Macroscopic Quantum Coherence in Small Antiferromagnetic Particle and the Quantum Interference Effects

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Abstract

Starting from the Hamiltonian operator of the noncompensated two-sublattice model of a small antiferromagnetic particle, we derive the effective Lagrangian of a biaxial antiferromagnetic particle in an external magnetic field with the help of spin-coherent-state path integrals. Two unequal level-shifts induced by tunneling through two types of barriers are obtained using the instanton method. The energy spectrum is found from Bloch theory regarding the periodic potential as a super-lattice. The external magnetic field indeed removes Kramers' degeneracy, however a new quenching of the energy splitting depending on the applied magnetic field is observed for both integer and half-integer spins due to the quantum interference between transitions through two types of barriers.

1 Introduction

The magnetization vector in solids is traditionally viewed as a classical variable. In recent years, theoretical and experimental works have demonstrated, however, that the vector

can tunnel quantum mechanically out of metastable magnetic states or resonate between two degenerate ground states[1-13] known as macroscopic quantum phenomena(MQP) which are distinguished into the macroscopic quantum tunneling (MQT) and the macroscopic quantum coherence (MQC) respectively. Quantum tunneling of the magnetization vector in small single-domain ferromagnetic (FM) particles[1,2], quantum nucleation of FM bubbles[3], and quantum depinning of a domain wall in bulk ferromagnets[4] are typical examples of the macroscopic quantum phenomena. Similar effect also exists in small single-domain antiferromagnetic (AFM) particles in which the Néel vector plays a role of macroscopic variable and can tunnel between orientations of lowest energy[5,6]. Since the tunneling rate in the AFM particles is much higher than that in the FM particles [7], the AFM particles are expected to be a better candidate for the observation of MQP than the FM particles. Another interesting phenomenon relating to tunneling in magnetization is that for spin systems with discrete rotation symmetry of two folds, the tunneling rate is completely suppressed for half-integer total spin known as Kramers' degeneracy[8]. Such an effect is called topological quenching in literature [9] and has been studied extensively[8-14].

In literature the AFM particle is usually described by the Néel vector of two collinear sublattices whose magnetizations are coupled by strong exchange interaction. External magnetic field does not play a role since the net magnetic moment vanishes for idealized sublattices. The quantum and classical transitions of the Néel vector in antiferromagnets has been well studied[15] in terms of the idealized sublattice model. The temperature dependence of quantum tunneling was also given for the same model[16] and the theoretical result agrees with the experimental observation[17]. A biaxial AFM particle with a small non-compensation of sublattices in the absence of external magnetic field was studied in Ref.[18] where it was shown that the noncompensated magnetic moment leads to a modification of oscillation frequency around the equilibrium orientations of the Néel vector. In the present paper we demonstrate that the small noncompensated magnetic moment obtains extra energy in magnetic field which changes the original equilibrium orientations of the Néel vector and results in interesting tunneling effects in AFM particles. With the help of spin-coherent-state path integrals we convert the spin system into a pseudoparticle

moving in a effective potential $-V(\phi)$ with a periodically recurring asymmetric twin barriers which lead to two kinds of instantons. The total effect of tunneling gives rise to the level splitting which is determined with Bloch theory regarding the periodic potential as a superlattice. We show explicitly that the external magnetic field removes the rotation symmetry of two-fold and , therefore, the Kramers' degeneracy[10]. The level splitting is not quenched any longer for half-integer spin. However a remarkable observation is that quantum interference between transitions through two-type of potential barriers results in an oscillation of level splitting with the external field. The splitting could be entirely suppressed at the certain value of magnetic field due to the disconstructive interference.

2 The effective Lagrangian of a biaxial AFM particle with a small non-compensated magnetic moment and the equilibrium orientations of the Néel vector

Consider a biaxial AFM particle having two collinear FM sublattices with a small non-compensation.We assume that the particle possesses a **x** easy axis and x-y easy plane, and the magnetic field H is applied along the **y** direction. Regarding each sublattice as a FM particle the Hamiltonian operator of the AFM particle has the form

$$\hat{H} = \sum_{\alpha=1,2} (k_\perp \hat{S}_\alpha^{z2} + k_\parallel \hat{S}_\alpha^{y2} - \gamma H S_\alpha^y) + J\hat{S}_1 \cdot \hat{S}_2, \tag{1}$$

where $k_\perp$, $k_\parallel > 0$ are the anisotropy constants, J is the exchange constant, γ is the gyromagnetic ratio, and $\hat{S}_1$, $\hat{S}_2$ denote the spin operators in two sublattices with the commutation relation $[S_\alpha^i, S_\beta^j] = i\hbar\epsilon_{ijk}\delta_{\alpha\beta}\hat{S}_\alpha^k$ $(i, j, k = x, y, z ; \alpha, \beta = 1, 2)$. Here we emphasize that because of the non-compensation of the two collinear FM sublattices the interaction terms with magnetic field, *i.e.* the third term in the summation of Eq.(1), do not vanish and result in the equilibrium-orientation change of the Néel vector. We begin with the evaluation of the matrix element of the evolution operator in spin- coherent-state representation by means of the coherent state path integrals

$$\langle \mathbf{N}_f | e^{-2i\hat{H}T/\hbar} | \mathbf{N}_i \rangle = \int \left[\prod_{k=M}^{M-1} d\mu(\mathbf{N}_k) \right] \left[\prod_{k=1}^{M} \langle \mathbf{N}_k | e^{-i\epsilon\hat{H}/\hbar} | \mathbf{N}_{k-1} \rangle \right]. \tag{2}$$

Here we define $|\mathbf{N}\rangle = |\mathbf{n}_1\rangle|\mathbf{n}_2\rangle$, $|\mathbf{N}_M\rangle = |\mathbf{N}_f\rangle = |\mathbf{n}_{1,f}\rangle|\mathbf{n}_{2,f}\rangle$, $|\mathbf{N}_0\rangle = |\mathbf{N}_i\rangle = |\mathbf{n}_{1,i}\rangle|\mathbf{n}_{2,i}\rangle$ and $t_f - t_i = 2T$, $\epsilon = 2T/M$,respectively. The spin coherent state is defined as

$$|\mathbf{n}_\alpha\rangle = \mathrm{e}^{-i\theta_\alpha \hat{A}_\alpha}|S_\alpha, S_\alpha\rangle , \quad (\alpha = 1,2), \tag{3}$$

where $\mathbf{n}_\alpha = (\sin\theta_\alpha\cos\phi_\alpha, \sin\theta_\alpha\sin\phi_\alpha, \cos\theta_\alpha)$ is the unit vector, $\hat{A}_\alpha = \sin\phi_\alpha\hat{S}_\alpha^x - \cos\phi_\alpha\hat{S}_\alpha^y$ and $|S_\alpha, S_\alpha\rangle$ is the reference spin eigenstate. The measure is defined by

$$\mathrm{d}\mu(\mathbf{N}_k) = \prod_{\alpha=1,2}\frac{2S_\alpha + 1}{4\pi}\mathrm{d}\mathbf{n}_{\alpha,k} , \quad \mathrm{d}\mathbf{n}_{\alpha,k} = \sin\theta_{\alpha,k}\mathrm{d}\theta_{\alpha,k}\mathrm{d}\phi_{\alpha,k}. \tag{4}$$

As $M \to \infty$, $\epsilon \to 0$, $\exp(-i\epsilon\hat{\mathrm{H}}/\hbar) \approx 1 - i\epsilon\hat{\mathrm{H}}/\hbar$, with

$$
\begin{aligned}
\hat{\mathrm{H}} &= \sum_{\alpha=1,2}\left[\frac{k_\parallel}{2}\hat{S}_\alpha^2 + \left(k_\perp - \frac{k_\parallel}{2}\right)\hat{S}_\alpha^{z2} - \frac{k_\parallel}{4}\left(\hat{S}_\alpha^{+2} + \hat{S}_\alpha^{-2}\right) - \frac{\gamma H}{2i}\left(\hat{S}_\alpha^+ - \hat{S}_\alpha^-\right)\right] \\
&\quad + \frac{J}{2}\left[\left(\hat{S}_1^-\hat{S}_2^+ + \hat{S}_1^+\hat{S}_2^-\right) + 2\hat{S}_1^z\hat{S}_2^z\right],
\end{aligned}
\tag{5}
$$

where $\hat{S}_\alpha^+ = \hat{S}_\alpha^x + i\hat{S}_\alpha^y$, $\hat{S}_\alpha^- = \hat{S}_\alpha^x - i\hat{S}_\alpha^y$. Making use of the following approximation

$$\langle\mathbf{N}_k|\hat{\mathrm{H}}|\mathbf{N}_{k-1}\rangle \approx \langle\mathbf{N}_k|\hat{\mathrm{H}}|\mathbf{N}_k\rangle\langle\mathbf{N}_k|\mathbf{N}_{k-1}\rangle \tag{6}$$

with

$$
\begin{aligned}
\langle\mathbf{N}_k|\mathbf{N}_{k-1}\rangle &= \prod_{\alpha=1,2}\langle\mathbf{n}_{\alpha,k}|\mathbf{n}_{\alpha,k-1}\rangle, \tag{7}\\
\langle\mathbf{N}_k|\hat{\mathrm{H}}|\mathbf{N}_k\rangle &= \sum_{\alpha=1,2}[S_\alpha^2(k_\perp\cos^2\theta_{\alpha,k} + k_\parallel\sin^2\theta_{\alpha,k}\sin^2\phi_{\alpha,k}) - \gamma H S_\alpha\sin\theta_{\alpha,k}\sin\phi_{\alpha,k}] \\
&\quad + JS_1 S_2[\sin\theta_{1,k}\sin\theta_{2,k}\cos(\phi_{1,k} - \phi_{2,k}) + \cos\theta_{1,k}\cos\theta_{2,k}], \tag{8}\\
\langle\mathbf{n}_{\alpha,k}|\mathbf{n}_{\alpha,k-1}\rangle &= \left(\frac{1 + \mathbf{n}_{\alpha,k}\cdot\mathbf{n}_{\alpha,k-1}}{2}\right)^{S_\alpha}\exp[-iS_\alpha A_\alpha(\mathbf{n}_{\alpha,k}, \mathbf{n}_{\alpha,k-1}, \mathbf{n}_0)] \\
&\approx \exp[-iS_\alpha(\phi_{\alpha,k} - \phi_{\alpha,k-1})(1 - \cos\theta_{\alpha,k})], \tag{9}
\end{aligned}
$$

and $A_\alpha(\mathbf{n}_{\alpha,k}, \mathbf{n}_{\alpha,k-1}, \mathbf{n}_0)$ being the area of the spherical triangle with vertices[19] at $\mathbf{n}_{\alpha,k}$, $\mathbf{n}_{\alpha,k-1}$ and $\mathbf{n}_0 = (0,0,1)$. Under the large S limit we obtain

$$\langle\mathbf{N}_f|\mathrm{e}^{-i\epsilon\hat{\mathrm{H}}T/\hbar}|\mathbf{N}_i\rangle = \mathrm{e}^{-i\sum_{\alpha=1,2}S_\alpha(\phi_{\alpha,f} - \phi_{\alpha,i})}\int\prod_{\alpha=1,2}\mathcal{D}[\phi_\alpha]\mathcal{D}[\theta_\alpha]\exp\left(\frac{i}{\hbar}\int_{t_i}^{t_f}\mathcal{L}\mathrm{d}t\right). \tag{10}$$

Where $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1$ is the Lagrangian with

$$
\begin{aligned}
\mathcal{L}_0 &= \sum_{\alpha=1,2}S_\alpha\dot{\phi}_\alpha\cos\theta_\alpha - JS_1 S_2[\sin\theta_1\sin\theta_2\cos(\phi_2 - \phi_1) + \cos\theta_1\cos\theta_2], \tag{11}\\
\mathcal{L}_1 &= -\sum_{\alpha=1,2}(k_\perp S_\alpha^2\cos^2\theta_\alpha + k_\parallel S_\alpha^2\sin^2\theta_\alpha\sin^2\phi_\alpha + \gamma H S_\alpha\sin\theta_\alpha\sin\phi_\alpha). \tag{12}
\end{aligned}
$$

For our interest of quantum transition between macroscopic states only the low energy trajectories with almost antiparallel S_1 and S_2 contribute to the path integral[18]. We therefore replace θ_2 and ϕ_2 by $\theta_2 = \pi - \theta_1 - \epsilon_\theta$ and $\phi_2 = \pi + \phi_1 + \epsilon_\phi$, where ϵ_θ and ϵ_ϕ denote small fluctuations. Working out the fluctuation integrations over ϵ_θ and ϵ_ϕ the transition amplitude Eq.(10) reduces to

$$\langle \mathbf{N}_f | e^{-i\hat{H}T/\hbar} | \mathbf{N}_i \rangle = e^{-iS_0(\phi_f - \phi_i)} \int \mathcal{D}[\theta]\mathcal{D}[\phi] \exp\left(\frac{i}{\hbar} \int_{t_i}^{t_f} \mathcal{L}' dt \right), \tag{13}$$

$$\mathcal{L}' = \Omega \left[\frac{m}{\gamma}\dot{\phi}\cos\theta + \frac{\chi_\perp}{2\gamma^2}(\dot{\theta}^2 + \dot{\phi}^2\sin^2\theta) \right] - V(\theta, \phi). \tag{14}$$

Where (θ_1, ϕ_1) has been replaced by (θ, ϕ). $V(\theta, \phi) = \Omega(K_\perp \cos^2\theta + K_\parallel \sin^2\theta \sin^2\phi - mH\sin\theta\sin\phi)$, $S_0 = S_1 + S_2$, $m = \gamma\hbar(S_1 - S_2)/\Omega$, Ω is the volume of the AFM particle. $K_\perp = 2k_\perp S^2/\Omega$ and $K_\parallel = 2k_\parallel S^2/\Omega$ are the trasnverse and longitudinal anisotropy constants, respectively. We have set $S_1 = S_2 = S$ except in the terms containing $S_1 - S_2$. The parameter $\chi_\perp = \gamma^2/J$ is introduced according to Ref.[20] for the problem at hand.

We consider a very strong transverse anisotropy $i.e.$ $K_\perp \gg K_\parallel$. In this case Néel vector is forced to lie in the x-y plane. Replacing θ by $\pi/2 + \eta_\theta$ where η_θ denotes the small fluctuation and carrying out integral over η_θ we obtain

$$\langle \mathbf{N}_f | e^{-i\hat{H}T/\hbar} | \mathbf{N}_i \rangle = e^{-iS_0(\phi_f - \phi_i)} \int \mathcal{D}[\phi] \exp\left(\frac{i}{\hbar} \int_{t_i}^{t_f} \mathcal{L}_{eff} dt \right), \tag{15}$$

where

$$\mathcal{L}_{eff} = (I_f + I_a)\frac{\Omega}{2}\left(\frac{d\phi}{dt} \right)^2 - V(\phi) \tag{16}$$

is the effective Lagrangian which is seen to be the Lagrangian of a plane rotor. Where $I_f = m^2/2\gamma^2 K_\perp$ and $I_a = \chi_\perp/\gamma^2$ are the effective FM and AFM moments of inertia, respectively[6]. $V(\phi) = \Omega K_\parallel(\sin\phi - \triangle)^2$ ($\triangle = H/H_c$ with a parameter $H_c = 2K_\parallel/m$) is the effective potential. It is seen that the net magnetic moment of the noncompensated sublattices in the applied magnetic field shifts the equilibrium orientations of Néel vector for corresponding angles $\pm\arcsin\triangle$ as shown in Fig.1-(b) besides the modification of FM moment of inertia I_f given in Refs.[6,18]. It may be worth while to compare our results with that in literature. In the absence of the magnetic field (namely $\triangle = 0$) the two degenerate equilibrium orientations return to the positive and negative x-axis (see Fig.1-(a)) respectively in agreement with the equilibrium phases of the AFM particle with

noncompensated sublattices[18]. The small oscillation frequency of Néel vector around its equilibrium orientations which serves as a characteristic parameter for the flip of Néel vector of the AFM particle is seen to be

$$\omega(H, m) = \left[\frac{2K_{\parallel}(1 - \triangle^2)}{I_f + I_a} \right]^{1/2} . \tag{17}$$

For $\triangle = 0$ it reduces exactly to

$$\omega(H = 0, m) = \left[\frac{2K_{\parallel}}{I_f + I_a} \right]^{1/2} \tag{18}$$

as given in Ref.[18]. If we consider idealized sublattices that $m = 0$ the frequency Eq.(17) goes back to the well known value

$$\omega(H = m = 0) = \gamma \left[\frac{2K_{\parallel}}{\chi_{\perp}} \right]^{1/2} = \left[2K_{\parallel} J \right]^{1/2} . \tag{19}$$

The effective potential of the plane rotor is plotted in Fig.2. The minima of the potential correspond to the equilibrium orientations of the Néel vector. The energy of net magnetic moment in the applied magnetic field lowers the barrier height in the direction of magnetic field while increases the barrier height in the opposite direction. We are interested in the quantum tunneling of the effective plane rotor through the barriers.

3   Two types of instantons and level shifts

In order to obtain the tunneling rate we evaluate the Euclidean path integrls in Eq.(15) with the Wick rotation $t = i\tau$. The Euclidean Lagrangian for the pseudoparticle moving in the classical forbidden region, namely, in the barrier is seen to be $L_E = (I_f + I_a)\frac{\Omega}{2} \left(\frac{d\phi}{d\tau} \right)^2 + V(\phi)$. The equation of motion of rotor at finite energy is

$$\frac{\Omega}{2}(I_f + I_a) \left(\frac{d\phi}{d\tau} \right)^2 - V(\phi) = -E , \tag{20}$$

The periodic potential $V(\phi) = V(\phi + 2n\pi)$ has an asymmetric twin barrier (Fig.2) .The two-fold rotation symmetry[10], namely, $V(\phi + \pi) = V(\phi)$ in the presence of magnetic field is removed . When the energy is higher than the ground sta8te tunneling is dominated by periodic instantons[21,22]. Thus there are two different periodic instantons corresponding

to two types of barriers. With the periodic boundary condition, two periodic instanton solutions of Eq.(17) are found to be

$$\phi_c^{(1)} = \frac{\pi}{2} + 2\arctan[\lambda_1 \mathrm{sn}(q\tau, k)] , \tag{21}$$

$$\phi_c^{(2)} = \frac{3\pi}{2} - 2\arctan[\lambda_2 \mathrm{sn}(q\tau, k)] , \tag{22}$$

where $\mathrm{sn}(q\tau, k)$ is elliptic function with modulus k and period $4\kappa(k)$. $\kappa(k)$ denotes the complete elliptic integral of the first kind, with

$$k = \left[\frac{(1-\eta)^2 - \triangle^2}{(1+\eta)^2 - \triangle^2}\right]^{1/2} , \quad \eta = \left(\frac{E}{\Omega K_\parallel}\right)^{1/2} .$$

The parameters q, λ_1 and λ_2 are defined by

$$q = \left(\frac{K_\parallel}{2(I_f + I_a)}\right)^{1/2} [(1+\eta)^2 - \triangle^2]^{1/2} , \quad \lambda_i = \left[\frac{(1-\eta)^2 - \triangle^2}{(1-(-1)^i \triangle)^2 - \eta^2}\right]^{1/2} , \quad (i = 1, 2)$$

The trajectories of instantons $\phi_c^{(1)}$ and $\phi_c^{(2)}$ are shown in Fig.2. At initial time τ_i, instantons $\phi_c^{(1)}$, $\phi_c^{(2)}$ start from the potential well at $\phi_i = \arcsin\triangle$ and reach the neighbouring well at $\phi_f = \pi - \arcsin\triangle$ at final time τ_f along the anticlockwise (through small barrier) and clockwise (through large barrier) paths respectively. In other words the Néel vector tunnels through a large barrier (or small barrier) between two angular positions with the lowest energy.

We assume that $|m, \phi_{2n}^{(1)}\rangle$ and $|m, \phi_{2n+1}^{(2)}\rangle$ denote the eigenstates of the harmonic oscillator approximated Hamiltonian in the potential wells at $\phi_{2n}^{(1)} = 2n\pi + \arcsin\triangle$ and $\phi_{2n+1}^{(2)} = (2n+1)\pi - \arcsin\triangle$, respectively, where m is the index of low-lying levels. The amplitudes tunneling through two different barriers are given by[21]

$$A_m^{(1)} = \langle m, \phi_0^{(1)}|e^{-\frac{2\beta\hat{H}}{\hbar}}|m, \phi_1^{(2)}\rangle = \exp\left(-\frac{2\beta\varepsilon_m}{\hbar}\right)\sinh\left(\frac{2\beta\triangle\varepsilon_m^{(1)}}{\hbar}\right) , \tag{23}$$

$$A_m^{(2)} = \langle m, \phi_1^{(2)}|e^{-\frac{2\beta\hat{H}}{\hbar}}|m, \phi_2^{(1)}\rangle = \exp\left(-\frac{2\beta\varepsilon_m}{\hbar}\right)\sinh\left(\frac{2\beta\triangle\varepsilon_m^{(2)}}{\hbar}\right) , \tag{24}$$

where $\triangle\varepsilon_m^{(1)}(\triangle\varepsilon_m^{(2)})$ is the level shift induced by tunneling through the small (large) barrier alone. $\triangle\varepsilon_m^{(i)}$ is actually the overlap integral defined in the following Eqs.(42),(43). Where $\beta = \tau_f - \tau_i$. With the help of the path integral, the matrix element in Eq.(23) and Eq.(24) can be rewritten as

$$A_m^{(1)} = \int \psi_m^*(\phi_0^{(1)}, \phi_f)\psi_m(\phi_1^{(2)}, \phi_i)\mathcal{K}^{(1)}(\phi_f, \tau_f; \phi_i, \tau_i)\mathrm{d}\phi_f \mathrm{d}\phi_i , \tag{25}$$

$$A_m^{(2)} = \int \psi_m^*(\phi_1^{(2)}, \phi_f)\psi_m(\phi_2^{(1)}, \phi_i)\mathcal{K}^{(2)}(\phi_f, \tau_f;\ \phi_i, \tau_i)\mathrm{d}\phi_f\mathrm{d}\phi_i\ , \tag{26}$$

where

$$\psi_m^*(\phi_0^{(1)}, \phi_f) = \langle m, \phi_0^{(1)}|\phi_f \rangle\ ,\quad \psi_m(\phi_1^{(2)}, \phi_i) = \langle \phi_i|m, \phi_1^{(2)} \rangle\ ,$$

$$\psi_m^*(\phi_1^{(2)}, \phi_f) = \langle m, \phi_1^{(2)}|\phi_f \rangle\ ,\quad \psi_m(\phi_2^{(1)}, \phi_i) = \langle \phi_i|m, \phi_2^{(1)} \rangle\ ,$$

$$\mathcal{K}^{(i)}(\phi_f, \tau_f;\ \phi_i, \tau_i) = \int_{\phi_i}^{\phi_f} \mathcal{D}[\phi] \exp\left(-\frac{S_E^{(i)}}{\hbar}\right)\ , \tag{27}$$

$$S_E^{(i)} = \int_{\tau_f}^{\tau_i} \left[\frac{\Omega}{2}(I_f + I_a)\left(\frac{\mathrm{d}\phi}{\mathrm{d}\tau}\right)^2 + V(\phi)\right]\mathrm{d}\tau\ ,\quad (i = 1, 2). \tag{28}$$

Here $S_E^{(i)}$ denotes the Euclidean action, and $\mathcal{K}^{(i)}(\phi_f, \tau_f;\ \phi_i, \tau_i)$ is Feynman propagator through two kinds of barriers. Substituting the periodic instanton solutions Eq.(21) and Eq.(22) into Eq.(28) the Euclidean action along the classical trajectory is found to be

$$S_{Ec}^{(i)} = 2E\beta + W^{(i)}\ , \tag{29}$$

$$W^{(i)} = \frac{4\Omega\chi_\perp q}{\gamma^2\lambda_i^2}\left[\lambda_i^2 E(k) + (k^2 - \lambda_i^2)\kappa(k) + (\lambda_i^4 - k^2)\Pi(k, \lambda_i)\right]\ , \tag{30}$$

where $E(k)$ is the complete elliptic integral of the second kind, and $\Pi(k, \lambda_i)$ is the complete elliptic integral of the third kind with the parameter λ_i. The level shift $\triangle\varepsilon_m^{(i)}$ can be determined by completing the integrals of (25) and (26) and comparing the result with Eq.(23) and Eq.(24). Using the method in Ref.[21], the transition amplitude is obtained as

$$A_m^{(i)} = \exp\left(-\frac{2E\beta}{\hbar}\right)\sinh\left\{\frac{\beta}{\sigma\kappa(k')}\left(\frac{2K_\parallel}{I_a + I_f}\right)^{1/2}\exp\left(-\frac{W^{(i)}}{\hbar}\right)\right\}\ ,\quad (i = 1, 2), \tag{31}$$

where $k' = (1 - k^2)^{1/2}$ and $\sigma = [(1 + \eta)^2 - \triangle^2]^{1/2}$. Comparing this expression with Eq.(23) and Eq.(24) we find that two types of level shifts are

$$\triangle\varepsilon_m^{(i)} = \frac{\hbar}{\sigma\kappa(k')}\left(\frac{2K_\parallel}{I_a + I_f}\right)^{1/2}\exp\left(-\frac{W^{(i)}}{\hbar}\right),\quad (i = 1, 2), \tag{32}$$

4   The magnetic field dependence of tunneling rates

It is easy to see that the difference between the heights of larger and small barriers increases with the external magnetic field . On the other hand, the effective frequency

of oscillator near the bottom of potential well given in Eq.(17) $i.\,e.\ \omega = \omega_0(1 - \triangle^2)^{1/2}$ decreases with the increasing field, where $\omega_0 = (\frac{2K_\parallel}{I_a+I_f})^{1/2}$ is the frequency in the absence of the magnetic field[18]. For the low energy case that the energy E is far below the barrier height , $i.e.\ \eta \ll 1 - \triangle, k \to 1,\ k' \to 0,\ E(k),\ \kappa(k)$ can be expanded as power series of k'. The complete elliptic integral of the third kind is expressed as

$$\Pi(k, \lambda_i) = \frac{k^2}{k^2 + \lambda_i^2} + \left[\frac{\lambda_i^2}{(1 + \lambda_i^2)(k^2 + \lambda_i^2)}\right]^{1/2} \left\{E(k)F(\alpha^i, k') + \kappa(k)[E(\alpha^i, k') - F(\alpha^i, k')]\right\},$$

where $\alpha^{(i)} = \arcsin(\lambda_i^2/(k^2 + \lambda_i^2))^{1/2}$. $F(\alpha^{(i)}, k'),\ \ E(\alpha^{(i)}, k')$ are the incomplete elliptic integrals of the first and second kinds, respectively. Thus $\Pi(k, \lambda_i)$ can be also expanded as the power series of k'. Then, the power series expression of $W^{(i)}$ reads

$$W^{(1)} = \frac{4K_\parallel \Omega}{\omega_0} \left\{(1 - \triangle^2)^{1/2} - \triangle \arccos \triangle - \frac{1}{16}(1 - \triangle^2)^{3/2}k'^4 \left[\ln \frac{4}{k'} + 1\right]\right\}, \qquad (33)$$

$$W^{(2)} = \frac{4K_\parallel \Omega}{\omega_0} \left\{(1 - \triangle^2)^{1/2} + \triangle \arccos(-\triangle) - \frac{1}{16}(1 - \triangle^2)^{3/2}k'^4 \left[\ln \frac{4}{k'} + 1\right]\right\}, \qquad (34)$$

In the low energy case, $k' = 4\eta/(1 - \triangle^2) \ll 1$,we may take the oscillator approximated energy-quantization $i.e.\ E \to E_m = (m + 1/2)\hbar\omega$. Taking note of limits $\kappa(k \to 0) \to \pi/2$ and $\sigma(\eta \to 0) \to (1 - \triangle^2)^{-1/2}$ we find

$$\triangle \varepsilon_m^{(1)} = F_m(1 - \triangle^2)^{5/4+3m/2} \exp\{-B[(1 - \triangle^2)^{1/2} - \triangle \arccos \triangle]\}, \qquad (35)$$

$$\triangle \varepsilon_m^{(2)} = F_m(1 - \triangle^2)^{5/4+3m/2} \exp\{-B[(1 - \triangle^2)^{1/2} + \triangle \arccos(-\triangle)]\}. \qquad (36)$$

Where

$$F_m = F_0 \frac{1}{n!}[4B]^n \ , \ B = \frac{4K_\parallel \Omega}{\omega_0 \hbar} \ , F_0 = \hbar\omega_0 \left[\frac{8B}{\pi}\right]^{1/2}.$$

Eq.(35) and Eq.(36) give rise to the field dependence of the level shift for low-lying excited states. There is an obvious difference between the level shifts induced by tunneling through two kinds of barriers. For a given excited state, $\triangle \varepsilon_m^{(i)}$ as a function of the external magnetic field is plotted in Fig. 3, with $k_\parallel = 10^6 erg/cm^3$, $K_\perp = 10^8 erg/cm^3$, $\chi_\perp = 10^4$, the excess of spin $S_1 - S_2 = 10$ and the AFM particle radius $r = 7.5nm$. It is clearly shown that the tunneling rate through a small barrier increases rapidly with the external magnetic field because the field reduces both the height and width of barrier. The situation is just opposite for the tunneling through the larger barrier . In addition, Fig.3 also shows

that the tunneling rate increases with the energy levels in the low-lying excited states. When $\triangle = H/H_c$ attends to 1 there is no tunneling at all since the small barrier shrinks to zero and only one easy direction remains. In the absence of applied magnetic field we have $(\triangle = 0)\triangle\varepsilon_m^{(1)} = \triangle\varepsilon_m^{(2)}$ and for the ground state tunneling,namely $E = \eta = 0$,the level shift $\triangle\varepsilon_0$ reduces to exactly the result in Ref.[18].

5   Level splitting and quantum interference effect

$\triangle\varepsilon_m^{(i)}$ is only the level shift induced by tunneling through a single barrier (smaller or larger). The periodic potential $V(\phi) = V(\phi + 2n\pi)$ can be regarded as a one-dimensional superlattice consisting of two sublattices. The general translation symmetry results in the energy band structure, and the energy spectrum could be determined with the Bloch theory. Let $|m, \phi_{2n}^{(1)}\rangle$ be the eigenstates of the zero order Hamiltonian $\hat{H}_0^{(1)}$ in the potential well which lies at $\phi_{2n}^{(1)} = 2n\pi + \arcsin\triangle$. $|m, \phi_{2n+1}^{(2)}\rangle$ denote the eigenstates of the zero order Hamiltonian $H_0^{(2)}$ in the well at $\phi_{2n+1}^{(2)} = (2n + 1)\pi - \arcsin\triangle$. Thus

$$H_0^{(1)}|m, \phi_{2n}^{(1)}\rangle = \varepsilon_m|m, \phi_{2n}^{(1)}\rangle , \tag{37}$$

$$H_0^{(2)}|m, \phi_{2n+1}^{(2)}\rangle = \varepsilon_m|m, \phi_{2n+1}^{(2)}\rangle . \tag{38}$$

Bloch state with 2π periodic boundary condition is written as

$$|\psi\rangle = \sum_n \left(e^{i(\xi+S_0)\phi_{2n}^{(1)}}|m, \phi_{2n}^{(1)}\rangle + e^{i(\xi+S_0)\phi_{2n+1}^{(2)}}|m, \phi_{2n+1}^{(2)}\rangle \right) , \tag{39}$$

where ξ is Bloch wave vector , $e^{iS_0\phi_{2n}^{(1)}}$ (or $e^{iS_0\phi_{2n+1}^{(2)}}$) is seen to be the topological phase from Eq.(15). Substituting Eq.(39) into the following stationary Schrödinger equation

$$\hat{H}|\psi\rangle = E|\psi\rangle , \tag{40}$$

and taking into account only the nearest neighbours yield the energy spectrum as

$$E = \varepsilon_m - \triangle\varepsilon_m^{(1)}\cos[(\xi + S_0)(\pi - 2\arcsin\triangle)]$$
$$-\triangle\varepsilon_m^{(2)}\cos[(\xi + S_0)(\pi + 2\arcsin\triangle)], \tag{41}$$

where the level shift $\triangle\varepsilon_m^{(i)}$ is actually the overlap integral defined by

$$\triangle\varepsilon_m^{(1)} = -\int u_m^*(\phi - \phi_{2n}^{(1)})\mathrm{H}u_m(\phi - \phi_{2n+1}^{(2)})\mathrm{d}\phi \ , \tag{42}$$

$$\triangle\varepsilon_m^{(2)} = -\int u_m^*(\phi - \phi_{2n}^{(1)})\mathrm{H}u_m(\phi - \phi_{2n-1}^{(2)})\mathrm{d}\phi \ . \tag{43}$$

The Bloch wave vector ξ can be assumed to take either of the two values 0 and 1 in the first Brillouin zone[21,23]. Thus the level splitting is seen to be

$$
\begin{aligned}
\triangle\varepsilon_m &= |\triangle\varepsilon_m^{(1)}\cos[2(1+S_0)\arccos\triangle] + (-1)^{2S_0}\triangle\varepsilon_m^{(2)}\cos[2(1+S_0)\arccos\triangle] \\
&\quad -\triangle\varepsilon_m^{(1)}\cos[2S_0\arccos\triangle] - (-1)^{2S_0}\triangle\varepsilon_m^{(2)}\cos[2S_0\arccos\triangle]| \\
&= E_m^{\pm}|\sin[(2S_0+1)\arccos\triangle]| \ , \tag{44}
\end{aligned}
$$

where

$$E_m^+ = R_m\cosh(B\pi\triangle/2) \ , \quad (S_0 = \text{integral}) \ , \tag{45}$$

$$E_m^- = R_m\sinh(B\pi\triangle/2) \ , \quad (S_0 = \text{half} - \text{integer}) \ , \tag{46}$$

$$R_m = 4F_m(1-\triangle^2)^{7/4+3m/2}$$

$$\exp\{-B[(1-\triangle^2)^{1/2} + \triangle\arcsin\triangle]\}. \tag{47}$$

When $H = 0, i.e. \arcsin\triangle = 0$, energy spectrum in Eq.(41) reduces to the result in Ref.[14], and for S_0 = half-integer the MQC is quenched in agreement with Kramers' theorem which can be well understood as two-fold discrete rotation-symmetry of Hamiltonian[10] . The applied magnetic field breaks the rotation symmetry and the Kramers' degeneracy is removed. Level splitting Eq.(44) shows the quantum interference effect depending on applied magnetic field. The level splitting increases with the magnetic field and whenever the magnetic field reaches some specific values which satisfy $H/H_c = \cos[l\pi/(2S_0+1)]$ (l is a integer), we have $\triangle\varepsilon_m = 0$ no matter S_0 is integer or half-integer. The quenching is similar to the case of the FM particle in Refs.[9,24] and is the result of quantum interference between transitions through the two kinds of barriers. Fig.4 shows the oscillation of the level splitting with the field for the ground state.

6 Conclusion

We present a full study of quantum tunneling effect for AFM particle with a small non-compensation of sublattices in an external magnetic field. The level splitting which is obtained only for ground state in literature has been extended to low-lying excited states with the help of periodic instanton method. The quantum interference effect, particularly, the entire suppression of tunneling may be of significance for practical application.

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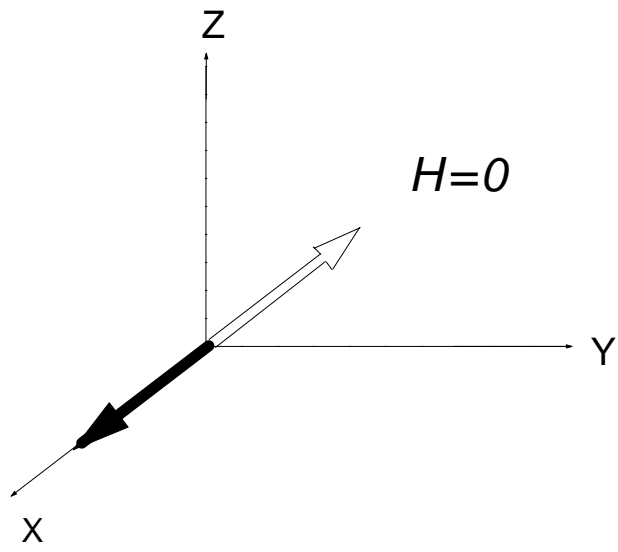24. E. M. Chudnovsky and David P. DiVincenzo, Phys. Rev. B 48(1993)10548.

Figure captions

Fig.1 (a) The two degenerate equilibrium orientations of Néel vector with noncompensated sublattices in an applied magnetic field. $\phi_+ = \arcsin \triangle$. (b) The equilibrium orientatons of Néel vector in the absence of applied magnetic field ($\triangle = 0$).
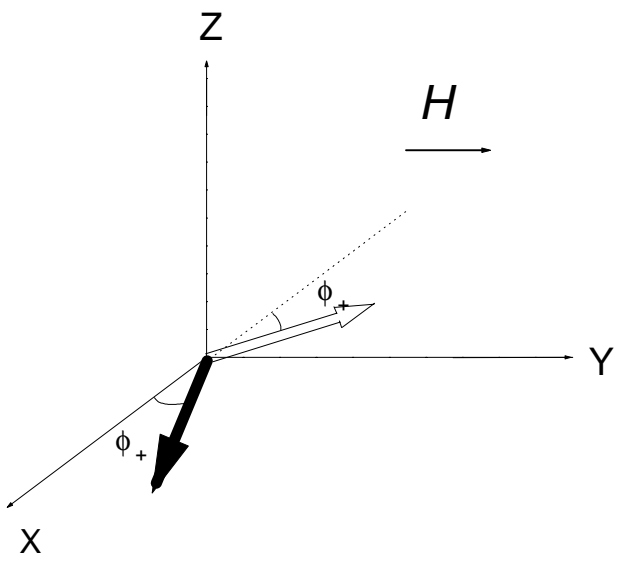
Fig.2 The periodic potential with asymmetric twin-barrier and the instanton trajectories.

Fig.3 The level shift $\triangle \varepsilon_m^{(i)}$ as a function of H/H_c. Solid line for $\triangle \varepsilon_m^{(1)}$ and dotted line for $\triangle \varepsilon_m^{(2)}$.

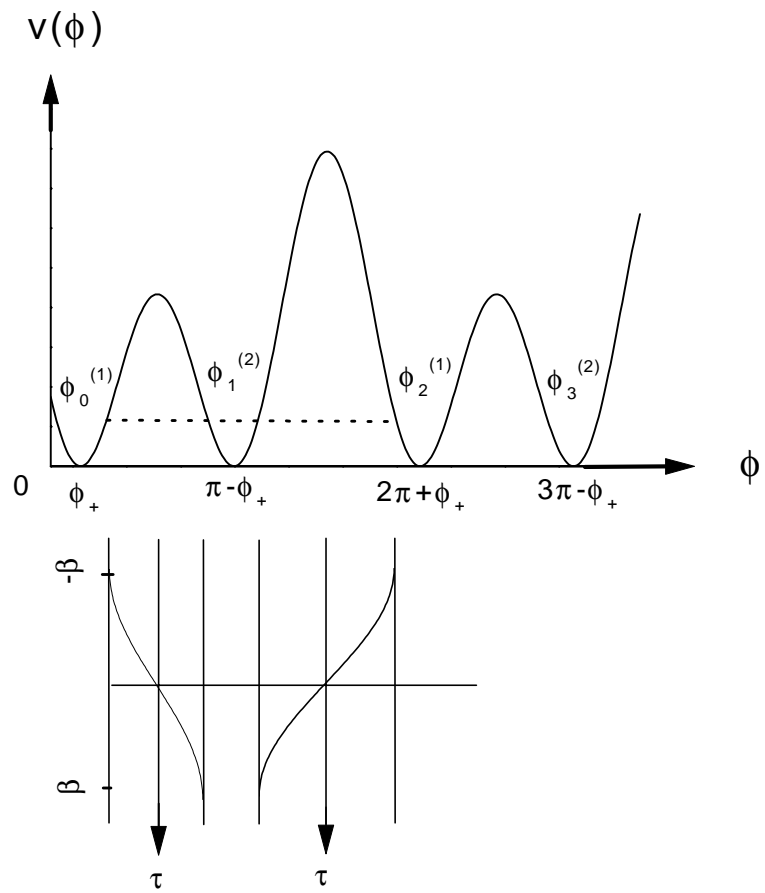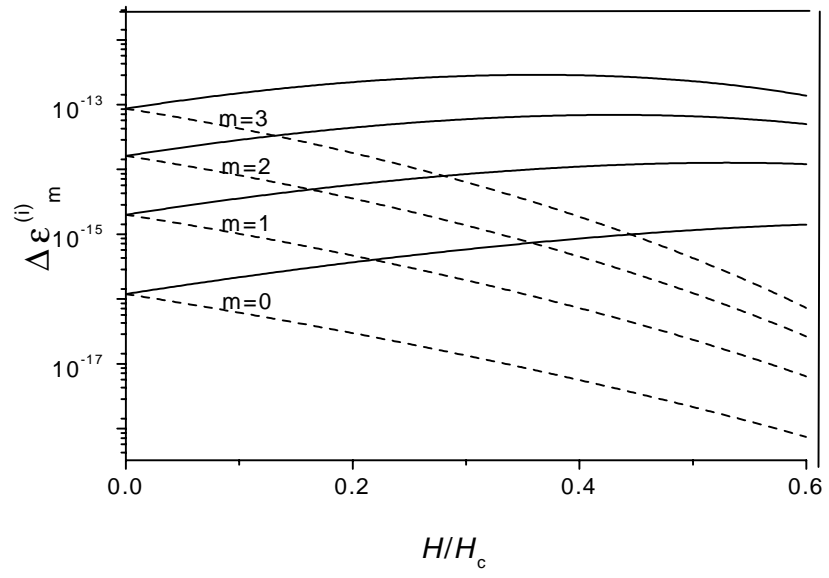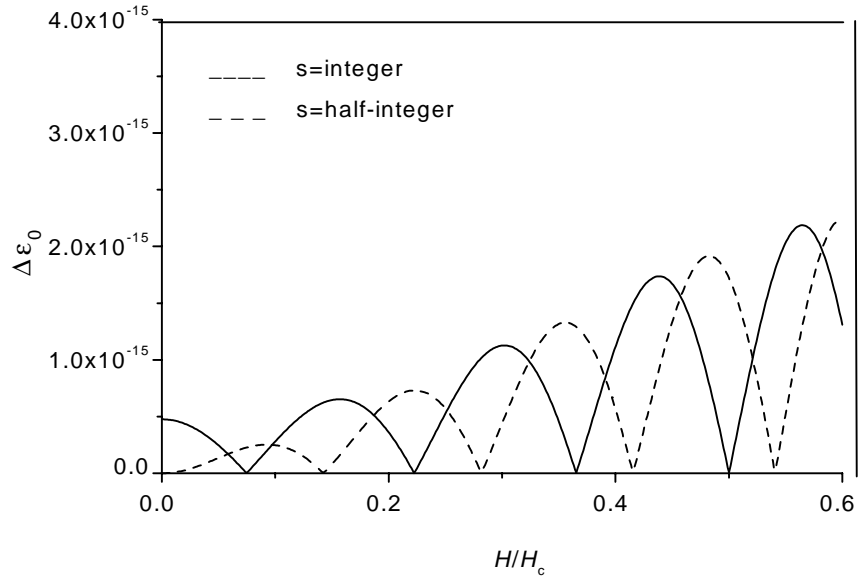Fig.4 The level splitting at ground state as a function of H/H_c.

Fig. 1

Fig. 2

Fig.3

Fig.4