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Macroscopic quantum coherence of the Neel vector in antiferromagnetic system without Kramers' degeneracy

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Abstract. At low temperatures the Neel vector in a small antiferromagnetic particle can possess quantum coherence between the classically degenerate minima. In some cases, the topological term in the magnetic action can lead to destructive interference between the symmetry-related trajectories for the half-integer excess spin antiferromagnetic particle. By studying a macroscopic quantum coherence problem of the Neel vector with biaxial crystal symmetry and a weak magnetic field applied along the hard axis, we find that the quenching of tunnel splitting could take place in the system without Kramers' degeneracy. Both the Wentzel-Kramers-Brillouin exponent and the pre-exponential factors are found exactly for the tunnel splitting. Results show that the tunnel splitting oscillates with the weak applied magnetic field for both the integer and half-integer excess spin antiferromagnetic particles, and vanishes at certain values of the field. All the calculations are performed based on the two sublattices model and the instanton method in spin-coherent-state path integral.

PACS. 75.10.Jm Quantized spin models – 73.40.Gk Tunneling – 75.50.Ee Antiferromagnetics

Macroscopic quantum phenomena (MQP) have been given extensive investigations for more than a decade since the fascinating prediction of Leggett and Caldeira. They found that the quantum tunneling could take place on the macroscopic scale if the dissipation due to the interactions of the macroscopic system with the environment was small enough [1,2]. MQP are largely classfied into macroscopic quantum tunneling (MQT) and coherence (MQC). MQT corresponds to the simple tunneling of a macroscopic variable through the barrier between two minima of the effective potential, while MQC corresponds to the resonance between the energetically degenerate states. The prediction of Leggett and Caldeira turned out to be in excellent agreement with the experiment carried out on the single electron tunneling at IBM, Yorktown Heights [3]. In recent years, owing mainly to the development in materials preparation techniques on nanometer-size magnetic particles, and in low-temperature magnetometry, there has been growing interest in observing the new MQP in magnetic systems. Particular cases of the magnetic MQP are quantum tunneling of the magnetization vector in small single-domain ferromagnetic (FM) particles [4–6], quantum nucleation of FM bubbles [7] and the depinning of FM domain walls from defects at low temperature [8–10]. MQP also exist in the small single-domain antiferromagnetic (AFM) particles in which the Neel vector can tunnel coherently between the low-energy directions at a temperature well below the anisotropy gap [11–15]. It has been suggested that the small single-domain AFM particle, which has a nonzero magnetic moment due to the irregular shape of the particle, is a better candidate for observing the MQP than the FM particle because of the much larger resonance frequency in one of the wells separated by the magnetic anisotropy. The MQC and MQT problems of the Neel vector were investigated based on the two sublattices model [11–13,15] and the anisotropic σ model [14] independently. And the quantum nucleation problems of the Neel vector were also studied in references [14,15].

One of the most striking effects in the magnetic MQP is that for some spin systems with high symmetry, the tunneling behaviors for the particle with half-integer total spin are much different from that for the particle with integer total spin. It has been theoretically demonstrated that the topological term in the magnetic action can lead to the destructive interference between the different symmetry-related tunneling paths for the half-integer total spin FM particle in the absence of a magnetic field. Such an effect gives a total tunneling amplitude that is exactly zero according to the Kramers' theorem [16,17]. But if the total spin of the FM particle is integer, the interference is constructive and the quantum tunneling is allowed [16,17]. The destructive quantum interference effect is known as topological quenching [18]. The topological quenching effect can also exist in the FM system without Kramers' degeneracy [18]. More recently, the quantum interference effect in resonant tunneling of the magnetization vector between nonequivalent wells formed by the applied

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magnetic field has been investigated theoretically for small single-domain FM particles [19,20].

Topological quenching effect can also take place in the small single-domain AFM particles [12,13]. It was pointed out that in a AFM system with time-reversal invariance the tunnel splitting of the ground state is suppressed to zero for the half-integer excess spin particle, but is nonzero for the integer excess spin particle [12,13]. In the present work we will emphasize that, similar to the FM system [18], the destructive interference or topological quenching effect is not necessarily related to the Kramers' degeneracy for the AFM system. We shall show this with the help of a specific example of MQC in a AFM system with biaxial crystal symmetry and a weak magnetic field applied along the hard axis. In this case the ground-state tunnel splitting can vanish even when the Kramers' theorem is inapplicable.

The system of interest is a small (~ 50 Å radius), single-domain, AFM particle at a temperature well below its anisotropy gap. According to the two sublattices model [12], there is a strong exchange energy $\mathbf{m}_1 \cdot \mathbf{m}_2/\chi_\perp$ between the two sublattices, where $\mathbf{m}_1$ and $\mathbf{m}_2$ are the magnetization vectors of the two sublattices with large, fixed and unequal magnitudes. In the following, we assume that $m_1 > m_2$ and $m = m_1 - m_2 \ll m_1$. The Lagrangian L of the system is given by

$$L = L_0 + L_1, \tag{1}$$

where L_0 is the magnetic Lagrangian without the anisotropy and Zeeman terms, which can be written as [12]

$$L_0=V\left\{\frac{m_1}{\gamma}\left(\frac{d\phi_1}{d\tau}\right)(\cos\theta_1-1)+\frac{m_2}{\gamma}\left(\frac{d\phi_2}{d\tau}\right)(\cos\theta_2-1)\right.$$
$$\left.-\frac{1}{\chi_\perp}m_1m_2\left[\sin\theta_1\sin\theta_2\cos(\phi_1-\phi_2)+\cos\theta_1\cos\theta_2+1\right]\right\}. \tag{2}$$

V is the volume of the AFM particle, γ is the gyromagnetic ratio and $\theta_{1,2}$, $\phi_{1,2}$ are the angular components of $\mathbf{m}_{1,2}$ in the spherical coordinate system. The topological terms have been included in the L_0 term. The anisotropy and Zeeman energies are included in the L_1 term. In order to obtain the tunneling rate for MQT or the tunnel splitting for MQC, we shall calculate the following path integral

$$\int D\{\theta_1\}D\{\phi_1\}D\{\theta_2\}D\{\phi_2\}\exp\left[\frac{i}{\hbar}\int dt(L_0+L_1)\right]. \tag{3}$$

The system we consider has an easy axis in the X–Y plane, and a hard axis in $\mathbf{z}$. In the presence of a weak magnetic field $\mathbf{H}$ along the hard axis, the L_1 term equals

$$L_1 = -V(K_\perp\cos^2\theta_1 + K_\parallel\sin^2\theta_1\sin^2\phi_1 - m_1H\cos\theta_1 - m_2H\cos\theta_2), \tag{4}$$

where $K_\perp$ and $K_\parallel$ are the transverse and longitudinal anisotropy coefficients, respectively. Like the problem studied in reference [12], in this paper we also assume that the transverse anisotropy coefficient is much larger than the longitudinal one, which agrees with the experimental condition on highly anisotropic materials (such as the rare-earth materials). When $H = 0$, equation (4) is reduced to the MQC problem of the Neel vector studied in reference [12]. It has been theoretically demonstrated that the tunnel splitting is suppressed to zero for the half-integer excess spin AFM particle when $H = 0$. Such a topological quenching effect of the AFM particle in the absence of the magnetic field is related to the Kramers' degeneracy due to the time-reversal invariance of the system. According to Kramers' theorem, the ground state is a Kramers doublet so long as the excess spin of the AFM particle is half-integer and so the rate of quantum tunneling is zero resulting from the destructive interference between the different paths of the clockwise and counterclockwise instantons. In real experiments, in order to detect the freezing of quantum tunneling in a small AFM particle with half-integer excess spin, one will always apply some weak magnetic fields to remove the Kramers' degeneracy. Therefore, we will investigate the tunneling behaviors of the Neel vector in the presence of a weak magnetic field, where the Kramers' theorem is inapplicable.

According to the two sublattices model for the AFM particles, only the low-energy trajectories with almost antiparallel $\mathbf{m}_1$ and $\mathbf{m}_2$ make the dominant contributions to the path integral in equation (3). Therefore, θ_2 and ϕ_2 can be eliminated by representing them as $\theta_2 = \pi - \theta_1 - \varepsilon_\theta$ and $\phi_2 = \pi + \phi_1 + \varepsilon_\phi$ ($|\varepsilon_\theta| \ll 1$, $|\varepsilon_\phi| \ll 1$) and performing the Gaussian integration over ε_θ and ε_ϕ. Then, equation (3) is reduced to the following path integral for a small non-compensated AFM particle

$$\int D\{\theta\}D\{\phi\}\exp[-S_E(\theta,\phi)], \tag{5}$$

where S_E is the effective Euclidean action which is given by

$$S_E(\theta,\phi) = \frac{V}{\hbar}\int d\tau\left\{i\frac{m_1+m_2}{\gamma}\left(\frac{d\phi}{d\tau}\right)\right.$$
$$\left.+\frac{\chi_\perp}{2\gamma^2}\left[\left(\frac{d\theta}{d\tau}\right)^2+\left(\frac{d\phi}{d\tau}-i\gamma H\right)^2\sin^2\theta\right]+E(\theta,\phi)\right\}. \tag{6}$$

When $H = 0$, the above action is consistent with the result in reference [12]. The $E(\theta, \phi)$ term in equation (6) is

$$\begin{aligned}E(\theta,\phi) &= K_\perp\cos^2\theta + K_\parallel\sin^2\theta\sin^2\phi - mH\cos\theta\\ &= K_\perp(\cos\theta-\cos\theta_0)^2 + K_\parallel\sin^2\theta\sin^2\phi.\end{aligned} \tag{7}$$

Now θ and ϕ are the angular components of $\mathbf{m}_1$, which can also determine the direction of the Neel vector. $\tau = it$ is the imaginary time and $m = m_1 - m_2 = \hbar\gamma s/V \ll m_1$, where s is the excess spin of the AFM particle due to the non-compensation of two sublattices. θ_0 in equation (7) is defined as $\cos\theta_0 = mH/2K_\perp$. It is noted that the first term in equation (6) is a total imaginary time derivative which does not make any contribution to the classical equations of motion. However, we shall show in the following that this term, known as the topological term, is of critical importance to the quantum properties of the AFM particles and makes the tunneling behaviors of the integer and half-integer excess spin particles strikingly different.

Now we ignore the quantum interference effect for the moment, but use the standard instanton method to evaluate the path integral in equation (5). The problem studied here is one of MQC, in which the Neel vector resonates between the energetically degenerate directions. When $H < H_c = 2K_\perp/m$, $E(\theta,\phi)$ in equation (7) has degenerate minima at $\theta = \theta_0$ and $\phi = 0, \pi$. H_c is the coercive field at which the initial state becomes classically unstable. We note that there also exists a spin-flop field which can destroy the spin configuration in the AFM particle. The magnitude of such a field is smaller than that of the coercive field for the small non-compensated AFM particle in general. However, of interest in this paper is the tunneling behaviors of the Neel vector in the presence of a weak magnetic field (*i.e.* $H/H_c \to 0$), where the applied magnetic field is smaller than the spin-flop field. So the two sublattices configuration is still valid for the AFM particle at $H \neq 0$. The calculation for the tunneling rate consists of two major steps. The first step is to find the classical or least-action path which gives the Wentzel-Kramers-Brillouin (WKB) exponent. The second step is to evaluate the Van Vleck determinant for the small fluctuations about the classical path, which gives the pre-exponential factors in the tunneling rate for MQT or in the tunnel splitting for MQC.

To execute the first step, we must find the classical path $(\bar\theta, \bar\phi)$ with the boundary conditions at $\tau = \pm T/2$. The classical path satisfies the following equations of motion

$$\frac{\chi_\perp}{\gamma^2}\frac{d^2\bar\theta}{d\tau^2} = \frac{\chi_\perp}{\gamma^2}\left(\frac{d\bar\phi}{d\tau} - i\gamma H\right)^2 \sin\bar\theta\cos\bar\theta + \frac{\partial E}{\partial\theta}$$

$$\frac{\chi_\perp}{\gamma^2}\frac{d}{d\tau}\left[\left(\frac{d\bar\phi}{d\tau} - i\gamma H\right)\sin^2\bar\theta\right] = \frac{\partial E}{\partial\phi}\ . \tag{8}$$

In the case of very strong transverse anisotropy $K_\perp$ and weak applied magnetic field, the Neel vector is forced to lie in the $X{-}Y$ plane and the fluctuations of θ about $\pi/2$ are small. Introducing $\theta = \pi/2 - \alpha$ ($|\alpha| \ll 1$), and then substituting equation (7) into the classical equations of motion, we obtain the following two equivalent paths in the small H/H_c limit,

$$\bar\phi = 2\arctan(e^{\omega_0\tau})$$

$$\bar\alpha = \frac{H}{H_c} + 2\left(\frac{K_\parallel}{K_\perp}\right)\left(\frac{H}{H_c}\right)\frac{1}{\cosh^2(\omega_0\tau)}, \tag{9}$$

and

$$\bar\phi = -2\arctan(e^{\omega_0\tau})$$

$$\bar\alpha = \frac{H}{H_c} + 2\left(\frac{K_\parallel}{K_\perp}\right)\left(\frac{H}{H_c}\right)\frac{1}{\cosh^2(\omega_0\tau)}, \tag{10}$$

where

$$\omega_0 = \gamma\sqrt{\frac{2K_\parallel}{\chi_\perp}}. \tag{11}$$

The classical path in equation (9) is defined as the instanton, which corresponds to the variation of $\bar\phi$ from $\bar\phi = 0$ at $\tau = -\infty$ to $\bar\phi = \pi$ at $\tau = +\infty$. The one in equation (10) is defined as the anti-instanton, which corresponds to the variation of $\bar\phi$ from $\bar\phi = 0$ at $\tau = -\infty$ to $\bar\phi = -\pi$ at $\tau = +\infty$. To the second order of H/H_c, the classical action for the instanton or anti-instanton is found to be

$$S_{cl} = 2^{3/2}\frac{V}{\hbar\gamma}\sqrt{\chi_\perp K_\parallel}\left[1 - \left(\frac{H}{H_c}\right)^2 - \frac{4}{3}\left(\frac{K_\parallel}{K_\perp}\right)\left(\frac{H}{H_c}\right)^2\right]. \tag{12}$$

In order to evaluate the Van Vleck determinant for small fluctuations about the classical path, we write

$$\theta(\tau) = \bar\theta(\tau) + \theta_1(\tau), \quad \phi(\tau) = \bar\phi(\tau) + \phi_1(\tau), \tag{13}$$

and expand the Euclidean action in equation (6) to the second order of θ_1 and ϕ_1, which gives the following expression

$$S_E(\theta,\phi) = S_{cl} + \delta^2 S, \tag{14}$$

where

$$\delta^2 S = \frac{V}{\hbar}\int d\tau\left\{\frac{\chi_\perp}{2\gamma^2}\left(\frac{d\theta_1}{d\tau}\right)^2 + \frac{\chi_\perp}{2\gamma^2}\sin^2\bar\theta\left(\frac{d\phi_1}{d\tau}\right)^2 + \frac{\chi_\perp}{\gamma^2}\sin 2\bar\theta\left(\frac{d\bar\phi}{d\tau} - i\gamma H\right)\left(\frac{d\phi_1}{d\tau}\right)\theta_1 + \frac{\chi_\perp}{2\gamma^2}\cos 2\bar\theta\left(\frac{d\bar\phi}{d\tau} - i\gamma H\right)^2\theta_1^2 + \frac{1}{2}(E_{\theta\theta}\theta_1^2 + 2E_{\theta\phi}\theta_1\phi_1 + E_{\phi\phi}\phi_1^2)\right\}. \tag{15}$$

$E_{\theta\theta}$, $E_{\theta\phi}$ and $E_{\phi\phi}$ in equation (15) are defined as $E_{\theta\theta} = \frac{\partial^2 E}{\partial\theta^2}|_{\theta=\bar\theta,\phi=\bar\phi}$, $E_{\theta\phi} = \frac{\partial^2 E}{\partial\theta\partial\phi}|_{\theta=\bar\theta,\phi=\bar\phi}$ and $E_{\phi\phi} = \frac{\partial^2 E}{\partial\phi^2}|_{\theta=\bar\theta,\phi=\bar\phi}$. We first note that, to the second order of H/H_c,

$$\frac{1}{2}E_{\theta\theta}+\frac{\chi_\perp}{2\gamma^2}\left(\frac{d\bar{\phi}}{d\tau}-i\gamma H\right)^2\cos 2\bar{\theta}=K_\perp-K_\perp\alpha_0^2-2K_\parallel\sin^2\bar{\phi}$$
$$+8K_\parallel\left(\frac{K_\parallel}{K_\perp}\right)\sin^2\bar{\phi}-K_\parallel\alpha_0^2\sin^2\bar{\phi}$$
$$-16K_\parallel\left(\frac{K_\parallel}{K_\perp}\right)\alpha_0^2\sin^2\bar{\phi}$$
$$-8K_\parallel\left(\frac{K_\parallel}{K_\perp}\right)\sin^4\bar{\phi}-16K_\parallel\left(\frac{K_\parallel}{K_\perp}\right)^2\sin^4\bar{\phi}$$
$$+26K_\parallel\left(\frac{K_\parallel}{K_\perp}\right)\alpha_0^2\sin^4\bar{\phi}$$
$$-32K_\parallel\left(\frac{K_\parallel}{K_\perp}\right)^2\alpha_0^2\sin^2\bar{\phi}+24K_\parallel\left(\frac{K_\parallel}{K_\perp}\right)^2\sin^6\bar{\phi}$$
$$+48K_\parallel\left(\frac{K_\parallel}{K_\perp}\right)\alpha_0^2\sin^6\bar{\phi}$$
$$=K_\perp+O(K_\parallel)>0, \tag{16}$$

where $\alpha_0 = H/H_c$. Therefore, we can integrate out θ_1 directly, which leads to the following effective action for ϕ_1 only

$$I(\phi_1)=\int\left[A\left(\frac{d\phi_1}{d\tau}\right)^2+B\phi_1\left(\frac{d\phi_1}{d\tau}\right)+C\phi_1^2\right]d\tau. \tag{17}$$

Here,

$$A=\frac{V}{\hbar}\frac{\chi_\perp}{2\gamma^2}\sin^2\bar{\theta}\left[1-\frac{4\frac{\chi_\perp}{\gamma^2}\cos^2\bar{\theta}(\frac{d\bar{\phi}}{d\tau}-i\gamma H)^2}{E_{\theta\theta}+\frac{\chi_\perp}{\gamma^2}\cos 2\bar{\theta}(\frac{d\bar{\phi}}{d\tau}-i\gamma H)^2}\right],$$

$$B=-\frac{V}{\hbar}\frac{\chi_\perp}{\gamma^2}\frac{E_{\theta\phi}\sin 2\bar{\theta}(\frac{d\bar{\phi}}{d\tau}-i\gamma H)}{E_{\theta\theta}+\frac{\chi_\perp}{\gamma^2}\cos 2\bar{\theta}(\frac{d\bar{\phi}}{d\tau}-i\gamma H)^2},$$

$$C=\frac{V}{2\hbar}\left[E_{\phi\phi}-\frac{E_{\theta\phi}^2}{E_{\theta\theta}+\frac{\chi_\perp}{\gamma^2}\cos 2\bar{\theta}(\frac{d\bar{\phi}}{d\tau}-i\gamma H)^2}\right]. \tag{18}$$

We now turn to the normalization factor for the remaining path integral over ϕ_1. In the spin-coherent-state representation, the measure of the path integral in equation (5) is defined as

$$\int D\{\theta\}D\{\phi\}=\lim_{n\to\infty}\prod_{k=1}^{n}\left[\frac{2S+1}{4\pi}\right]\int\sin\bar{\theta}_k d\theta_{1,k}d\phi_{1,k}, \tag{19}$$

where $\theta_k = \theta(-T/2+k\eta)$, $\phi_k = \phi(-T/2+k\eta)$. $\eta = T/(n+1)$ is the width of the imaginary time slices. S in equation (19) is the total spin in one sublattice for the AFM particle. In addition to generating contributions to the B and C terms in equation (17), the Gaussian integration over $\theta_{1,k}$ will yield a factor of

$$\left\{\frac{2\pi\hbar}{\eta V[E_{\theta\theta}(\bar{\theta}_k,\bar{\phi}_k)+\frac{\chi_\perp}{\gamma^2}\cos 2\theta(\frac{d\phi}{d\tau}-i\gamma H)^2|_{\theta=\bar{\theta}_k,\phi=\bar{\phi}_k}]}\right\}^{1/2}. \tag{20}$$

Then the path integral in equation (5) can be written as

$$N'e^{-S_{cl}}\int[d\phi_1]e^{-I[\phi_1(\tau)]}, \tag{21}$$

where

$$N'=\lim_{n\to\infty}\prod_{k=1}^{n}\left[\frac{2S+1}{2}\right]\times\sqrt{\frac{\hbar}{\eta 2\pi V[E_{\theta\theta}(\bar{\theta}_k,\bar{\phi}_k)+\frac{\chi_\perp}{\gamma^2}\cos 2\theta(\frac{d\phi}{d\tau}-i\gamma H)^2|_{\theta=\bar{\theta}_k,\phi=\bar{\phi}_k}]}}\times\sin\bar{\theta}_k. \tag{22}$$

It is easy to obtain the following relation for the transverse susceptibility $\chi_\perp$ with the exchange energy density J between the two sublattices [13]

$$\chi_\perp=\frac{\hbar^2\gamma^2}{JV^2}S^2. \tag{23}$$

In the limit of large S, equation (22) is reduced to

$$N'=\lim_{n\to\infty}\prod_{k=1}^{n}(A_k'/\pi\eta)^{1/2}, \tag{24}$$

where

$$A_k'=J\frac{V}{\hbar}\frac{\chi_\perp}{2\gamma^2}\times\frac{\sin^2\bar{\theta}_k}{E_{\theta\theta}(\bar{\theta}_k,\bar{\phi}_k)+\frac{\chi_\perp}{\gamma^2}\cos 2\theta(\frac{d\phi}{d\tau}-i\gamma H)^2|_{\theta=\bar{\theta}_k,\phi=\bar{\phi}_k}}\cdot \tag{25}$$

Next, we change τ to a new time variable ζ, which is defined by

$$d\zeta=d\tau/2A'(\bar{\theta}(\tau),\bar{\phi}(\tau)). \tag{26}$$

Then, in terms of the discretized variables, the path integral in equation (5) can be cast in the standard form for a one-dimensional motion problem [6,21–23],

$$e^{-S_{cl}}\lim_{n\to\infty}\left[\prod_{k=1}^{n}\int\frac{d\phi_{1,k}}{\sqrt{2\pi\Delta_k}}\right]\times\exp\left\{-\sum_{k=1}^{n}\left[\frac{1}{2\Delta_k}\left(\frac{A_k}{A_k'}\right)(\phi_{1,k}-\phi_{1,k-1})^2+2\Delta_k A_k'C_k'\phi_{1,k}^2\right]\right\}, \tag{27}$$

where $\phi_{1,0}=0$ and Δ_k, the width of the kth imaginary time slice in the new time variable ζ, is given by

$$\Delta_k=\zeta_k-\zeta_{k-1}=\eta/2A_k'. \tag{28}$$

We have defined $A_k = A(\bar{\theta}_k,\bar{\phi}_k)$ and $C_k' = C'(\bar{\theta}_k,\bar{\phi}_k)$ in equation (27), where

$$C'=C+\frac{V}{\hbar}\frac{\chi_\perp}{\gamma^2}\frac{d}{d\tau}\left[\frac{E_{\theta\phi}\sin 2\bar{\theta}(\frac{d\bar{\theta}}{d\tau})}{E_{\theta\theta}+\frac{\chi_\perp}{\gamma^2}\cos 2\bar{\theta}(\frac{d\bar{\phi}}{d\tau}-i\gamma H)^2}\right]. \tag{29}$$

The remaining procedure to evaluate the Van Vleck determinant of the quadratic form of ϕ_1 in equation (27) for the AFM particles is very similar to that for the FM particles [6]. Here we only give a summary on how to evaluate the tunneling rate or the tunnel splitting for the AFM particles. The first step is to find the classical path which satisfies the boundary conditions from the equations of motion. The second step is to differentiate the classical path to obtain $d\bar{\phi}/d\tau$, then convert from τ to the new time variable ζ according to the relation in equation (26), which gives

$$\frac{d\bar{\phi}}{d\tau} = ae^{-\mu\zeta} \qquad \text{as} \quad \zeta \to \infty. \tag{30}$$

Then the tunnel splitting for MQC (not including the contributions of topological term) equals [6]

$$\Delta = k_\zeta |a| (\mu/\pi)^{1/2} e^{-S_{cl}}, \tag{31}$$

where k_ζ is the number of the equivalent escape directions, *i.e.* the number of paths which have the same classical action. We note that only the asymptotic relation in equation (30) is needed for calculating the tunnel splitting, and this is usually easy to obtain. The tunneling rate for MQT can be evaluated by using similar techniques, and we will not discuss it any further.

For the MQC problem studied in the present work, we find the following relation between τ and the new time variable ζ,

$$\tau = \frac{\hbar}{2VK_\perp} S^2 \zeta + \frac{\hbar}{VK_\perp}\sqrt{\frac{2K_\parallel}{J}} \left[2 + \frac{40}{3}\left(\frac{K_\parallel}{K_\perp}\right) + 3\left(\frac{H}{H_c}\right)^2 + \frac{4}{3}\left(\frac{K_\parallel}{K_\perp}\right)\left(\frac{H}{H_c}\right)^2\right]. \tag{32}$$

From equation (9) or equation (10), it is a simple matter to show that

$$\frac{d\bar{\phi}}{d\tau} = 2^{3/2}\frac{V}{\hbar S}\sqrt{K_\parallel J} \exp\left\{-\left(\frac{K_\parallel}{K_\perp}\right)\left[2 + \frac{40}{3}\left(\frac{K_\parallel}{K_\perp}\right) + 3\left(\frac{H}{H_c}\right)^2 + \frac{4}{3}\left(\frac{K_\parallel}{K_\perp}\right)\left(\frac{H}{H_c}\right)^2\right]\right\} \times \exp\left(-\sqrt{\frac{K_\parallel J}{2K_\perp^2}} S\zeta\right), \quad \text{as} \quad \zeta \to \infty. \tag{33}$$

Thus,

$$|a| = 2^{3/2}\frac{V}{\hbar S}\sqrt{K_\parallel J} \exp\left\{-\left(\frac{K_\parallel}{K_\perp}\right)\left[2 + \frac{40}{3}\left(\frac{K_\parallel}{K_\perp}\right) + 3\left(\frac{H}{H_c}\right)^2 + \frac{4}{3}\left(\frac{K_\parallel}{K_\perp}\right)\left(\frac{H}{H_c}\right)^2\right]\right\},$$

and

$$\mu = \sqrt{\frac{K_\parallel J}{2K_\perp^2}} S. \tag{34}$$

Substituting equation (34) into the general formula (31), using $k_\zeta = 2$ and including the contributions of the topological term, we obtain the tunnel splitting for this MQC problem in the weak field limit,

$$\Delta = \frac{2^{13/4}}{\pi^{1/2}} \frac{V}{\hbar} K_\perp \left(\frac{K_\parallel J}{K_\perp^2}\right)^{3/4} S^{-1/2} \times \exp\left\{-\left(\frac{K_\parallel}{K_\perp}\right)\left[2 + \frac{40}{3}\left(\frac{K_\parallel}{K_\perp}\right) + 3\left(\frac{H}{H_c}\right)^2 + \frac{4}{3}\left(\frac{K_\parallel}{K_\perp}\right)\left(\frac{H}{H_c}\right)^2\right]\right\} \left|\cos\left\{\left[s + 2\,\frac{K_\perp}{J}\left(\frac{S^2}{s}\right)\left(\frac{H}{H_c}\right)\right]\pi\right\}\right| e^{-S_{cl}}, \tag{35}$$

where S is the total spin in one sublattice and s is the excess spin in the AFM particle. It is clearly shown that the tunnel splittings for both the integer and half-integer excess spin AFM particles oscillate with the weak magnetic field. In terms of the exchange energy density J and the total spin in one sublattice S, the classical action in equation (12) can be rewritten as

$$S_{cl} = 2^{3/2}\sqrt{\frac{K_\parallel}{J}} S \left[1 - \left(\frac{H}{H_c}\right)^2 - \frac{4}{3}\left(\frac{K_\parallel}{K_\perp}\right)\left(\frac{H}{H_c}\right)^2\right]. \tag{36}$$

For $H = 0$, the tunnel splitting in equation (35) is reduced to

$$\Delta = \frac{2^{13/4}}{\pi^{1/2}} \frac{V}{\hbar} K_\perp \left(\frac{K_\parallel J}{K_\perp^2}\right)^{3/4} S^{-1/2} \exp\left[-2\left(\frac{K_\parallel}{K_\perp}\right) - \frac{40}{3}\left(\frac{K_\parallel}{K_\perp}\right)^2\right] |\cos(s\pi)| e^{-S_{cl}(H=0)}, \tag{37}$$

where

$$S_{cl}(H=0) = 2^{3/2}\sqrt{\frac{K_\parallel}{J}} S. \tag{38}$$

The factor $\cos(s\pi)$ in equation (37) represents the quantum interference between the different paths of clockwise ($\Delta\phi = -\pi$) and counterclockwise ($\Delta\phi = \pi$) instantons for the Neel vector in small AFM particle. If the excess spin of the AFM particle is half-integer, the suppression of tunnel splitting is evident [12,13]. If the excess spin is integer, the tunnel splitting is nonzero and of the order of single-instanton splitting. The classical action, *i.e.* the WKB exponent at $H = 0$ in equation (38) is in good agreement with the result in reference [12]. However, the tunnel splitting in reference [12] is obtained only from the contribution of the classical path, which gives the WKB exponential factor and leaves the prefactors incomplete. Here, both the WKB exponent and the pre-exponential factors are found exactly for the tunnel splitting, which will be helpful for the observation of such topological quenching effect in experiments.

When $H = 0$, it has been demonstrated that the tunnel splitting is completely suppressed for the half-integer excess spin AFM particle (see references12 and 13, or equation (37) in this paper). However, a weak magnetic field applied along the hard axis can lead to the oscillation of tunnel splitting with the field for both the integer and half-integer excess spin AFM particles. The tunnel splitting is thus quenched whenever

$$\frac{H}{H_c} = \frac{J}{2K_\perp}\left(\frac{s}{S^2}\right)\left(n + \frac{1}{2} - s\right), \tag{39}$$

where n is an integer.

In summary, the macroscopic quantum coherence of the Neel vector in a AFM system without Kramers' degeneracy is considered in the present work. In the absence of an applied magnetic field, the suppression of tunnel splitting for the half-integer excess spin AFM particle is evident. Furthermore, the detailed prefactors in the tunnel splitting are found exactly, compared with the results in reference [12]. The system at $H = 0$ has time-reversal invariance and all eigenstates are doubly degenerate for the half-integer excess spin AFM particle according to Kramers' theorem. This implies that the tunnel splitting between the energetically degenerate states at $\phi = 0$ and $\phi = \pi$ vanishes. When a weak magnetic field is applied along the hard axis, the time-reversal invariance of the system is broken, but the quenching of tunnel splitting is preserved at certain values of the field. Another important result is that the tunnel splitting oscillates with the weak magnetic field for both the integer and half-integer excess spin AFM particles. The definite values of the magnetic field at which the quenching of tunnel splitting occurs are clearly shown. Both the WKB exponent and the pre-exponential factors are found exactly for the tunnel splitting in the weak field limit. After investigating this specific example of macroscopic quantum coherence of the Neel vector in the presence of a weak magnetic field, we conclude that the quenching of tunnel splitting for the AFM particle need not be related to the Kramers' degeneracy of the system. We hope that the theoretical results obtained in this paper will stimulate more experiments to observe the quantum interference, or spin-parity effect in the small single-domain antiferromagnets.

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