as in the case of an $S = 1/2$ Heisenberg antiferromagnetic chain. In the case where $S < S'$, there exists a spin degeneracy corresponding to the effective spin $(S' - S)$ in the ground state. Due to the spin degeneracy, $D_0(\epsilon)$ shows a logarithmic behaviour in the low-energy region:

$$D_0(\epsilon) \sim \frac{1}{2}(S' - S) \frac{1}{\epsilon \left[\ln(\epsilon/\pi)\right]^2}. \tag{14}$$

This kind of logarithmic behaviour appears in the susceptibility of an impurity spin in the small-field region, $\chi \sim S(S' - S)/[H(\ln H)^2]$ [8]. When $S > S'$, properties of the ground state are rather peculiar in contrast to the above two cases as seen in the residual entropy shown in (1). This peculiar spin degeneracy induces a power-law behaviour in $D_0(\epsilon)$ in the low-energy region:

$$D_0(\epsilon) \sim \begin{cases} \dfrac{1}{2\pi^2 S} \sin\left(\dfrac{S'}{S}\pi\right)\left(\dfrac{\epsilon}{\pi}\right)^{1/S-1} & (S > 1) \\[2ex] -\dfrac{1}{\pi^3} \ln\left(\dfrac{\epsilon}{\pi}\right) & (S = 1,\ S' = 1/2). \end{cases} \tag{15}$$

It is noted that the exponent depends only on the host spin S. In the case where $S = 1$ and $S' = 1/2$, the exponent vanishes, and a logarithmic divergence emerges. The kind of behaviour is seen also in physical quantities such as the low-field susceptibility of an impurity spin: $\chi \sim H^{1/S-1}$ (for $S > 1$) and $-\ln H$ (for $S = 1$ and $S' = 1/2$), and the low-temperature susceptibility: $\chi \sim T^{-1+4/(2S+2)}$ (for $S > 1$) and $-\ln T$ (for $S = 1$ and $S' = 1/2$) [8]. Our results indicate that so far as the low-energy behaviour is concerned, the spectral density for the dressed-hole excitation reflects conspicuously features of physical quantities which are caused by the many-body effect.

We now compare our results with the spectral density for the multichannel Kondo model. In the low-energy region, the spectral density for the dressed-hole excitation of the n-channel Kondo model takes the form [16]

$$D(\epsilon) \sim \begin{cases} \dfrac{1}{\pi} \dfrac{T_\mathrm{K}}{\epsilon^2 + {T_\mathrm{K}}^2} & (n = 2S') \\[2ex] \dfrac{1}{4}(2S' - n) \dfrac{1}{\epsilon[\ln(\epsilon/T_\mathrm{K})]^2} & (n < 2S') \\[2ex] \dfrac{\sin(2S'\pi/n)}{n\pi \cos(\pi/n) T_\mathrm{K}} \left(\dfrac{\epsilon}{T_\mathrm{K}}\right)^{2/n-1} & (n > 2S') \end{cases} \tag{16}$$

where S' is the magnitude of an impurity spin and T_K is the Kondo temperature. In the low-energy region, the spectral densities of the present system in the cases where $S < S'$ and $S > S'$ show similar energy dependences to those of the underscreened ($n < 2S$) and the overscreened ($n > 2S$) cases, respectively. In the higher-energy region, the spectral densities of the present model diverge as will be seen in figures 1(a)–2(b), although they do not diverge in the multichannel Kondo model. It is considered that this divergence comes from the properties of the spectral density for the bulk system in the higher-energy region.

3. Elementary excitations at finite temperatures

3.1. Formulation

We now extend the calculation of the elementary excitation to the case of finite temperatures, applying the method developed by Yang and Yang [12–15]. Other kinds of string solution are introduced in order to formulate the thermodynamics of the system. We recall here that the ground state of the model is given only by the $2S$-string solution, and that the leading contribution to thermodynamic quantities in the low-temperature region is from the $2S$-string solution [8]. Therefore, it is considered that a simple excitation is given by removing one of the $2S$-string solutions at thermal equilibrium. We refer to this as a dressed-hole excitation at finite temperatures, which is characterized by the real part of the removed solution. The backflow effect rearranges the distribution of rapidities; hence, the energy shifts from the value at thermal equilibrium. The excitation energy renormalized by the backflow effect is given in terms of the pseudo-energy at thermal equilibrium corresponding to the $2S$-string solution

$$\Delta E(q) = -\epsilon_{2S}(q) + \epsilon_{2S}(-\infty) \tag{17}$$

where q is the real part of the $2S$-string solution removed. The pseudo-energy defined as $\epsilon_n(\Lambda) = T \ln[\sigma_n^h(\Lambda)/\sigma_n(\Lambda)]$ $(n = 1, 2, \ldots)$ is determined by a set of coupled integral equations [8]:

$$\epsilon_n(\Lambda) = \frac{T}{2}\operatorname{sech}(\pi\Lambda) * \left\{\ln\left[1 + \exp\left(\frac{\epsilon_{n-1}}{T}\right)\right]\left[1 + \exp\left(\frac{\epsilon_{n+1}}{T}\right)\right]\right\} - \delta_{n,2S}\frac{\pi}{2}\operatorname{sech}(\pi\Lambda) \tag{18}$$

where the asterisk denotes convolution. The impurity parts of the density functions of particles $\sigma_{n,I}(\Lambda)$ and of holes $\sigma_{n,I}^h(\Lambda)$ for n-string solutions are obtained from the following set of coupled integral equations [8]:

$$\sigma_{n,I}(\Lambda) + \sigma_{n,I}^h(\Lambda) = \frac{1}{2}\operatorname{sech}(\pi\Lambda) * \left[\sigma_{n+1,I}^h(\Lambda) + \sigma_{n-1,I}^h(\Lambda)\right] + \delta_{n,2S'}\frac{1}{2}\operatorname{sech}(\pi\Lambda). \tag{19}$$

In the limit of zero temperature, $\Delta E(q)$ coincides with the excitation energy from the ground state shown in (11).

At finite temperatures, the contribution from an impurity spin to the spectral density is expressed in terms of the excitation energy $\epsilon = -\epsilon_{2S}(q) + \epsilon_{2S}(-\infty)$:

$$D(\epsilon) = \frac{\sigma_{2S,I}(q)}{|\mathrm{d}\epsilon_{2S}(q)/\mathrm{d}q|}. \tag{20}$$

In order to see the behaviour of $D(\epsilon)$ clearly, we introduce the *whole* excitation spectrum, defined as

$$\rho(\epsilon) = \frac{\sigma_{2S,I}(q) + \sigma_{2S,I}^h(q)}{|\mathrm{d}\epsilon_{2S}(q)/\mathrm{d}q|}. \tag{21}$$

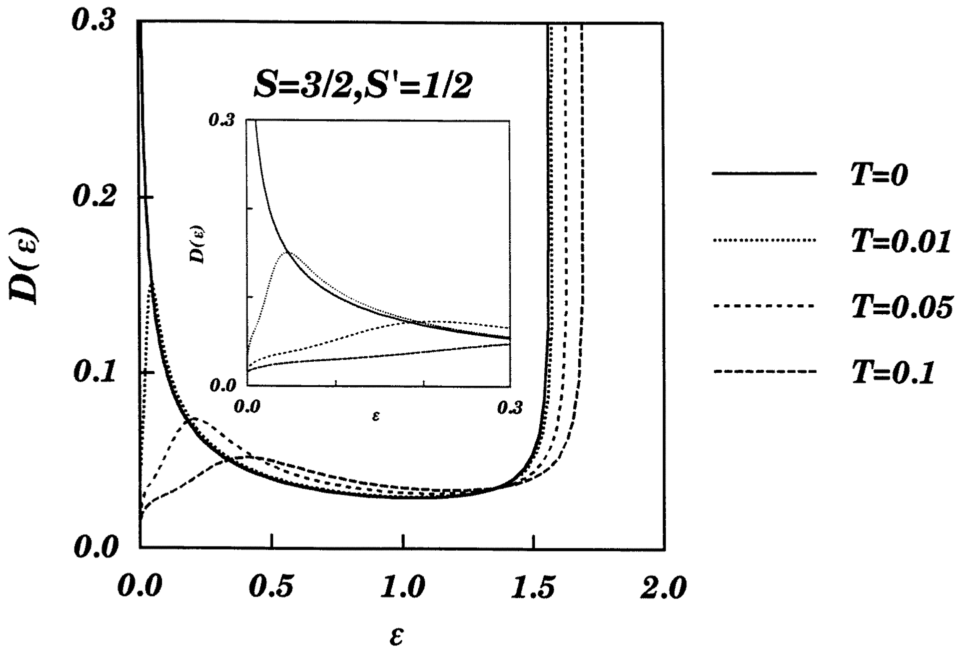
These spectral densities satisfy the relation

$$D(\epsilon) = \frac{1}{1 + \exp\{(-\epsilon + \epsilon_{2S}(-\infty))/T\}}\rho(\epsilon). \tag{22}$$

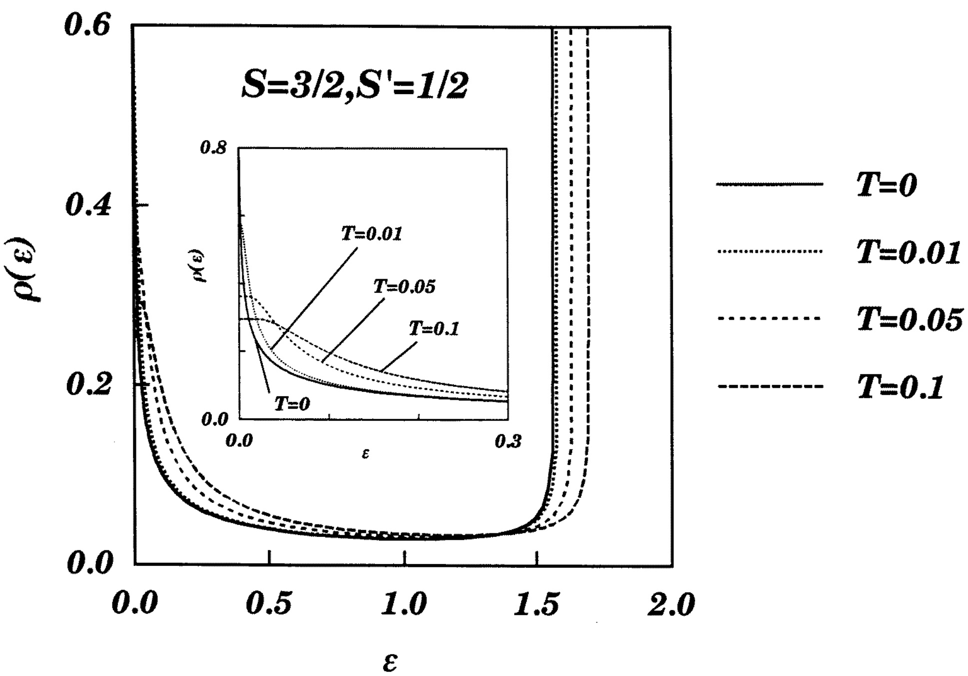
The total weight of the dressed-hole excitation depends on the temperature and satisfies the following relation:

$$\int_0^\infty D(\epsilon)\ \mathrm{d}\epsilon = \frac{\min(S, S')}{2S} - \sum_{n\neq 2S} n\int_{-\infty}^\infty \sigma_{n,I}(\Lambda)\ \mathrm{d}\Lambda. \tag{23}$$

It is seen that the total weight takes the maximum value $\min(S, S')/2S$ at zero temperature, and decreases as the temperature is increased.



(*a*)



(*b*)

Figure 2. (*a*) Plots of the spectral density for the dressed-hole excitation for several temperatures in the cases where $S = 3/2$ and $S' = 1/2$. (*b*) Plots of the whole excitation spectrum for several temperatures in the cases where $S = 3/2$ and $S' = 1/2$.

3.2. Numerical results

Here, we show the numerical results for the elementary excitation spectrum in the cases where $S < S'$ and $S > S'$. When $S < S'$, the partial compensation of an impurity spin takes place, leaving the spin degeneracy $\ln[2(S' - S) + 1]$ at zero temperature. The divergence property of the spectral densities in the low-energy region in figures 1(*a*) and 1(*b*) can be understood from this remaining spin degeneracy. It is seen that the temperature dependence of $\rho(\epsilon)$ is not so conspicuous in contrast to $D(\epsilon)$, and $\rho(\epsilon)$ shifts slightly to the higher-energy region as the temperature is increased.

In the case where $S > S'$, the remaining spin degeneracy is rather peculiar as in (1). The numerical results for $D(\epsilon)$ and $\rho(\epsilon)$ are shown in figures 2(*a*) and 2(*b*), respectively, in the cases where $S = 3/2$ and $S' = 1/2$. Judging from the numerical results, $D(0)$ and $\rho(0)$ do not diverge and increase as the temperature is decreased. The peak structure in $D(\epsilon)$ in the low-energy region grows and shifts towards the lower-energy region, as the temperature is decreased. This pattern of behaviour can be interpreted in terms of the increment of the low-energy state which compensates an impurity spin S'.

From the numerical results, we can see that the spectral densities approach those of zero temperature, when the temperature is decreased. This means that the present formulation of finite temperatures is a reasonable extension from the zero-temperature case. In the case where $S < S'$, the temperature dependence of $\rho(\epsilon)$ is very weak in the low-energy region. Therefore, the characteristic temperature dependence of $D(\epsilon)$ in the low-energy region is well described by multiplying the spectral density at zero temperature by the Fermi distribution function. In the case where $S > S'$, on the other hand, the temperature dependence of $D(\epsilon)$ cannot be described by using only the Fermi distribution function.

In the higher-energy region, the spectral densities diverge in both cases. The energy values where the spectra diverge coincide with each other in the two cases at a given temperature, if the magnitudes of the host spins are the same. Therefore, it is considered that the divergence property in the higher-energy region reflects the property of the excitation spectrum for the host spin not only at zero temperature but also at finite temperatures.

4. Summary

We have investigated the elementary excitation for the integrable spin-S Heisenberg chain with an impurity spin, introducing a dressed hole. We have shown that the spectral densities of an impurity spin show characteristic behaviours in the low-energy region depending on the values of S and S'.

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