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Spin-Wave-Spin-Wave Interaction and the Thermodynamics of the Heisenberg Spin Chain

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Abstract. The low-temperature free energy of the spin S quantum Heisenberg ferromagnetic chain in a strong magnetic field is obtained within the two-particle approximation by using the exact solution of the two-spin-wave problem. The result is beyond perturbation theory because it incorporates both the bound and scattering state contributions, and the scattering effect is essential, as well as the bound state one. In particular, main temperature renormalization of the exchange constant is found to be temperature-linear, instead of $T^{3/2}$ dependence corresponding to the perturbation theory result.

1 Introduction

The low-dimensional spin systems show many special features in thermodynamics. Some of them are the result of a large number of excitations in the system, e.g., the destruction of a long-range order that the well-known Mermin and Wagner theorem states [1]. Also these features are often coupled with the failure of the free-spin-wave-based consideration for the low-dimensional systems. In this communication we would like to note that the exchange interaction of even two spin waves in the Heisenberg chain shows an effect which is beyond perturbation theory. In fact, this property is connected with the well-known peculiarity of the low-dimensional quantum mechanical problem, such as formation of the bound state and

strong scattering within the long-wave limit in a weak potential [2]. Though, when spin $S \rightarrow \infty$, it is a weak coupling limit, perturbation theory is not correct for the long-wave excitations, which dominate at low temperatures. The consideration of the $1/S$ corrections was noted earlier to be essential for the low-dimensional spin systems [3, 4].

2 Spectrum and density of states for two spin waves

We explore a pure exchange Heisenberg ferromagnetic spin chain with an arbitrary spin, S , in a strong magnetic field within the limit of low temperatures. The Hamiltonian is as follows

$$H = -J \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j - h \sum_i S_i^z. \quad (2.1)$$

In the first term, the sum runs over different pairs of the nearest neighboring sites where quantum spins \mathbf{S}_i are located. For $S = 1/2$, this system can be solved by the Bethe Ansatz method [5]. When $S > 1/2$, there is no exact solution. On the other hand, it is usually assumed that perturbation theory is correct when $S \rightarrow \infty$ [6]. We show below that this statement is wrong for a spin chain. Other known methods also do not allow to consider specific features of low-dimensional systems [7, 8].

The Zeeman energy of a ferromagnetic spin system in the magnetic field depends only on the number of excitations. That allows us to consider separately the states with one, two or more spin deviations. We are interested in the correction to the free energy due to interaction, which arises from the two-spin-wave sector at first. The two-spin-wave problem was exactly solved for an arbitrary spin, S [9]. The energy spectrum of two spin waves in the finite chain of size N follows from the eigenvalue equation [9]

$$D(p, q) = 1 - \frac{1}{N} \sum_k \frac{2J \cos(k)(\cos(k) - \cos(p/2))}{2S \cos(p/2)(\cos(k) - \cos(q))} = 0, \quad (2.2)$$

where $k = 2\pi n/N$, $n = 0, 1, \dots, N - 1$, and p is center mass momentum of the two-spin-wave state. The energy spectrum of the state is parametrized by q as follows

$$E(p, q) = 4SJ(1 - \cos(p/2) \cos(q)) + 2h. \quad (2.3)$$

Let us consider the function D versus q at fixed center of mass momentum p . While the chain is finite, $D(q)$ is a meromorphic function with N poles and N zeros, where the poles correspond to free-spin waves and the zeros correspond to real energy levels. As $N \rightarrow \infty$, the function D changes its analytical properties. Within the limit of a large N , it gives an isolated zero beyond the continuous spectrum and a cut which corresponds to the scattering states. Within this limit, the difference between scattering state energy levels and the free-spin-wave energy levels is $\sim 1/N$. It is this small value that gives a perturbation of the free

energy by spin-wave-spin-wave scattering, because the number of scattering states is $\sim N^2$ and, therefore, the scattering contributes to the order of N .

The finite sum in Eq.(2.2) is calculated directly, and we obtain

$$D(p, q) = 1 - \frac{1}{2S} \left(1 - \frac{\cos(q)}{\cos(p/2)} \right) \left(1 + \cot(q) \cot\left(\frac{Nq}{2}\right) \right). \quad (2.4)$$

The state out of the continuum corresponds to an imaginary parameter q . We use $q = i\alpha$. Then, as $N \rightarrow \infty$, Eq.(2.4) gives the bound state condition which is the same as in [9]

$$1 - \frac{1}{2S} \left(1 - \frac{\cosh(\alpha)}{\cos(p/2)} \right) (1 - \coth(\alpha)) = 0. \quad (2.5)$$

Within the long-wave limit we obtain $\alpha = (p/2)^2/4S + O(p^4)$. Thus, the coupling energy is $E_b(p) - E(p, 0) = -4SJ(p/2)^4/32S^2$.

To find the perturbation of the continuum, we use $q = 2\pi(n + \Delta)/N$ where n is an integer and Δ characterizes the energy level shift. Then, from Eq.(2.4) we obtain the equation for Δ

$$1 - \frac{1}{2S} \left(1 - \frac{\cos(q)}{\cos(p/2)} \right) \left(1 + \cot(q) \cot(\pi\Delta(q)) \right) = 0. \quad (2.6)$$

Therefore,

$$\Delta(q) = \frac{1}{2} - \frac{1}{\pi} \arctan \left\{ \tan(q) \left(\frac{2S}{1 - \frac{\cos(q)}{\cos(p/2)}} - 1 \right) \right\} \quad (2.7)$$

Function $\Delta(q)$ is essentially different when $S = 1/2$ and $S > 1/2$. This function is periodic for $S > 1/2$ and multivalued for $S = 1/2$. In the last case, $\Delta(\pi) - \Delta(0) = 1$; that provides the correct reduction of the number of states for $S = 1/2$.

3 Free energy expansion

After elementary transformations by keeping the terms of the order of N we obtain the spin-chain free energy f which is formed from one- and two-spin-wave states at the temperature T

$$\begin{aligned} -\frac{f}{T} = Ne^{-h/T} \int_{-\pi}^{\pi} \frac{dk}{2\pi} e^{-\varepsilon_1(k)/T} - \frac{N}{2} e^{-2h/T} \int_{-\pi}^{\pi} \frac{dp}{2\pi} \int_0^{\pi} dq \frac{d\Delta}{dq} e^{-\varepsilon_2(p,q)/T} + \\ \frac{N}{2} e^{-2h/T} \int_{-\pi}^{\pi} \frac{dp}{2\pi} e^{-\varepsilon_b(p)/T}, \end{aligned} \quad (3.1)$$

where $\varepsilon_1(k) = 2SJ(1 - \cos(k))$ and $\varepsilon_2(p, q) = 4SJ(1 - \cos(p/2)\cos(q))$ are one- and two-spin-wave energies and $\varepsilon_b(p)$ is the bound state energy without the Zeeman term. The factor $1/2$ in the two-spin-wave terms follows from the permutation symmetry of this state. We note that the zero q state is not realized as follows from Eq.(2.6).

We calculate the scattering term using Eq.(2.7) and the bound state term, using the bound state energy from Eq.(2.5). Then we obtain

$$-\frac{f_{scatt}}{NT} = e^{-\frac{2h}{T}} \left\{ -\frac{1}{2\sqrt{2}} \left(\frac{T}{4\pi SJ} \right)^{1/2} \left[1 + \frac{2\pi}{16} \left(\frac{T}{4\pi SJ} \right) \left(1 + \frac{3}{(2S)^2} \right) + \frac{2\pi\sqrt{2}}{16(2S)} \left(\frac{T}{4\pi SJ} \right)^{3/2} \left(1 + \frac{4}{2S} - \frac{15}{2(2S)^2} \right) \right] + O(T^{5/2}) \right\}; \quad (3.2)$$

$$-\frac{f_{bound}}{NT} = e^{-\frac{2h}{T}} \left\{ \frac{1}{\sqrt{2}} \left(\frac{T}{4\pi SJ} \right)^{1/2} + \frac{2\pi}{16\sqrt{2}} \left(\frac{T}{4\pi SJ} \right)^{3/2} \left(1 + \frac{3}{(2S)^2} \right) + O(T^{5/2}) \right\}. \quad (3.3)$$

We note that the bound state and scattering contributions are of the same order. The free-spin-wave theory gives

$$-\frac{f_{FSW}}{NT} = - \int_{-\pi}^{\pi} \frac{dk}{2\pi} \ln \left(1 - e^{-\varepsilon_1(k)/T} \right) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left(e^{-h/T - \varepsilon_1(k)/T} + \frac{1}{2} e^{-2h/T - 2\varepsilon_1(k)/T} + \dots \right). \quad (3.4)$$

Thus, the deviation from the free-spin-wave free energy is

$$-\frac{f - f_{FSW}}{N} = T \left\{ \frac{2\pi}{32\sqrt{2}} \frac{3}{(2S)^2} \left(\frac{T}{4\pi SJ} \right)^{3/2} - \frac{2\pi}{32(2S)} \left(\frac{T}{4\pi SJ} \right)^2 \left(1 + \frac{4}{2S} - \frac{15}{2(2S)^2} \right) \right\} e^{-\frac{2h}{T}} + O(T^{7/2}) e^{-\frac{2h}{T}}. \quad (3.5)$$

We note that this temperature expansion of the free energy does not contain the T^2 term. It is in agreement with the results for 1D ferromagnetic spin 1/2 Heisenberg system [10]. The term T^3 which corresponds to the perturbation theory is also present. It is interesting to note how this term depends on the spin value S . When $S = 1/2$, it has the same sign as the main contribution and for all other spins it has the opposite sign.

4 Conclusion

There is a number of exact results for the spin 1/2 Heisenberg chain. Low-temperature expansion of the free energy for the ferromagnetic chain in a small magnetic field was obtained in the work of Johnson and Bonner[11] by using the Gaudin formalism[12] up to order of $e^{-h/T}$. However, we are interested in the interaction effects which appear for the first time in the terms of the order of $e^{-2h/T}$. Thus, we can not use the exact results for spin 1/2[11] and compare them with the above expression in the Eq.(3.5).

It is interesting to consider the temperature renormalization of the exchange parameter which characterizes the temperature correction to the energy spectrum. In order to define this renormalization, we reduce the real free energy to the free-spin-wave form. Then we obtain

$$\frac{\Delta J}{J} = -\frac{3T}{16\sqrt{2}J(2S)^3} e^{-\frac{h}{T}} \left(1 + \frac{2h}{3T + 2h} \right). \quad (4.1)$$

Thus, the spin-wave-spin-wave exchange interaction gives a linear temperature factor in the effective exchange parameter. A similar result follows from the consideration of the classical spin system. Within the large spin limit at the fixed temperature, the leading temperature term will be suppressed due to the extra factor $1/S$. So other contributions will become more essential. This fact means that the low-temperature expansion is divergent when the spin is large. It is easy to see that the use of the $1/S$ expansion for the exact scattering spectrum in Eq.(2.7) gives divergencies in the expression for the free energy. It explains the failure of perturbation theory for a spin chain.

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