

Critical behavior of Tan's contact for bosonic systems with a fixed chemical potential

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Abstract

The temperature dependence of Tan's contact parameter C and its derivatives for spin gapped quantum magnets are investigated. We use the paradigm of Bose–Einstein condensation (BEC) to describe the low temperature properties of quasiparticles in the system known as triplons. Since the number of particles and the condensate fraction are not fixed we use the μVT ensemble to calculate the thermodynamic quantities. The interactions are treated at the Hartree–Fock–Bogoliubov approximation level. We obtained the temperature dependence of C and its derivative with respect to temperature and applied magnetic field both above and below T_c of the phase transition from the normal phase to BEC. We have shown that C is regular, while its derivatives are discontinuous at T_c in accordance with Ehrenfest's classification of phase transitions. Moreover, we have found a sign change in $\partial C/\partial T$ close to the critical temperature. As to the quantum critical point, C and its derivatives are regular as a function of the control parameter r , which induces the quantum phase transition. At very low temperatures, one may evaluate C simply from the expression $C = m^2 \mu^2 / \tilde{a}^4$, where the only parameter effective mass of quasiparticles should be estimated. We propose a method for measuring of Tan's contact for spin gapped dimerized magnets.

Keywords: Tan's contact, spin gapped quantum magnets, triplons

(Some figures may appear in colour only in the online journal)

1. Introduction

Some years ago, Tan derived a set of exact relations that link the short distance large-momentum correlations to the bulk thermodynamic properties of a fermionic system with short-range inter-particle interactions [1–3]. They are connected by a single coefficient C , referred to as the integrated contact intensity or 'contact'. Further, Tan's ideas were developed [4, 5] and extended to Bose systems also [6–9]. It has been established that Tan's contact measures the density of pairs at short distances and determines the exact large-momentum or high frequency behavior of various physical observables. It serves

as an important quantity to characterize strongly interacting many-body systems [10].

Experimentally, Tan's relations have been confirmed both for fermions (especially for quasi-1D systems) [11–13] and Bose gases [14–18].

Although, there are several theoretical studies of contact of low dimensional Fermi systems even at finite temperatures [4, 19–24], the temperature dependence of bosonic contact in three dimensions is mostly unknown.

Studying the temperature dependence of contact parameter gives an opportunity to know its critical behavior near phase transitions. For example, Chen *et al* [25] have shown that contact and its derivatives are uniquely determined by the universality class of the phase transition for fermions in the critical

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region. In a system of bosons, critical behavior of thermodynamic quantities have some specifics due to Bose–Einstein condensation (BEC) at low temperatures. For instance, the specific heat is discontinuous at the critical temperature T_c , and the Grüneisen parameter changes its sign [26, 27].

The main goal of the present work is to study the temperature dependence of Tan’s contact for bosons, as well as its derivatives, to draw conclusions about their critical behavior near T_c and close to the quantum critical point (QCP) of the quantum phase transition (QPT).

It is well known that physical systems at equilibrium are studied in statistical mechanics through statistical ensembles. For example, a system that the canonical ensemble exchanges only energy with the surroundings is called NVT , where N is the number of atoms of a gas in the volume V at temperature T . On the other hand, a grand canonical ensemble also makes it possible for particles to exchange, with the parameter μ , which may be interpreted as the chemical potential, and is called μVT . In the former case, N or $\rho = N/V$ is fixed and the chemical potential is determined by the equation of state, while in the latter case μ is fixed as an input parameter which defines number of particles through a thermodynamic equation [28]. Tan’s relations including the contact have been thoroughly studied for NVT ensembles, however, the investigations of contact for a μVT ensemble is still missing. In this work, we choose a system of bosonic quasiparticles introduced in bond operator formalism [29, 30] to describe the singlet–triplet excitations in spin gapped magnetic materials [31]. It is well established that low temperature properties of such a class of quantum magnets could be described within the paradigm of BEC of these quasiparticles called triplons. Therefore, one may conclude that, at low temperature, thermodynamic properties of such materials are mainly determined (but not only) by the condensation (and depletion) of triplons [27, 31–33]. Triplon concept has found application in other spin-gapped models as well [34].

There is one more reason of our choice of spin gapped quantum magnets to study Tan’s contact. In such systems, the number of particles N and the condensate fraction N_0/N can be directly evaluated by measuring the uniform magnetization M and staggered magnetization M_\perp respectively, as $N = M/g\mu_B$, $N_0^2 = 2M_\perp^2/(g\mu_B)^2$ [35], where g is the electron Landé factor and μ_B is the Bohr magneton. Evidently, the final analytic expression for C will include M and M_\perp , making the contact parameter to be easily measured.

In practice, Tan’s contact for bosons with zero range interaction may be evaluated by any of following Tan’s relations [10]. For example,

- (a) By the asymptotic behavior of momentum distribution n_k ,

$$C = \lim_{k \rightarrow \infty} k^4 n_k. \quad (1.1)$$

- (b) By Tan’s sweep theorem as

$$C = \frac{8\pi m a^2}{V} \begin{cases} \left(\frac{\partial F}{\partial a} \right)_{N,T} & \text{for } NVT \text{ ensembles,} \\ \left(\frac{\partial \Omega}{\partial a} \right)_{\mu,T} & \text{for } \mu VT \text{ ensembles,} \end{cases} \quad (1.2)$$

where F and Ω are the free energy and the grand canonical potential, respectively [36]; a is the scattering length and m is the effective mass of the particle.

- (c) By using Hellman–Feynman theorem [4]

$$C = \frac{16\pi^2 a^2}{V} \int d\vec{r} \langle \psi^\dagger(\vec{r}) \psi^\dagger(\vec{r}) \psi(\vec{r}) \psi(\vec{r}) \rangle. \quad (1.3)$$

In our previous paper [37], it has been shown that if one uses mean field theory (MFT), evaluation of C from equation (1.2) will be the most convenient and reliable. Consequently, we study C of a triplon gas at finite temperature in the framework of MFT, namely in the Hartree–Fock–Bogoliubov (HFB) approximation [38]. We stress here that below we shall discuss C only for homogeneous systems. For inhomogeneous systems, especially at very low temperatures, one may also use the Gross–Pitaevskii equation to study the dynamics of the condensate [39, 40] as well as that of the Tan’s contact.

For convenience, we adopt units such that $\hbar = 1$, $k_B = 1$ and $V = 1$ in the following text. In these units C is dimensionless. In natural units C may be obtained further by dividing it by \bar{a}^4 , getting it in $(\text{length})^{-4}$ where \bar{a} is the average lattice parameter, $\bar{a} = V^{1/3}$, and V is the unit cell volume of the crystal.

This article is organized as follows. In section 2, we outline main equations for a triplon gas at finite temperature in the HFB approximation, which will be used to evaluate the Tan’s contact and its derivatives in section 3. Our discussions and conclusions will be presented in section 4.

2. Triplon density in the HFB approximation

We start with the effective Hamiltonian of triplons as a non-ideal Bose gas with contact repulsive interaction

$$\hat{H} = \int d\vec{r} \left[\psi^\dagger(\vec{r}) (\hat{K} - \mu) \psi(\vec{r}) + \frac{U}{2} (\psi^\dagger(\vec{r}) \psi(\vec{r}))^2 \right], \quad (2.1)$$

where $\psi(\vec{r})$ is the bosonic field operator, $U = 4\pi a/m$ is the interaction strength, and \hat{K} is the kinetic energy operator which defines the bare triplon dispersion $\varepsilon_{\vec{k}}$ in momentum space. Since the triplon BEC occurs in solids, the integration is performed over the unit cell of the crystal with the corresponding momenta defined in the first Brillouin zone [41]. The parameter μ characterizes an additional direct contribution to the triplon energy due to the external field

$$\mu = g\mu_B H - \Delta \quad (2.2)$$

and it can be interpreted as the chemical potential of the $S_z = -1$ triplons [42]. In equation (2.2), $\Delta = g\mu_B H_c$, is the spin gap separating the ground-state from the lowest energy triplet excitation and H_c is the critical external magnetic field [43]. The effective Hamiltonian \hat{H} has the following free parameters characterizing a given material: g , H_c , U and possibly, an effective triplon mass m for the case of a simple bare dispersion given as $\varepsilon_{\vec{k}} = \vec{k}^2/2m$.³

³ In general, a realistic $\varepsilon_{\vec{k}}$ includes several other parameters [44].

In general the Hamiltonian in equation (2.1) is invariant under global $U(1)$ gauge transformation $\psi(\vec{r}) \rightarrow e^{i\alpha}\psi(\vec{r})$ with a real number α . However, this symmetry is broken in the condensate phase, where $T < T_c$, and it is restored in the normal phase, $T \geq T_c$.

This transition temperature T_c , which corresponds to the vanishing of the condensate density $\rho_0(T_c) = 0$ may be calculated from the following equation

$$\sum_k \frac{1}{e^{\varepsilon_k/T_c} - 1} = \frac{\mu}{2U} \equiv \rho_c. \quad (2.3)$$

Note that for existing quantum magnets with a spin gap T_c is rather large, $T_c \approx 2$ K, in contrast to the critical temperature of BEC in atomic gases, where the number of particles is fixed and the critical temperature is of the order of nanokelvins. However, in the μVT ensemble under discussion, the particle density depends on the external magnetic field through the chemical potential μ as

$$\rho(T \geq T_c) = \sum_k \frac{1}{e^{\beta\omega_k} - 1}, \quad \omega_k = \varepsilon_k - \mu + 2U\rho, \quad (2.4)$$

in the normal phase. In the BEC phase, an explicit expression for $\rho(T < T_c)$ strongly depends on the chosen version of an approximation. For example, in the HFB approximation, which is employed here, the particle density and condensate fraction are given by the following set of equations [45]

$$\begin{aligned} \rho(T < T_c) &= \rho_0 + \rho_1 = \frac{\mu + \mu_{\text{eff}}}{2U}, \\ \mu_{\text{eff}} &= \mu + 2U(\sigma - \rho_1), \\ \rho_1 &= \frac{1}{2} \sum_k \left[\frac{\coth(\beta E_k/2)(\varepsilon_k + \mu_{\text{eff}})}{E_k} - 1 \right], \\ \sigma &= -\frac{\mu_{\text{eff}}}{2} \sum_k \frac{\coth(\beta E_k/2)}{E_k}, \end{aligned} \quad (2.5)$$

where ρ_1 and σ correspond to the density of non-condensed particles and anomalous density, respectively. The hyperbolic function in equation (2.5) can be represented also as $\coth(\beta x/2) = 1/2 + f_B(x)$, where $f_B(x) = 1/(\exp(\beta x) - 1)$ is the Bose distribution function.

Note that neglecting σ leads to an unexpected cusp in magnetization [46]. In equation (2.5), E_k is the dispersion of quasi-particles (bogolons) given as $E_k = \sqrt{\varepsilon_k^2 + 2\mu_{\text{eff}}\varepsilon_k}$ with the speed of sound $c = \sqrt{\mu_{\text{eff}}/m}$, where m has the meaning of the triplon effective mass, corresponding to the limit of small momenta $\varepsilon_k \approx \vec{k}^2/2m$. The typical value of m , used in the literature, [31] is rather small, $m \approx 0.02$ K.

3. Tan's contact for a triplon gas

As it is pointed out in the introduction, for the μVT ensemble it is convenient to calculate C using

$$C = 2U^2 m^2 \left(\frac{\partial \Omega}{\partial U} \right)_{T, \mu}, \quad (3.1)$$

where the grand thermodynamic potential Ω has the following total derivative [10, 32, 33]

$$d\Omega = -SdT - PdV - Nd\mu - MdH + \frac{Cda}{8\pi m a^2}, \quad (3.2)$$

in which S is the entropy and P is the pressure. Note that the relation between the magnetization M and the triplon density may be directly obtained from equation (3.2) as $M = g\mu_B\rho$. Moreover, using equation (3.2) one may find useful expressions for the derivatives of C as

$$\begin{aligned} \left(\frac{\partial C}{\partial T} \right) &= -2U^2 m^2 \left(\frac{\partial S}{\partial U} \right), \left(\frac{\partial C}{\partial \mu} \right) \\ &= \frac{1}{g\mu_B} \left(\frac{\partial C}{\partial H} \right) = -2U^2 m^2 \left(\frac{\partial \rho}{\partial U} \right). \end{aligned} \quad (3.3)$$

It is well known that from BEC to a normal phase transition is a second order phase transition, in which the entropy $S(T, H, a)$ is continuous across the critical temperature i.e.

$$\begin{aligned} dS(T = T_c^-) &= dS(T = T_c^+) = \left(\frac{\partial S}{\partial T} \right)_{H,a} dT \\ &+ \left(\frac{\partial S}{\partial H} \right)_{T,a} dH + \left(\frac{\partial S}{\partial a} \right)_{H,T} da. \end{aligned} \quad (3.4)$$

Therefore, using equations (3.2)–(3.4) leads to an extended Ehrenfest relation:

$$\begin{aligned} T_c^{-1} \Delta[C_H] &= -\Delta \left[\left(\frac{\partial M}{\partial T} \right)_{H,U} \right] \left(\frac{dH}{dT} \right) \\ &+ \frac{1}{2U^2 m^2} \Delta \left[\left(\frac{\partial C}{\partial T} \right)_{H,U} \right] \left(\frac{dU}{dT} \right), \end{aligned} \quad (3.5)$$

where $C_H = T(\partial S/\partial T)$ is the heat capacity and $\Delta[f] \equiv f(T = T_c^-) - f(T = T_c^+)$ is the jump in the function f at $T = T_c$.⁴

In the following we discuss the normal and BEC phases, separately.

3.1. Normal phase ($T \geq T_c$)

In the normal phase Ω is given by

$$\Omega(T \geq T_c) = -U\rho^2 + T \sum_k \ln(1 - e^{\beta\omega_k}), \quad (3.6)$$

where ρ and ω_k are defined in equation (2.4). Now, taking the derivative of Ω and using equation (2.4) one may easily find

$$\left(\frac{\partial \Omega}{\partial U} \right)_{T \geq T_c} = -\rho^2 - 2U\rho\rho' + (2\rho + 2U\rho') \sum_k \frac{1}{e^{\beta\omega_k} - 1} = \rho^2, \quad (3.7)$$

⁴ A similar relation for NVT ensembles will be $T_c^{-1} \Delta[C_P] = -\Delta \left[\left(\frac{\partial P}{\partial T} \right)_{V,U} \right] \left(\frac{dV}{dT} \right) + \frac{1}{2U^2 m^2} \Delta \left[\left(\frac{\partial C}{\partial T} \right)_{V,U} \right] \left(\frac{dU}{dT} \right)$ when the entropy is considered as a function of temperature, volume and the strength of the contact interaction.

and hence

$$C(T \geq T_c) = 2U^2 m^2 \rho^2 = \frac{2U^2 m^2 M^2}{(g\mu_B)^2}. \quad (3.8)$$

The derivatives of C can be evaluated using equation (3.3) or directly from equation (3.8) as

$$\begin{aligned} \left(\frac{\partial C}{\partial T}\right)_{T \geq T_c} &= 4U^2 m^2 \rho \left(\frac{\partial \rho}{\partial T}\right) = -2m^2 U^2 \left(\frac{\partial S}{\partial U}\right), \\ \left(\frac{\partial C}{\partial \mu}\right)_{T \geq T_c} &= 4U^2 m^2 \rho \left(\frac{\partial \rho}{\partial \mu}\right) = -2m^2 U^2 \left(\frac{\partial \rho}{\partial U}\right), \end{aligned} \quad (3.9)$$

where [27]

$$\left(\frac{\partial S}{\partial U}\right)_{T \geq T_c} = \frac{2\rho\beta I_1}{1-2I_2}, \quad \left(\frac{\partial \rho}{\partial U}\right)_{T \geq T_c} = \frac{2\rho I_2}{U[1-2I_2]}, \quad (3.10)$$

and the integrals I_1 and I_2 are given in the appendix A. Note that equation (3.9) lead to the following relations for the susceptibility, $\chi = (\partial M / \partial H)$ in the normal phase

$$\begin{aligned} \left(\frac{\partial C}{\partial H}\right)_{T \geq T_c} &= \frac{4U^2 m^2}{(g\mu_B)^2} (M\chi)_{T \geq T_c}, \chi(T \geq T_c) \\ &= -\frac{(g\mu_B)^2}{2M} \left(\frac{\partial M}{\partial U}\right)_{T \geq T_c}. \end{aligned} \quad (3.11)$$

3.2. Condensed phase ($T < T_c$)

In the condensed phase the thermodynamic potential is given by [30, 32, 33]

$$\begin{aligned} \Omega(T < T_c) &= \frac{U\rho_0^2}{2} - \mu\rho_0 - \frac{U}{2}(2\rho_1^2 + \sigma^2) \\ &+ \frac{1}{2} \sum_k (E_k - \varepsilon_k - \mu_{\text{eff}}) + T \sum_k \ln(1 - e^{-\beta E_k}) \end{aligned} \quad (3.12)$$

with μ_{eff} , ρ_1 and ρ are given by equation (2.5), $\rho_0 = \rho - \rho_1 = \mu_{\text{eff}}/U - \sigma$ and $E_k = \sqrt{\varepsilon_k^2 + 2\mu_{\text{eff}}}$. For simplicity, one may start with the well-known Bogoliubov approximation, where the depletion and anomalous density are completely neglected. For atomic gases, this leads to the Gross–Pitaevskii equation which is successfully used in a lot of systems [10]. In the present case Bogoliubov approximation corresponds to $\rho_0 \approx \rho$, $\mu_{\text{eff}} \approx \mu = U\rho$ and hence

$$\begin{aligned} \Omega_{\text{Bogoliubov}}(T < T_c) &= -\frac{\mu^2}{2U} + \frac{1}{2} \sum_k [E_k - \varepsilon_k - \mu] \\ &+ T \sum_k \ln(1 - e^{-\beta E_k}). \end{aligned} \quad (3.13)$$

Since in μVT ensembles the chemical potential does not depend on the inter-particle interaction, i.e. $(\partial \mu / \partial U) = 0$, one

Table 1. Material parameters used in our numerical calculations. The parameters g , H_c , \bar{a} and Δ are taken directly from the experimental measurements, while m and U are optimized to fit experimental magnetizations (see reference [27] for details).

	g	$H_c[\text{T}]$	$m[\text{K}^{-1}]$	$U[\text{K}]$	$\Delta[\text{K}]$	$\bar{a}[\text{\AA}]$
Ba ₃ Cr ₂ O ₈	1.95	12.10	0.2	20	15.85	3.97
Sr ₃ Cr ₂ O ₈	1.95	30.40	0.06	51.2	39.8	3.82
TlCuCl ₃	2.06	5.1	0.02	315	7.1	7.93

immediately obtains from equation (3.13) Tan's contact in the Bogoliubov approximation as⁵

$$C_0 = m^2 \mu^2. \quad (3.14)$$

From this equation, it is seen that in this simple approximation Tan's contact does not depend on temperature, which means that in μVT ensembles Bogoliubov approximation is not applicable to finite temperatures. The quality of this approximation at $T = 0$ is tested below. In figure 1, Tan's contact as a function of the magnetic field is presented for two different compounds TlCuCl₃ (figure 1(a)) and Ba₃Cr₂O₈ (figure 1(b)) in natural units, i.e. in \AA^{-4} . It is seen that for both compounds, the difference between the exact HFB (solid lines) and simple Bogoliubov approximation (dashed lines) is rather small, especially for small chemical potentials. Remarkably, the contact given by equation (3.14) does not include the scattering length of triplon interaction but includes only the effective mass as an internal microscopic parameter of the system. This is why the contact for TlCuCl₃ at the same magnetic field e.g. at $H = 13.5$ T, is much smaller than that for Ba₃Cr₂O₈. In fact, as it is seen from table 1 the ratio of effective masses is of the order of $m(\text{Ba}_3\text{Cr}_2\text{O}_8)/m(\text{TlCuCl}_3) \approx 10$.

Although C_0 in equation (3.14) is not good at finite temperatures, it may serve as a characteristic scale for the contact C . Thus, differentiating Ω in equation (3.12) with respect to U we obtain the following explicit expression for the contact in HFB approximation

$$\begin{aligned} C(T < T_c) &= C_0 \left\{ \tilde{\rho} - \frac{\tilde{\rho}_1^2 + \tilde{\rho}^2 - \tilde{\sigma}^2}{4} + 2\rho_c \mu'_{\text{eff}} [I_3 - 1 - U\tilde{\sigma}\sigma'] \right. \\ &\left. + \frac{\tilde{\rho}_0}{2} + U\rho'_1(2 - \tilde{\rho}_1 - \tilde{\rho}) \right\}, \end{aligned} \quad (3.15)$$

where $\tilde{\rho} = \rho/\rho_c$, $\tilde{\rho}_1 = \rho_1/\rho_c$, $\tilde{\rho}_0 = \rho_0/\rho_c$, $\tilde{\sigma} = \sigma/\rho_c$, $\rho'_1 = (\partial \rho_1 / \partial \mu_{\text{eff}})$, $\sigma' = (\partial \sigma / \partial \mu_{\text{eff}})$, $\mu'_{\text{eff}} = (\partial \mu_{\text{eff}} / \partial U) = (\tilde{\sigma} - \tilde{\rho}_1) / [1 + 2U(\rho'_1 - \sigma')]$ and $\rho_c = \mu/2U$. The explicit expressions for I_3 , ρ'_1 and σ' are given in the appendix A. Note that, due to the factoring out of C_0 , the quantity in curly brackets is dimensionless.

Now, using equations (3.3) and (3.12), yields

⁵ In natural units $C_0 = m^2 \mu^2 / \bar{a}^4$, where the average lattice parameter \bar{a} can be taken from table 1.

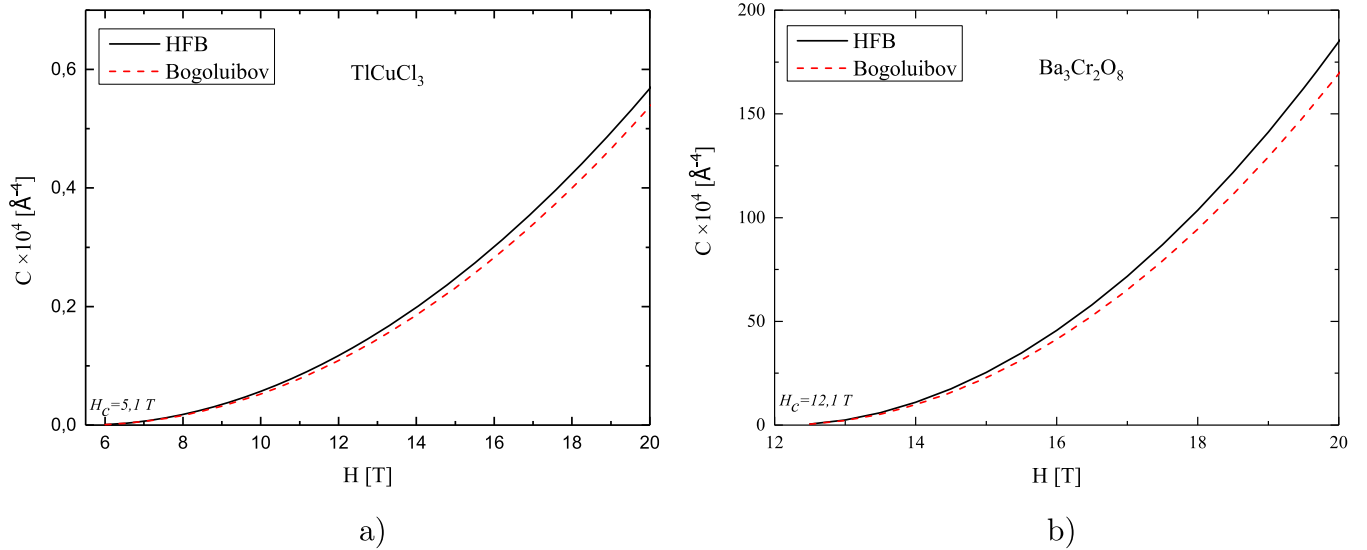


Figure 1. Tan's contact at zero temperature for TiCuCl_3 (a) and $\text{Ba}_3\text{Cr}_2\text{O}_8$ (b) in \AA^{-4} in HFB (solid lines) and Bogoliubov approximations (dashed lines). The input parameters are given in table 1.

$$\begin{aligned}
S(T < T_c) &= -\sum_k \ln(1 - e^{-\beta E_k}) \\
&+ \beta \sum_k E_k f_B(E_k), \left(\frac{\partial C}{\partial T} \right)_{T < T_c} \\
&= -2m^2 U^2 \left(\frac{\partial S}{\partial U} \right) \\
&= 8\beta (Um\rho_c)^2 \rho_c I_4 \mu'_{\text{eff}}, \left(\frac{\partial C}{\partial H} \right)_{T < T_c} \\
&= \frac{1}{g\mu_B} \left(\frac{\partial C}{\partial \mu} \right) = -\frac{2m^2 U^2}{g\mu_B} \left(\frac{\partial \rho}{\partial U} \right) \\
&= \frac{m^2 \mu (\tilde{\rho} - 2\rho_c \mu'_{\text{eff}})}{g\mu_B} = -\frac{2m^2 U^2}{(g\mu_B)^2} \left(\frac{\partial M}{\partial U} \right). \tag{3.16}
\end{aligned}$$

Unlike in the normal phase, for $T < T_c$ we failed to find a simple relation between susceptibility and $(\partial C/\partial \mu)$ similar to equation (3.11).

In the previous subsection we have shown that at zero temperature the contact may be conveniently approximated as $C(T = 0) \approx C_0 = m^2 \mu^2$. We now analyze the temperature dependence of $C(T < T_c)$ given in equation (3.15) which requires solving the set of equations (2.5). In figure 2(a), we present $C(T)$ for three compounds $\text{Ba}_3\text{Cr}_2\text{O}_8$, $\text{Sr}_3\text{Cr}_2\text{O}_8$, and TiCuCl_3 calculated in the HFB approximation (solid curves) using equations (3.8) and (3.15). It is seen that contact at finite temperature can be at least qualitatively approximated as

$$C(T) \approx 2U^2 m^2 M^2 / (g\mu_B)^2, \tag{3.17}$$

(dashed lines) which coincides with the exact one in the normal phase. In figure 2(b) the magnetizations for the same compounds as a function of temperature are also presented for completeness.

3.3. Contact and its derivatives near critical temperature

The crude approximation in equation (3.17) is also useful to explain the temperature dependence of $(\partial C/\partial H)$ and $(\partial C/\partial T)$ presented in figures 3(a) and (b), respectively. In fact, it follows that

$$\begin{aligned}
\left(\frac{\partial C}{\partial H} \right) &\propto \left(\frac{\partial M^2}{\partial H} \right) \propto M\chi, \left(\frac{\partial C}{\partial T} \right) \\
&\propto \left(\frac{\partial M^2}{\partial T} \right) = 2M \left(\frac{\partial M}{\partial T} \right). \tag{3.18}
\end{aligned}$$

The experimental susceptibilities of quantum magnets with a spin gap show a well-pronounced maximum at $T = T_c$, and they decrease exponentially at low temperatures indicating the existence of a gap Δ between the ground-state and first excited triplet states [35, 47, 48], while the magnetization has a local minimum i.e. $(\partial M/\partial T)|_{T=T_c} = 0$ at the critical point (see figure 2(b)). This is in good agreement with our predicted temperature dependence of derivatives of the contact: $(\partial C/\partial H)$ has a maximum and $(\partial C/\partial T)$ changes its sign near the phase transition from BEC to a normal phase.

On the other hand, it is well established that the heat capacity C_V has a cusp near the transition point [49–52]. Therefore, we ask whether the quantities under consideration have a jump near T_c . To study this question we consider equations (3.8) and (3.15). From equation (3.8) one may see that $C(T \rightarrow T_c^+) = 2U^2 m^2 \rho_c^2$. On the other side, setting in (3.15) $\tilde{\rho}_1 = \tilde{\rho} = 1$, $\sigma = 0$, $\mu_{\text{eff}} = 0$ and $E_k = \varepsilon_k$, one obtains $C(T \rightarrow T_c^-) = m^2 \mu^2 [1/2 + (I_3 - 1)2\rho_c \mu'_{\text{eff}}] = 2U^2 m^2 \rho_c^2$, where we used $I_3(T = T_c) = \sum_k f_B(\varepsilon_k) = \rho_c$ and $\mu = 2U\rho_c$. Therefore, Tan's contact is continuous at the critical temperature: $C(T \rightarrow T_c^-) = C(T \rightarrow T_c^+) = 2(Um\rho_c)^2$. As to its derivatives, using explicit expression for $(\partial C/\partial \mu)$ and $(\partial C/\partial T)$ given by equations (3.9) and (3.16), it can be demonstrated that they have a cusp at $T = T_c$. Presenting the details in the appendix A, we bring here the final expression for the discontinuities in dimensionless units

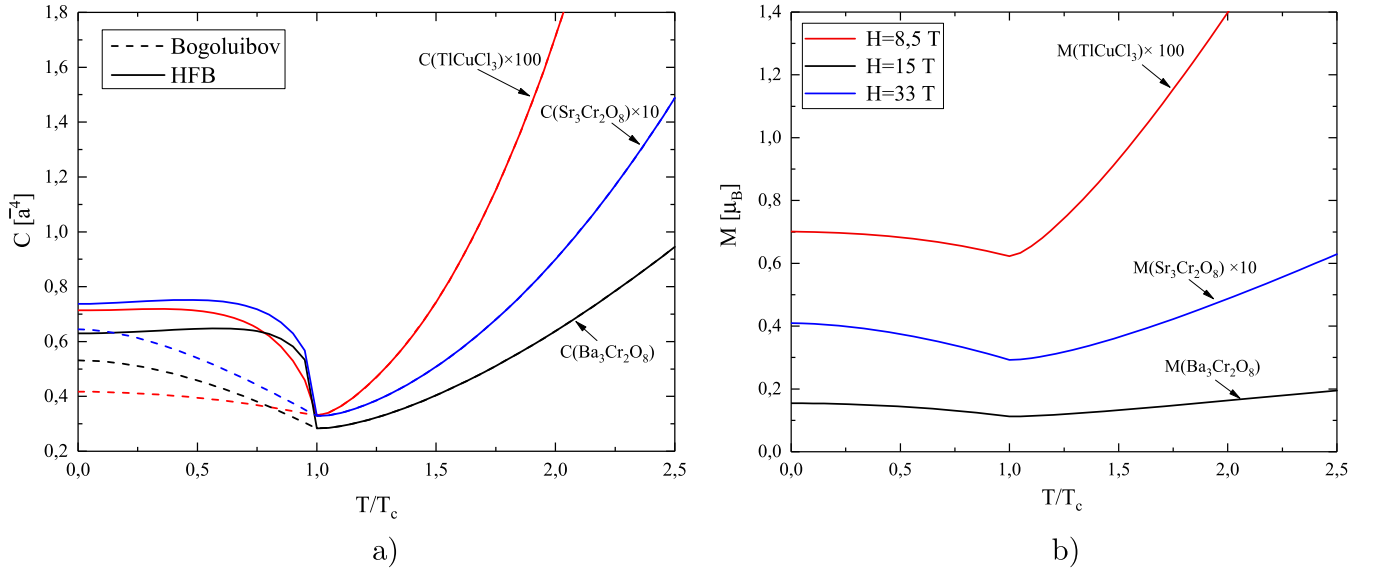


Figure 2. (a) Contact for spin gapped magnets in dimensionless units. The solid lines are for HFB approximation. The dashed lines correspond to the classic approximation given in equation (3.17); (b) the magnetizations $M(T)$ per dimer.

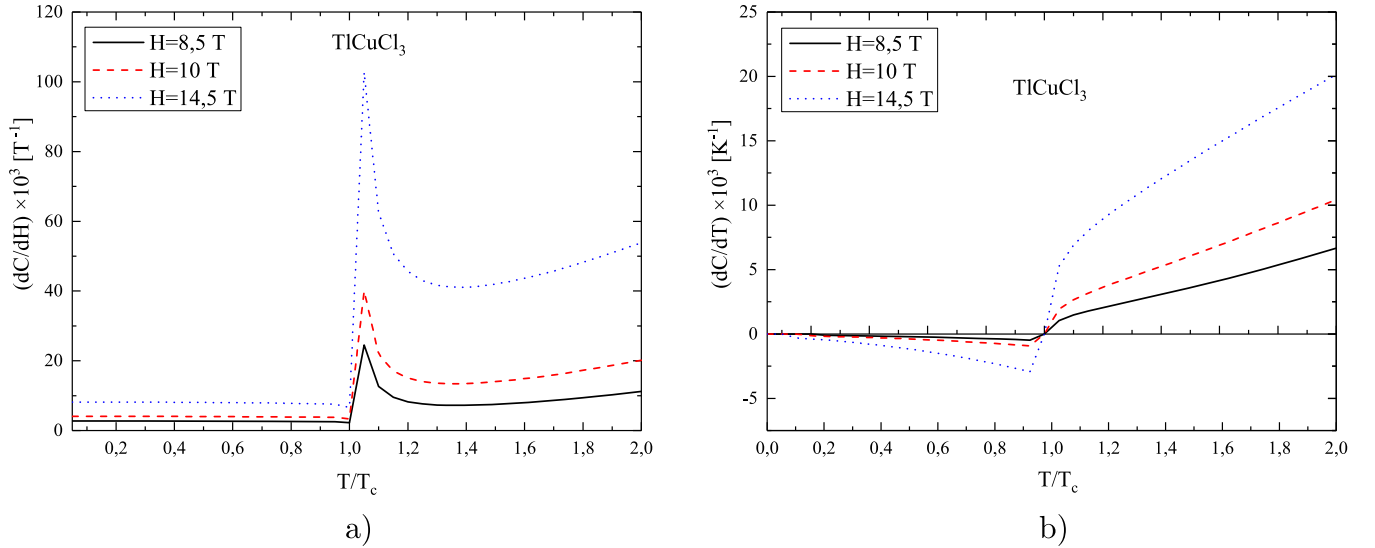


Figure 3. Derivatives of contact with respect to magnetic field (a) and to temperature for TiCuCl_3 . Here we use $V = 1$ units, so $(\partial C/\partial H)$ and $(\partial C/\partial T)$ are given in T^{-1} and K^{-1} , respectively. The curves are obtained from equations (3.16).

$$\begin{aligned}
 R_H &\equiv \frac{H_c}{C_0} \left\{ \left(\frac{\partial C}{\partial H} \right)_{T=T_c-0} - \left(\frac{\partial C}{\partial H} \right)_{T=T_c+0} \right\} \\
 &= \frac{4T_c}{U} \left\{ \sum_k \left[1 + \frac{4f_B(\varepsilon_k)T_c}{\varepsilon_k} - 4f_B^2(\varepsilon_k) \right] \right\}^{-1}, \\
 R_T &= \frac{T_c}{C_0} \left\{ \left(\frac{\partial C}{\partial T} \right)_{T=T_c-0} - \left(\frac{\partial C}{\partial T} \right)_{T=T_c+0} \right\} \\
 &= -\frac{R_H}{\rho_c T_c} \sum_k \varepsilon_k e^{\beta \varepsilon_k} f_B(\varepsilon_k).
 \end{aligned} \tag{3.19}$$

The numerical values of discontinuities R_H and R_T for TiCuCl_3 for some values of the magnetic field are presented in

table 2. From table 2 it may be concluded that the jump in $(\partial C/\partial T) \propto R_T$ is negative ($R_T < 0$), in contrast to the jump in $(\partial C/\partial \mu) \propto R_\mu > 0$, and in the heat capacity as well as in the Grüneisen parameter [27]. Thus, from the relation $R_T \approx -2m^2 U^2 (\partial S/\partial U)|_{T=T_c}$ one may conclude that, in μVT ensembles entropy increases with increasing repulsive interaction strength, i.e. $(\partial S/\partial U) > 0$. Next, we discuss another critical phenomenon, which is related to the low temperature critical behavior.

3.4. Low temperature expansion and QPT

In a μVT ensemble, studied in the present work, a QPT occurs at zero temperature upon tuning the external magnetic field or equivalently the chemical potential. At $T = 0$ the distance to

Table 2. Some critical parameters of TiCuCl_3 .

$H[\text{T}]$	$T_c[\text{K}]$	ρ_c	$C(T = T_c)[\text{nm}^{-4}]$	R_T	R_μ
6.0	2.15	0.001 20	0.000 384	−0.0245	0.0134
6.5	3.06	0.002 30	0.001 40	−0.0365	0.0190
7.0	3.73	0.003 40	0.003 07	−0.0458	0.0230
7.5	4.28	0.004 50	0.005 37	−0.0540	0.0263
8.0	4.75	0.005 59	0.008 31	−0.0609	0.0290
8.5	5.16	0.006 69	0.0119	−0.0671	0.0314
9.0	5.54	0.007 79	0.0161	−0.0727	0.0336
9.5	5.88	0.008 89	0.0210	−0.0779	0.0355
10.0	6.20	0.009 99	0.0265	−0.0826	0.0373
10.5	6.49	0.0111	0.0326	−0.0870	0.0390
11.0	6.77	0.0122	0.0394	−0.0911	0.0405
11.5	7.04	0.0133	0.0468	−0.0950	0.0420
12.0	7.28	0.0144	0.0549	−0.0986	0.0420

the QCP is determined by a control parameter, $r(H)$. Near the QCP the control parameter can be linearized around the critical magnetic field H_c as $r(H) = (H - H_c)/H_c$, which corresponds to $\mu = r\Delta$ (where $\Delta = g\mu_B H_c$ is the spin gap). It is expected that some thermodynamic quantities will diverge at QPT. For example, the Grüneisen parameter which plays an important role in magnetocaloric effect diverges as $\Gamma_H|_{r \rightarrow 0} \sim 1/r$ [26, 53]. In the following we address the critical behavior of Tan's contact and its derivatives close to QCP.

The case of C and $(\partial C/\partial \mu)$ is rather straightforward. Actually, in section 2, we have shown that at $T = 0$ the contact can be simply approximated as $C|_{T=0} = m^2 \mu^2$, especially at weak magnetic fields, i.e. as $r \rightarrow 0$ (see figure 1). Thus, one directly obtains

$$C(T = 0)|_{r \rightarrow 0} = m^2 r^2 \Delta^2 + O(r^{5/2}), \quad \left(\frac{\partial C}{\partial \mu} \right) |_{T=0, r \rightarrow 0} = 2m^2 r \Delta + O(r^{3/2}), \quad (3.20)$$

to show that in contrast to Γ_H , contact and its derivative $(\partial C/\partial H)$ are regular near QCP.

The case of $(\partial C/\partial T)$ is a little more complicated. Here, one has to find the low temperature expansion for $(\partial S/\partial U)$, as well as small r expansion for the effective chemical potential $\mu_{\text{eff}}(r)$. This leads to following expressions [27]

$$\begin{aligned} \left(\frac{\partial S}{\partial U} \right) &= -\mu'_{\text{eff}} \beta^2 \sum_k \varepsilon_k e^{\beta E_k} f_B^2(E_k) \\ &= -\frac{\mu'_{\text{eff}} \pi^2 T^3}{15 m s_0^5} + O((Tm)^5), \quad \mu'_{\text{eff}} = \left(\frac{\partial \mu}{\partial U} \right) \\ &= -\frac{r Q_0 m \Delta_1}{\pi \Delta} + O(r^{3/2}), \quad \mu_{\text{eff}} = r \Delta_1 + r^{3/2} \Delta_{32}, \end{aligned} \quad (3.21)$$

where $s_0 = \sqrt{\mu_{\text{eff}}/m}$ is the sound velocity at $T = 0$, $\Delta_1 = \Delta \pi / (\pi + Q_0 U m)$, $\Delta_{32} = 4(\Delta m)^{3/2} \sqrt{\pi} U / 3(Q_0 U m + \pi)^{5/2}$ and $Q_0 = (6/\pi)^{1/3}$ is the Debye momentum [27]. Then, the low temperature expansion for $(\partial C/\partial T)$ near QCP can be directly obtained as

$$\left(\frac{\partial C}{\partial T} \right) = -2m^2 U^2 \left(\frac{\partial S}{\partial U} \right) = -\alpha \frac{T^3}{r^{3/2}} + O((Tm)^5), \quad (3.22)$$

where $\alpha = m^{9/2} U^2 \pi Q_0 / 15 \Delta \sqrt{\Delta_1}$. It is seen that at low but finite temperatures $(\partial C/\partial T)$ diverges as $1/r^{3/2}$, but there is no divergence at exactly $T = 0$, where QPT occurs. Numerical estimations show that α is positive and rather small and hence, at low temperatures the contact decreases very slowly as seen in figure 2(a).

4. Discussion and conclusion

We have studied the Tan's contact for spin-gapped quantum magnets, assuming that their low temperature properties are related to that of a triplon gas. To the best of our knowledge, this is the first time the parameter C and its dependence on temperature is investigated for a solid. Naturally, it will be interesting to compare our results with existing ones in the literature. However, there is neither a theoretical nor an experimental study of Tan's contact for μVT ensembles at finite temperatures and most of the literature on $C(T)$ concern 1D gases in NVT ensembles.

The temperature dependence of C of harmonically trapped 1D Leib–Liniger Bose gas has been studied by Yao *et al* [54]. They have found that contact increases at low temperatures, reaches a maximum at $T = T^*$ and then starts to decrease, i.e. $(\partial C/\partial T)|_{T < T^*} > 0$, $(\partial C/\partial T)|_{T = T^*} = 0$ and $(\partial C/\partial T)|_{T > T^*} < 0$. From figures 1 and 2, one may note that for a 3D system of bosons the situation is quite the opposite; $(\partial C/\partial T)|_{T < T_c} < 0$ and $(\partial C/\partial T)|_{T > T_c} > 0$. But at the critical temperature T_c , in both cases $C(T)$ exhibits an extremum as a function of temperature, maximum for 1D bosons and minimum for triplons, i.e. in both cases $(\partial C/\partial T)$, changes its sign near the critical temperature. Bearing in mind the relation $(\partial C/\partial T) \sim (\partial S/\partial U)$, one may conclude that at $T = T_c$ the interaction dependence of the entropy displays a maximum. Note that in the case of 1D bosons this maximum provides a signature of the crossover to the fermionized regime, while in the case of quantum magnets it corresponds just to the point of finite temperature phase transition, where accumulation of entropy occurs [26].

In the present work the temperature dependence of $C(T)$ at large temperatures $T > T_c$, is found to be almost linear. This is to be compared with the results by Vignolo and Minguzzi [55] who obtained the large temperature behavior as $C \sim \sqrt{T}$ for a 1D Bose gas in the Tonks–Girardeau limit. It would be interesting to study the effect of dimensionality on $C(T)$ in μVT ensembles also [56].

We have studied the critical behavior of C at the QPT and found that C and $(\partial C/\partial \mu)$ are regular at QCP which is in good agreement with predictions made by Chen *et al* [25].

In conclusion it should be underlined that our analytical expressions for Tan's contact of spin gapped compounds are expressed in terms of magnetizations which are directly observable. For example, at very low temperatures, $T \ll T_c$, one evaluates C simply from the expression $C = m^2 \mu^2 / \bar{a}^4$, where the only parameter, effective mass should be estimated. Note that, in this region contact of a μVT ensemble is almost not sensitive to the strength of the boson-boson interaction U , while the dependence on U of the contact of an NVT ensemble

is rather strong even in the classical approximation, when C is given by $C(NVT) \approx 16\pi^2 a^2 \rho^2 = U^2 m^2 \rho^2$ [10, 37].

Finally, we venture to suggest a way to measure C in quantum magnets, which can be performed in a similar way as it was done in reference [17] (see appendix B for details).

We hope our work will stimulate more studies, especially experimental ones exploring the universality of μVT ensembles in quantum magnets. Results presented here will deepen our understanding of the connection between short-ranged two-body correlations and magnetic phase transitions in antiferromagnetic materials, which have the potential to be used in developing the next generation of spintronic devices.

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Data availability statement

The data that support the findings of this study are available upon reasonable request from the authors.

Appendix A

In this appendix we provide explicit expressions for the integrals introduced in equations (3.10), (3.15) and (3.16):

$$\begin{aligned} I_1 &= -\beta \sum_k \omega_k f_B^2(\omega_k) e^{\beta \omega_k}, & I_2 &= -U\beta \sum_k f_B^2(\omega_k) e^{\beta \omega_k}, \\ I_3 &= \rho_c^{-1} \sum_k \left(\frac{\varepsilon_k W_k}{E_k} - \frac{1}{2} \right), & I_4 &= \beta \sum_k f_B^2(\omega_k) \varepsilon_k e^{\beta \omega_k}, \end{aligned} \quad (\text{A.1})$$

where $f_B(x) = 1/(e^{\beta x} - 1)$, $W_k = (1/2 + f_B(E_k))$, $\omega_k = \varepsilon_k - \mu + 2U\rho$ and $E_k^2 = \varepsilon_k(\varepsilon_k + 2\mu_{\text{eff}})$.

Equation (3.15) includes $(\partial \rho_1 / \partial \mu_{\text{eff}})$, $(\partial \sigma / \partial \mu_{\text{eff}})$ and $(\partial \mu_{\text{eff}} / \partial U)$. The derivatives with respect to μ_{eff} can be found by differentiating equations (2.5) to give

$$\left(\frac{\partial \rho_1}{\partial \mu_{\text{eff}}} \right) = \sum_k \frac{\varepsilon_k}{E_k^2} \left[\frac{\mu_{\text{eff}} W_k}{E_k} + \frac{(\varepsilon_k + \mu_{\text{eff}}) W'_k}{4} \right], \quad (\text{A.2})$$

$$\left(\frac{\partial \sigma}{\partial \mu_{\text{eff}}} \right) = -\sum_k \frac{\varepsilon_k}{E_k^2} \left[\frac{\mu_{\text{eff}} W'_k}{4} + \frac{(\varepsilon_k + \mu_{\text{eff}}) W_k}{E_k} \right], \quad (\text{A.3})$$

where $W'_k = \beta(1 - 4W_k^2)$.

As to $(\partial \mu_{\text{eff}} / \partial U)$, it can be obtained by differentiation of both sides of the equation $\mu_{\text{eff}}(U) =$

$\mu + 2U[\sigma(\mu_{\text{eff}}(U)) - \rho_1(\mu_{\text{eff}}(U))]$ with respect to U and then solving it for $(\partial \mu_{\text{eff}} / \partial U)$. This leads to

$$\left(\frac{\partial \mu_{\text{eff}}}{\partial U} \right) = \frac{\mu_{\text{eff}} - \mu}{UD}, \quad (\text{A.4})$$

$$D = 1 + 2U \left[\left(\frac{\partial \rho_1}{\partial \mu_{\text{eff}}} \right) - \left(\frac{\partial \sigma}{\partial \mu_{\text{eff}}} \right) \right]. \quad (\text{A.5})$$

Now, we proceed to evaluate $(\partial C / \partial H) = -2m^2 U^2 g \mu_B (\partial \rho / \partial U)$ and $(\partial C / \partial T) = -2m^2 U^2 (\partial S / \partial U)$ near the critical temperature T_c .

From the explicit expression

$$S(T > T_c) = \sum_k \ln(1 - e^{-\beta \omega_k}) + \beta \sum_k \omega_k f_B(\omega_k), \quad (\text{A.6})$$

where $\omega_k = \varepsilon_k - \mu + 2U\rho(U)$, one obtains

$$\left(\frac{\partial S}{\partial U} \right)_{T=T_c+0} = -\beta^2 \sum_k e^{\beta \omega_k} \omega_k \omega'_k f_B^2(\omega_k), \quad (\text{A.7})$$

where $\omega'_k = (\partial \omega_k / \partial U) = 2\rho + 2U(\partial \rho / \partial U)$ and $(\partial \rho / \partial U)$ is given by equation (3.10). It is straightforward to show that the integral I_2 in equation (3.10) is divergent at $T = T_c$, where $\omega_k = \varepsilon_k \sim k^2/2m$, and hence $(\partial \rho / \partial U)|_{T=T_c} = -\rho/U$. This means that $\omega'_k(T = T_c^+) = 0$ and $(\partial S / \partial U)|_{T=T_c^+} = 0$. Therefore $(\partial C / \partial T)|_{T=T_c^+} = 0$ and $(\partial \rho / \partial U)|_{T=T_c^+} = -\rho/U$.

Replacing ω_k by E_k in equation (A.6) and taking the derivative one finds

$$\left(\frac{\partial S}{\partial U} \right)_{T < T_c} = -\beta^2 \left(\frac{\partial \mu_{\text{eff}}}{\partial U} \right) \sum_k \varepsilon_k e^{\beta E_k} f_B^2(E_k). \quad (\text{A.8})$$

Now, taking into account that $\mu_{\text{eff}}(T_c) = 0$, $\rho(T_c) = \rho_c = \mu/2U$, $E_k(T_c) = \varepsilon_k$ and using equation (A.5) we obtain

$$\left(\frac{\partial S}{\partial U} \right)_{T=T_c^-} = \frac{\mu \beta^2}{UD} \sum_k \varepsilon_k e^{\beta \varepsilon_k} f_B^2(\varepsilon_k) \quad (\text{A.9})$$

which proves the equation (3.19). The derivative $(\partial \rho / \partial U)|_{T=T_c^-}$ may be obtained from $\rho(U) = (\mu_{\text{eff}} + U)/2U$ as

$$\left(\frac{\partial \rho}{\partial U} \right)_{T=T_c^-} = -\frac{\mu(1+D)}{2U^2 D}, \quad (\text{A.10})$$

where D is given by equation (A.5) and $(\partial \mu_{\text{eff}}) / (\partial U)$ should be evaluated at $T = T_c$.

The expansion of entropy and the effective chemical potential near QCP may be found in the appendix of reference [27].

Appendix B

Here we outline a sketch of a possible method of measuring Tan's contact for spin gapped magnets. We presume that this can be achieved in a similar way to that for atomic gases.

Wild et al [17] measured C for ^{85}Rb atoms in a gas with a 60% condensate fraction. The atoms are in the $|F = 2, m_F = -2\rangle$ state, where F is the total atomic spin and m_F is

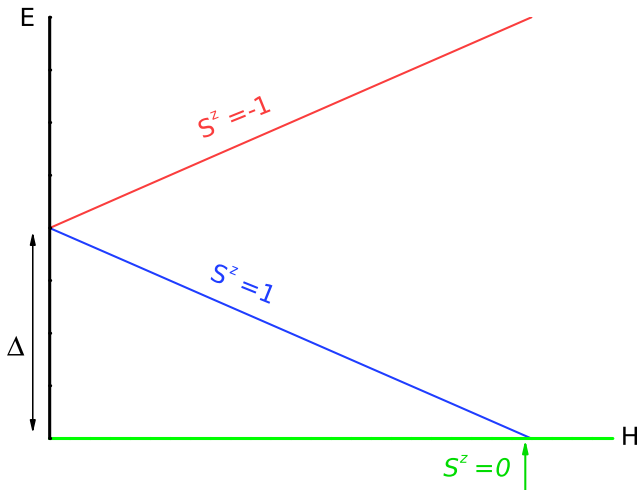


Figure 4. Cartoon of the spin levels of a typical spin gapped quantum magnet showing that there are $S_z = \pm 1$ excited doublet and $S_z = 0$ ground states. They are separated by a gap $\Delta = g\mu_B H_c$, which can be collapsed due to Zeeman effect for $H > H_c$.

the spin projection. Then by applying an rf pulse the atoms are driven from $|2, -2\rangle$ to $|2, -1\rangle$ state. The rate for transferred atoms to the final spin state is given by [5, 17]

$$\lim_{\omega \rightarrow \infty} \Gamma(\omega) = \frac{\Omega^2}{4\pi} F(a, \omega, m) C, \quad (\text{B.1})$$

where Ω is the Rabi frequency, $F(a, \omega, m)$ is a given function of scattering length a , the frequency ω , and the atomic mass m . Tan's contact has been extracted from this equation after a direct measurement of Γ as a function of ω .

Now we consider the spin gapped magnets. Here for $H > H_c$ we have two spin levels with $S_z = 1$ (ground state) and $S_z = -1$ (nearest excited state), as illustrated in figure 4. The direct transition between the spin singlet and triplet states is, in principle, forbidden in magnetic dipole transitions. Nonetheless, such transitions have been observed in many spin gapped systems by means of high frequency electron spin resonance measurements [57–60]. It was shown that, these transitions are, in fact, driven by ac electric fields, and observed electric dipole transitions can be explained by spin dependent polarization. Very recently, Matsumoto *et al* [60] developed a theoretical description of singlet–triplet transitions in spin gapped magnet KCuCl_3 in the framework of spin-wave theory, and proposed practical formulas for the transition probability W , using Fermi's golden rule (see e.g. equation (18) of reference [60]). We surmise that if one uses an effective Hamiltonian similar to equation (2.1) the transition probability from reference [60] can be related to the Tan's contact as in equation (B.1), and hence one will be able to obtain C from measurements of W , using proper normalization of observed quantities.

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