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Field-induced superfluid state of magnons in the two-dimensional spin-1/2 quantum XY model

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Abstract

A field-induced superfluid state of magnons is exhibited in the two-dimensional spin-1/2 quantum XY model in a strong magnetic field h ($h/J \leq 2$) along \hat{z} below a critical temperature T_c by using the renormalized field theory and the running coupling constant method. In such a state, there exist several distinctive phenomena: spins are aligned better in a constant magnetic field as the temperature increases; and entropy rises with increasing strength of the magnetic field at constant temperature. Mechanisms which lead to the above phenomena are proposed, and the distinctive curve of $\langle S_z \rangle$ versus *T* in XCuCl₃ can also be explained accordingly. Similarities and differences between our system and XCuCl₃ are also discussed.

1. Introduction

Recently, field-induced magnetic ordering has attracted considerable interest in studying quantum phase transitions in spin systems composed of three-dimensional crystalline networks of dimers like TlCuCl₃ and KCuCl₃ [1–5]. As the applied magnetic field H is larger than a critical value, an unusual magnetic ordering occurs as a quantum phase transition. Such field-driven quantum phase transitions can be controlled precisely, and provide unrivalled opportunities for studying collective phenomena in strongly correlated 3D quantum systems.

On the other hand, the quantum spin system in lower dimensions (d < 3) has also been one of the most intensively studied topics in condensed matter physics. Rich physics are connected with many modern quantum statistical phenomena such as the low dimensional (antiferro-)magnetism [6] and the high T_c superconductivity [7]. Further, the quantum spin-1/2 system in lower dimensions itself is of fundamental interest as a quantum many-body system. For example, the two-dimensional spin-1/2 quantum XY model ($2DS_{1/2}QXYM$) [8–11] is one of the simplest models supporting topological excitations. In this model, the topological excitation (vortex) plays an important role in its statistical behaviour, and results in the Kosterlitz–Thouless (KT) transition at temperature $T_{KT,h=0} = 0.35J$ [8] when no magnetic field is present.

The $2DS_{1/2}QXYM$ is equivalent to a lattice boson system with infinite on-site repulsion (hard-core lattice boson) [12, 13]; this theorem has been proved *rigorously* [13], and applied to several spin models successfully [14, 15]. The hard-core bosonic property of the spin-1/2 magnons (spin waves) of the $2DS_{1/2}QXYM$ may be reminiscent of that of the triplet magnons of the 3D XCuCl₃ [4]. In XCuCl₃ the ground state of the magnon is a non-magnetic state with zero magnetization, while in the $2DS_{1/2}QXYM$ the ground state of the spin-1/2 magnon is a fully polarized ferromagnetic state. In addition to the statistical property (bosonic or fermionic), fluctuation is also essential in many-body phenomena. Literally, the statistical behaviour of a many-body bosonic system at low temperatures is governed by the competition between the quantum collective behaviour of the Bose statistics and the coupled classical and quantum fluctuations. In XCuCl₃, being in three dimensions, fluctuation is small; thus there is Bose– Einstein condensation (BEC) at low temperatures, while in the $2DS_{1/2}QXYM$ fluctuation is enhanced due to low dimensionality; thus there is no BEC at temperature $T \neq 0$ [16]. Nevertheless, if they are in external magnetic fields, the above two quantum spin systems still have some collective behaviour in common-superfluidity (SF). However, most theoretical and numerical efforts have not been directed toward the study of the finite-temperature behaviour of the $2DS_{1/2}QXYM$ in a magnetic field. We will show later that due to SF, some seemingly anomalous *field-induced* phenomena would appear in the $2DS_{1/2}QXYM$ at finite temperatures. Associated mechanisms would be proposed as well. The distinctive curve of $\langle S_z \rangle$ versus T in XCuCl₃ [1] can also be explained accordingly.

In a ferromagnetic state, normally, fluctuations grow with temperature and therefore decrease the magnetization [18]; and ordering of spins grows with increasing strength of the magnetic field, and this would usually decrease the entropy. In this paper we would like to report that at temperature below a critical value $T_c \leq T_{\text{KT}}$ an anomalous ferromagnetic state which is a field-induced magnon superfluid state can be exhibited in the $2DS_{1/2}QXYM$ in a magnetic field along \hat{z} : in this state, the magnetization $\langle S_z \rangle$ grows as the temperature *increases* in a constant magnetic field, and entropy *rises* with *increasing* magnetic field at constant temperature.

It should be noted that, at temperature T below T_{KT} , the vortex density is small and weakly dependent on T; and it rises considerably above T_{KT} [8]. Thus the effect due to the vortex can be ignored at $T < T_{\text{KT}}$, within which discussions in the rest of this paper are focused.

On the other hand, analytical studies of quantum spin systems at finite temperatures in lower dimensions are rather difficult. This is because the spin operator is neither purely boson-like nor fermion-like [13]. In addition, even though the spin algebra is compact, the algebra generated by the spin wave annihilation and creation operators is not [13]. Therefore, the conventional field theoretical techniques constructed for the boson and fermion cannot be directly applied to quantum spin systems. Thanks to the equivalence between spin-1/2 systems and their corresponding hard-core lattice boson theory, which can then be converted back to the original spin theory afterwards. But field theoretical studies of bosonic systems in lower dimensions (at finite temperatures) are more difficult than those done in three dimensions for the following reasons: the conventional calculations of interacting boson systems in three dimensions at finite temperatures [19, 20] are based on two facts.

- (i) BEC occurs at finite temperatures in three dimensions (and also at T = 0 in two dimensions), i.e., $\langle \phi \rangle > 0$, where ϕ is the boson field.
- (ii) The *t*-matrix [19–21] is nonzero at long wavelengths and zero particle density ($t_0 \neq 0$).

Thus one may perturb around $\langle \phi \rangle$ with expansion parameter t_0 . But in two dimensions (at finite temperatures) the standard perturbation calculation breaks down [22] because the phase

fluctuation destroys the BEC at finite temperatures [23], and the *t*-matrix vanishes at low k and ω ($t_0 = 0$) [21, 24]. We circumvent the difficulty of $\langle \phi \rangle = 0$ by adopting polar coordinates, $\phi = \sqrt{\rho}e^{i\theta}$ such that $\langle \rho \rangle = \langle \phi^{\dagger}\phi \rangle \neq 0$. However, the renormalization of the coupling v, necessary to cancel an ultraviolet divergence, introduces in two dimensions an infrared logarithmic divergence associated with the vanishing of t_0 . We instead renormalize v at ρ ($\neq 0$). This leads to a 'running' coupling constant v_{ρ} . Thus the non-vanishing ρ_c (the classical value of ρ) and v_{ρ} take the roles of $\langle \phi \rangle$ and t_0 , respectively, in the standard perturbative calculations. In the v_{ρ} expansion we do not encounter an infrared divergence.

The outline of this paper is as follows. The model and renormalization calculations to the one-loop order are given in section 2. Discussions of some distinctive physical phenomena together with their physical interpretations will be made in sections 3.1 and 3.2. Similarities and differences between our system and XCuCl₃ will be discussed in section 3.3. Conclusions, further applications and future work will be mentioned in section 4.

2. The model, and calculations to the one-loop order

The Hamiltonian of the $2DS_{1/2}QXYM$ in a magnetic field along the *z*-direction on a simple cubic lattice is

$$\mathcal{H} = -J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y) - h \sum_j S_j^z, \tag{1}$$

$$= -\frac{J}{2} \sum_{\langle ij \rangle} (S_i^+ S_j^- + S_j^+ S_i^-) - h \sum_j \left(\frac{1}{2} - S_j^+ S_j^-\right), \tag{2}$$

in terms of the spin raising and lowering operators S^+ and S^- (creation and annihilation operators of spin waves, respectively), with

$$S_i^{\pm} \equiv S_i^x \mp S_i^y, \qquad S_i^+ S_i^- = \frac{1}{2} - S_i^z,$$
(3)

and *J* the exchange constant. By the Friedberg–Lee–Ren theorem [13], the lattice boson system equivalent to equation (1) is constructed by first expressing the spin-wave Hamiltonian by the normal ordering of S^+ and S^- , as in equation (2), and then replacing them by those of the lattice boson, b^{\dagger} and *b*, respectively,

$$\begin{pmatrix} S_i^+\\ S_i^- \end{pmatrix} \longleftrightarrow \begin{pmatrix} b_i^\dagger\\ b_i \end{pmatrix},$$

with an infinite on-site repulsion $G/2 \cdot b^{\dagger 2}b^2$ being added finally,

$$H(b^{\dagger}, b) = \mathcal{H}(b_i, b_i^{\dagger}) + \frac{G}{2} \sum_i b_i^{\dagger 2} b_i^2,$$
(4)

where G would be set to infinity finally. Define \mathcal{N} as the number of lattice sites, and $\mu \equiv 2J - h$, which will be identified below as the chemical potential of the lattice boson. Then the Hamiltonian \mathcal{H} in equation (2) is equivalent to the following one:

$$H(b^{\dagger}, b) = -\frac{J}{2} \sum_{\langle ij \rangle} (b_i^{\dagger} b_j + b_j^{\dagger} b_i) + (2J - \mu) \sum_j b_j^{\dagger} b_j + \frac{G}{2} \sum_j b_j^{\dagger 2} b_j^2,$$
(5)

which describes a two-dimensional system of a lattice boson with a hard-core interaction when G is set to ∞ . To handle such a hard-core boson, the *binary collision method* has been well developed since 1959 [25, 26]. The idea is that we sum up all diagrams representing repeated and continuous scatterings between two particles (also called the *t*-matrix [26]) as the new coupling which keeps finite after the limit $G \rightarrow \infty$ is taken.

As has been shown by Friedberg [27], through a careful treatment of path integration, or normal ordering in the operator formulation, only the coupling constant in equation (5) needs to be renormalized. Then we can write the *bare* Hamiltonian H_b for renormalization from equation (5) as

$$H_{\rm b} = -\frac{J}{2} \sum_{\langle ij \rangle} (b_i^{\dagger} b_j + b_j^{\dagger} b_i) + (2J - \mu) \sum_j b_j^{\dagger} b_j + \frac{v_{\rm b}}{2} \sum_j b_j^{\dagger 2} b_j^2, \tag{6}$$

where v_b is the bare coupling constant, and an unimportant constant $-\frac{h}{2}N$ has been discarded. Apart from renormalization corrections which are already contained in the *t*-matrix, the *renormalized* coupling *v* is equal to the *t*-matrix; this point will be further explored later.

The partition function $\mathcal{Z} \equiv \text{Tr } e^{-\beta H_b}$ can be expressed in the path-integral formulation as

$$\mathcal{Z} = \int \prod_{i} \mathrm{D}b_{i}^{*} \mathrm{D}b_{i} \exp\left\{-\frac{1}{l}S[b_{i}(\tau), b_{i}^{*}(\tau)]\right\},\tag{7}$$

where τ is the imaginary time, $b_i(\tau)$ is restricted by the periodic boundary condition for boson $b_i(\beta) = b_i(0)$, and

$$S = \int_0^\beta \mathrm{d}\tau \left[\sum_i b_i^*(\tau) \partial_\tau b_i(\tau) + H_\mathrm{b}^c(b^*(\tau), b(\tau)) \right],\tag{8}$$

with H_b^c the classical version of H_b . The parameter *l* in equation (7) is there to keep track of the 'loop expansion' defined by expanding the thermodynamic (grand) potential (of the lattice boson system)

$$W = -l\beta^{-1}\ln\mathcal{Z} \tag{9}$$

in ascending powers of *l*; and will be set equal to unity afterwards.

In two dimensions, lacking a constant long range order (or, in the boson language, the Bose–Einstein condensate $\langle b_i \rangle$ is absent at finite temperatures [23, 22]), we cannot perform perturbation around $\langle b_i \rangle$ as in the three dimensions. To circumvent this difficulty, we shall adopt polar coordinates and parametrize b_j s as

$$b_j = \sqrt{\rho_j} e^{i\theta_j}, \qquad b_j^* = \sqrt{\rho_j} e^{-i\theta_j}.$$

Rewritten in the polar coordinates, $H_{\rm b}^c$ in equation (8) is

$$H_{\rm b}^c = (2J - \mu) \sum_j \rho_j - J \sum_{\langle ij \rangle} \sqrt{\rho_i} \sqrt{\rho_j} \cos(\theta_i - \theta_j) + \frac{v_{\rm b}}{2} \sum_j \rho_j^2.$$
(10)

To zeroth order in l (tree level) we have simply

$$w \equiv \mathcal{N}^{-1}W = w_0 = (\beta \mathcal{N})^{-1} S_0, \tag{11}$$

where w is the grand potential per site, w_0 the zeroth order term of w, and S_0 the minimum value of $S[b_j, b_j^*]$, obtained by setting the b_j equal to a constant such that $|b_j|^2 = \rho_c$, and minimizing with respect to ρ_c . The results are

$$S_0 = \beta \mathcal{N} \left(-\mu \rho_{\rm c} + \frac{v_{\rm b}}{2} \rho_{\rm c}^2 \right);$$
$$\rho_{\rm c} = \frac{\mu}{v_{\rm b}}, \qquad w_0 = -\frac{\mu^2}{2v_{\rm b}}.$$

To first order in l (the 'one-loop order') we have

$$w \approx w_0 + lw_1 = -\frac{\mu^2}{2v_b} + lw_1, \tag{12}$$

where w_1 is to be obtained by expanding the Hamiltonian in equation (10) to the second order in θ_j and $\xi_j \equiv \rho_j - \rho_c$; and the action S in equation (8) is

$$S \simeq S_0 + \int_0^\beta \mathrm{d}\tau \sum_i \left[\mathrm{i}\xi_i \partial_\tau \theta_i + J\rho_\mathrm{c} a^2 (\nabla_\mathrm{D}\theta_i)^2 + \frac{J a^2}{4\rho_\mathrm{c}} (\nabla_\mathrm{D}\xi_i)^2 + \frac{v_\mathrm{b}}{2} \xi_i^2 \right], \quad (13)$$

where $\nabla_{\rm D}$ is the two-dimensional discrete gradient operator, and *a* the lattice spacing. One might proceed *natively* by expanding θ_j and ξ_j in Fourier series in τ as well as in *j*, and integrating over the Fourier components in equation (7). Then w_1 can be obtained as

$$w_1^{\text{native}} = \frac{1}{\mathcal{N}} \sum_k \left[\frac{\omega_k}{2} + \beta^{-1} \ln(1 - e^{-\beta \omega_k}) \right],\tag{14}$$

where
$$\omega_{\vec{k}} = \sqrt{\epsilon_{\vec{k}}(\epsilon_{\vec{k}} + 2\mu)},$$

and $\epsilon_{\vec{k}}$ is the famous Bloch spectrum of spin wave defined as

$$\epsilon_{\vec{k}} = J\left(2 - \sum_{x,y} \cos k_{\alpha} a\right), \quad \text{and} \quad \epsilon_{\vec{k}} \stackrel{|\vec{k}| \sim 0}{\approx} \frac{J a^2 k^2}{2}.$$
 (16)

Nevertheless, following a careful definition of path integral [27], or the normal ordering of the operator formalism as mentioned earlier, the one-loop calculation leads not to equation (14) but to (note that $\mathcal{N}^{-1}\sum_{\vec{k}} \rightarrow \int_{-\pi}^{\pi} \frac{d^2(\vec{k}a)}{(2\pi)^2}$)

$$w_1 = \int \int_{-\pi}^{\pi} \frac{\mathrm{d}^2(\vec{k}a)}{(2\pi)^2} \frac{\omega_k - \epsilon_k - \mu}{2} + w_\beta, \tag{17}$$

with

$$w_{\beta} = \frac{1}{\beta} \int \int_{-\pi}^{\pi} \frac{\mathrm{d}^{2}(\vec{k}a)}{(2\pi)^{2}} \ln(1 - \mathrm{e}^{-\beta\omega_{k}}).$$

Next we need to check if the above thermodynamic potential density w is consistent with the lattice boson model. In the discrete regime, equation (17) behaves well and does not suffer any ultraviolet (UV) or IR divergence. On the other hand, in the continuum limit, the lattice boson model becomes the two-dimensional hard disk boson model which is a well defined physical system and its thermodynamic potential should also be finite. But in such a limit (with $a \rightarrow 0$, and $\epsilon_{\vec{k}} \rightarrow Ja^2 \vec{k}^2/2$), the grand potential density $w^{\text{continuum}} (\equiv W/(Na^2))$ at zero temperature is (while keeping Ja^2 and μ fixed)

$$w_{T=0}^{\text{continuum}} = \lim_{a \to 0} \frac{w_{1,T=0}}{a^2} = \int \int_{-\infty}^{\infty} \frac{\mathrm{d}^2 \vec{k}}{(2\pi)^2} \frac{Ja^2}{4} \left(k\sqrt{k^2 + \frac{4\mu}{Ja^2}} - k^2 - \frac{2\mu}{Ja^2} \right),$$

with $k\sqrt{k^2 + \frac{4\mu}{Ja^2} - k^2 - \frac{2\mu}{Ja^2}} \sim -\frac{2\mu^2}{J^2a^2k^2}$ at large k, and it diverges logarithmically after integration. Therefore, to get a consistent theory, w_1 (equation (17)) needs to be renormalized and this can be accomplished by renormalizing the coupling v as follows.

Defining $f \equiv w + \mu \bar{\rho}$ as the free energy per site, then by taking the idea of v as an effective potential between particles, the renormalized coupling v can be defined as

$$v_{\hat{\rho}} = \left(\frac{\partial^2 f}{\partial \bar{\rho}^2}\right)_{\substack{T=0,\\ \bar{\rho}=\hat{\rho}}}, \quad \text{or} \quad v_{\hat{\rho}}^{-1} = -\left(\frac{\partial^2 w}{\partial \mu^2}\right)_{\substack{T=0,\\ \bar{\rho}=\hat{\rho}}}, \quad (18)$$

where we have adopted the idea of running coupling constant by taking $\hat{\rho}$ as some arbitrary fixed *nonzero* density. Were $\hat{\rho}$ taken as zero in equation (18), it would lead to the IR divergence. By equation (18), equations (12) and (17), it can be obtained that

$$v_{\rm b}^{-1} - v_{\hat{\rho}}^{-1} = \frac{l}{\mathcal{N}} \sum_{k} \frac{1}{2} \left(\frac{\partial^2 \omega_k}{\partial \mu^2} \right)_{\bar{\rho} = \hat{\rho}} = -\frac{l}{\mathcal{N}} \sum_{k} \frac{\epsilon_k^2}{2\hat{\omega}_k^3},\tag{19}$$

(15)

where $\hat{\omega}_k = \sqrt{\epsilon_k(\epsilon_k + 2\hat{\mu})}$, and $\hat{\mu}$ is not the actual chemical potential μ but the chemical potential that would correspond thermodynamically to zero temperature and particle density $\hat{\rho}$. Then by equations (12) and (19), we have

$$w = -\frac{\mu^2}{2v_{\hat{\rho}}} + \frac{l}{2\mathcal{N}} \sum_k \left[\omega_k - \epsilon_k - \mu + \frac{1}{2} \mu^2 \frac{\epsilon_k^2}{\hat{\omega}_k^3} \right] + l w_\beta, \tag{20}$$

where the last term $\frac{1}{2}\mu^2\epsilon_k^2/\hat{\omega}_k^3$ within the square parenthesis in the above summation is from the renormalization correction and remains finite at small k. Therefore we have escaped the IR divergence. Briefly speaking, the UV divergence in the continuum limit of the lattice model calls for renormalization for the sake of consistency between the unrenormalized grand potential w and the lattice boson model; and the IR divergence arouses the use of the running coupling constant $v_{\hat{\rho}}$.

By equation (19), for different renormalization points $\hat{\rho}$ and $\hat{\rho}'$, we observe that

$$-\frac{1}{v_{\hat{\rho}'}} + \frac{l}{\mathcal{N}} \sum_{k} \frac{\epsilon_k^2}{2\hat{\omega}_k'^3} = -\frac{1}{v_{\hat{\rho}}} + \frac{l}{\mathcal{N}} \sum_{k} \frac{\epsilon_k^2}{2\hat{\omega}_k^3}.$$

Thus the grand potential density w in equation (20) is invariant under changing the running renormalization point from $\hat{\rho}$ to $\hat{\rho}'$. Therefore, to the one-loop order ($\mathcal{O}[l^1]$), all the physical quantities derived from w are *renormalization invariants*; for example, the particle density $\bar{\rho}$ given by $\bar{\rho} = -\partial w/\partial \mu$,

$$\bar{\rho} \approx \frac{\mu}{v_{\hat{\rho}}} - \frac{l}{2\mathcal{N}} \sum_{k} \left[\frac{\epsilon_{k}}{\omega_{k}} - 1 + \frac{\mu \epsilon_{k}^{2}}{\hat{\omega}_{k}^{3}} \right] - l \frac{\partial w_{\beta}}{\partial \mu}.$$
(21)

It is noteworthy that the elementary excitation in this model is a 'phonon like quasi-particle (PLQP)' with linear spectrum at small momentum,

$$\omega_{\vec{k}} \stackrel{\kappa \sim 0}{\approx} v_{\rm s} k = \sqrt{J a^2 \mu} k. \tag{22}$$

To the tree level, the renormalized potential $v_{\bar{\rho}}$ and the *t*-matrix $t(\mu(\bar{\rho}))$ is basically the same. Therefore the differences between them are the renormalization (loop) corrections $(v_b - v_{\bar{\rho}})$ except that the divergent diagrams of ladder type which have already been handled in $t(\mu)$ should be excluded. To $O[l^1]$, this is the one-loop ladder diagram with its analytical expression as

$$l\frac{v_{\bar{\rho}}^2}{\mathcal{N}}\sum_{\vec{k}}\int_{-\infty}^{\infty}\frac{\mathrm{d}\omega}{2\pi}\frac{1}{\omega-(\epsilon_{\vec{k}}-\mu)+\mathrm{i}\delta}\frac{1}{-\omega-(\epsilon_{\vec{k}}-\mu)+\mathrm{i}\delta} = -l\frac{v_{\bar{\rho}}^2}{2\mathcal{N}}\sum_{\vec{k}}\frac{1}{\epsilon_{\vec{k}}-\mu}.$$
(23)

Thus, to the one-loop order, we have

1 0

$$v_{\bar{\rho}} - t(\mu(\bar{\rho})) = -\frac{lv_{\bar{\rho}}^2}{2\mathcal{N}} \sum_{\vec{k}} \left(\frac{\epsilon_k^2}{\omega_k (\mu(\bar{\rho}))^3} - \frac{1}{\epsilon_k - \mu(\bar{\rho})} \right).$$
(24)

The *t*-matrix of the lattice boson system $H(b^{\dagger}, b)$ (equation (5)) is [31]

$$t(\mu) = \frac{2Ja^2}{\frac{1}{2N}\sum_{\vec{k}}(2 - \sum_{x,y}\cos k_{\alpha}a - \frac{\mu}{J})^{-1}};$$
(25)

with
$$t(\mu) \sim \frac{8\pi J}{\ln \frac{2Ja^2}{\mu} - 1} \ll 1$$
, as $\mu \sim 0 \quad (h \to 2J)$, (26)

and
$$t(\mu) \to \infty$$
 monotonically, as $\mu \to 2J$ $(h \to 0)$. (27)

Unlike the field theories in real time (T = 0), in which loop expansion is a power series of a natural parameter \hbar [28], the expansion parameter l defined in equation (7) (a finitetemperature field model) is only a bookkeeping notation and should be set to be *unity* finally. Thereafter, the above loop expansions (equations (7), (9), and (20)) would then be identified as expansions in powers of $v_{\bar{\rho}}$ (or t); and they would still be valid *only if* $v_{\bar{\rho}}$ (or t) is a small quantity. This is the situation when μ is small ($h \rightarrow 2J$), and so is the density of the lattice boson $\bar{\rho}$ (noting that $\bar{\rho} \ll 1$, as $\mu \ll 1$). Thus, it corresponds to the *dilute boson approximation* which has been adopted in most analytical treatments of the three-dimensional hard-core boson model as well [13, 26, 29, 30, 19, 32]. Note that the dilute boson approximation (ρ , $\mu \ll 1$) in the lattice boson system is equivalent to the requirement that the strength h of the external magnetic field is close to 2J ($h \rightarrow 2J$) in the spin system.

The magnetization $\langle S_z \rangle = 1/2 - \bar{\rho}$ in the spin system can be obtained by combining equations (21), (24) and (25),

$$\langle S_z \rangle = \frac{1}{2} - \frac{\mu}{t(\mu)} - \frac{1}{2\mathcal{N}} \sum_{\vec{k}} \left[\frac{\epsilon_k}{\omega_k} - 1 + \frac{\mu}{\epsilon_k - \mu} \right] + \frac{1}{\mathcal{N}} \sum_{\vec{k}} \frac{\epsilon_k}{\omega_k} \frac{1}{e^{\beta\omega_k} - 1}, \qquad \text{for } h/J < 2.$$
(28)

In obtaining equation (28), we have set $\hat{\mu} = \mu$, and l = 1. Thus to the one-loop order, the magnetization $\langle S_z \rangle$ (equation (28)) is obtained and is finite in both the discrete case and the continuum limit. Please notice that at T = 0 both the second and the third terms on the RHS of the above equation contain the quantum corrections. By using the standard spin-wave approach [33] to the 2DS_{1/2}QXYM (equation (2)), the magnetization $\langle S_z \rangle_{sw}$ at T = 0 can be obtained,

$$\langle S_{z} \rangle_{\rm sw} = \frac{1}{2} - \frac{\mu}{4J} - \frac{1 - \frac{\mu}{2J}}{4\mathcal{N}} \sum_{k} \gamma_{k} \left\{ \sqrt{\frac{2 - \gamma_{k}}{2 - (1 - \frac{\mu}{2J})^{2} \gamma_{k}}} - 1 \right\},\tag{29}$$

where $\gamma_k = \cos(k_x) + \cos(k_y)$. On the RHS of equation (29), the first two terms are the result of the mean field calculation, and the third term is the spin wave correction, which is small in the limit $\mu \to 0$ ($h \to 2J$).

By noting that the grand potential density w (equations (11) and (9)) of the lattice boson system is, in fact, the free energy density of the spin system, the entropy per site s can then be obtained as

$$s = -\left(\frac{\partial w}{\partial T}\right)_{\mathcal{N}a^2 \text{ fixed}} = \frac{1}{\mathcal{N}} \sum_{k} \left[\frac{\beta \omega_k}{e^{\beta \omega_k} - 1} - \ln(1 - e^{-\beta \omega_k})\right].$$
 (30)

3. Discussions

By equations (28) and (30), some very distinctive phenomena can be predicted in the magnon superfluid state. In equation (28), the temperature correction term grows with increasing temperature, and so does the magnetization $\langle S_z \rangle$ (figure 1). For example, when h = 1.65J, $\langle S_z \rangle$ is increased by 5% as temperature increased from 0 to 0.34J. On the other hand, at constant temperature below T_c , the entropy per site *s* (equation (30)) grows with rising magnetization $\langle S_z \rangle$ driven by increasing the strength of the magnetic field (figure 2). For example, when *h* is increased from 1.5J to 1.9J, the entropy per site *s* is increased almost threefold while $\langle S_z \rangle$ is increased from 0.42 to 0.49.

The behaviours of magnetization $\langle S_z \rangle$ and entropy density *s* mentioned above seem abnormal but are not impossible, and are closely connected to the superfluidity of magnons; but before we make further explorations, it would be better to discuss the critical temperature



Figure 1. $\bar{\rho}$, ρ_n , ρ_s , and $\langle S_z \rangle$ versus T with h/J = 1.65 and $T_c/J = 0.34$.



Figure 2. $\langle S_z \rangle$, δS_z , and entropy per site $s \times 10$ versus *h* at T = 0.1J.

 T_c first. Two temperatures are responsible for determining T_c , the temperature T_S at which the supercomponent of magnon $\rho_s(T)$ (defined later in equation (33)) depletes (figure 3), i.e.,

$$\rho_{\rm s}(T_{\rm S}) = 0,\tag{31}$$

and $T_{\rm KT}$, the transition temperature of the Kosterlitz–Thouless transition occurring in a magnetic field. By numerical calculations of the above equation in different *h*, the thermal energy $T_{\rm S}$ can be fitted as $T_{\rm S} \approx 0.7 \times (2 - h/J) = 1.4 \times mv_{\rm s}^2/2$ (figure 3), where $m = (Ja^2)^{-1}$ is the 'mass' of magnons obtained from equation (16), while by a classical mean-field approximation the temperature $T_{\rm KT} \approx \frac{\pi J}{4}(1 - \frac{h^2}{4J^2})$ (figure 3). Both $T_{\rm S}$ and $T_{\rm KT}$ approach zero at the limit $h/J \rightarrow 2$. In the three-dimensional superfluid systems, there is only one transition temperature [29]. In our case, nevertheless, it is not clear yet whether $T_{\rm S}$ and $T_{\rm KT}$ are the same or not before we have included the vortex and do an analytical calculation or a quantum Monte Carlo computation of $T_{\rm KT}$ in an external magnetic field at finite temperature. But anyway, $T_{\rm c}$ should be the smaller one between $T_{\rm S}$ and $T_{\rm KT}$ if they are different.

On the other hand, those seemingly abnormal phenomena mentioned above can be understood in the following ways: the fact that the Mermin–Wagner theorem [16] rules out the presence of BEC in the two-dimensional boson system at finite temperatures does not exclude the possibility of the existence of superfluidity [17]. In the $2DS_{1/2}QXYM$ (equations (2)–(5)),



Figure 3. $T_{\rm S}$ versus *h* (when no vortex is present), and the classical mean field approximation of $T_{\rm KT}$ versus *h* ($T_{\rm KT} \approx \frac{\pi J}{4} (1 - \frac{h^2}{4J^2})$).

magnons are like hard-core bosons with elementary excitations of both PLQP and vortex. At temperature below T_c , the vortex density is very small and can be ignored [8]; then the partition function equation (7) can be viewed as that of a *grand* canonical ensemble of magnons with PLQP excitations only. In such a low-temperature region, almost all magnons move with speed less than v_s . By Landau's famous argument [29, 30], because of the *linearity* of the spectrum $\omega(\vec{k})$ at low momenta (equation (22)), the PLQP will not be excited if the speed of the disturbance is less than v_s . Therefore, magnons form a superfluid state. Due to SF, magnons can hence be divided into the *normal* component with density ρ_n , which has entropy, and the *super* component with density ρ_s , which has no entropy,

$$\rho_{\rm n} = \frac{\beta}{2Na^2} \sum_{\vec{k}} \frac{k^2 {\rm e}^{\beta \omega_k}}{({\rm e}^{\beta \omega_k} - 1)^2},\tag{32}$$

$$\rho_{\rm s} = \rho - \rho_{\rm n},\tag{33}$$

obtained by following a treatment analogous to that in [29].

3.1. $\langle S_z \rangle$ increases with T at constant h

As we mentioned earlier in the previous paragraph, at low temperatures, the partition function equation (7) can be viewed as that of a *grand* canonical ensemble of magnons. Accordingly, the average energy and magnon number are determined by conditions of the *reservoir* with which our system of magnons is in contact.

Below T_c , as the temperature T increases, the super component density ρ_s decreases, and the normal component density ρ_n increases, in order to increase the averaged entropy. This process can be viewed as exchanging magnons of the system with the reservoir: as temperature increases, the super component flows into the reservoir and decreases ρ_s ; and the normal component flows from the reservoir and increases ρ_n . Thus the system will warm up. But the super component flows with no viscosity and depletes faster than the supply of the normal component of magnons from the reservoir. This makes the total density $\bar{\rho} (=\rho_n + \rho_s)$ of magnons decrease as the system attains the new temperature. The fewer magnons, the less deviation of the spins, and this causes larger $\langle S_z \rangle (\langle S_z \rangle = 1/2 - \bar{\rho})$. Therefore the magnetization $\langle S_z \rangle$ increases with T (figure 1). As temperature approaches T_c , a finite fraction (~ several per cent) of magnons are heated up to move with speed larger than v_s . Thus a considerable number of PLQPs are excited, and this makes the thermal fluctuation intensified and decisive at $T \ge T_c$. At temperature above T_c , the superfluid component is exhausted, and the total density $\bar{\rho}$ (= ρ_n) increases with T. Thus $\langle S_z \rangle$ decreases as for normal spin systems (figure 1).

3.2. Entropy grows with h at constant T

In the magnon superfluid state, when the strength of the magnetic field *h* increases, $\langle S_z \rangle$ grows and $\bar{\rho}$ decreases. As in the usual gas system, the velocity of the PLQP, v_s , is proportional to the total density $\bar{\rho}$ of magnons ($v_s \propto \sqrt{\bar{\rho}}$, equations (22) and (21)); therefore, v_s decreases as *h* increases. Then it becomes easier to excite the PLQP by Landau's argument, and there exist more magnons moving faster than v_s . Thus the normal density ρ_n increases, and so does the entropy per site *s*. Therefore, the entropy per site *s* grows with the magnetization $\langle S_z \rangle$ as *h* increases (figure 2). But this does not violate the second law of thermodynamics: as *h* increases, the fluctuation of S_z , $\delta S_z \equiv \sqrt{\langle S_z^2 \rangle - \langle S_z \rangle^2}$ also rises (though slowly) with entropy (figure 2).

Note that it is because of the existence of ρ_s and the fact that it depletes faster than the supply of ρ_n from the reservoir that the decrease of $\bar{\rho}$ and the increase of ρ_n can occur simultaneously. As $T > T_c$, there is only ρ_n . Thus, like normal systems, as *h* increases, $\bar{\rho} = \rho_n$ decreases, and so does the entropy per site *s*.

3.3. Comparisons between the $2DS_{1/2}QXYM$ and $XCuCl_3$

In the above discussions, the 2DS_{1/2}QXYM is in a strong external magnetic field in \hat{z} so that the dilute limit of magnons can be met from the perspective of calculation. From the point of view of symmetry, an external magnetic field in \hat{z} can break the *mirror* symmetry in \hat{z} $(S_z \leftrightarrow -S_z)$; and the 2DS_{1/2}QXYM is then in an *ordered* state with a constant order parameter $\langle S_z \rangle \neq 0$ at low temperatures. 'Owing to symmetry breaking, the systems gain rigidity' [34]; hence, fluctuations in the ordered state may result in situations quite different from those in the *disordered* state. When no external magnetic field is present, the system is in a state with no (constant) long range order because of the symmetry property of the Hamiltonian and the fact that the low dimensionality causes strong classical fluctuation which is coupled with the enhanced quantum fluctuation due to the small spin (S = 1/2) [8]. Therefore, the magnetic field plays an essential role here. It should be noted that even though the mirror symmetry of S_{z} is broken by an external magnetic field in the z-direction, the U(1) symmetry of the Hamiltonian is still preserved in the $2DS_{1/2}QXYM$. Thus a superfluid state may exist. This is also due to the hard-core bosonic property of the magnon, and hence the excitation spectrum ω_k is linear at low k. The linearity of ω_k is essential to SF [29, 30]. This property is shared by both $2DS_{1/2}QXYM$ and $XCuCl_3$ [5].

Though the external field *h* is essential in forming quantum transitions in both $2DS_{1/2}QXYM$ and XCuCl₃, nevertheless, the functionality of the external field *h* is a bit different in the above two models. In XCuCl₃, the effect of *h* is to close the energy gap and a non-magnetic (singlet) state is the ground state of the magnon; while in the $2DS_{1/2}QXYM$, it is to break the mirror symmetry of S_z (and $-S_z$) to form a fully polarized ferromagnetic state with a constant long-range order $\langle S_z \rangle$ as the ground state. For this reason, $\langle S_z \rangle \propto \rho$ in XCuCl₃, and $\langle S_z \rangle \propto \frac{1}{2} - \rho$ in our model. But the qualitative behaviours of the magnon density ρ versus *T* in the above two systems are similar. The curve of the total density of magnons versus *T* in figure 1 may be reminiscent of the characteristic cusplike curve of magnetization versus *T* in XCuCl₃ [1].

4. Conclusions and future works

By using the equivalence between the spin 1/2 system and the lattice hard-core boson, and by applying the renormalization technique to the one-loop order, we have shown that there is a magnon superfluid state in the $2DS_{1/2}QXYM$ in a strong magnetic field along \hat{z} at low temperatures. In such a state, there appear some distinctive phenomena like magnetization increasing with temperature, and entropy growing with the magnetic field. Related physical interpretations are given. Our results are based on the dilute boson approximation in the lattice boson system, and this corresponds to the requirement that the strength of the external magnetic field in the spin system (equation (1)) is close to 2J.

Please notice that the one-loop renormalization corrections to both $\langle S_z \rangle$ (equation (28)) and *s* (equation (30)) are small (<1%). As we mentioned in section 2, the loop expansions should be identified as expansions in powers of $v_{\bar{\rho}}$ or $t(\mu)$ as *l* has been set as unity; and both parameters ($v_{\bar{\rho}}$ and $t(\mu)$) are small in the dilute approximation. Therefore, the one-loop calculation suffices for our study of those phenomena mentioned above.

We believe that by suitably defining the vacuum of magnons, the mechanism proposed in section 3.1 (magnon density first decreases and then increases as temperature increases at constant magnetic field) may also be relevant in understanding the field-induced magnetic ordering in the spin-gap systems like TlCuCl₃, KCuCl₃ [1], and other systems in which there is a superfluid state of magnons.

It is worth noting that in equation (1) the applied magnetic field *h* can be an external field, or an internal effective field due to some internal interactions. For a two-dimensional spin-1/2 ferromagnetic system with J = 0.55 meV, and an external magnetic field of 8 T, the critical temperature T_c is about 2.0–2.5 K.

In this paper, for simplicity, we have restricted our analysis within the range in which the temperature *T* is below T_c to avoid complications which may be caused by vortices. In the future, we plan to investigate situations $T \sim T_c$ to see how vortices would influence the magnon superfluid state, and to clarify what the transition temperature T_c should be (T_s or T_{KT}). Besides, there is a critical value $h_c(T)(\sim h_c(0) + \mathcal{O}[T^2])$ of the external field to close the energy gap for the field-induced ordering in XCuCl₃. The form of $h_c(T)$ for the field-induced superfluid state in our model will be left for further explorations.

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References

- [1] Oosawa A et al 1999 J. Phys.: Condens. Matter 11 265
- [2] Nikuni T et al 2000 Phys. Rev. Lett. 84 5868
- [3] Vyaselev O et al 2004 Phys. Rev. Lett. 92 207202
- [4] Rice T M 2002 Science **298** 760
- [5] Rüegg Ch et al 2003 Nature **423** 62
- [6] Endoh Y et al 1988 Phys. Rev. B 37 7443
- [7] Anderson P W 1987 Science 235 1196
- [8] Makivic M S 1992 Phys. Rev. B 46 3167
- [9] Sandvik A and Hamer C 1999 Phys. Rev. B 60 6588
- [10] Cuccoli A et al 2003 Phys. Rev. B 67 104414
 Cuccoli A et al 2003 Phys. Rev. Lett. 90 167205

- [11] Betts D D 1974 Phase Transitions and Critical Phenomena vol 3, ed C Domb and M S Green (London: Academic)
- [12] Matsubara T and Matsuda H 1956 Prog. Theor. Phys. 16 569
- [13] Friedberg R, Lee T D and Ren H C 1993 Ann. Phys. 228 52
- [14] Ma Y-Q 1998 Phys. Rev. B 58 282
- [15] Chang C C 2001 Ann. Phys. 293 111
- [16] Mermin N D and Wagner H 1966 Phys. Rev. Lett. 17
- [17] Crowell P A and Reppy J D 1993 Phys. Rev. Lett. 70 3291
- [18] Kittel C 1976 Introduction to Solid State Physics 5th edn (New York: Wiley) and references therein
- [19] Beliaev S T 1958 JETP USSR 34 417
- [20] Hugenholtz N M and Pines D 1959 Phys. Rev. 116 489
- [21] Chang C C and Friedberg R 1994 Phys. Rev. A 49 913
- [22] Fisher D S and Hohenberg P C 1988 Phys. Rev. B 37 4936
- [23] Hohenberg P C 1967 Phys. Rev. 158 383
- [24] Schick M 1971 Phys. Rev. A 3 1067
- [25] Lee T D and Yang C N 1959 Phys. Rev. 113 1165
- [26] Abrikosov A A, Gor'kov L P and Dzyaloshinsky I E 1965 Quantum Field Theoretical Methods in Statistical Physics (New York: Pergamon)
- [27] Friedberg R 1995 J. Math. Phys. 36 2675
- [28] Itzykson C and Zuber J-B 1985 Quantum Field Theory (New York: McGraw-Hill)
- [29] Landau L D and Lifshitz E 1980 Statistical Physics Part 2 (Oxford: Pergamon)
- [30] Huang K 1987 Statistical Mechanics 2nd edn (New York: Wiley)
- [31] Chang C C 2005 in preparation for publication
- [32] Wu T T 1959 Phys. Rev. 115 1390
- [33] Bernardet K et al 2002 Phys. Rev. B 65 104519 and [15] therein
- [34] Nagaosa N 1999 Quantum Field Theory in Condensed Matter Physics (Berlin: Springer)