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Macroscopic Quantum Coherence of an Antiferromagnetic Spin Chain with Biaxial Anisotropy in an External Magnetic Field

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Abstract We in this paper provide a sine-Gordon model of (1 + 1)-dimensions in which macroscopic quantum coherence of domain walls may be observed. The tunneling amplitude in field models of (1 + 1)-dimensions, such as sine-Gordon, is negligible small at zero temperature. In the *long, but finite-length* chain at finite temperature it is possible to have a *finite, but still very small* one. In the present model of the antiferromagnetic spin chain with biaxial anisotropy in an external magnetic field, in which the height of the sine-Gordon barrier can be tuned, the tunneling amplitude is shown to be enhanced by adjusting the external parameter.

Keywords Macroscopic quantum coherence · Antiferromagnetic spin chain

1 Introduction

Macroscopic quantum tunneling phenomena have attracted considerable interest because of its wide application in areas ranging from condensed matter to high energy physics and cosmology [1]. The two main types of phenomenon considered in literature are macroscopic quantum tunneling in which the system in question tunnels out of a metastable potential well into a true ground state, and macroscopic quantum coherence in which it performances coherent oscillations between two degenerate wells separated by a classically impenetrable barrier.

The instanton method [2, 3] is a powerful tool for the calculation of tunneling effects. Instantons, which are classical Euclidean configurations with finite Euclidean action, are seen to be just the classical trajectories of pseudoparticles existing in the potential barrier region and not actual field configurations of real time. The tunneling amplitude between two relevant states is, however, dominated by the instanton configurations in the semiclassical expansion of the functional integral. In the context of quantum mechanics the instantons, which are obtained from (1 + 0)-dimensional Euclidean equation of motion, have been well

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studied for various potentials such as double-well [4], sine-Gordon [5] etc. Recently the quantum tunneling of magnetization vector in single domain ferromagnetic grain and Néel vector in single domain antiferromagnetic grain has become an active research field [6, 7] both theoretically and experimentally. With the help of spin-coherent-state path integrals the spin systems can be converted to typical potential tunneling models of $(1+0)$-dimension.

Although quantum tunneling in the context of field theory, for instance the tunneling of domain walls [8–18], has been investigated, the explicit, multidimensional (time-space) instanton configurations have not been studied extensively. In almost all the literature, a collective coordinate of the domain wall is introduced to describe the behavior of quantum tunneling, or the situation is simplified to the case of a uniform spin configuration, namely, single domain magnetic grain. In fact, it has been reduced to the one-particle problem of quantum mechanics in these description. In the present paper we give the instanton configuration of $(1+1)$-dimensions and demonstrate the macroscopic quantum coherence of the degenerate orientations of the Néel vectors in a continuous antiferromagnetic spin chain of biaxial anisotropy with an external magnetic field. In [17], the authors have studied the macroscopic quantum tunneling in an antiferromagnetic spin chain and given the pure-quantum-tunneling configuration for the sine-Gordon model. But in this paper, we investigate the finite-temperature effects, namely, the thermally assisted quantum tunneling. Furthermore, the tunneling amplitude we obtained explicitly can be controlled by the external field.

The paper is organized as follows: in Sect. 2, we introduce the model of antiferromagnetic spin chain with biaxial anisotropy in an external magnetic field and the equation of motion is reduced to the $(1+1)$-dimensional sine-Gordon field equation in strong-anisotropy limit. In Sect. 3, the instanton configuration and the corresponding tunneling amplitude are obtained analytically. Finally, we summarize our result in Sect. 4.

2 Model

We consider an antiferromagnetic spin chain with biaxial anisotropy in an external magnetic field, which is oriented along the x direction. A model Hamiltonian is described by

$$\hat{H} = J\Sigma_n \hat{S}_n \cdot \hat{S}_{n+1} + K_1 \Sigma_n \left(\hat{S}_n^z\right)^2 - K_2 \Sigma_n \left(\hat{S}_n^x\right)^2 - g\mu_B B_x \Sigma_n \hat{S}_n^x, \tag{1}$$

where $J > 0$ is the exchange parameter, K_1 and K_2 are the anisotropy parameters with $K_1 > K_2 > 0$, g is the Landé factor, μ_B is the Bohr magneton.

In the large-spin limit, the spin operators can be treated as fixed-length classical vectors, with spherical coordinate [19]

$$\hat{S}_n = \vec{S}_n = (-1)^n \hbar S \left(\sin\theta_n \cos\varphi_n, \sin\theta_n \sin\varphi_n, \cos\theta_n\right), \tag{2}$$

where $S = s(s+1)\hbar$ with s the spin quantum number.

The classical equations of motion for the dynamical variables θ_n and φ_n are easily obtained from (1) by using the Poisson-bracket $\{\varphi_n, S_{n'}^z\} = \delta_{nn'}$, $\dot{\varphi}_n = \{\varphi_n, H\}$, etc.,

$$\begin{aligned}\frac{\partial\theta_n}{\partial t} = -\frac{1}{2}\omega(-1)^n \Sigma_\pm \Big[&\sin\theta_{n\pm1}\sin\left(\varphi_{n\pm1} - \varphi_n\right) \\ &- \frac{\kappa_2}{2}\sin\theta_n \sin\varphi_n \cos\varphi_n - (-1)^n \frac{b_x}{2}\sin\varphi_n\Big],\end{aligned} \tag{3}$$

$$\frac{\partial \varphi_n}{\partial t} = -\frac{1}{2}\omega(-1)^n \Sigma_{\pm}\Big[\cos\theta_{n\pm1} - \cot\theta_n \sin\theta_{n\pm1}\cos(\varphi_{n\pm1}-\varphi_n) - \frac{\kappa_1}{2}\cos\theta_n - \frac{\kappa_2}{2}\cos\theta_n\cos^2\varphi_n - (-1)^n\frac{b_x}{2}\cos\varphi_n\cot\theta_n\Big], \tag{4}$$

where we have introduced the notation

$$\omega = 2J\hbar S, \qquad \kappa_1 = \frac{2K_1}{J}, \qquad \kappa_2 = \frac{2K_2}{J}, \qquad b_x = \frac{g\mu_B B_x}{J\hbar S}. \tag{5}$$

To make progress with these equations, we assume that θ_n and φ_n vary slowly with n, with a small superimposed staggered-fluctuation components; this should be valid at low temperatures [19, 20]:

$$\theta_n = \theta(x) + a(-1)^n\alpha(x), \qquad \varphi_n = \varphi(x) + a(-1)^n\beta(x), \quad x = na, \tag{6}$$

where a is the lattice constant. $\theta(x)$ and $\varphi(x)$ are continuous varying angle fields, while $\alpha(x)$ and $\beta(x)$ are small staggered-fluctuation fields, chosen to have dimensions of density.

The variables at nearest-neighboring sites can be expressed through Taylor-series expansion about $x = na$. Up to second order in α, β, and $\frac{\partial}{\partial x}$, each equation (3) and (4) yields two independent equations of motion (for the uniform and staggered parts):

$$\frac{2}{c}\left(\frac{\partial\theta}{\partial t}\right) = 4\beta\sin\theta + \kappa_2\left(\frac{\alpha}{2}\cos\theta\sin 2\varphi + \beta\sin\theta\cos 2\varphi\right) + b_x\sin\varphi, \tag{7}$$

$$\frac{2}{c}\left(\frac{\partial\varphi}{\partial t}\right) = -\frac{4\alpha}{\sin\theta} - \kappa_1\alpha\sin\theta - \kappa_2\left(\beta\cos\theta\sin 2\varphi + \alpha\sin\theta\cos^2\varphi\right) + b_x\cot\theta\cos\varphi, \tag{8}$$

$$\frac{2}{c}\left(\frac{\partial\alpha}{\partial t}\right) = -4\alpha\beta\cos\theta - 2\cos\theta\left(\frac{\partial\theta}{\partial x}\right)\left(\frac{\partial\varphi}{\partial x}\right) - \sin\theta\frac{\partial^2\varphi}{\partial x^2} + \frac{\kappa_2}{2}\sin\theta\sin 2\varphi + b_x\beta\cos\varphi, \tag{9}$$

$$\frac{2}{c}\left(\frac{\partial\beta}{\partial t}\right) = 4\alpha^2\frac{\cos\theta}{\sin^2\theta} - \cos\theta\left[\left(\frac{\partial\varphi}{\partial x}\right)^2 + 4\beta^2\right] + \frac{1}{\sin\theta}\frac{\partial^2\theta}{\partial x^2} + \kappa_1\cos\theta\left(\frac{1}{a^2} - \frac{\alpha^2}{2}\right) + \kappa_2\cos\theta\cos^2\varphi - b_x\left(\alpha\frac{\cos\varphi}{\sin^2\theta} + \beta\cot\theta\sin\varphi\right), \tag{10}$$

where $c = \omega a$ is the long-wavelength spin-wave velocity [20]. Here and after, we take a as unit of length.

In terms of the fields introduced above and applying continuum approximation to the Hamiltonian given in (1) we rewrite

$$H = J\hbar^2 S^2 + \frac{1}{2}J\hbar^2 S^2\int dx\,[h_{\mathrm{exc}}(x) + h_{\mathrm{aniso}}(x) + h_{\mathrm{Zeeman}}(x)], \tag{11}$$

where

$$h_{\text{exc}} = \left(\frac{\partial\theta}{\partial x}\right)^2 + 4\alpha^2 + \sin^2\theta\left[\left(\frac{\partial\varphi}{\partial x}\right)^2 + 4\beta^2\right],$$
$$h_{\text{aniso}} = \kappa_1\left[\cos^2\theta + \alpha^2(1-2\cos^2\theta)\right] - \kappa_2\sin^2\theta\cos^2\varphi, \tag{12}$$
$$h_{\text{Zeeman}} = 2b_x\left(\beta\sin\theta\sin\varphi - \alpha\cos\theta\cos\varphi\right).$$

In the strong-anisotropy limit $K_1 \gg K_2$, the spins are nearly confined to the xy plane and our equations of motion can be further linearized about $\theta = \frac{\pi}{2}$. Introducing that $\theta_s = \frac{\pi}{2} - \theta$ and linearize (7) and (8) in θ_s, we obtain

$$\frac{\partial\theta_s}{\partial t} = -\frac{c}{2}[4\beta + b_x\sin],$$
$$\frac{\partial\varphi}{\partial t} = -\frac{c}{2}(4+\kappa_1)\alpha, \tag{13}$$

where we have assumed that b_x is small.

Before discussing the remaining equations of motion, it is instructive to consider the Hamiltonian density following from (11) after using the equations above to eliminate α and β:

$$h(x) = h_{\theta_s}(x) + h_\varphi(x), \tag{14}$$

where

$$h_{\theta_s}(x) = \frac{1}{2}J\hbar^2S^2\left[\frac{1}{c^2}\left(\frac{\partial\theta_s}{\partial t}\right)^2 + \left(\frac{\partial\theta_s}{\partial x}\right)^2 + \kappa_1\theta_s^2\right],$$
$$h_\varphi(x) = \frac{1}{2}J\hbar^2S^2\left[\frac{1}{c_t^2}\left(\frac{\partial\varphi}{\partial t}\right)^2 + \left(\frac{\partial\varphi}{\partial x}\right)^2 + \left(\kappa_2 - \frac{1}{4}b_x^2\right)\sin^2\varphi\right], \tag{15}$$

where $c_t = (4+\kappa_1)^{1/2}c/2$ and we have neglected higher-order coupling terms. Here and after, all the constant terms are omitted.

The corresponding Lagrangian density is easily obtained

$$\pounds = \pounds_{\theta_s}(x) + \pounds_\varphi(x), \tag{16}$$

where

$$\pounds_{\theta_s}(x) = J\hbar^2S^2\left[\frac{1}{2c^2}\left(\frac{\partial\theta_s}{\partial t}\right)^2 - \frac{1}{2}\left(\frac{\partial\theta_s}{\partial x}\right)^2 - \frac{1}{2}\kappa_1\theta_s^2\right],$$
$$\pounds_\varphi(x) = J\hbar^2S^2\left[\frac{1}{2c_t^2}\left(\frac{\partial\varphi}{\partial t}\right)^2 - \frac{1}{2}\left(\frac{\partial\varphi}{\partial x}\right)^2 - V(\varphi)\right], \tag{17}$$

where $V(\varphi) = \frac{m}{4}(1-\cos 2\varphi)$ with $m = (\kappa_2 - \frac{1}{4}b_x^2)$. A quasi-classical rotation of Néel vector may occur in any plane θ_s=constant [17, 18] and we take it to be zero in the limit of strong anisotropy. The dynamics of the in-plane degree of freedom is therefore reduced to the sine-Gordon model with mass parameter m. The equation of motion for φ then is

$$\frac{\partial^2\varphi}{\partial x^2} - \frac{1}{c_t^2}\frac{\partial^2\varphi}{\partial t^2} = \frac{m}{2}\sin 2\varphi. \tag{18}$$

In the absent of the external field, the sine-Gordon model is just the same with that in the ferromagnetic spin chain with biaxial anisotropy [21]. As a consequence of the square term $(\hat{S}_i^x)^2$, the two equilibrium orientations of the magnetization along the $\pm x$ directions are degenerate, despite the ferromagnetic or antiferromagnetic interactions. The effect of the external magnetic field is dramatically different for ferromagnetic or antiferromagnetic ones. For antiferromagnetic spin chain, the external field oriented along the $+x$ direction forces the sublattice magnetization into the $\pm x$ directions [20] and hence lowers the barrier height of the sine-Gordon potential density effectively. This allow us to obtain the tunneling rate explicitly. But for ferromagnetic spin chain, the same external field configuration would result in a rather complicated effective potential density [8].

3 Instanton and Macroscopic Quantum Coherence of Domain Walls

The instanton is a solution of Euclidean field equation of motion

$$\frac{\partial^2\varphi}{\partial x^2}+\frac{\partial^2\varphi}{c_t^2\partial\tau^2}=\frac{m}{2}\sin(2\varphi), \tag{19}$$

for the Euclidean Lagrangian density $\pounds_e = J\hbar^2 S^2[\frac{1}{2c_t^2}(\frac{\partial\varphi}{\partial\tau})^2+\frac{1}{2}(\frac{\partial\varphi}{\partial x})^2+V(\varphi)]$, where $\tau = it$ is imaginary time. We look for the trial solution $\varphi(\xi)$ with $\xi = x - v\tau$, where v is the velocity of the instanton. Then we have

$$\left[1+\left(\frac{v}{c_t}\right)^2\right]\left(\frac{d^2\varphi}{d\xi^2}\right)=\frac{m}{2}\sin(2\varphi). \tag{20}$$

Multiplying with the term $(\frac{d\varphi}{d\xi})$ and integrating over the variable ξ, the equation of motion is seen to be

$$\frac{1}{2}\left[1+\left(\frac{v}{c_t}\right)^2\right]\left(\frac{d\varphi}{d\xi}\right)^2-V(\varphi)=-E_{cl}, \tag{21}$$

where the integration constant E_{cl} plays the role of dimensionless energy density. We want to get the instanton configuration with the energy parameter confined in the region $0 < E_{cl} < \frac{m}{2}$, namely, $E_{cl} = \frac{m}{2}(1-k^2)$ with $0 < k < 1$. Then we get

$$\left(\frac{d\varphi}{d\xi}\right)^2=\frac{m}{[1+(v/c_t)^2]}\left(k^2-\cos^2\varphi\right). \tag{22}$$

By direct integration [22], the instanton configuration is obtained as

$$\cos[\varphi(x,\tau)] = k\,\mathrm{sn}\left[\pm\frac{\sqrt{m}(x-v\tau-x_0)}{\sqrt{1+(v/c_t)^2}},k\right], \tag{23}$$

where sn is Jacobian elliptic function [22] with modulus $k=\sqrt{1-2E_{cl}/m}$. The integration constant x_0 is the centre position of the instanton at $\tau = 0$. Under the initial condition that $\varphi(x=0,\tau=0)=\pi/2$, it is zero.

We demand that $\varphi(x, \tau)$ be periodic with period L along the spin chain, $\varphi(x,\tau) = \varphi(x+L,\tau)$, where L denotes the dimensionless length of the chain measured in unit of lattice constant. This leads to the condition

$$\frac{\sqrt{m}L}{\sqrt{[1+(v/c_t)^2]}} = 4nK(k), \tag{24}$$

where $n = 1, 2, 3, \ldots$ are positive integer and $K(k)$ denotes the complete elliptic integral of the first kind [22].

The periodic solution in 1-dimensional space with spatial period L are equivalent to the solution in a ring of circumstance L. It then can be viewed as in the spin chain ring. We also would like to note here that the length of the chain should be large enough to meet the periodic condition.

In statistical mechanics, the mathematical analogy of the density matrix [23] and the transition amplitude in imaginary time offer the period of the periodic instanton at given temperature T [7]

$$p = \frac{\hbar}{K_B T} = \frac{4K(k)\sqrt{[1+(v/c_t)^2]}}{\sqrt{m}v}, \tag{25}$$

where $\hbar$ and K_B are the Planck and the Boltzmann constant, respectively. The parameter k is to be determined from the above two equations. Then we have

$$v = \frac{K_B T L}{n\hbar}, \tag{26}$$

namely, the velocity of the instanton is quantized due to the periodic boundary condition.

Inserting (26) into (25), we obtain the dependence relation of k on temperature T

$$K(k) = \frac{L\sqrt{m}}{4n}\frac{1}{\sqrt{[1+(\frac{K_B T L}{n\hbar c_t})^2]}}. \tag{27}$$

Then we have the T-dependent energy density $E_{cl}(T) = \frac{m}{2}(1-k^2)$.

For $k \to 0$, the energy parameter $E_{cl} \to m/2$. In this limit, the configuration tends to the top of the potential density $V(\varphi)$,

$$\varphi^t = \frac{\pi}{2}, \tag{28}$$

and for $k \to 1$, i.e., $E_{cl} \to 0$, the solution becomes

$$\varphi^0(x,\tau) = \arccos\left\{\tanh\left[\pm\frac{\sqrt{m}(x-v\tau)}{\sqrt{1+(v/c_t)^2}}\right]\right\}. \tag{29}$$

The tunneling amplitude for the domain wall is

$$\Gamma(T) \sim \exp\left(-\frac{W(T)}{\hbar}\right), \tag{30}$$

where the Euclidean action for the periodic instanton configuration (23) is

$$\begin{aligned} W(T) &= \int_0^p d\tau \int_0^L dx \pounds_e \\ &= \frac{2n\sqrt{m}J\hbar^3 S^2}{K_B T}\left[2E(k) - k'^2 K(k)\right]\sqrt{1+\left(\frac{K_B T L}{n\hbar c_t}\right)^2} \\ &= \frac{2n\sqrt{m}J\hbar^3 S^2}{K_B} F(k)\sqrt{\frac{1}{T^2}+\left(\frac{K_B L}{n\hbar c_t}\right)^2}, \end{aligned} \tag{31}$$

where $k' = \sqrt{1-k^2}$ and $E(k)$ denotes the complete elliptic integral of the second kind.

The function $F(k) = 2E(k) - k'^2 K(k)$ is monotonic and increase from $\pi/2$ to 2 for $0 < k < 1$. Thus it can be treated as a constant when analyzing the dependence relation of the Euclidean action W on T and L. The lower the temperature is, the smaller the tunneling amplitude of the domain wall is. In the limit of $T \to 0$, we have an infinite action, implying that the energy splitting of the degenerate vacuum states, which is proportional to Γ, is negligible small, in accord with the existing results in literature [3] and [17] (in the limit of $\Delta V \to 0$ of (24) there). Similarly, the longer the spin chain is, the smaller the tunneling amplitude is. It is possible to have a *finite, but still very small* tunneling amplitude in a *long, but finite-length* antiferromagnetic spin chain with biaxial anisotropy in a weak external field at finite temperature.

It is interesting to find that the Euclidean action $W(T) \propto \sqrt{m} = \sqrt{\kappa_2 - \frac{1}{4}b_x^2}$, which can be controlled by adjusting the intensity of the external magnetic field. With the increase of the intensity, namely, the decrease of $\sqrt{m}$, we have smaller Euclidean action, consequently, larger tunneling amplitude. The above result can also be understood in terms of the potential density $V(\varphi) = \frac{m}{4}(1 - \cos 2\varphi)$. Obviously, the height of the barrier is determined by the parameter m. The lower the barrier is, the easier the tunneling happens.

4 Summary

We in the present paper provide a model of $(1+1)$-dimensions in which macroscopic quantum coherence of domain walls may be observed. The tunneling amplitude obtained explicitly can be enhanced by adjusting the external parameter. This should be in other branches of the macroscopic quantum effect [1].

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