The Heisenberg Model

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Abstract

This is a summary of the talk I gave in the Statistical Physics seminar by Prof. A. Mielke.
In the first part the quantum Heisenberg model is introduced. Then a short overview of the ferromagnetic and antiferromagnetic ordering of the Heisenberg model is given. In last part the spin wave approximation for the antiferromagnetic case is outlined.

1. Motivation

The Heisenberg model is an effective model to describe ferro- and antiferromagnetic solids. It is suited for the description of insulators rather than metals [2]. Nevertheless it is used to describe real materials e.g. the insulator La_2CuO_4 which is important in the topic of superconductors. The Heisenberg model can only be exactly solved in one dimension. For higher dimensions one has to rely on analytic approximation or numerical methods. One of these is the spin wave approximation.

2. The Heisenberg Model

The model is defined on a d-dimensional lattice with N sites. To each site i the spin operators $\mathbf{S_i} = (S_i^x, S_i^y, S_i^z)$ are assigned. Only nearest neighbor interactions between the spins are considered. The hamiltonian reads as follows.

$$H = \sum_{<i,j>} J_x S_i^x S_j^x + J_y S_i^y S_j^y + J_z S_i^z S_j^z - h \sum_i S_i^z \tag{1}$$

The last term of the hamiltonian describes the lowering of the energy by an external magnetic field h.

For each spin $S = \frac{1}{2}, 1, \frac{3}{2}, ...$ there exists a set of $(2S+1) \times (2S+1)$ spin matrices $\mathbf{S}$. Thus H is defined on the Hilbert space $\mathcal{H} = \bigotimes_N \mathbb{C}^{2S+1}$ with $S_i^m = \mathbb{I} \otimes \mathbb{I} \otimes ... \otimes \mathbb{I} \otimes S^m \otimes \mathbb{I} \otimes ...\mathbb{I}$, where S^m is at the i-th position. The spin matrices satiesfy the commutation relation $[S^m, S^n] = i\epsilon_{mno}S^o$. Furthermore S^z has $2S$ eigenvectors $|s_z\rangle$ with eigenvalues $-S, -S+1, ...S$. For simplicity we set $J = J^x = J^y = J^z$.

3. Ferro- and Antiferromagnetism

3.1. Ferromagnetism

A spin system is said to be ferromagnetic, if the ground state has a ferromagnetic order. This means that the state is similiar to the classical ferromagnetic state, in which all spins point in to the same direction. This is said to be true, if for the magnetisation per site $< m > \neq 0$ holds.

For $J > 0$ the Heisenberg model is ferromagnetic. In demension $d = 1$ and $d = 2$ however there is no ferromagnetic order for finite temperatures $T > 0$. In dimension $d \geq 3$ there exist a critical temperature T_c, so that for temperatures $T \leq T_c$ the Heisenberg model is ordered.

3.2. Antiferromagnetism

A spin system is said to antiferromagnetic, if the ground state has an antiferromagnetic order. This means it is similiar to the classical antiferromagnetic state, in which neighbouring spins point exactly in opposite direction. The lattice of the system is devided into two sublattices A and B. On A the spins point into S^z direction and on B they point into the opposite direction. To measure the ordering one looks on the magnetisation $< m_{St} >$ of the the sublattice A. If it is nonzero the system is ordered.

For $J < 0$ the Heisenberg model is in most cases antiferromagnetic depending on the dimension d and the specific lattice. In dimension $d = 1$ it is assumed that there is no odering. Whereas in dimension $d = 2$ it is assumed that there is ordering only for the temperature $T = 0$. As in the ferromagnetic case, for

$d \geq 3$ there exists a critical temperature T_N. For temperature $T \leq T_N$ the Heisenberg model is ordered.

(a) the classical ferromagnetic state for a 2d cubic lattice

(b) the classical antiferromagnetic state for a 2d cubic lattice

Figure 1

Source: https://en.wikipedia.org/wiki/Ferromagnetism#/media/File:Ferromagnetic_ordering.svg, https://en.wikipedia.org/wiki/Antiferromagnetism#/media/File:Antiferromagnetic_ordering.svg

4. The Spin Wave Approximation

One can not solve the Heisenberg model exactly for $d \geq 2$. But for system with ferro- or antiferromagnetic ordered ground state and particular for large S and small temperatures one can use the so-called spin wave aprroximation. In the following we derive this approximation for the antiferromagnetic Heisenberg model on a cubic lattice in the limit $h \to 0$.
First one defines ladder operators $S^{\pm}$ to rewrite the hamiltonian (1).

$$\begin{aligned} S_i^{\pm} &\equiv S_i^x \pm S_i^y \\ H &= \sum_{<i,j>} \frac{J}{2}(S_i^+ S_j^- + S_i^- S_j^+) + J S_i^z S_j^z - h \sum_i S_i^z \end{aligned} \tag{2}$$

Then we define the operator

$$\hat{n}_i = \begin{cases} S - S_i^z & i \in A \\ S - (-S_i^z) & i \in B \end{cases} \tag{3}$$

, which measures the difference of a state from the classical antiferromagnetic state. From the definition it follows that the eigenvectors of S_i^z are eigenvectors

$|n_i\rangle$ of $\hat{n}_i$ with eigenvalues $n_i = 0, 1, ..., 2S$. $S^\pm$ are ladder operators and one can show that

$$
\begin{aligned}
S_i^+ |n_i\rangle &= \sqrt{2S(1 - \frac{n_i - 1}{2S})n_i}\, |n_i - 1\rangle \\
S_i^- |n_i\rangle &= \sqrt{2S(n_i + 1)(1 - \frac{n_i}{2S})}\, |n_i + 1\rangle
\end{aligned} \tag{4}
$$

for an $i \in A$. For an $i \in B$ S^+ and S^- are interchanged. The idea is now to rewrite $S^\pm$ in terms of boson creation and annihilation operators c_i^+ and c_i.

$$
\begin{aligned}
c_i^+ |n_i\rangle &= \sqrt{n_i + 1}\, |n_i + 1\rangle \\
c_i |n_i\rangle &= \sqrt{n_i}\, |n_i - 1\rangle \\
[c_i, c_j^+] &= \delta_{ij}
\end{aligned} \tag{5}
$$

The relations (5) are similiar to the $S^\pm$ relations (4) and yield

$$\hat{n}_i = c_i^+ c_i.$$

Then we rename $a_i \equiv c_i$ on A and $b_i \equiv c_i$ on B to obtain an expression of $S^\pm$ for an $i \in A$.

$$
\begin{aligned}
S_i^+ &= \sqrt{2S}\sqrt{1 - \frac{\hat{n}_i}{2S}}a_i \\
S_i^- &= \sqrt{2S}a_i^+\sqrt{1 - \frac{\hat{n}_i}{2S}}
\end{aligned}
$$

For $i \in B$ one interchanges $a_i \leftrightarrow b_i$ and $S_i^+ \leftrightarrow S_i^-$. This is known as the Holstein-Primakoff transformation. Inserting it into (2) yields

$$
\begin{aligned}
H =& NdJS^2 \\
&- 2dJ(\sum_i \hat{n}_i)S - J\sum_{<i,j>}(f_S(\hat{n}_i)a_i f_S(\hat{n}_j)b_j + a_i^+ f_S(\hat{n}_i)b_j^+ f_S(\hat{n}_j))S \\
&+ J\sum_{<i,j>}\hat{n}_i\hat{n}_j
\end{aligned} \tag{6}
$$

with

$$f_S(\hat{n}_i) = \sqrt{1 - \frac{\hat{n}_i}{2S}} \approx 1 - \frac{\hat{n}_i}{4S} - \frac{\hat{n}_i^2}{32S^2} - .... \tag{7}$$

To simplify the hamiltonian we approximate $f_S(\hat{n}_i) \approx 1$ and neglect the term quadratic in $\hat{n}_i$, which yields

$$\begin{aligned} H =& NdJS^2 \\ &- 2dJ(\sum_i \hat{n}_i)S - J \sum_{<i,j>} (a_i b_j + a_i^+ b_j^+)S \end{aligned} \tag{8}$$

On the one hand this is valid in the limit $S \to \infty$, because the quadratic term is only of order S^0. On the other hand one can argue as follows: (7) is an exspansion in $\frac{\hat{n}_i}{2S}$ and not only in $\frac{1}{S}$. For small temeperature the relevant states are small exitiation of the ground state $|0\rangle$. So, if $\frac{\langle 0|\hat{n}_i|0\rangle}{2S} \ll 1$, $f_S(\hat{n}_i) \approx 1$ should hold and the quadratic term can be neglected.
To diagonalize (8) we write it in terms of a pair of new creation and annihilation operators α_k and β_k.

$$\begin{aligned} \alpha_k &= cosh(\theta_k) a_k + sinh(\theta_k) b_k^+ \\ \beta_k &= sinh(\theta_k) a_k^+ + cosh(\theta_k) b_k \end{aligned}$$

The θ_k is some real constant choosen in such a way, that (8) becomes diagonal. The a_k and b_k are the fourier transformations of a_i and b_i with k in the Brillouin zone of the sublattices A or B [1]. The hamiltonian (8) becomes:

$$H_{LSW} = E_0 + \sum_k \omega(k)(\alpha_k^+ \alpha_k + \beta_k^+ \beta_k) \tag{9}$$

Then with $E_0 < 0$ and $\omega(k) > 0$ the ground state $|0\rangle$ is define by

$$\alpha_k |0\rangle = 0, \quad \beta_k |0\rangle = 0$$

and exitation are given by

$$\alpha_k^+ |0\rangle, \quad \beta_k^+ |0\rangle,$$

the so-called spin waves or magnons.
To measure the validity of the approximation in (8) one can look if $\frac{\langle 0|\hat{n}_i|0\rangle}{2S} \ll 1$ really holds. For $S = \frac{1}{2}$ in the limit $N \to \infty$ one finds:

$$\frac{1}{N} \sum_i \frac{\langle 0| \hat{n}_i |0\rangle}{2S} = \begin{cases} \leq 0,2 & d = 2,3 \\ \infty & d = 1 \end{cases}$$

So in dimension $d = 2, 3$ one can assume that the approximation holds, but in one dimension it is clearly wrong. This is due to the fact that only in dimensions $d \geq 2$ the model has an ordered ground state, which is necassary for $\hat{n}_i$ to be small.

In conclusion we rewrote our system of interactiong spin into a system of non interaction bosons. The eigenvalues and eigenstates in the spin wave approximation are easily computable. But one has to check in the end, if it is really a valid approximation.

References

[1] E. Manousakis, The spin- heisenberg antiferromagnet on a square lattice and its application to the cuprous oxides, Rev. Mod. Phys. 63 (1991) 1–62. doi:10.1103/RevModPhys.63.1.
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[2] W. Nolting, Viel-Teilchen-Theorie, 8th Edition, Springer Spektrum, Berlin, 2015.