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On coherent states and the Self-Consistent Harmonic Approximation

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ABSTRACT

We used the Self-Consistent Harmonic Approximation (SCHA) to study the thermodynamics of the precession magnetization in a two-dimensional isotropic ferromagnet. The SCHA treats the Hamiltonian in terms of the canonically conjugate operators S^z and φ (the azimuth angle) including renormalized temperature dependent parameters to take into account higher order interactions. It is well-known that in right conditions, a dynamic magnetic field is able to provide spin pumping and drives the system to a magnon Bose-Einstein condensation. The magnon condensate is a coherent state that presents minimal uncertainty for the S^z and φ operators. Consequently, $\langle S^z\rangle$ and $\langle\varphi\rangle$ should constitute natural fields to describe the model, which justifies the SCHA formalism. The results obtained are consistent with other theoretical and experimental works.

1. Introduction and motivation

Macroscopic quantum effects are one of the more fascinating phenomena of quantum physics. The main idea, theorized by Schrödinger in 1926, is to represent the quantum state of the harmonic oscillator model by coherent states where the momentum and position uncertainties are minimal. In this way, the coherent states are the closest states to classical physics that also keep their full quantum nature. Bose-Einstein condensation (BEC), superfluid helium-4, and superconductivity are consequences of quantum coherent states [1]. More recently, magnon Bose-Einstein condensation (mBEC) [2–8] and spin-superfluidity [9–11] have been used to arouse interest in the physics community due to the fast development of spintronic [12,13]. However, different from the more traditional models, which treat real particle systems, the magnetic condensed matter models consider the controversial BEC and superfluidity of spin collective modes (magnons in general). The ephemeral lifetime and the non-conservation of the collective modes make the observation of coherence phenomena in magnetic materials a laborious process. Demokritov et al. have experimentally shown the condensation of magnons in a quasi-equilibrium process at room temperature [2,6]. Using the microwave pumping technique in yttrium-iron-garnet (YIG) films, they created a gas of magnons where the number of excited modes is conserved for a very short time. Therefore, as long the chemical potential is finite, the magnon BEC state occurs but after some hundred microseconds, magnon-phonon scatterings dissipate the spin fluctuations and the model reaches the thermodynamic equilibrium. Representing the spin operator by Holstein-Primakoff bosons and adopting coherent states, Rezende presented a model for magnon BEC in YIG films [14–16]. In this case, all spins coherently process around a static planar magnetic field and the magnetization can be considered as a classical vector. The spin-superfluidity is a more delicate question. Different from the helium atoms in mass superfluidity and electrons in superconductivity, the spin conservation is not guaranteed and there is no consensus as to how define a spin current density [11]. However, if one considers models where processes that violate spin law conservation are weak, the adoption of a spin continuity equation as well as a spin current density is natural and the development of spin-superfluidity is similar to mass superfluidity [17].

In this work, we applied the coherent states formalism and the Self-Consistent Harmonic Approximation (SCHA) [18–23] to describe the thermodynamics of two-dimensional ferromagnets in a coherent state. When compared with other bosonic formalisms, the SCHA has the advantage of including higher order interactions by introduction of renormalized temperature dependent parameters and, at the same time, keeps the quadratic structure of the Hamiltonian. Besides, in many situations, the SCHA is an efficient method to determine the Berezinskii-Kosterlitz-Thouless (BKT) temperature [20,21]. The magnetic model is described by the time-independent Heisenberg Hamiltonian

$$H = -J\sum_{\langle ij\rangle}\vec{S}_i\cdot\vec{S}_j - g\mu_B B_s\sum_i S_i^x, \tag{1}$$

where the first sum is done over nearest neighbors and the second term is the Zeeman energy associated with a uniform static magnetic field $\vec{B} = B_s\hat{x}$. Here, we adopted the z-axis perpendicular to the plane defined by the two-dimensional ferromagnet. A dynamic magnetic field is required to generate a magnetization precession, so we added the time-dependent interaction $V(t) = -g\mu_B\sum_i B_i(t)\theta(t-t_0)S_i^z$, which will be

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treated as a perturbation in Section (3). In YIG films, the most used ferromagnetic insulator in experiments due to its small magnetic losses, it is also necessary to consider dipolar interactions to properly describe the magnon spectrum [14,15]. However, we considered a simpler ferromagnet model where the exchange interaction is dominant. Despite small differences that should appear in the magnon spectrum due to dipolar interactions, the results obtained from Eq. (1) are according to the expected ones. It is important to note that we have considered a two-dimensional model but the method is general and can be applied to three-dimensional model as well.

In the imaginary time path integral formalism, the partition function for a spin model is expressed as $\mathscr{Z} = \int D\Omega e^{-\mathscr{S}}$, being the action given by

$$\mathscr{S} = \int_0^{\beta\hbar} d\tau \left(\left\langle \vec{\Omega} \middle| \partial_\tau \vec{\Omega} \right\rangle + \frac{1}{\hbar} \left\langle \vec{\Omega} \middle| H \middle| \vec{\Omega} \right\rangle \right), \tag{2}$$

where $|\vec{\Omega}\rangle$ represents the spin coherent state [24]. The integration measure $D\Omega$ includes integration over all closed paths with $\vec{\Omega}_i(0) = \vec{\Omega}_i(\beta\hbar)$ for each site i. The first term, the so-called Berry phase, carries all quantum information about the model. This phase describes the solid angle subtended by the closed path when the vector $|\vec{\Omega}\rangle$ evolves from $\tau = 0$ to $\tau = \beta\hbar$. If quantum fluctuations are not relevant and the phase is not considered, the action becomes a classical model in (d + 1)-dimensional space. The second term in $\mathscr{S}$ is the representation of the Hamiltonian in spin coherent states, where spin operators are replaced by spin fields. In the classical point of view, the spin fields can be parameterized by the S^z component and the azimuth angle φ, which obey the Poisson bracket $\{\varphi_i, S_j^z\} = \delta_{ij}$. Hence, φ and S^z are canonically conjugate variables and they should play a role similar to position and momentum. Indeed, when we treat S^z and φ as operators, they satisfy the commutation relationship $[\varphi_i, S_j^z] = i\hbar\delta_{ij}$. It is a straightforward procedure to show that the Berry phase can be written as $-iS_i^z\partial_\tau\varphi_i$, identical to the term $-ip\partial_\tau x$ present in the path integral for particles. Therefore, it would be convenient to express $\langle\vec{\Omega}|H|\vec{\Omega}\rangle$ also in terms of φ and S^z, which is provided by the SCHA. Besides, the coherent state yields expected values $\langle\vec{\Omega}|S^z|\vec{\Omega}\rangle$ and $\langle\vec{\Omega}|\varphi|\vec{\Omega}\rangle$ with minimal uncertainties and so it is natural to consider the φ and S^z fields as the most appropriated classical fields to describe the quantum model in a coherent space.

In Fig. (1) we show the dynamic of spin precession along the x-axis. In the absence of magnetic fields, the Hamiltonian (1) has an O(3) symmetry but when the static magnetic field is turned on, the symmetry is broken and, in the ground state, the spins align along the x-axis. The new O(2) symmetry is associated with the angle ϕ of the precession induced by the magnetic field $\vec{B}(t) = B(t)\hat{z}$. It is important to note that the energy is invariant to the precession angle and any point on the ring defined by the fixed polar angle has the same energy, as shown in Fig. (1)b. Naturally, the precession state is not an equilibrium state due to the spin relaxation and continuous spin pumping is required to conserve the precession dynamic. If we consider that the relaxation spin

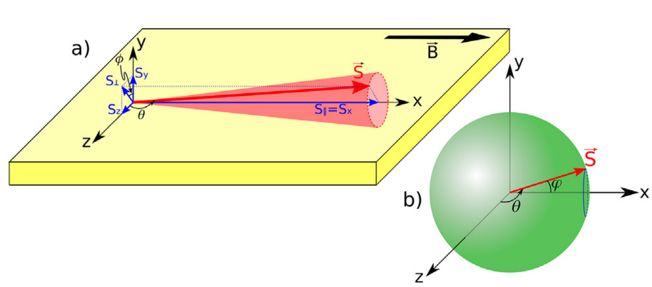

Fig. 1. (a) The precession dynamic of a spin subject to a static magnetic field oriented along the x-axis. (b) Representation of the internal spin space. During the precession, the spin rotates along the x-axis at a constant θ angle.

processes are weak, we can adopt the precession as a quasi-equilibrium state. Hence, we treated $\vec{S}$ as a classical vector and wrote $\vec{S}_{\rm cl} = (S_\parallel, S_\perp\cos\phi, S_\perp\sin\phi)$, where $S_\parallel$ and $S_\perp$ are respectively the longitudinal and transverse component and ϕ is the precession angle. Here, the precession O(2) symmetry is equivalent to the U(1) symmetry of the wave function of the particles in a bosonic system of real particles. It is well known that the U(1) symmetry is spontaneously broken in the mass superfluid phase and a similar spontaneous broken symmetry should occur in a spin superfluid phase [11].

2. Self-Consistent Harmonic Approximation

The structure of the path integral for spin models suggests us to represent the spin operators S^x and S^y a as function of S^z and φ (different from the precessing angle ϕ). Therefore, we adopted the Villain representation [18] $S_i^+ = e^{i\varphi_i}\sqrt{\tilde{S}^2 - S_i^z(S_i^z+1)}$ and $S_i^- = \sqrt{\tilde{S}^2 - S_i^z(S_i^z+1)}\,e^{-i\varphi_i}$, where $\tilde{S} = \sqrt{S(S+1)}$. Due to the static magnetic field along the x-axis, we considered $S^z/\tilde{S} \ll 1$ as well as $\varphi \ll 1$ and, after performing an expansion until the second order in S^z and φ, we obtained the quadratic Hamiltonian

$$H_0 = J\sum_{\langle ij\rangle}\left[\frac{\rho\tilde{S}^2}{2}(\varphi_j-\varphi_i)^2 - S_i^z S_j^z + S_i^z S_i^z\right] + g\mu_B B_s\sum_i\left[\frac{1}{2\tilde{S}}(S_i^z)^2 + \frac{\zeta\tilde{S}}{2}\varphi_i^2\right] \tag{3}$$

where ρ and ζ are temperature dependent parameters added to take into account higher order terms in the harmonic approximation [14]. They are determined through the Bogoliubov variational principle. If we define F as the Helmholtz free energy for the original Hamiltonian and F_0 as the free energy for the quadratic Hamiltonian then, ρ and ζ should be chosen to satisfy the inequality $F \leqslant F_0 + \langle H - H_0\rangle_0$, where the mean-value is evaluated using the harmonic Hamiltonian. Such a procedure provides the self-consistent equations

$$\rho = \left[1 - \left\langle\left(\frac{S_i^z}{\tilde{S}}\right)^2\right\rangle_0\right] e^{-\frac{1}{2}\left\langle\left(\varphi_j-\varphi_i\right)^2\right\rangle_0} \tag{4}$$

and

$$\zeta = \left[1 - \frac{1}{2}\left\langle\left(\frac{S_i^z}{\tilde{S}}\right)^2\right\rangle_0\right] e^{-\frac{1}{2}\left\langle\varphi_i^2\right\rangle_0} \tag{5}$$

The Hamiltonian H_0 can be diagonalized by Fourier transformation in space and the definition of new bosonic operators a_q and $a_q^\dagger$

$$\varphi_q = \frac{1}{\sqrt{2}}\left(\frac{H_q^z}{H_q^\varphi}\right)^2\left(a_q^\dagger + a_{-q}\right) \tag{6}$$

$$S_q^z = \frac{i}{\sqrt{2}}\left(\frac{H_q^\varphi}{H_q^z}\right)^2\left(a_q^\dagger - a_{-q}\right), \tag{7}$$

where we defined the coefficients $H_q^\varphi = 4J\tilde{S}^2\rho(1-\gamma_q) + \zeta\tilde{S}g\mu_B B_s/2$ and $H_q^z = 4J[1-\gamma_q] + g\mu_B B_s/2\tilde{S}$ with $\gamma_q = (\cos q_x + \cos q_y)/2$ being the structure factor for the two-dimensional square lattice (we adopted unitary lattice parameter). Note that if we write the action as

$$\mathscr{S} = \sum_q \int_0^{\beta\hbar} d\tau \begin{pmatrix}\varphi_{-q} & S_{-q}^z\end{pmatrix} G_q^{-1}(\tau) \begin{pmatrix}\varphi_q \\ S_q^z\end{pmatrix} \tag{8}$$

then H_q^z and H_q^φ are the time-independent part of the Green's function defined by