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LETTER TO THE EDITOR

Macroscopic quantum tunnelling in antiferromagnets

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Abstract. Macroscopic quantum tunnelling in a single-domain antiferromagnetic particle is considered using different models for the antiferromagnet: an effective two-spin model and an anisotropic σ-model (large-spin continuum limit of the Heisenberg Hamiltonian). For both models the probability of tunnelling at low temperatures has been calculated. The tunnelling rates obtained in these cases agree qualitatively when expressed in the terms of the corresponding quantities. We have also estimated the tunnelling rate for a false-vacuum decay in an antiferromagnet with a small fourth-order anisotropy.

Quantum mechanics is applicable to both macroscopic and microscopic objects. Recently this well known fact was experimentally confirmed in studying the phenomenon of macroscopic quantum tunnelling (MQT) (Leggett *et al* 1987). One must distinguish between two types of tunnelling process. The first (MQT) is a false(metastable)-vacuum decay at low temperatures, while the second is tunnelling in small systems. The false-vacuum decay brings about the formation of an energy-favourable (stable) phase. The tunnelling in finite systems results in a small splitting of the ground-state energy (macroscopic quantum coherence).

Recently another rich field for MQT study has appeared—spin tunnelling. The magnetization in small ferromagnetic particles can tunnel through a classically forbidden region owing to subbarrier rotation as a single quantum variable, when the dynamics of the individual spins are suppressed (Chudnovsky and Gunter 1988a). This type of tunnelling differs somewhat from the usual mechanism in quantum mechanics owing to the quantum nature of spin compared with that of ordinary coordinate variables (van Hemmen and Süto 1986). Nevertheless, for a wide class of anisotropic spin systems, finding the energy spectrum and the problem of spin tunnelling can be approximately (Enz and Schilling 1986a, b) or even rigorously (Zaslavskii *et al* 1983, Scharf *et al* 1987, Zaslavskii 1990) reduced to the usual picture of a particle moving in a double well. A similar situation arises in the many-particle case (the Heisenberg model with weak anisotropy), when the exchange interaction causes the formation of a collective magnetic moment proportional to the total particle number. Meanwhile, the dynamics of such an effective-spin system are governed by the usual one-dimensional Schrödinger equation (Vekslerchik *et al* 1989). (Note that another type of rigorous application of the one-dimensional Schrödinger equation to many-particle systems is in the Lipkin–Meshkov–Glick model (Zaslavskii 1985).)

Quantum nucleation of magnetic bubbles is another type of tunnelling process, which can occur in continuous models. These bubbles correspond to domains of magnetization

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in a stable phase surrounded by a metastable phase. The decay rate of a false vacuum has been calculated by Chudnovsky and Gunter (1988b) and Caldeira and Furuya (1988) for anisotropic ferromagnetic systems.

The purpose of our paper is to discuss both the tunnelling effects described above (macroscopic quantum coherence and the decay of a false vacuum) for antiferromagnetic (AFM) systems (neglecting dissipation). The discrete symmetry of anisotropic infinite AFM systems is broken spontaneously in the Néel phase. In small AFM particles, tunnelling removes the degeneracy of the ground state and restores the full symmetry of the Lagrangian.

The role of the macroscopic variable tunnelling through the barrier between two minima of the corresponding effective potential is now played by the AFM vector. The Lagrangian for the AFM vector is known to be quadratic in the time derivative and thus is suitable for instanton method calculations.

First we present a simple 'toy' model of an antiferromagnet for which the MQT reduces to the well known quantum mechanical problem. Then a vacuum-to-vacuum tunnelling in a finite-length AFM chain is considered using a realistic continuum model–σ-model with θ-term. The resulting expressions for the tunnelling rate are proved to be equal for both models. Tunnelling in small particles involves a splitting of the ground state and in this way affects the low-frequency properties of such samples.

We begin with the formation of a simple model of two interacting spins of the same value S_0. This can correspond, for example, to two sublattices in small AFM particles. The Hamiltonian has the form

$$H = \tfrac{1}{2}J[\tfrac{1}{2}(M^2 - L^2) - 2\alpha L_z^2]. \tag{1}$$

Here $M = S_1 + S_2$, $L = S_1 - S_2$, M being the magnetization and L the AFM vector, while $J > 0$ and $\alpha > 0$. The last term in (1) is connected with magnetic anisotropy.

Parametrizing L by the spherical angles θ and φ, one can easily obtain that for $\alpha \ll 1$ and $M^2 \ll L^2$ the classical equations of motion take the form

$$\dot\varphi \sin^2\theta = \text{constant} \qquad \ddot\theta = \tfrac{1}{2}\sin(2\theta)(\dot\varphi^2 - \omega_0^2) \tag{2}$$

where $\omega_0 = 2^{3/2} J S_0 \alpha^{1/2}$.

These classical equations can be derived using the Lagrangian

$$\mathcal{L} = J^{-1}[(\tfrac{1}{2}\sin^2\theta)\dot\varphi^2 + \tfrac{1}{2}\dot\theta^2 - \tfrac{1}{2}\omega_0^2\sin^2\theta]. \tag{3}$$

According to equation (3), a classical ground state of the system turns out to be twofold degenerate (φ = constant, $\theta = 0$ or $\theta = \pi$). It corresponds to two energy-equivalent directions of L (along the z axis and in the opposite direction). When quantum tunnelling is taken into account, one can obtain the ground-state splitting ΔE_0. This value is determined by the tunnelling action W:

$$W = \frac{\omega_0}{J}\int_0^\pi d\theta\,\sqrt{2U(\theta)} \tag{4}$$

($U(\theta) = \tfrac{1}{2}\sin^2\theta$ being the dimensionless potential energy). Following Coleman (1979), we have

$$\Delta E_0 \sim \omega_0 W^{1/2}\exp(-W) \sim J S_0^{3/2}\alpha^{3/4}\exp(-4\sqrt{2\alpha}S). \tag{5}$$

If the anisotropy has a two-axis nature so that the term $J\beta L_x^2$ ($\beta > \theta$) in equation (1) is included, one must change α to $\alpha + \beta$ in equation (5). Note that the parameters of the problem must satisfy the conditions $S^{-2} \ll \alpha \ll 1$ since equation (5) is described in the quasiclassical approximation ($\Delta E_0 \ll E_0$).

The Hamiltonian (1) is the quantum mechanical 'toy' model for a Néel antiferromagnet. Nevertheless it describes correctly, as we shall see below, the tunnelling processes in small AFM particles. In the microscopic approach we must start from the Heisenberg Hamiltonian

$$H = J \sum_{\langle i,j \rangle} [\boldsymbol{S}_i \cdot \boldsymbol{S}_j + aS_i^z S_j^z - b(S_i^z)^2] \tag{6}$$

where a, b and J are all positive quantities, $S^2 = S(S+1)$ and the sum is over near-neighbour sites only.

We are interested in the long-wave (semiclassical) limit of the model (6) when the quantum lattice Hamiltonian may be changed for the simple continuum classical Hamiltonian.

Let us consider first a one-dimensional spin chain in the large-S limit. According to Haldane (1983) and Affleck (1985, 1986), the low-energy part of the quantum Hamiltonian (6) coincides in this approximation with the well known O(3) σ-model with θ-vacuum. The Lagrangian density of this model assumes the following standard form (Rajaraman 1982):

$$\mathcal{L} = (1/2g)(|\partial_\mu \boldsymbol{n}|^2 + m^2 n_z^2) + (\theta_S/8\pi)\varepsilon^{\mu\nu}\boldsymbol{n} \cdot (\partial_\mu \boldsymbol{n} \times \partial_\nu \boldsymbol{n}). \tag{7}$$

Here $\boldsymbol{n}$ is the AFM vector, $\mu = (t, x)$ and $\varepsilon^{\mu\nu} = -\varepsilon^{\nu\mu}$. The couplings in (7) are connected with the parameters of the Heisenberg Hamiltonian by the simple relations (Affleck 1985)

$$1/g = S/2 \qquad \theta_S = 2\pi S \qquad m = \sqrt{\tfrac{1}{2}(a+b)}\Delta^{-1} \qquad c = 2SJ\Delta \tag{8}$$

where Δ is the lattice spacing. We have adopted in (7) convenient units with $\hbar = C = 1$.

The quantities m and C in (7) and (8) are the mass and velocity of the small fluctuations of the AFM vector (spin waves), as can be seen from (7). The coefficient by which L_z^2 is multiplied in the Hamiltonian (1) corresponds to the following values of the Ising anisotropy in (6): $a = 2\alpha$, $b = \alpha$. In this case the activation energy of the spin waves given by $\omega_s = mc = \sqrt{6\alpha}SJ$ coincides with the characteristic energy ω_0 in (2) up to a numerical factor.

In terms of the angle variables $\theta(x, t)$ and $\varphi(x, t)$ the Lagrangian (7) takes the form

$$\begin{aligned} \mathcal{L} = (1/g)[(\tfrac{1}{2}\sin^2\theta)(\partial_\mu\varphi)^2 + \tfrac{1}{2}(\partial_\mu\theta)^2 - \tfrac{1}{2}m^2\sin^2\theta] \\ + (\theta_S/4\pi)\varepsilon^{\mu\nu}\partial_\nu(\cos\theta\,\partial_\mu\varphi). \end{aligned} \tag{9}$$

The equations of motion for the dynamical variables (which are spatially homogeneous fields $\theta(t)$, $\varphi(t)$) derived from equation (9) are identical with equation (2) as the last term in (9) (θ-vacuum) does not disturb the local dynamics of the system that we are dealing with. It is precisely this fact that justified the usefulness of the 'toy' model (1) for describing the tunnelling in the small AFM particles.

For a finite-length (L) spin chain, the classical vacua φ = constant, $\theta = 0$ and φ = constant, $\theta = \pi$ are separated by the potential barrier of finite approximate value Lm^2/g and vacuum-to-vacuum tunnelling is possible. It is plausible to assume (we prove this assumption below) that the minimum of the Euclidean action is realized for the spatially homogeneous instanton trajectories (the imaginary time solutions of the Euler–Lagrange equations)

$$\varphi = \text{constant} \qquad \cos[\theta(\tau)] = \tanh(m\tau). \tag{10}$$

The action for this trajectory can be expressed as

$$W_0 = LE_s \qquad E_s = 2m/g \tag{11}$$

where E_s is the rest energy of the AFM vector topological soliton (kink) (Mikeska 1980, Affleck 1985).

Because of the vacuum tunnelling the ground-state energy of the spin chain is described by the value

$$\Delta V_t \sim (m/L)W_0^{1/2}\exp(-W_0). \tag{12}$$

It should be compared with the tunnelling splitting for the two-spin model (1). Note that both actions will agree numerically when S_0 in (5) is replaced by the effective total 'spin':

$$S_0 = S_{\text{eff}} = (\sqrt{3}/8)NS \tag{13}$$

where $N = L/\Delta$ is the number of sites in the spin chain. One now must prove that the spatially inhomogeneous instantons increase the Euclidean action. The exact solution of the Euler–Lagrange equations in the imaginary time describing the inhomogeneous instanton has the form

$$\Phi(x,\tau) = kx + \text{constant} \qquad \cos[\theta(x,\tau)] = \tanh(m\tau). \tag{14}$$

In the finite chain the momentum k is quantized and for the periodic boundary condition $\boldsymbol{n}(\tau,0) = \boldsymbol{n}(\tau,L)$, which is the only one compatible with vacuum homogeneity ($\boldsymbol{n}$ = constant), is given by

$$k_n = (2\pi/L)n \qquad n = 0, \pm1, \pm2, \dots. \tag{15}$$

Using (14) and (15) we obtain the following Euclidean action:

$$W_n = -E_sL - (L/gm)k_n^2 + \mathrm{i}\theta_S n. \tag{16}$$

We now demonstrate that the tunnelling splitting will not depend on the vacuum angle θ_S, even though the one-instanton action (16) is a function of θ_S. The corresponding calculations include the summation over all instanton and anti-instanton trajectories with a finite action compatible with the boundary conditions. For our double-well potential, each instanton is accompanied by the anti-instanton (with opposite-sign vacuum angle in the action) and the resulting formula for the tunnelling splitting turns out to be θ_S independent.

The zero mode ($n = 0$) in (15) and (16) gives the action of the spatially homogeneous instanton trajectory. For $n \neq 0$, $|W_n| > |W_0|$, the probability of vacuum-to-vacuum tunnelling peaks for the instanton solution (10).

Let us now consider the AFM system with a metastable state and calculate the decay rate. The corresponding Lagrangian is

$$\mathcal{L} = (1/g)[(\dot\theta^2 + \dot\varphi^2\sin^2\theta)/2c^2 - \tfrac{1}{2}(|\nabla\theta|^2 + |\nabla\varphi|^2\sin^2\theta) - U]$$
$$U = (\omega_0^2/2c^2)\sin^2\theta - (\omega_1^2/4c^2)\sin^4\theta. \tag{17}$$

Here c is the speed of the spin waves, and the number n ($= 1, 2, 3, \dots$) of space dimensions is arbitrary. Such a Lagrangian is very similar to that in equation (7) but in contrast with equation (7) it is phenomenological for $n \neq 1$. The term proportional to ω_1^2 appears because of the fourth-order anisotropy in the n_i-power expansion. Although such terms are small in general, they must be taken into account for substances with second-order anisotropy to be anomalously small.

One can easily see that a metastable state exists for $\omega_1 > \omega_0$. Note that, in contrast with the ferromagnetic case, a magnetic field (described by a term $-\boldsymbol{B} \cdot \boldsymbol{S}$) does not cause the system to have a metastable state since in the main approximation the magnetic moments of sublattices are compensated. In fact, the inclusion of a magnetic external field leads to a redefinition of the generalized velocity $\dot{\varphi} \to \dot{\varphi} - \Omega$ (Ω being the precession frequency) only. The above assertion is valid for the collinear phase of an antiferromagnet. The case of the spin-flop phase is a separate problem.

If $\omega_1 > \omega_0$, $\theta = \frac{1}{2}\pi$ for the metastable state and $\theta = 0$ for the true ground state. Owing to quantum tunnelling, a metastable state decays, forming true-vacuum bubbles. The corresponding calculation technique is well known (Coleman 1979). To calculate the tunnelling probability one has to find the Euclidean action for spherically symmetric solutions of the equation

$$\mathrm{d}^2\theta/\mathrm{d}r^2 + (n/r)\,\mathrm{d}\theta/\mathrm{d}r = \sin\theta\cos\theta\,(m^2 - \mu^2\sin^2\theta)$$
$$r = \sqrt{\tau^2c^2 + x^2} \qquad m = \omega_0/c \qquad \mu = \omega_1/c \tag{18}$$

where τ is the Euclidean time.

Let us restrict ourselves to the thin-wall approximation where the energy difference ΔV between a true vacuum and a false vacuum is small:

$$\omega_1^2 = 2\omega_0^2(1-\varepsilon) \qquad \Delta V = \varepsilon\omega_0^2/2gc^2 = m^2/2gc^2 \qquad 0 < \varepsilon \ll 1. \tag{19}$$

Since in real substances the anisotropy constants cannot be changed by the experimenter, the relation (19) is not valid in general. Therefore calculations have an illustrative character. They permit us to obtain simple analytical expressions. (In general, one needs to calculate the decay rate numerically.)

The tunnelling probability per unit n-dimensional volume has the form

$$\Gamma/V_n = A\exp(-W). \tag{20}$$

Here the Euclidean action equals

$$W = \tfrac{1}{2}\omega_0[d_n/(n+1)](r_0^n/gc^2) \qquad A \sim (W/2\pi)^{(n+1)/2}c(\omega_0/c)^{n+1} \tag{21}$$

and the radius of the bubble is

$$r_0 = (n/\varepsilon)c/\omega_0.$$

Depending on the number of dimensions, d_n equals different values: $d_1 = 2\pi$, $d_2 = 4\pi$ and $d_3 = 2\pi^2$. Note that in the one-dimensional case ($n = 1$) for $\omega_1^2 = 2\omega_0^2$ our model (17) reduces to the sine–Gordon model. It has exact solutions (in particular, kinks, i.e. topologically stable solitons)

$$\theta(x,t) = \tfrac{1}{2}\cos^{-1}\{\mp\tanh[m(x - Vt)/\sqrt{1 - V^2/c^2}]\}$$
$$= \tan^{-1}\{\exp[\pm m(x - Vt)/\sqrt{1 - V^2/c^2}]\} \tag{22}$$

which connect the vacuum $\theta = 0$ with the vacuum $\theta = \frac{1}{2}\pi$ at space infinities. The rest energy of the soliton (22) equals

$$E_k = \omega_0/2gc = m/2g. \tag{23}$$

In one-dimensional problems ($n = 1$) the tunnelling action (21) can be rewritten in terms of the soliton energy (23) and the vacuum energy difference ΔV to take the well known form

$$W_{n=1} = \pi E_k^2 / c\,\Delta V. \tag{24}$$

It is interesting that the consideration of quantum tunnelling in antiferromagnets turns out to be simpler than that for ferromagnets (Chudnovsky and Gunter 1988b, Caldeira and Furuya 1988). This is because classical equations of motion for the AFM vector are of second order. The corresponding Lagrangian has the form (17) which allows us to use the well known instanton method immediately. Meanwhile, the equations of motion of magnetic moments in ferromagnets (the Landau–Lifshitz equation) are first order. Therefore additional efforts are necessary to derive the corresponding second-order equations (Chudnovsky and Gunter 1988b, Caldeira and Furuya 1988).

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