
FIP10604 – Text 11 — ONE-DIMENSIONAL HEISENBERG MODEL

We mentioned at the end of Text 10 that the one-dimensional Heisenberg model can be exactly solved. We must add that this applies only to $S = 1/2$. One of the formulations of the solution method will be briefly present here, together with some results for physical quantities.

The system consists of spins localized at the sites of a linear chain with lattice parameter a . As usual, we consider a finite lattice of N sites with periodic boundary conditions, so that site $N + 1$ coincides with site 1. The exchange interaction is restricted to nearest neighbors, which allows to write the Hamiltonian as

$$\mathcal{H} = -J \sum_{n=1}^N \mathbf{S}_n \cdot \mathbf{S}_{n+1} = -J \sum_{n=1}^N \left[S_n^z S_{n+1}^z + \frac{1}{2} (S_n^+ S_{n+1}^- + S_n^- S_{n+1}^+) \right]. \quad (1)$$

This Hamiltonian commutes with any component α of the total spin, $S_T^\alpha = \sum_{n=1}^N S_n^\alpha$, which means that its eigenvectors may be selected as belonging to orthogonal subspaces where S_T^z has a definite value. The maximum value of S_T^z is $N/2$, corresponding to the state $|F\rangle$, which is the ground state **if** $J > 0$ (FM case). In general, we will write $S_T^z = N/2 - r$, where r is the number of spin deviations in relation to the **reference state** $|F\rangle$.

The $r = 0$ subspace is one-dimensional, with the eigenvalue $E_0 = -NJS^2 = -NJ/4$.

The $r = 1$ subspace has dimension N since a local spin deviation can be at any one of the N lattice sites. A possible **basis** for the $N \times N$ block of the Hamiltonian in this subspace can be the set of vectors

$$|n\rangle = S_n^- |F\rangle, \quad n = 1, \dots, N. \quad (2)$$

The Hamiltonian is not diagonal in this basis, as we saw in Text 07, when we studied magnons. Following the same procedure employed there, we take lattice-translation symmetry into account, defining vectors

$$|k\rangle = \frac{1}{\sqrt{N}} \sum_{n=1}^N e^{ikn} |n\rangle, \quad (3)$$

that are energy eigenvectors associated to the eigenvalues

$$E_k = E_0 + J(1 - \cos k). \quad (4)$$

Here we have chosen $a = 1$, meaning that all distances are measured in units of the lattice parameter. Periodic boundary conditions determine that k can assume N independent values which we write as $k = (2\pi\lambda)/N$, with $\lambda = 0, 1, \dots, N - 1$. Note that the $|k\rangle$ states are exactly the spin waves defined in Text 07, and the last term in Eq. (4) reproduces the magnon dispersion relation for our present choice of parameters and spatial dimension.

For any subspace with $r > 1$ we depart from the independent-magnon approach, since $(S_n^-)^2 = 0$ for $S = 1/2$.

Bethe ansatz¹

In search of an exact solution, we will look for a systematization of the method allowing to obtain energy eigenvalues without violating any restrictions implied by spin-deviation operators. As a preliminary step, we will revisit the case $r = 1$ with a different approach.

We want to solve the eigenvalue equation

$$\mathcal{H}|\psi\rangle = E|\psi\rangle \quad (5)$$

using the $\{|n\rangle\}$ basis, i.e.,

$$|\psi\rangle = \sum_{n=1}^N a_n |n\rangle, \quad (6)$$

with $|n\rangle$ given by Eq. (2). Explicitly applying the Hamiltonian (1), we obtain the recursion relations

$$2[E - E_0]a_n = J[2a_n - a_{n-1} - a_{n+1}], \quad a_{n+N} = a_n. \quad (7)$$

It is easy to verify that a solution to these equations is

$$a_n = e^{ikn}, \quad k = (2\pi\lambda)/N, \quad \lambda = 0, 1, \dots, N-1, \quad (8)$$

as obtained before.

Going to $r = 2$, we write

$$|\psi\rangle = \sum_{\substack{n_1, n_2 \\ (1 \leq n_1 < n_2 \leq N)}} a_{n_1 n_2} |n_1 n_2\rangle, \quad (9)$$

where

$$|n_1 n_2\rangle = S_{n_1}^- S_{n_2}^- |F\rangle. \quad (10)$$

The vectors $|n_1 n_2\rangle$ define a subspace of dimension $N(N-1)$. Now, the recursion relations become

$$2[E - E_0]a_{n_1 n_2} = J[4a_{n_1 n_2} - a_{n_1-1, n_2} - a_{n_1+1, n_2} - a_{n_1, n_2-1} - a_{n_1, n_2+1}], \quad (11)$$

for $n_2 > n_1 + 1$, and

$$2[E - E_0]a_{n_1 n_2} = J[2a_{n_1 n_2} - a_{n_1-1, n_2} - a_{n_1, n_2+1}], \quad (12)$$

for $n_2 = n_1 + 1$.

These equations can be solved through the **Bethe ansatz**. Our discussion will be restricted to the form originally proposed by Bethe,² often called *coordinate Bethe ansatz*, in contrast

¹M. Karbach and G. Müller, “Introduction to Bethe Ansatz I”, Computers in Physics **11**, 36 (1997) [cond-mat/9809162].

²H. Bethe, Z. Phys. **71**, 205 (1931).

to the *algebraic Bethe ansatz*, which became more popular. The latter makes use of a methodology employed in inverse-scattering problems, falling into the more general context of *integrable* systems. In its coordinate version, the *ansatz* consists in assuming that

$$a_{n_1 n_2} = A e^{i(k_1 n_1 + k_2 n_2)} + A' e^{i(k_1 n_2 + k_2 n_1)} . \quad (13)$$

This form satisfies Eq. (11) if we choose

$$E_{k_1, k_2} = E_0 + J \sum_{j=1}^2 (1 - \cos k_j) . \quad (14)$$

On the other hand, noticing that Eq. (11) is also satisfied if $n_2 = n_1 + 1$, Eq. (12) implies the condition

$$2a_{n_1, n_1+1} = a_{n_1 n_1} + a_{n_1+1, n_1+1} . \quad (15)$$

This leads to a relation between the coefficients A and A' which can be written as

$$\frac{A}{A'} \equiv e^{i\theta} = -\frac{e^{i(k_1+k_2)} + 1 - 2e^{ik_1}}{e^{i(k_1+k_2)} + 1 - 2e^{ik_2}} . \quad (16)$$

We can then rewrite Eq. (13) as

$$a_{n_1 n_2} = e^{i(k_1 n_1 + k_2 n_2 + \theta_{12})} + e^{i(k_1 n_2 + k_2 n_1 + \theta_{21})} , \quad (17)$$

with $\theta_{12} = -\theta_{21} = \theta$. After some algebra, Eq. (16) results in

$$2 \cot \frac{\theta}{2} = \cot \frac{k_1}{2} - \cot \frac{k_2}{2} . \quad (18)$$

Periodic boundary conditions imply that

$$e^{ik_1 N} = e^{i\theta} , \quad e^{ik_2 N} = e^{-i\theta} , \quad (19)$$

leading to

$$k_1 = \frac{2\pi\lambda_1 + \theta}{N} , \quad k_2 = \frac{2\pi\lambda_2 - \theta}{N} , \quad \lambda_i \in \{0, 1, \dots, N-1\} . \quad (20)$$

It is important to remark that, among all possible k_i of the sets defined in Eq. (20), only pairs k_1, k_2 that satisfy Eq. (18) are solutions.

In the absence of the *phase shift* θ , Eq. (17) corresponds to an independent-magnon solution. Therefore, a non-zero θ appears as an effect of magnon interaction. In the case of spin 1/2, this interaction is of *hard-core* type, i.e., we cannot have two magnons (spin deviations) at the same site.

The solutions of Eqs. (18) and (20) fall into three categories:

- 1) a branch identical to the single-magnon spectrum for either k_1 or k_2 , the other being null;
- 2) a branch of two-magnon **bound states**, when the equations present complex solutions for k_1 and k_2 (complex conjugate pairs);
- 3) a continuum of two-magnon **scattering states**, with real k_1 and k_2 .

Generalization for any r

In the general case, an energy eigenvector is written as

$$|\psi\rangle = \sum_{\substack{n_1 \dots n_r \\ 1 \leq n_1 < \dots < n_r \leq N}} a_{n_1 \dots n_r} |n_1 \dots n_r\rangle. \quad (21)$$

The Bethe *ansatz* (BA) becomes

$$a_{n_1 \dots n_r} = \sum_{\mathcal{P}} \exp \left(i \sum_{j=1}^r k_{\mathcal{P}_j} n_j + \frac{i}{2} \sum_{i < j} \theta_{\mathcal{P}_i \mathcal{P}_j} \right), \quad (22)$$

where each \mathcal{P} is one of the possible permutations of $\{1, 2, \dots, r\}$.

The energy eigenvalue corresponding to $|\psi\rangle$ is

$$E_{\{k_i\}} = E_0 + J \sum_{j=1}^r (1 - \cos k_j), \quad (23)$$

the k_i 's and θ_{ij} 's being determined by the equations

$$\begin{aligned} Nk_i &= 2\pi\lambda_i + \sum_{j \neq i} \theta_{ij}, \quad \lambda_i \in \{0, 1, \dots, N-1\}, \\ 2 \cot \frac{\theta_{ij}}{2} &= \cot \frac{k_i}{2} - \cot \frac{k_j}{2}, \quad i, j = 1, \dots, r. \end{aligned} \quad (24)$$

We will not discuss the solutions in detail. We will just comment on some of their characteristics.

- Since the Heisenberg Hamiltonian also preserves the total spin, each subspace with a given r (i.e., given S_T^z) may be further divided into subspaces corresponding to possible values of S_T .
- There is always a state with all k_i 's null and energy equal to E_0 , corresponding to the maximum value of S_T (i.e., $N/2$). This state has r spin deviations **uniformly distributed** on the lattice, which is nothing but a **rotation** of the state $|F\rangle$.
- Subspaces with intermediate values of S_T , i.e., $N/2 - r < S_T < N/2$, have at least one k_i null (but not all).
- The subspace corresponding to the smallest possible value of S_T , that is, $N/2 - r$, has all k_i 's non-zero, both real values and complex-conjugate pairs.

AF Heisenberg chain

All the BA equations obtained for the one-dimensional Heisenberg model are independent of the sign of J . Therefore, in contrast to what was done for magnons in the AF system in three dimensions, we do not use the Néel state as a reference, but describe the states in terms of spin deviations (independent or **not**) relative to the completely aligned (FM) state.

From now on we focus on the AF case, changing $J \rightarrow -J$ everywhere (including the Hamiltonian), and treating J as a positive quantity.

The AF ground state (for N even) certainly has S_T^z null, corresponding to $r = N/2$. Numerical studies on finite lattices indicate that the $N/2$ quantum numbers λ_i associated to this state are the odd numbers $1, 3, \dots, N - 1$.

It is possible to analytically determine the asymptotic value of the ground-state energy in the thermodynamic limit, which can be expressed by the relation

$$\frac{E_{\text{AF}} - E_{\text{F}}}{N} = -J \ln 2, \quad (25)$$

Where E_{F} is the energy of the FM state, previously denoted by E_0 .

Unfortunately, it is not possible to build a simple image describing the nature of the ground state. We know that it has zero total spin and **no magnetic long-range order**. It is possible (although the complexity exceeds the level of our discussion) to evaluate spin correlation functions, which show a power-law decay with the inter-site distance. It should be noted that in a “normal” system, without magnetic order (e.g., the PM phase of a 3D ferromagnet), this decay is exponential. In theories of phase transitions, correlation functions with power-law decay are associated to critical phenomena. One can then say that the ground state of the AF Heisenberg chain is a “critical state”.

Effect of a uniform magnetic field

Applying a uniform field H to the AF chain, the Hamiltonian becomes

$$\mathcal{H} = \mathcal{H}_{\text{AF}} - HS_T^z. \quad (26)$$

Since S_T^z commutes with \mathcal{H}_{AF} , the eigenvectors remain the same, but the energy eigenvalues vary linearly with H with a slope given by the corresponding eigenvalue of S_T^z . The AF ground state, for which $S_T^z = 0$, remains unchanged in the presence of field. However, all the other states, which have higher energies when $H = 0$, will have these energies reduced as H increases, crossing the original ground state and one another. Eventually, the uppermost one at zero field, state $|F\rangle$, will become the ground state. The last interchange will be with the state having a single spin deviation. The energy difference between final two lowest states is $2J$, which means that the **saturation field**, above which all spins are aligned, is $H_s = 2J$.

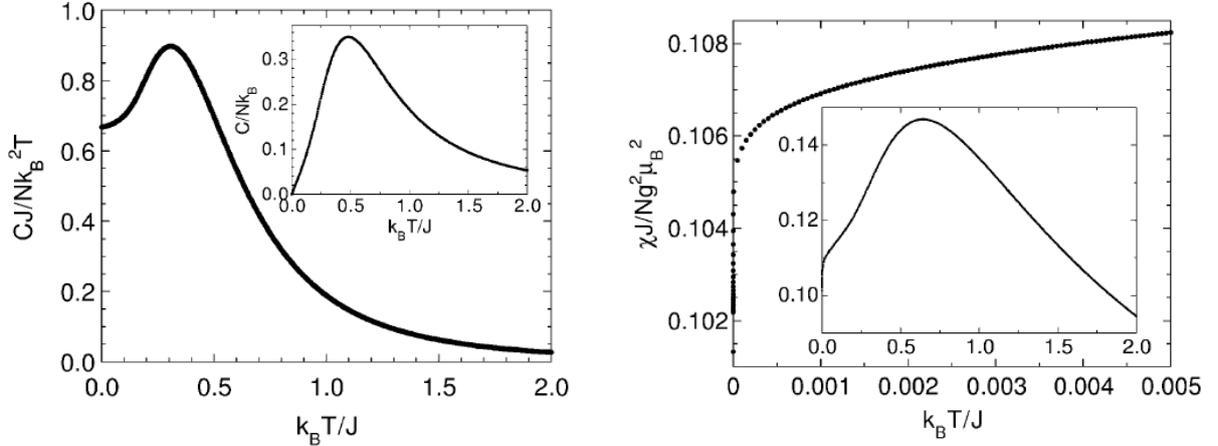


Figure 1: Specific heat (left) and uniform magnetic susceptibility (right) of the AF Heisenberg chain. [Extracted from: A. Klümper and D. C. Johnson, Phys. Rev. Lett. **84**, 4701 (2000).]

Thermodynamic properties

The BA equations allow, in principle, to obtain the entire energy spectrum. We can thus build up the partition function (even in the presence of applied field) and evaluate thermodynamic properties. As we have already hinted, even though the equations are exact, their solution and the evaluation of other quantities must be done numerically. Without going into practical details, and in order to illustrate what can be obtained with the method, we present plots of the specific heat and uniform magnetic susceptibility as functions of temperature in Fig. 1 (where the constants N , g , μ_B and k_B appear explicitly).

Some interesting observations can be made about these results:

- Both specific heat and susceptibility present broad maxima in the same region of temperatures (see the figure insets).
- The specific heat is **linear** in T for $T \rightarrow 0$ (the c/T vs. T plot has a finite limit at $T = 0$).
- The susceptibility shows singular behavior for $T \rightarrow 0$, although with a finite limit. This limit is $J\chi(0) = 0.101321\dots = 1/\pi^2$. Field-theory methods⁴ yield an analytic relation in this region,

$$J\pi^2\chi \simeq 1 + \frac{1}{2\ln(T_0/T)}. \quad (27)$$

It is possible to fit the BA results with this equation for $T_0 \simeq 7.7J$.

⁴S. Eggert, I. Affleck, and Takahashi M., Phys. Rev. Lett. **73**, 332 (1994).