On the Functional Integral Theory of Systems with Kinematical Interaction

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We propose a systematic way to investigate the low-temperature thermodynamic properties of quantum spin systems subject to the restriction that only a finite number of bosons may occupy a single lattice site. Such a kinematical interaction results in appearance of a temperature dependent chemical potential. Its low-temperature asymptotics is calculated self-consistently using the functional integration technique.

To systematically calculate the thermodynamic properties of a two-dimensional (2D) quantum ferromagnet at low temperatures remains an unsolved problem of the spin wave theory \cite{1}. The main difficulty is in how to consistently calculate both dynamical and kinematical interactions of magnons. Such interactions are believed to vanish the average spin (magnetization) of a system, as it naturally follows from the absence of long range order in 2D systems at low temperatures.

Recently, a few different approaches to this problem have been developed. In his “modified spin wave theory”, Takahashi \cite{4} uses the Holstein-Primakoff representation to introduce \( \text{(by hands)} \) a chemical potential for a system of bosons. This chemical potential is essentially nonzero in 2D systems, even in the absence of magnetic field. Thus, the zero magnetization condition, \( \langle S_z \rangle = 0 \), is enforced. Despite good agreement with numerical calculations, such an approach seems to be not ultimately self-consistent. In another approach by Arovas and Auerbach \cite{5}, a functional integral for a partition function is constructed using the generalized bosonic SU(\( N \) \( \rightarrow \) \( 2 \)) representation of spin algebra. Being calculated self-consistently using the functional integration technique, its low-temperature asymptotics is calculated subject to the restriction that only a finite number of particles per site is, in fact, closely related to the para-statistics theory \cite{6} with essentially similar “exclusion” principles.

We demonstrate the method on a simple model with the Hamiltonian:

\[
H = \sum_k \omega_k b_k^+ b_k , \quad \omega_k = \frac{JK^2 a^2}{2} , \quad [b_k, b_k^+ \rangle = \delta_{kq} \quad (1)
\]

on a square lattice, where \( a \) is a lattice constant, \( \beta = 1/t \) is the inverse temperature, and \( b \) and \( b^+ \) are the Bose operators.

As mentioned above, we consider the system of bosons with kinematical interaction. In other words, each lattice site can be occupied by no more than \( L \) bosons. Thus, we need a projecting operator to eliminate all unphysical states with \( n \geq L + 1 \) (see Fig. \( 1 \)), while all physical states \( 0 \leq n \leq L \) are to remain unchanged. Heuristically, we define the projecting operator \( P = \prod_i P_i \) as follows:

\[
P_i = : e^{-b_i^+ b_i} \sum_{n=0}^{L} \frac{(b_i^+ b_i)^n}{n!} : , \quad (2)
\]

where \( O \) is normally ordered form of an operator \( O \). Here we used a useful identity:

\[
e^{ab^+ b} = : e^{(a-1)b^+ b} : \quad (3)
\]

which can be proved straightforwardly.

Now the partition function of the system is:

\[
Z = Sp\{Pe^{-\beta H}\} . \quad (4)
\]
To obtain the functional representation for the partition function \(Z\), it is instructive to transform to the coherent basis \(|\rangle\) :

\[
|u\rangle = e^{-\frac{\beta H}{2}} \sum_{n=0}^{\infty} \frac{u^n}{\sqrt{n!}} |n\rangle ,
\]

with the properties:

\[
\begin{align*}
\int |u\rangle \langle u| \frac{dx^* du}{\pi} &= \sum_{n=0}^{\infty} \langle n| |n\rangle = \hat{1} , \\
b|u\rangle &= u|u\rangle , \\
\langle u|b^+ &= \langle u|u^* , \\
\langle v|u\rangle &= e^{-\frac{1}{2} (u^* u + v^* v) + \beta H} .
\end{align*}
\]

Using identity \(\langle 0|\rho|0\rangle\), we rewrite the partition function as follows:

\[
Z = \int \langle v|P|u\rangle \langle u|e^{-\beta H}|v\rangle DuDv. 
\]

Since all the operators are in normal ordered form, we use Eqs. (6b) to obtain the following matrix elements:

\[
\begin{align*}
\langle v_i|P_i|u_i\rangle &= e^{-\frac{1}{2} (v_i^* u_i + v_i^* v_i)} \sum_{n=0}^{L} \frac{(v_i^* u_i)^n}{n!} , \quad (8a) \\
\langle u|e^{-\beta H}|v\rangle &= e^{-\sum_k \langle \frac{1}{2} (v_k^* u_k + v_k^* v_k) - e^{-\beta \omega k} u_k v_k \rangle} , \quad (8b)
\end{align*}
\]

Thus, the exact partition function becomes:

\[
Z = \int e^{-S(u,v)} DuDv , 
\]

where the “action” \(S(u,v)\) is

\[
S(u,v) = \sum_k (u_k^* u_k + v_k^* v_k - e^{-\beta \omega_k} u_k v_k)
- \sum_i \ln \left( \sum_{n=0}^{L} \frac{(v_i^* u_i)^n}{n!} \right)
\]

In the mean field approximation, we expand the logarithm up to the first nonlinear term:

\[
\ln \sum_{n=0}^{L} \frac{x^n}{n!} = \ln (e^x - \sum_{n=L+1}^{\infty} \frac{x^n}{n!})
= x + \ln \left( 1 - e^{-x} \sum_{n=L+1}^{\infty} \frac{x^n}{n!} \right)
\approx x - \frac{x^{L+1}}{(L + 1)!}.
\]

It can be shown that the higher order terms omitted in Eq. (11) give only small corrections to the expressions obtained at low temperatures, because of the small parameter \(|\log T|^{-1} \ll 1\). Now the action \(S(u,v)\) reads as

\[
S(u,v) \approx S_0(u,v) + S_{int}(u,v) ,
\]

where

\[
\begin{align*}
S_0(u,v) &= \sum_k (u_k^* u_k + v_k^* v_k - e^{-\beta \omega_k} u_k v_k) , \quad (13a) \\
S_{int}(u,v) &= \sum_i \frac{(v_i^* u_i)^{L+1}}{(L + 1)!} . \quad (13b)
\end{align*}
\]

The term \(S_{int}(u,v)\) is of fundamental importance. Indeed, omitting it from Eq. (12) yields the partition function:

\[
Z_0 = \int e^{-S_0(u,v)} DuDv ,
\]

which suffers from infrared divergences in the thermodynamic average for the one- and two-dimensional cases:

\[
\langle v_i^* u_i \rangle_0 = \frac{1}{N} \sum_k \frac{1}{e^{\beta \omega_k} - 1} = \infty .
\]

Thus, it is equivalent to the omission of the projection operator from Eq. (13).

We now linearize the “action” Eq. (12) as follows:

\[
S_{int}(u,v) \rightarrow \sum_i \left( (L + 1) \Delta^L e_i^* u_i - L \Delta^{L+1} \right)
\]

and introduce the mean field partition function

\[
Z_{mf}(\Delta) = \int e^{-S_{mf}(u,v,\Delta)} DuDv ,
\]

with

\[
S_{mf}(u,v,\Delta) = \sum_k (u_k^* u_k + v_k^* v_k - e^{-\beta \omega_k} u_k v_k)
- \sum_i \frac{(v_i^* u_i)^{L+1}}{(L + 1)!} .
\]

Here we defined the thermodynamic average:

\[
\Delta = \langle v_i^* u_i \rangle_{mf} ,
\]

Thus, in the mean field approximation, we have the quadratic mean field “action” \(S_{mf}(u,v,\Delta)\) instead of nonlinear the “action” \(S(u,v)\). The parameter \(\Delta\) will be self-consistently obtained below, in accordance with Eq. (15). The simplicity of the mean field “action” \(\langle v_i^* u_i \rangle_{mf}\) allows us to perform functional integration in the partition function to yield:

\[
Z_{mf}(\Delta) = \prod_k \frac{e^L e^{\Delta^{L+1}}}{1 - e^{-\beta \omega_k} (1 - (L + 1) \Delta L)} = e^{-\beta F_{mf}(\Delta)} .
\]

Here

\[
F_{mf}(\Delta) = \frac{1}{\beta} \sum_k \left( - L \Delta^{L+1} \right.
+ \ln \left( 1 - e^{-\beta \omega_k} (1 - (L + 1) \Delta L) \right) .
\]
The temperature dependence of $\Delta_0$ for two cases: $L = 1$ and $L \gg 1$.

From the condition:

$$\frac{\partial F_{m.f}(\Delta)}{\partial \Delta} \bigg|_{\Delta_0} = 0 ,$$

we obtain the self-consistent equation for $\Delta_0$:

$$\Delta_0 = \frac{1}{N} \sum_k e^{\beta \omega_k} - (1 - (L + 1)\Delta_0^L) .$$

In the two-dimensional case at low temperature (and for $\Delta_0 \ll 1$), it reduces to

$$\Delta_0 = \frac{T}{2\pi J} \ln \left( \frac{(L + 1)\Delta_0^L}{1 - (L + 1)\Delta_0^L} \right) \simeq \frac{T}{2\pi J} \ln \left( (L + 1)\Delta_0^L \right) .$$

The temperature dependence for $\Delta_0$ is presented in Fig. 2 for two limiting cases: $L = 1$ and $L \gg 1$ (here $L = 500$). The thermodynamic average $\Delta_0$ vanishes at $T = 0$ and rapidly grows as temperature increases. When $T_\ast = T/2\pi J \ll 1$,

$$\Delta_0 \simeq -T_\ast L \ln (T_\ast) .$$

Now, it is obvious that we can exclude the projecting operator from Eq. (4), but simultaneously we must introduce the chemical potential

$$\mu = T(L + 1)\Delta_0^L = Te^{-2\pi J\Delta_0/T}$$

in Eq. (4). This is precisely the Takahashi’s assumption that results in very good agreement with the Bethe-ansatz for an one-dimensional ferromagnet at low temperature. Note, $\mu$ decreases with $L$ and vanishes in the absence of the kinematical interaction, $L = \infty$ (i.e., non-interacting bosons). From Eqs. (23), (24), we obtain the low-temperature asymptotics:

$$\mu \simeq 2\pi J T_\ast^{L+1} .$$

To conclude, we have shown that a kinematical interaction in 2D magnon systems can be compensated via introducing a “fictitious” chemical potential into their effective dispersion law, and proposed a systematic, self-consistent procedure of calculating its low-temperature dependence in the one-loop approximation.

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