BOSE-EINSTEIN CONDENSATION OF MAGNONS

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We use the Renormalization Group method to study the Bose-Einstein condensation of the interacting dilute magnons which appears in three dimensional spin systems in magnetic field. The obtained temperature dependence of the critical field \( H_c(T) - H_c(0) \sim T^2 \) is different from the recent self-consistent Hartree-Fock-Popov calculations (cond-matt 0405422) in which a \( T^{3/2} \) dependence was reported. The origin of this difference is discussed in the framework of quantum critical phenomena.

1. INTRODUCTION

Bose-Einstein condensation (BEC) remains one of the most exotic predictions of the quantum mechanics. In the last half-decade a continue interest have been shown with respect to this phenomena because of its experimental evidence in ultra-cooled diluted atomic gases. It is also known that a quantum spin system can be mapped onto an interacting Bose gas. The analogy between a quantum spin system which presents long-range order, and an interacting Bose gas, which presents BEC, is well known for a long time [1]. Recently, these systems became of great interest because the experimental data on the ladder systems showed the possibility of a quantum phase transition (QPT) driven by the magnetic field [2].

A quantum spin liquid is characterized by a finite magnetic correlation length, which is inversely proportional to the energy gap, \( \Delta \), between the singlet ground state and the lowest triplet excitation. The effect of a magnetic field on a gapped system is especially interesting for a small gap. Application of an external magnetic field cause a linear reduction of \( \Delta \) by the Zeeman effect. The ground state become gapless and the system can undergo 3D magnetic ordering.

The existence of the magnetic order in the spin-gap magnetic compounds was predicted by a standard mean-field theory for spins [3]. However, several characteristic features cannot be explained by this theory. For example, the cusplike minimum of the magnetization as a function of the temperature at the transition, and the power-law like dependence of the critical field

\[
H_c(T) - H_c(0) \sim T^\Phi
\]  

(1)
in the low temperature regime. A monotonic decrease of the magnetization and an exponentially approach of the critical field $H_c(T)$ to its zero-temperature limit $H_c(0)$ are rather predicted by the mean-field theory.

These features were better interpreted, at least qualitatively, as a Bose-Einstein condensation (BEC) of the spin triplet excitations (magnons) [4]. As the temperature is lowered a decrease of the number of the non-condensed magnons together with an increase of the condensed magnons below the transition give rise to the cusp-like minimum of the magnetization. The self-consistent Hartree-Fock-Popov (HFP) theory predicted a power-low dependence with the exponent $\Phi = 3/2$ [5].

In the case of quantum spin liquid systems it is possible to tune the density of magnons by magnetic field [5, 6] or pressure [7]. As the magnetic field can be easily controlled – which correspond to the chemical potential of the magnons - these systems provide new possibilities for the study of BEC in grand-canonical ensemble with a tunable chemical potential.

The $\text{XCuCl}_3$ compounds, with X = Tl, K, and MH[4] realize especially interesting systems. Magnetization plateaus are observed in $\text{NH}_4\text{CuCl}_3$, while $\text{KCuCl}_3$ and $\text{TlCuCl}_3$ show magnetic-field induced critical phenomena. The quantum magnetism is based on $S = 1/2$ spins of Cu$^{2+}$ ions, arranged as planar dimmers of Cu$_2\text{Cl}_6$.

The compound which offered the possibility of performing many measurements is $\text{TiCuCl}_3$ which is composed of a chemical double chain Cu$_2\text{Cl}_6$. The magnetic susceptibility, measured as function of temperature $T$ for three different directions of the magnetic field, exhibit a broad maxima at $T = 38$ K, decreasing to zero with the temperature decreasing [5]. This result indicates that the compound has an excitation gap $\Delta \approx 7$ K above the singlet ground state. This gap may by attributed to the anti-ferromagnetic dimer coupling in the double chain [6]. In a magnetic field $H$ the gap for $S_z = -1$ excitations is reduced as $\Delta - g\mu_B H$. Reaching a field of $H_c = \Delta/(g\mu_B)$ the gap collapse.

The magnon dispersion has been investigated theoretically [8] and experimentally by inelastic neutron scattering [9]. The experiments showed that the magnon modes are split into three by magnetic field with the splitting proportional to the field, and the lower modes becomes soft at the critical field $H_c$.

An important result has been obtained by Sherman et al. [10] by sound attenuation in TiCuCl$_3$ in magnetic field at low temperatures. The occurrence of the sharp peak in the sound attenuation near the BEC critical temperature and the Drude form of the sound dumping suggested a constant weak magnon-magnon coupling. The sound attenuation suggested a magnons dispersion like $\omega^2 = \Delta^2 + \frac{J^2 k^2}{4}$ (here $J$ is the exchange interaction) for small wave vector “k”,
approximation valid if $T_c$ and $\Delta$ are of the order of $T_c \sim 7$ K and $\Delta \sim 7$ K as for the case of TlCuCl$_3$.

The form of the magnon dispersion (called “relativistic”) changes the dynamics of the system and we expect $\Phi = 2$. This conjecture is one of the most important result of Ref. [10] and we will use it for the model of the magnon condensation.

The existence of an induced magnetic field-spin transition has been proposed by Giamarchi and Tsvelik [11] considering as a possible mechanism the BEC of the soft mode. The Hartree-Fock approximation using the Hamiltonian from the theory of BEC in dilute bosonic gases with effective chemical potential $\mu = \mu_B g(H - H_c)$ has been applied [4] to calculate the temperature dependence of magnetization. Near the critical temperature $T_c$ this approximation breaks down and the magnetization is expected to behave like $M \sim (T - T_c)^{\beta}$ where $\beta = \frac{3}{2}$. The temperature dependence of the critical field has the form $[H_c(T) - H_c(0)] \sim T^{\Phi}$ where $\Phi = \frac{3}{2}$ but the best fit [6, 4, 12] is obtained for $\Phi = 2.2$.

We can conclude that the system analyzed here has some important characteristics. First, we mention the small three-dimensional (3D) character of the system which leads to a small gap. Another important feature is the decreasing of the number of thermal excitations with the increasing of the magnetic field, and as a consequence the driving of the condensate to $T = 0$ behavior.

The outline of this paper is as follows. In Sect. II we present the model based on the already presented experimental data. The Sect. III is devoted to the Renormalization Group (RNG) formulation and to present the low temperature quantum critical properties of the system. Sec. IV contain the main results of the paper, the relevant thermodynamic quantities next to the quantum critical point. Finally, in the last section we will discuss the results and compare with other theoretical approaches and experimental evidence.

2. MICROSCOPIC MODEL

For the theoretical description of the physical properties of TlCuCl$_3$ system close to the quantum critical point we will use the general formalism of the RNG applied for bosonic systems [13, 14, 15, 16, 17, 18] and recently reconsidered for the spin systems [19].

The general form of the action, generated by a Hubbard-Stratonivich transformation used to describe the magnon condensation in magnetic field can be written as:
\[ S_{\text{eff}} = S_{\text{eff}}^{(2)} + S_{\text{eff}}^{(4)} \]  

where:

\[ S_{\text{eff}}^{(2)} = \frac{1}{2} \sum_k \chi^{-1}(k) |\phi(k)|^2 \]  

\[ S_{\text{eff}}^{(4)} = \frac{u_0}{16} \sum_{k_1} \ldots \sum_{k_4} \phi(k_1) \ldots \phi(k_4) \delta(k_1 + \ldots + k_4) \]  

Here \( \phi(k) \) is a bosonic field associated to the order parameter fluctuations and we introduced the notations \( k = (k, \omega_n) \), \( \omega_n \) being the bosonic Matsubara frequency and

\[ \sum_k = T \sum_n \frac{d^d k}{(2\pi)^d} \]  

Higher order terms in the action given by Eq. (3) are neglected.

In Eq. (3) \( \chi(k) \) is the magnon propagator and \( u_0 \) the bare coupling constant. Using [10] we write the magnon propagator as

\[ \chi(k, \omega_n) = \frac{1}{\omega_n^2 + k^2 + r_0} \]  

where \( r_0 = \Delta - \mu_B g H \) is the effective chemical potential associated to the magnons and \( H \) is the external magnetic field.

### 3. Renormalization Group Equations

We follow the standard Wilson RNG scaling procedure for this action in the \((k, \omega_n)\) Fourier space. Reducing the degrees of freedom and re-scaling the wave vectors \( k = k'/b \), the Matsubara frequencies \( \omega_n = \omega_n'/b^z \), and the fluctuation fields \( \phi(k) \), for the 3-dimensional case to one loop approximation we obtain the following renormalization group equations at finite temperature \( T \):

\[ \frac{dT(l)}{dl} = T(l) \]  

\[ \frac{du(l)}{dl} = - \frac{(n+8)K_3}{8} u^2(l) F_1[r(l), T(l)] \]  

\[ \frac{dr(l)}{dl} = 2r(l) + \frac{(n+2)K_3}{8} u(l) F_2[r(l), T(l)] \]  

where \( n \) is the number of components of the fluctuation field \( \phi(k) \), \( K_3 = \frac{1}{2\pi^2} \).
and we use the dynamical critical exponent $z = 1$ for this quantum model. The functions $F_{1,2}$ are characteristic functions for the model [16].

In order to extract all the possible information about criticality and thermodynamic properties of the model here considered, we have to solve the system of eqs. (6), (7) and (8) using a set of initial conditions $u(l = 0) = u_0$, $r(l = 0) = r_0$, and $T(0) = T_0 \equiv T$. One expects both $r_0$ and $u_0$ to depend on temperature, but this dependence is usually negligible in comparison to that near criticality, so we will not use it explicitly in this paper.

It is a difficult task to solve the RNG equations with such initial conditions. In the original pioneering treatment [22] a so called “quantum” regime at $T = 0$ and a “classical” one as $T \to \infty$ were considered in order to iterate the RNG transformation. The critical behavior in the classical regime is governed by the finite-temperature fixed point which are usually expressed in terms of a new coupling parameter $v = u \cdot T$. In this situation the quantum degrees of freedom are suppressed and any quantum system behaves as a classical one in terms of distance from the critical point $r_0 - r_c$. Quantum effects becomes relevant when we approach $T \to 0$.

In the case of a $T = 0$ fixed point $(r^*, u^*)$ the related eigenvalues up to the first order in $\epsilon = 4 - (d + z)$ can be expressed:

$$\lambda_r = 2 - \frac{n + 2}{16} K_3 u^*$$

$$\lambda_u = \epsilon - \frac{n + 8}{8} K_3 u^*$$

(9)

with $r^* = u^* = 0$ for the Gaussian fixed point and

$$r^* = -\frac{n + 2}{n + 8} \epsilon / \epsilon, \quad u^* = \frac{16}{(n + 8)K_3} \epsilon$$

for the non-Gaussian one.

The same technique, developed in [16], allows us to solve the RNG equations in certain conditions. Note that the temperature $T$ as well as the parameter $r$, is a relevant scalar field $(T(l) = T\epsilon^l)$. Although, a small but finite value of $T$ measure a deviation from the critical surface, the parameter $T$ cannot be treated as $r$ since functions $F_{1,2}(r, T)$ cannot be expanded in power series of $T$. Because of this we need to solve the RNG equations in the low-temperature regime.

We can approximate $F_2[r(l), T(l)] = \frac{1}{4}$ within this limit, and consequently the equation for $u$ can be linearized. The solution of Eq. (7) has the simple form:

$$u(l) = \frac{1}{C_0(l + l_0)}$$

(10)
with $C_0 = \frac{(n + 8)K_3}{16}$. Following the same approximation we can write down a low-temperature solution for $r(l)$, namely

$$r(l) = n_0 e^{\Lambda_r(l)} h(l)$$

(11)

with

$$\Lambda_r(l) = 2l - \frac{n + 2}{4} K_3 \int_0^l dx u(x) F^{(0)}_2(x)$$

$$h(l) = 1 + \frac{1}{n_0} \frac{n + 2}{4} K_3 \int_0^l dx e^{-\Lambda_r(x)} u(x) F^{(0)}_1(x)$$

(12)

and $F^{(0)}_{1,2}(x) \equiv F^{(0)}_{1,2}(0, T(x))$.

In order to describe the physics near the QCP we define a linear scaling field $t_r(l)$:

$$t_r(l) = r(l) + bu(l) = n_0 e^{\Lambda_r}$$

(13)

with $b = \frac{n + 2}{16} K_3$. We can in this way determine the critical line by imposing that the scalar field is zero $t_r(l) = 0$. The expression of $t_r(l)$ has been calculated in Ref. [16] for the three dimensional case as:

$$t_r(l) = e^{\Lambda_r(l)} \left\{ t_r(0) + \frac{n + 2}{4} K_d \int_0^l dx \frac{e^{-2s u(x)}}{e^{1/T(x)} - 1} \right\}$$

(14)

where for the case $d = 3$, $\Lambda_r(l)$ reduces to:

$$\Lambda_r(l) = 2l - \frac{n + 2}{n + 8} \ln \left( \frac{l_0}{l_0 + 1} \right)$$

(15)

Using these results we will calculate the thermodynamic quantities near the critical point. The basic idea of the method is to stop the renormalization procedure close enough to this point that the system can see the influence of the quantum effects. This matching condition is in fact equivalent to stop the renormalization when a scale $l = l^*$, where $l^*$ is reached at which $t_r(l^*) = 1$.

In the approximation $l^* \gg 1$ and $T(l^*) \ll 1$ we obtain from Eq. (15) to the order of interest, the relation:

$$\exp(l^*) = [t_r(T)]^{\frac{-1}{l_0}}$$

(16)

where for the three-dimensional case and $\epsilon = 0$ we can approximate the eigenvalue of the relevant parameter $r$ as $\lambda_r = 2$ and $t_r(T)$ is given by the relation [16]:

"


\[ t_n(T) = r_0 - r_{0c} + \frac{n + 2}{128} u_0 T^2 \]  

(17)

By following an iterative method (see for example [17]) we can compute now the critical value of the scale \( T^* \) as:

\[ T^* = \frac{1}{2} \ln \frac{1}{T} \]  

(18)

4. THERMODYNAMIC QUANTITIES

Using these results we shall calculate the relevant thermodynamic quantities near the quantum critical point, but in the disordered state. The temperature dependence of the number of magnons is defined as:

\[ n(T) = \exp(-3 n^*) \int \frac{d^3 k}{(2\pi)^3} J_0[T(P^*)] \]  

(19)

This equation gives for \( n(T) \) a temperature dependence of the form:

\[ n(T) \propto T^{\frac{1}{2}} \]  

(20)

This result is in agreement with the behavior of magnetization at very low temperatures.

First, we define the critical line by \( t_n(T) = 0 \) and we obtain:

\[ H_c(T) - H_c(0) = C_0 T^2 \]  

(21)

where \( C_0 \propto u_0 \) is a constant. From Eq. (17) we calculate the critical line in the \((r_0, T)\) plane using the condition \( t_n(T) = 0 \). This gives:

\[ r_{0c}(T) = r_{0c} - \frac{(n + 2)}{128} u_0 T^2 \]  

(22)

and for \( r_0 \leq r_{0c} \) we get the general equation

\[ T_c(r_0) = \left[ \frac{128}{(n + 2) u_0} \right]^{1/2} (r_{0c} - r_0)^{1/2} \]  

(23)

Using now the definition (see Ref. [16]) of \( r_{0c} \)

\[ r_{0c} = -\frac{(n + 2)}{32\pi^2} u_0 \]  

(24)

we obtain

\[ T_c(H) \sim |H - \tilde{H}_c|^{\frac{1}{2\alpha}} \]  

(25)
with $\alpha = 2$ and

$$\tilde{H}_c = H_c + \frac{(n + 2)}{32\pi^2} u_0.$$  

Equations (20), (21) and (25) are the main results of this paper.

The specific heat can be also calculated for the important case $r_0 \neq r_0c$ but $T \rightarrow T_c^+ (r_0)$ using the singular part of the free energy reported in [16] as:

$$F_c (T) \sim \left[ T - T_c (H) \right]^2 \left[ \ln (T - T_c (H)) \right]^{\frac{2 + \xi}{2 + \gamma}}$$  

and it gives us a logarithmic behavior:

$$\frac{C_c (T)}{T} \sim \left[ \ln (T - T_c (H)) \right]^{\frac{-2 + \xi}{2 + \gamma}}$$  

We will discuss these results in connection with the existent theoretical approaches and the experimental data for TlCuCl$_3$.

### 5. DISCUSSIONS

The occurrence of BEC induced by the magnetic field in a spin-gap system has been predicted by Giamarki and Tsvelik [11] in order to explain the three-dimensional ordering in coupled ladders. Nikuni et al. [4] applied Popov theory (see for example [20]) for the BEC obtaining a temperature dependence for magnetization in agreement with the experimental data, of the form $T^{3/2}$.

However, as it was mentioned in Ref. [4] the critical exponent $\Phi$ of the critical field $[H_c (T) - H_c (0)] - T^\Phi$ was obtained as $\Phi = 3/2$, but the experimental data shows $\Phi = 2.2$.

Recently Misguich and Oshikawa [21] reconsidered the self-consistent Hartree-Fock-Popov (HPF) method using a realistic dispersion for magnons [8] and they reobtained $\Phi = 3/2$. They also calculated the specific heat and obtained a $\lambda$-shape.

We would like to mention several basic points related to this problem. In the HPF theory the effect of fluctuations have been neglected and consequently the thermodynamic quantities on the critical line have wrong critical exponents. Although, the changing of the dispersion law for the magnon can improve the HPF results, it still does not affect the basic approach. We can also notice that in both papers [4] and [20] a QPT driven by the temperature was considered, and in fact it is induced by the magnetic field. These observations justify the application of the RNG method in the version proposed by Caramico D’Auria et al. [16] to study the magnon condensation.
Our main result can be summarized as follows. We obtained the critical exponent $\Phi = 2$, which is in a better agreement with existent experimental data ($\Phi = 2.2$). The magnetization calculated in our approach is $T^{5/2}$ dependent. The critical temperature $T_c(H)$ has a dependence given by Eq. (25) with $\alpha = 2$ in agreement with [6].

The specific heat calculated by RNG method has a logarithmic correction as was expected. The $T$ dependence of $C_\nu$ is not relevant if we consider a magnetic field driven QPT, then we consider it by respect to the dependence of $H(T)$. Such an experiment has been done [6] and we can notice a small anomaly in this dependence. But a final decision about the $H(T)$ dependence of our Eq.(25) cannot be taken.

The agreement between the experimental data and the theory presented in [21] appears in our opinion due to the fact that the authors considered, on a very narrow interval, a linear dependence between the critical field $H_c(T)$ and the critical density $n_c$. This approximation can be valid for $n_c < 0.002$ which describes a part of the real temperature dependence of $H_c(T)$.

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REFERENCES