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LETTER TO THE EDITOR

Tunnelling of a large spin at finite temperature

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Abstract. The spin system with two-axis anisotropy is considered. The temperature dependence of the probability of transition from the metastable state due to quantum and thermal fluctuations is determined. The method of calculation is based on exact correspondence between the spin system and a particle moving in a potential field.

Tunnelling between two classical degenerate states in a double well and the decay of the metastable state are known effects in quantum mechanics. But it is only recently that such tunnelling has begun to be investigated for spin systems (van Hemmen and Süto 1986, Enz and Schilling 1986a, b, Scharf *et al* 1987, Chudnovsky and Gunther 1988a). This question needs special methods to be developed. One of them is connected with accounting for the contribution of sub-barrier instanton trajectories. Such a method (which is physically relevant for the consideration of tunnelling) enables one to calculate the energy splitting of the ground state, including the pre-exponential factor (Enz and Schilling 1986b). But it is rather complicated, deals with the phase variable (which is not a well defined quantity in quantum mechanics—Carruthers and Nieto 1968) and is not convenient for generalisation at finite temperatures.

I develop in this Letter another approach, which is connected with exact correspondence between the spin systems and a particle moving in a potential field. It provides the possibility of using quantum mechanical methods directly, and of investigating spin tunnelling at a finite temperature, $T \neq 0$.

Let us consider the spin system with a Hamiltonian

$$H = BS_z^2 - AS_x^2 - hS_y. \tag{1}$$

The energy levels E_n of such system correspond to the boundaries of bands for a particle described by the Schrödinger equation (Zaslavskii and Ulyanov 1987)

$$(S+\tfrac{1}{2})^{-2}\,\mathrm{d}^2\Psi/\mathrm{d}x^2 + \Psi(\kappa - V) = 0 \qquad E = \kappa(S+\tfrac{1}{2})^2(A+B) \tag{2}$$

$$V = \frac{2a}{1+b}\frac{\operatorname{cn} x}{\operatorname{dn}^2 x} + \frac{\operatorname{sn}^2 x}{\operatorname{dn}^2 x}\frac{1}{(1+b)^2}\left(a^2 - b\frac{S(S+1)}{(S+\frac{1}{2})^2}\right) \tag{3}$$

$$a = h/A(2S+1) \qquad b = B/A$$

the modulus of the elliptic functions being $k = (1+b)^{-1/2}$.

The value $(S+\frac{1}{2})^{-1}$ plays the role of the Planck constant $\hbar$. For large spin $S \gg 1$ it is possible to ignore the difference between $(S+\frac{1}{2})^2$ and $S(S+1)$, which simplifies calculations.

If $h > h_0 = B(2S+1)$ the system has the metastable state. It corresponds, for example, to the point $x_0 = 0$ in the potential picture.

Now one can use the results of calculations of the transition probability for such potential directly in a WKB approximation (Noble 1979, Affleck 1981) or in terms of instanton technique (Weiss and Haeffner 1983). Consider the case $h - h_0 \ll h_0$, so $a \simeq b$. One can then use a power expansion of the potential

$$V(x) - V(0) = cx^2 - dx^4 + \dots \tag{4}$$

Following the last mentioned paper, the temperature dependence of the transition probability

$$\Gamma(T)/\Gamma(0) = (1 - e^{-\omega/T}) \exp[(D^2/2\omega)\, e^{-\omega/T}]. \tag{5}$$

Here $\hbar = 1$, ω being the frequency of small oscillations near the minimum

$$\Gamma(0) = (\omega/\pi)^{1/2}\tfrac{1}{2}D \exp(-W) \tag{6}$$

W is the whole Euclidean action along the instanton trajectory, the constant D is determined by the asymptotic form of this trajectory

$$x(\tau) \simeq x_0 + (D/2\omega m^{1/2}) \exp(-\omega\tau) \qquad \tau \to \infty$$
$$x(-\infty) = x_0 \qquad x(0) = x_1 \tag{7}$$

m is the particle mass, x_1 is the turning point. One can find

$$\omega = 2c^{1/2}(A+B)(S+\tfrac{1}{2}) \qquad W = \tfrac{4}{3}(c^{3/2}/d)(S+\tfrac{1}{2})$$
$$D = 2^{5/2}c[(A+B)/d]^{1/2}(S+\tfrac{1}{2}). \tag{8}$$

Equations (5)–(8) are applicable to any potential of the form (4), if $T < T_1 = \hbar\omega/2\pi$. In our case

$$c = (a-b)/(1+b) \qquad d = b/4(1+b). \tag{9}$$

For $T \gtrsim T_1$ we have, according to Affleck (1981),

$$\Gamma = [TT_1/\pi\hbar(T - T_1)] \sinh\frac{\hbar\omega}{2T} \exp(-T_2/T) \qquad T_2 = (A+B)(S+\tfrac{1}{2})^2c^2/4d. \tag{10}$$

In the high-temperature limit $T \gg T_1$ the transitions of magnetisation are determined by the thermal fluctuations. The corresponding probability has the form

$$\Gamma = (\omega/2\pi)\exp(-T_2/T). \tag{11}$$

The general expression for the crossover region where $T \simeq T_1$ between the quantum and thermal fluctuations can be obtained in a similar manner. But it is rather cumbersome (Affleck 1981) and is omitted here.

The potential (3) contains, besides spin states, 'superfluous' states with numbers $n > 2S$. But at temperatures $T \ll T_2$ ($T_2 \gg T_1$ since $S \gg 1$) the relative contribution of such states to the transition probability is negligible.

Note that for one-axis anisotropy ($B = 0$) the effective potential was obtained in Zaslavskii *et al* (1983) and then rediscovered in Scharf *et al* (1987) where it was used in a WKB approximation†.

† The rules of quantisation of the Bohr–Sommerfeld type with quantum corrections were derived for a spin Hamiltonian of general form in Zaslavskii (1984).

The results of this work can be useful, for example, in the investigation of the switching of the magnetic moment in small ferromagnetic particles (Bean and Livingston 1959, Chudnovsky and Gunther 1988a).

Strictly speaking the results obtained described only the initial stage of the decay time $t \sim \Gamma^{-1}$ due to reflection at the walls. In the thermodynamical equilibrium state the transition probability calculated above is compensated by the flux of the opposite sign. Such a situation was discussed in Noble (1979) where only outgoing waves have been taken into account.

I did not discuss here a quantum tunnelling in many-particle spin systems which is a separate question (Chudnovsky and Gunther 1988b, Caldeira and Furuya 1988, Vekslerchik *et al* 1989).

The interesting problem is the effective potential approach for describing the effects of dissipation (Legget *et al* 1987).

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