Quantum mechanical tunneling in the Heisenberg model with weak anisotropy

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(Submitted 12 October 1988)
Zh. Eksp. Teor. Fiz. **95**, 1820–1825 (May 1989)

It is shown that the energy levels of low lying states in the Heisenberg model with weak anisotropy can be found as eigenvalues of a paramagnetic Hamiltonian whose anisotropy constants have been renormalized relative to the original ones and whose spin is proportional to the number of particles. The spectrum of such a system is rigorously described with the help of a simple effective potential permitting the use of familiar quantum-mechanical methods. Using instanton techniques, the splitting of the ground state energy due to tunneling is calculated and found to be quite sensitive to all parameters in the problem except the isotropic exchange constant.

These days investigation of tunneling effects is of considerable interest in various areas of condensed matter physics. As a rule one studies the interaction with the reservoir of a particle in a double-well potential (the resultant splitting of the ground states due to tunneling is described by an effective spin $\frac{1}{2}$). Recently investigation of tunneling effects of a different kind has been undertaken, connected to the quantum nature of spin in magnetic systems.[1–6] (A description of tunneling in such systems was already attempted in Ref. 7. Since, however, the interaction Hamiltonian commutes with the Hamiltonian of the quantum top considered there, no tunneling transitions are possible in that model.) Moreover, only one-particle Hamiltonians were considered. At the same time more realistic cases are of special interest, when interaction between spins plays a substantial role.

In this paper we calculate the energy splitting of the ground state due to tunneling in the Heisenberg model. This becomes possible because the system under consideration, as will be shown below, reduces in a well-defined sense to a one-particle system, whose parameters are renormalized relative to the original ones.

An important separate question involves the development of special methods for the description of quantum-mechanical properties of spin systems, in particular tunneling. Thus, instanton techniques for calculations in spin systems were developed in Ref. 4, but the corresponding method is rather complicated and difficult to control, involving, for example, the use of an exponential phase operator (for a discussion of the difficulties associated with this see Ref. 8). In Ref. 5 use was made in the main approximation of the WKB method, which is only one applicable, strictly speaking, to the analysis of excited states. (We note that an analog of the WKB method with account of the main quantum correction was developed for spin Hamiltonians of a general form in Ref. 9.) We emphasize that the point is the need for taking into account very subtle effects, since the sharp exponential dependence of tunneling on the spin L means that the difference between, say, L and $L+\frac{1}{2}$ may turn out to be significant even for $L\gg 1$. Notwithstanding the special attention paid to this circumstance in Ref. 3, the corresponding results[3,4] are not free of this shortcoming.

Here we shall exploit the possibility, discovered in Refs. 10–12, of reducing certain spin systems to the motion of a particle in an effective potential field, thus permitting the use of familiar methods of quantum mechanics and providing at the same time a clear picture of the process.

We consider a spin system described by the Hamiltonian

$$H=\alpha\sum_{\mathbf{n}}S_{\mathbf{n}}^{z2}-\beta\sum_{\mathbf{n}}S_{\mathbf{n}}^{y2}+h\sum_{\mathbf{n}}S_{\mathbf{n}}^{x}-J\sum_{\mathbf{n},\boldsymbol{\delta}}\mathbf{S}_{\mathbf{n}}\mathbf{S}_{\mathbf{n}+\boldsymbol{\delta}}. \tag{1}$$

Here the exchange constant $J>0$ (the ferromagnetic case), S^i is the operator for the ith component of the spin S, $\alpha\geqslant 0$ and $\beta\geqslant 0$ are single-ion anisotropy constants, h is the magnetic field strength in corresponding units, and $\boldsymbol{\delta}$ labels nearest neighbors.

The investigation of the energy spectrum of such a Hamiltonian (and, in particular, of tunneling, if the classical ground state is degenerate) is in general fraught with difficulties. We shall confine ourselves to the case of weak anisotropy of α and β, and small values of the field h/S, when the single-ion part of the Hamiltonian may be treated as a perturbation in comparison with the exchange part.

As is well-known,[13] the ground state of an isotropic ferromagnet corresponds to the value $L=NS$ of the total angular momentum (where N is the number of nodes) and is $(2L+1)$-fold degenerate in one of its components (say L^z). Therefore in the leading approximation the correction to the energy levels is determined from the secular equation, and to zeroth order the wave functions are constructed as

$$|\Psi\rangle=\sum_{\sigma=-L}^{L}c_\sigma|\sigma\rangle,\qquad L^z|\sigma\rangle=\sigma|\sigma\rangle. \tag{2}$$

The only nonvanishing matrix elements are the diagonal ones and the off-diagonal ones for the transitions $\sigma\to\sigma\pm 2$. Taking it into account that

$$|\sigma\rangle=\left(\frac{(L+\sigma)!}{(2L)!\,(L-\sigma)!}\right)^{1/2}(L^-)^{L-\sigma}|L\rangle, \tag{3}$$

where $L^+=L^x+iL^y$ is the lowering operator, and applying the commutation rules for components of spin, we find for the diagonal matrix elements

$$f_\sigma=\langle\sigma|\sum_{\mathbf{n}}S_{\mathbf{n}}^{z2}|\sigma\rangle$$

the recurrence relation

$$f_\sigma=2S\sigma-NS^2+\frac{NS-\sigma}{NS+\sigma+1}[NS(S+1)+\sigma+1-f_{\sigma+1}]. \tag{4}$$

Its solution has the form

$$f_\sigma=\frac{2S-1}{2NS-1}(\sigma^2-N^2S^2)+NS^2. \tag{5}$$

 0038-5646/89/051052-04$04.00

The off-diagonal elements are evaluated analogously.

As a result it turns out that the sought-for corrections, corresponding to the splitting of the original multiplet, are found as eigenvalues of the Hamiltonian

$$H=BL_z^2-AL_y^2+hL_x+\frac{N(N-1)}{2NS-1}S^2(\alpha-\beta), \tag{6}$$

which describes a paramagnet with spin $L = NS$ and anisotropy constants

$$B=\alpha(2S-1)/(2NS-1),\ A=\beta(2S-1)/(2NS-1). \tag{7}$$

Thus it can be said that the exchange interaction creates the resulting spin and leads to a renormalization of the anisotropy constants, but otherwise is not directly manifested in the dynamic properties of the system in this approximation for the low-lying states.

We consider first the case of uniaxial anisotropy of the "easy axis" type, when $\alpha = 0, \beta > 0$. Then, as was shown in Refs. 10 and 11 (and thereafter in Ref. 5), the energy spectrum of such a system coincides with the $2L + 1$ low-lying levels of a particle moving in a potential

$$U(x)=\frac{h^2}{4A}\,\mathrm{sh}^2 x-h\left(L+\frac{1}{2}\right)\mathrm{ch}\,x. \tag{8}$$

Here the role of the Planck constant $\hbar$ is played by $(L+\frac{1}{2})^{-1}$, and that of the mass m by A^{-1}. For $h < h_0$

$$h_0=(2L+1)A=\frac{(2S-1)(2NS+1)}{2NS-1}\beta, \tag{9}$$

the potential has two minima and the corresponding classical ground state is twofold degenerate.

At this point one may employ directly the instanton method.[14,15] The energy splitting of the ground state equals

$$\Delta E_0=(\hbar\omega/\pi)^{1/2}M\exp(-W/\hbar). \tag{10}$$

Here W is the Euclidean action along the trajectory connecting the two minima and ω is the frequency of small oscillations in them. We note that at the same time the concept of an instanton in a spin system acquires a simple and clear meaning (compare with Ref. 4). The asymptotic form of the instanton trajectory (say, going from the left minimum x_- to the right x_+) permits the determination of the value of the coefficient of the exponential:

$$x(\tau)\approx x_+-\frac{M}{2\omega m^{1/2}}\exp(-\omega\tau), \tag{11}$$

for Euclidean time $\tau\to\infty$. The instanton trajectory for the case under consideration has the form

$$\mathrm{th}\frac{x}{2}=\left(\frac{1-a}{1+a}\right)^{1/2}\mathrm{th}\frac{(1-a^2)^{1/2}\tau}{2},\qquad a=\frac{h}{h_0}, \tag{12}$$

whence we obtain, with Eqs. (7)–(11) taken into account,

$$\Delta E_0=\frac{8\beta}{\pi^{1/2}}\frac{(2S-1)}{(2NS-1)}\frac{(NS+{}^1/_2)^{3/2}(1-a^2)^{5/4}a^{2NS}}{(1+(1-a^2)^{1/2})^{2NS+1}}$$

$$\times \tag{13}$$

The effective potential method permits the determination of not only the size of the tunneling splitting for the ferromagnet, but also the actual value of the energy of the ground state, similarly to what has been done for the paramagnet in Ref. 10. We give, as an example, this value [accurate up to the exchange term and the c-number part in (6)] for the critical value of the magnetic field, when the double minimum disappears, and the potential reduces (for large values of the effective spin) to a pure quartic oscillator:

$$\Delta E_0=-\frac{2\beta(NS+{}^1/_2)^2(2S-1)}{2NS-1}+\frac{0{,}668\beta(2S-1)}{2NS-1}\left(NS+\frac{1}{2}\right)^{2/3}. \tag{14}$$

The characteristic change in the magnetic susceptibility occurs in the neighborhood of the critical field

$$|\gamma|\sim 1,\qquad \gamma=\frac{h-h_0}{h_0}\left(NS+\frac{1}{2}\right)^{2/3},$$

where it can be found with the help of numerical methods, and is substantially different from the classical step-like behavior (calculational details and the corresponding figure are given in Ref. 10).

It should be pointed out that for $N\gg 1$ the conditions for applicability of perturbation theory to the energy values themselves—smallness of matrix elements of the perturbation compared to differences in energy levels—are violated. However, for the size of the splitting ΔE_0 the results remain valid, as in the evaluation of the gap in the theory of superconductivity.[16]

We consider now the case of biaxial anisotropy. In that case the Schrödinger equation that provides a realization of the spin-coordinate correspondence has the form[12]

$$(A+B)\frac{d^2\Psi}{dx^2}+\Psi(E-U)=0, \tag{15}$$

$$U=(A+B)^{-1}\left[\frac{h^2}{4}-ABL(L+1)\right]\frac{\mathrm{sn}^2 x}{\mathrm{dn}^2 x}+\frac{h(L+{}^1/_2)\,\mathrm{cn}\,x}{\mathrm{dn}^2 x},$$

with the modulus of the elliptic functions $k=A^{1/2}/(A+B)^{1/2}$ and the spin levels corresponding to the edges of the band.

Let us analyze first the case $h = 0$. If S is half-integer and N is odd then the effective spin $L = NS$ is half-integer and the degeneracy is not removed.[12] We shall therefore consider NS to be integer (let us note that in this manner the structure of low-lying levels in the case of half-integer spin depends on the parity of their number even in the case of arbitrarily large N). Then, as was shown in Ref. 12, the ground state of the spin system corresponds to the lower edge of the first energy band, and the first excited state to the upper edge of the same band. The problem therefore reduces to the quasiclassical calculation of the width of the band, which can be done with the help of formulas of the type (10), which now have for the periodic case an additional factor 2.[14] The role of the Planck constant is now played by $[NS(NS+1)^7]^{-1/2}$.

The instanton trajectory is expressed in terms of elliptic functions:

$$\mathrm{sn}\,x=\mathrm{th}\,2\left(\frac{\beta}{\alpha+\beta}\right)^{1/2}\tau, \tag{16}$$

and the expression for the tunneling splitting has the form

$$\Delta E_0=\frac{16}{\pi^{1/2}}\frac{[NS(NS+1)]^{3/4}}{2NS-1}(2S-1)\frac{(\alpha+\beta)^{3/4}\beta^{3/4}}{\alpha^{1/2}}\times\left(\frac{(\alpha+\beta)^{1/2}-\beta^{1/2}}{(\alpha+\beta)^{1/2}+\beta^{1/2}}\right)^{(NS(NS+1))^{1/2}} \tag{17}$$

Let us consider another special case: $h = 2(AB)^{1/2}(L(L+1))^{1/2}$, so that the first term in the potential (15) vanishes. The effective Planck constant now equals $[NS(NS+1)]^{-1/4}(NS+\frac{1}{2})^{-1/2}$. Let $\beta > \alpha$, so that the potential has a double minimum in a cell (see Fig. 1, Ref. 12). The ground spin state belongs to the first energy band, and the first excited state to the second band.[12]

As can be verified by direct calculation, the Euclidean action is larger for an instanton trajectory through a barrier between cells (which exists also in the absence of two minima) than for a trajectory between the two minima in the same cell. Therefore, in the quasiclassical case under consideration, the width of both energy bands is exponentially small to higher order than the distance between them. This means that one may ignore details of distribution of levels within a band, i.e., ignore the band nature of the spectrum connected with the periodicity of the potential. Then the difference between the energies of the first excited and ground spin states can be calculated as the splitting of a level in an isolated cell directly from formulas (10) and (11).

The formulas for the instanton trajectory and the size of the splitting have respectively the form

$$\frac{1+\operatorname{cn} x}{1-\operatorname{cn} x} = \frac{\beta^{1/2}-\alpha^{1/2}}{\beta^{1/2}+\alpha^{1/2}} \operatorname{th}^2\left(\frac{\beta-\alpha}{\beta+\alpha}\right)^{1/2} \tau, \tag{18}$$

$$\Delta E_0 = \frac{2^{5/2}}{\pi^{1/2}} \frac{\tilde{L}^{3/2}(2S-1)}{(2NS-1)} \frac{(\alpha+\beta)^2}{(\alpha\beta)^{1/2}} \times \left(\frac{(\alpha+\beta)^{1/2}-(\beta-\alpha)^{1/2}}{(\alpha+\beta)^{1/2}+(\beta-\alpha)^{1/2}}\right)^{\tilde{L}} \times \exp(2\varphi\tilde{L}) \left(\frac{\beta-\alpha}{\beta+\alpha}\right)^{5/4}, \tag{19}$$

$$\varphi = \arccos\left(\frac{\alpha+\beta}{2\beta}\right)^{1/2}, \quad \tilde{L} = [NS(NS+1)]^{1/4}\left(NS+\frac{1}{2}\right)^{1/2}.$$

Finally, let us consider the general case. It is only possible to find the instanton trajectory and to calculate the Euclidean action if one ignores in the potential (15) the difference between $L(L+1)$ and $(L+\frac{1}{2})^2$, which does not affect substantially the exponential dependence. The double minimum exists if $h < h_0$.

We give right away the result (compare with Ref. 4):

$$\Delta E_0 = \frac{8}{\pi^{1/2}} \frac{\beta(NS+1/2)^{3/2}(2S-1)}{(2NS-1)} \frac{(1-a^2)^{5/4}(1+b)^{3/4}}{(b+a^2)^{1/2}} \times \left(\frac{(1+b)^{1/2}-(1-a^2)^{NS+1/2}}{(1+b)^{1/2}+(1-a^2)^{1/2}}\right)^{NS+1/2} e^{(2NS+1)\varphi\lambda}, \tag{20}$$

$$\varphi = \arccos\frac{a(1+b)^{1/2}}{(a^2+b)^{1/2}}, \quad a = \frac{h}{h_0}, \quad b = \frac{\alpha}{\beta}, \quad \lambda = \frac{a}{b^{1/2}}$$

We have been assuming throughout single-ion anisotropy. Let us consider now the case of inter-ion anisotropy, when the perturbation Hamiltonian has the form (for simplicity we shall speak of one chain only)

$$V = J_1 \sum_{n=1}^{N-1} S_n^z S_{n+1}^z - J_2 \sum_{n=1}^{N-1} S_n^y S_{n+1}^y. \tag{21}$$

Proceeding in a manner analogous to the above within the framework of perturbation theory we find that the effective Hamiltonian has the same structure (6), with the effective anisotropy constants expressed in terms of the constants of the anisotropic part of the exchange interaction as follows:

$$A = \frac{2S}{2NS-1} J_2(1-N^{-1}), \qquad B = \frac{2S}{2NS-1} J_1(1-N^{-1}) \tag{22}$$

[if both single-ion and inter-ion anisotropy is present, one should take the sum of the expressions (7) and (22)].

The tunneling splitting is obtained from the formulas derived above by appropriate replacements of the effective anisotropy constants. Let us note that aside from a different character of the quantum renormalization connected with the individual spin of the particles, the effective anisotropy constant contains now an additional factor. It takes into account edge effects for a finite open chain (in the case of a closed chain this factor becomes unity).

We emphasize that all these factors—quantum renormalization of the effective total angular momentum and anisotropy constants, including those due to topology—are substantial as a result of the sharp exponential dependence in ΔE_0; changing N by a finite number may give rise to the appearance of additional factors of the order of unity. Therefore, an experiment on the determination of the frequency of tunneling transitions $\Delta E_0/\hbar$ (for example, in studying small ferromagnetic particles[7]) should be very sensitive to the dimensions of the interaction region, being in this sense mesoscopic.

The results have no dependence whatsoever (in contradiction with the assertions in Ref. 7) on the exchange constant J. This circumstance is connected not so much with the approximation of weak anisotropy as with the fact that the Hamiltonian of the isotropic exchange part commutes with the total spin. It therefore does not contribute to the equations of motion of the angular momentum as a whole and has no effect on the size of the Euclidean action for the corresponding instanton, if the problem is viewed in the spirit of Ref. 6. However, in comparison with the approach of Ref. 6, where equations of motion were solved for two angular variables determining the direction of the magnetic moment, the method developed in this article has the advantage, due to the introduction of the effective potential, of working with a one-dimensional rather than two-dimensional system, not to mention the evaluation of the coefficient of the exponential and the automatic taking into account of the quantum renormalization of the primary Hamiltonian.

We note that since the tunneling exponential contains the product NS, the condition of being quasiclassical, needed for the validity of all the formulas, may in fact be already satisfied for systems of finite size and relatively small particle spins $S > 1$.

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Translated by Adam M. Bincer