MACROSCOPIC QUANTUM TUNNELING IN MAGNETIC NANOSTRUCTURES

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Abstract. Theoretical foundations of the problem of quantum spin tunneling in magnetic nanostructures are presented. Several model problems are considered in detail, including recent new results on tunneling in antiferromagnetic nanoparticles and topologically nontrivial magnetic structures in systems with reduced dimension.

1. Introduction

It is well known that magnetic ordering is an essentially quantum phenomenon. According to the Bohr – van Leeuwen theorem (see, e.g., [1]), the magnetization of a thermodynamically equilibrium classical system of charged particles is zero even in presence of an external magnetic field. Classical theories of magnetic properties were based on certain assumptions going beyond the limits of classical physics (e.g., the existence of stable microparticles with nonzero magnetic moment assumed in Langevin’s theory of paramagnetism [1]). The nature of magnetic ordering was revealed only after the discovery of modern quantum mechanics in the works of Heisenberg, Frenkel and Dorfman. In 30s, many remarkable results were obtained within the microscopic quantum theory: Bloch [2] predicted the existence of magnons and low-temperature behavior of magnetization; Bethe [3] was able to construct the complete set of excited states for a spin-\(\frac{1}{2}\) chain, including nonlinear soliton-type excitations (spin complexes).

The ‘undivided rule’ of the quantum theory of magnetism lasted only till 1935, when in the well-known work Landau and Lifshitz [4] formulated the equation describing the dynamics of macroscopic magnetization of a ferromagnet (FM). When deriving the Landau-Lifshitz (LL) equation, a
quantum picture of magnetic ordering was used, particularly, the exchange nature of spin interaction, but the LL equation itself has the form of a classical equation for the magnetization $\vec{M}$. Later on the basis of the LL equation the macroscopic theory of magnetism was developed and enormous number of various phenomena were described \[5, 6\] (an overview of modern phenomenological theory of magnetically ordered media can be also found in this book in the lecture by V.G.Bar’yakhtar).

This lecture presents an introduction to the foundations of a new, fast-developing topic in the physics of magnetism, Macroscopic Quantum Tunnelling (MQT). Let us first address briefly the scope of problems belonging to this field. MQT problems can be roughly divided into two main types. First of all, there are phenomena connected with the underbarrier transition from a metastable state, corresponding to a local minimum of the magnet energy, to a stable one. Such effects were observed in low-temperature remagnetization processes in small FM particles as well as in macroscopic samples (due to the tunneling depinning of domain walls), see the recent review \[7\]. Such phenomena of “quantum escape” are typical not only for magnets, e.g., quantum depinning of vortices contributes significantly to the energy losses in HTSC materials \[8\].

Here we will concentrate on another type of phenomena, the so-called coherent MQT. To illustrate their main feature, let us consider a small FM particle with the easy axis along the $Oz$ direction. If the particle size is small enough (much less than the domain wall thickness $\Delta_0$), the particle is in a single-domain state, because the exchange interaction makes the appearance of a state with magnetic inhomogeneities energetically unfavorable. Then, from the point of view of classical physics, the ground state of the particle is twofold degenerate. Those two states correspond to two local minima of the anisotropy energy and are macroscopically different since they have different values of macroscopic magnetization $\vec{M} = \pm M_0 \vec{e}_z$. The situation is the same as in the elementary mechanical problem of a particle in two-well potential $U(x)$ having equivalent minima at $x = \pm a$, see Fig. 1. In classical mechanics the minimum of energy corresponds to a particle located in one of the two local minima of the potential.

However, from quantum mechanics textbooks it is well known that the actual situation is qualitatively different: the particle is “spread” over two wells, and the ground state is nondegenerate \[9\]. One can expect that the same should be true for a FM particle: its correct ground state will be a superposition of “up” and “down” states, and the mean value of magnetization will be zero. Such picture was first proposed by Chudnovsky \[10\]; further calculations showed \[11\] that such effects are possible for FM particles with rather large number of spins (about $10^3 \div 10^4$). The tunneling effects, according to the theoretical estimates \[12, 13\], should be even
more important for small particles of antiferromagnet (AFM); the effects of quantum coherence in AFM particles were observed in Ref. [14].

Thus, an important feature of quantum mechanics, a possibility of underbarrier transitions, can manifest itself in magnetic particles on a macroscopic (strictly speaking, mesoscopic) scale. Maybe even more interesting is the manifestation of another characteristic feature of quantum physics, viz. the effects of quantum interference. Such effects arise in the problem of MQT in magnetic nanostructures and can partially or completely suppress tunneling, restoring the initial degeneracy of the ground state [15, 16]. We wish to remark that understanding that motion of particles along very different classical trajectories can “sum up” in some sense and yield an interference picture was one of the crucial points in the development of quantum mechanics, and a considerable part of the well-known discussion between Bohr and Einstein was devoted to this problem. Besides the importance of the tunneling phenomena in magnets from the fundamental point of view, they are potentially important for the future magnetic devices working on a nanoscale.

In the present lecture we restrict ourselves to discussing the problems of coherent MQT in various mesoscopic magnetic structures. The paper is organized as follows: Sect. 2 contains the elementary description of the instanton formalism, traditionally used in the theoretical treatment of MQT problems. Since the instanton approach, though being the most straightforward one, is based on rather complicated mathematical formalism, we will discuss it in parallel with simple and widely known semiclassical approximation of quantum mechanics. The point is that those two approaches are equally adequate for treating the problem of MQT in small particles, and the “standard” semiclassical calculations, easily reproducible by anybody who learned foundations of quantum mechanics, may be helpful for understanding the structure of the results derived within the instanton technique. Further, in Sections 3 and 4 we discuss the problem of MQT in ferro- and antiferromagnetic small particles, with a special attention to the interference effects. For the description of AFM we use simple but adequate approach based on the equations for the dynamics of the antiferromagnetism vector $\vec{l}$. This approach easily allows one to keep trace of the actual magnetic symmetry of the crystal; the symmetry is lowered when external magnetic field is applied or when certain weak interactions, e.g., the so-called Dzyaloshinskii-Moriya (DM) interaction, are taken into account, which leads to quite nontrivial interference phenomena. Section 5 is devoted to the analysis of coherent MQT in “topological nanostructures,” i.e. static inhomogeneous states of magnets with topologically nontrivial distribution of magnetization; among the examples considered there are domain walls in one-dimensional (1D) magnets [17, 18, 19], magnetic vortices [20]
and disclinations [21] in 2D antiferromagnets, and antiferromagnetic rings with odd number of spins [22]. For those problems, when the description of tunneling involves multidimensional (space-time) instantons, there is no alternative to the instanton approach and its use is decisive. Finally, Section 6 contains a brief summary and discussion of several problems which are either left out of our consideration or unsolved.

2. Basics of Tunneling: With and Without Instantons

For the sake of the presentation completeness, let us recall briefly the main concepts of the instanton technique, since we will extensively use them below.

In quantum field theory, the propagator, i.e., the amplitude of probability $P_{AB}$ of the transition from any given state with the field configuration $\varphi_A(x)$ at $t = 0$ to another state $\varphi_B(x)$ at $t = t_0$ is determined by the path integral

$$P_{AB} = \langle \varphi_A | e^{i \hat{H} t_0 / \hbar} | \varphi_B \rangle = \int D\varphi(x,t) \exp \{ i A[\varphi] / \hbar \},$$

where

$$A[\varphi] = \int_0^{t_0} dt \int dx \mathcal{L}[\varphi(x,t)]$$

is the action functional. Here $\mathcal{L}$ is the Lagrangian density, and the integration in (1) goes over all space-time field configurations $\varphi(x,t)$ satisfying the boundary conditions $\varphi(x,0) = \varphi_A(x)$ and $\varphi(x,t_0) = \varphi_B(x)$. (We leave out the problem of a consistent definition of the measure $D\varphi$ that arises for systems with infinitely many degrees of freedom, keeping in mind that we are going to talk about the application of field theory to the physics of spin systems on a discrete lattice, and thus all necessary regularizations are provided by the lattice in a natural way.)

Instead of working with the propagator (1) in usual Minkovský’s spacetime, it is convenient to make the Wick rotation $t \rightarrow i \tau$ (essentially this procedure is an analytical continuation in $t$), passing to the Euclidean space-time. Then one has the Euclidean propagator

$$P_{AB}^{\text{eucl}} = \langle \varphi_A | e^{-\hat{H} \tau_0 / \hbar} | \varphi_B \rangle = \int D\varphi \exp \{ - A_{\text{eucl}} / \hbar \}.$$  

The main contribution to the path integral comes from the global minimum of the Euclidean action functional $A_{\text{eucl}}$. This minimum corresponds to a trivial solution $\varphi = \varphi_0 = \text{const}$, where $\varphi_0$ determines the minimal energy of the system. However, if several different values of $\varphi_0$ are possible, it is often important to take into account the contribution from the local minima.
of the Euclidean action as well. Such a local minimum can correspond, e.g., to a trajectory $\varphi = \varphi_{\text{inst}}(\tau)$ connecting two possible $\varphi_0$ values; it is clear that the probability $P_{AB}$ will contain the factor $\exp\{-A_{\text{eucl}}[\varphi_{\text{inst}}]/\hbar\}$. Such a contribution can be calculated in a semiclassical approximation and describes effects which cannot be accessed by means of the perturbation theory.

We will illustrate the above arguments on the example of a simple quantum-mechanical problem. Consider the motion of a particle of mass $m$ in a symmetric two-well potential $U(x)$ of the type shown in Fig. 1, with two equivalent minima at $x = \pm a$. Following the popular choice \cite{23}, we will assume this potential in the form

$$ U(x) = \lambda(x^2 - a^2)^2, \quad (2) $$

where the parameters $\lambda$ and $a$ determine the height and width of the barrier between two wells. This model is described by the Lagrangian

$$ L = \frac{m}{2} \left( \frac{dx}{dt} \right)^2 - U(x). \quad (3) $$

After passing to the imaginary time, the Euclidean action is easily obtained in the form

$$ A_{\text{eucl}} = \int_{\tau_0}^{\tau} d\tau \left\{ \frac{1}{2}m \left( \frac{dx}{d\tau} \right)^2 + U(x) \right\}. \quad (4) $$

The classical (global) minimum of this functional is reached at $x = a$ or $x = -a$. Equations of motion for the action (4)

$$ m \frac{d^2x}{d\tau^2} = \frac{dU}{dx} $$

correspond to the particle moving in the potential $-U(x)$, so that $x = \pm a$ are maxima of this effective potential, and there exist classical low-energy trajectories connecting them. Such trajectories represent local minima of the Euclidean action functional and are called instantons. They can be easily found in implicit form,

$$ \int dx \left( \frac{m}{2U(x)} \right)^{1/2} = \tau - \tau_0, \quad (5) $$

where $\tau_0$ is an arbitrary parameter determining the “centre” of instanton solution. For many potentials the integration can be performed explicitly, e.g., in case of (2) one obtains

$$ x = \pm a \tanh[\omega_0(\tau - \tau_0)/2], \quad (6) $$
where $\omega_0 = (8\lambda a^3/m)$ is the frequency of linear oscillations around one of classical minima. Euclidean action for the instanton trajectory can be written as

$$A_0 = \int_{-a}^{+a} \sqrt{2mU(x)} \, dx.$$  \hspace{1cm} (7)

For the model (2) one has $A_0 = 8a^3\sqrt{\lambda m}/3$. Thus, instantons are very much like solitons with the difference that they are localized in time. Trajectories (6) begin at $\tau \to -\infty$ in one of the minima of $U(\phi)$ and end at $\tau \to +\infty$ in the other one; the contribution of those trajectories is responsible for the tunneling splitting of the lowest energy level in the two-well potential. Indeed, the tunneling level splitting is proportional to the matrix element $t_{12}$ of the transition from one well to the other, and the probability amplitude of such a transition is given by the path integral from $x = a$ to $x = -a$. It is thus clear that the contribution of a single instanton to the transition amplitude is proportional to $e^{-A_0/\hbar}$.

The full calculation of this amplitude, however, is more complicated and should take into account not only the instanton trajectories but all trajectories close to them. Further, the full variety of multiinstanton paths
which bring the particle from one well to the other should be taken into account. If the problem is semiclassical, i.e. $A_0/h$ is large and the probability of tunneling is small, integration over “close” trajectories can be described as an effect of small fluctuations above the instanton solution. Even this, usually elementary, problem of integrating over small (linear) fluctuations is nontrivial in case of instantons, because some of those fluctuations do not change the action. Particularly, from (6) it is easy to see that changing the position of instanton centre $\tau_0$ has no effect on $A_0$. Such “zero modes” always arise in instanton problems and their contribution requires a special analysis. Detailed description of this technique would take us out of the space limits, and we refer the interested reader to textbooks and review articles (see, e.g., [24, 23]).

We will attempt to get the correct result for the probability amplitude $P_{AB}$ by means of the “traditional” quantum mechanics (without use of path integrals and instantons). First, let us note that, due to the symmetry of the potential $U(-x) = U(x)$, two lowest levels correspond to even and odd eigenfunctions $\psi_s(x)$ and $\psi_a(x)$, with the energies $E_s$ and $E_a$, respectively. Multiplying the Schrödinger equation for $\psi_s$ by $\psi_a$ and vice versa, then taking the difference of those two equations and finally integrating over $x$ from 0 to $\infty$, one obtains the relation

$$(E_a - E_s) \left[ \psi_s \frac{d\psi_a}{dx} \right]_{x=0} = \int_0^\infty \psi_a \psi_s \, dx,$$

which is exact and is nothing but a mere consequence of the symmetry properties.

It is natural to try to use a semiclassical approximation. The semiclassical result is given, e.g., in a popular textbook by Landau and Lifshitz ([9], see the problem 3 after §50). According to that result, $E_s - E_a = (\hbar \omega_0 / \pi) \exp\{-A'_0/h\}$, where $\omega_0 = [k/m]^{1/2}$, $k \equiv (d^2U/dx^2)_{x=a}$ and $A'_0 = \int_a^{a'} [2m(U(x) - E)]^{1/2}$, here $a'$ is the turnover point of the classical trajectory with energy $E$ (corresponding to a non-split level) defined by the equation $U(a') = E$. However, this result is not adequate for our problem, and it does not coincide with the result of instanton calculation. The point is that, surprisingly, the problem of tunneling from one classical ground state to another is not semiclassical: semiclassical approximation cannot be directly applied to the ground state wavefunction inside one well.

Therefore we will do as follows: let us represent the wavefunctions inside the barrier region as symmetric and antisymmetric combinations of the WKB exponents,

$$\psi_s = \frac{C_s}{\sqrt{|p|}} \cosh \left\{ \frac{1}{\hbar} \int_0^x |p| \, dx \right\}$$
ψ_a = \frac{C_a}{\sqrt{|p|}} \sinh \left\{ \frac{1}{\hbar} \int_0^a |p| dx \right\} 

where \(|p| = \sqrt{2m[U(x) - E]}\). Those wavefunctions can be used inside the entire barrier region, except narrow intervals \(|x \pm a| < \delta\) near the well minima, where \(\delta = (\hbar/m\omega_0)^{1/2}\) is the amplitude of zero-point fluctuations.

On the other hand, if the condition \(a \gg \delta\) is satisfied, then for the description of the wavefunction inside the well any reasonable potential \(U(x)\) can be replaced by the parabolic one, \(U(x) \rightarrow (k/2)(x \pm a)^2\). Then in “non-semiclassical” regions one may use well-known expression for the ground state wavefunction of a harmonic oscillator,

\[\psi \rightarrow (\pi \delta^2)^{-1/4} \exp[(x \pm a)^2/2\delta^2].\]  

Thus, in the regions \(a^2 \gg (x \pm a)^2 \gg \delta^2\) both the expressions (9) and (10) are valid. Then, normalization factors \(C_{s,a}\) can be determined from the condition of matching (9) and (10) in the two above-mentioned regions, and after that the integration in (8) can be performed explicitly. After some amount of algebra the tunneling level splitting can be represented in the form

\[E_a - E_s = 4\hbar \omega \sqrt{\frac{2}{\pi}} \exp \left\{ \int_0^{a-\delta} dx \sqrt{\frac{U''(a)}{2U(x)}} \right\} \exp \left\{ -\frac{1}{\hbar} A_0 \right\},\]  

where the quantity \(A_0 = \int_0^{a-\delta} dx \sqrt{2mU(x)}\) coincides with the Euclidean action for the instanton trajectory.

One can see that the difference between the formula (11) and the usual semiclassical result consists in the pre-exponential factor containing the integral of the type \(\int dx U^{-1/2}(x)\). It is clear that the main contribution into this prefactor comes from the region \(x \sim a\), where the integral can be approximated as \(\int_0^{a-\delta} dx /|a - x|\), so that it diverges logarithmically at \(\delta \rightarrow 0\). Thus for any potential \(U(x)\) the prefactor can be represented in the form \(\tilde{C}(a/\delta)\) or, equivalently, \((CA_0/\hbar)^{1/2}\). Here \(C\) is a numerical constant of the order of unity, it can be easily calculated for any given potential \(U(x)\). So, finally we arrive at the following universal formula:

\[E_a - E_s = 4\hbar \omega_0 \left( \frac{2C}{\pi} \right)^{1/2} \left( \frac{A_0}{\hbar} \right)^{1/2} \exp \left\{ -\frac{A_0}{\hbar} \right\} .\]  

For the model potentials \(U = \lambda(x^2 - a^2)\) and \(U = 2U_0 \sin^2 x\) the value of \(C\) is equal to \(\sqrt{3}\) and \(\sqrt{2}\), respectively.

The formulas (11,12) give the desired result for any two-well potential with sufficiently large barrier. The main feature of this result is the presence of an exponentially small factor. The small parameter of the MQT
problem is $h/A_0$, which can be represented as a ratio of the zero-point fluctuations amplitude to the distance between wells, $(h/A_0) \sim (\delta/a)^2$. The expression $e^{-a^2/\delta^2}$ is non-analytical in the small parameter, and thus the MQT phenomenon cannot be obtained in any order of the perturbation theory. We wish to emphasize that the correct result is roughly $(A_0/h)^{1/2}$ times greater than that following from “naive” semiclassical formula. This large additional factor appears due to the contribution from the regions close to the minima of the potential, where the motion is not semiclassic. Let us try to understand this in the instanton language.

As we mentioned before, the small exponential factor $\exp(-A_0/h)$ arises immediately in the instanton approach; the main problem is to compute the pre-exponential factor, which is determined by the integration over all small deviations from the instanton solution. Those deviations are of two types: real fluctuations of the instanton structure, which increase the Euclidean action, and “zero modes” which correspond to moving the instanton centre. It is rather clear that “nonzero” modes have a characteristic energy of the order of $\hbar \omega_0$, and that the quantity $\omega_0$ has nothing to do with the zero mode. Thus, it is obvious that the factor $\hbar \omega_0$ arises from the integration over all “nonzero” modes, and the large factor $(A_0/h)^{1/2}$ arises due to the zero (in our case – translational) mode. Such a “separation” naturally arises in rigorous calculations [23, 24].

It is remarkable that the above result can be generalized to the case of much more complicated problems involving space-time instantons (which, as we will see later, is important for the problem of MQT in topological nanostructures). For any instanton all nonzero modes yield a factor like $\hbar \omega_0$, and each of the zero modes yields the factor $(A_0/h)^{1/2}$ [23, 24], so that the final result can be reconstructed practically without calculations (up to a numerical factor of the order of unity).

To illustrate one more feature typical for tunneling problems, let us consider another model [24]: a particle of mass $m$ which can move along the circle of radius $R$, so that its coordinate is determined by a single angular variable $\varphi$, $0 \leq \varphi \leq 2\pi$, in the two-well potential

$$U(\varphi) = U_0(1 - \cos 2\varphi).$$

The model is described by the following Lagrangian:

$$L = \frac{1}{2} m R^2 \left( \frac{d\varphi}{dt} \right)^2 - U(\varphi).$$  \hspace{1cm} (14)

The classical Lagrangian can be modified by adding the arbitrary full derivative term, e.g.,

$$L \rightarrow L + \gamma \frac{d\varphi}{dt},$$  \hspace{1cm} (15)
which of course does not change the corresponding classical equations of motion. However, adding the full derivative (15) changes the definition of the canonical momentum conjugate to \( \varphi \), which, as one can easily check, leads to a considerable change in the Hamiltonian of the corresponding quantum-mechanical system after canonical quantization: for nonzero \( \gamma \) the correct Hamiltonian would be
\[
\hat{H} = \frac{1}{2mR^2} \left( i\hbar \frac{d}{d\varphi} + \gamma \right)^2 + U(\varphi). 
\]
(16)

Thus, there is no one-to-one correspondence between classical and quantum-mechanical systems: several quantum systems can have the same classical system as a classical limit.

For this model problem the instanton trajectories can be written down explicitly:
\[
\cos \varphi = \sigma_i \tanh[\omega(\tau - \tau_i)],
\]
\[
\omega = \left( \frac{4U_0}{mR^2} \right)^{1/2},
\]
(17)

where \( \tau_i \) is the arbitrary parameter determining the instanton position in the imaginary time axis and \( \sigma_i = \pm 1 \) is the topological charge distinguishing instantons and antiinstantons; the instanton action is finite and is given by \( A_0 = (8mR^2U_0)^{1/2} \).

The importance of the full derivative term (15) can be most easily understood in terms of instantons. Indeed, let us consider the tunneling amplitude \( P_{12} \) from the \( \varphi = 0 \) well to \( \varphi = \pi \) one: it is clear that the contribution to this amplitude is made equally by instantons (with \( \varphi \) changing from 0 to \( \pi \)) and antiinstantons (with \( \varphi \) changing from 0 to \( -\pi \)). However, the term (15) becomes an imaginary part of the Euclidean action and leads to the additional factor \( e^{i\pi \gamma/\hbar} \) associated with the instanton contribution and a similar factor \( e^{-i\pi \gamma/\hbar} \) for antiinstanton paths. Thus, the resulting transition amplitude for nonzero \( \gamma \) is modified as follows:
\[
P_{12} = [P_{12}]_{\gamma=0} \cos(\pi \gamma / \hbar),
\]
(18)

where \( [P_{12}]_{\gamma=0} \propto \omega (A_0 / \hbar)^{1/2} e^{-A_0 / \hbar} \), according to the general result described above. One can see that for half-integer \( \gamma / \hbar \) the interference of instanton and antiinstanton paths is destructive, so that at \( \gamma = \pm \frac{h}{2}, \pm \frac{3h}{2}, \ldots \) the tunneling between two wells is completely suppressed. This effect is essentially topological because the topological charge appears in the answer: the contribution of configurations with different topological charge is different. The same result can be obtained directly by solving the Schrödinger equation with the Hamiltonian (16): for half-integer \( \gamma / \hbar \) it can be mapped to the Mathieu equation with antiperiodic boundary conditions, and the
corresponding energy levels are known to be doubly degenerate [25], which also means absence of tunneling.

3. Field-Theoretical Description of a Small Ferromagnetic Particle

In this section we consider the basic technique of field-theoretical description for spin systems on the simplest example, namely a nanoparticle of a ferromagnetic material. Such an object may be viewed as a zero-dimensional magnetic system, because at very low temperature all spins in the particle can be considered as pointing in the same direction.

It is worthwhile to consider first the dynamics of a single spin $S$. In order to obtain the effective Lagrangian describing the spin dynamics, it is convenient to use a coherent state path-integral approach (see, e.g., the excellent textbook by Fradkin [26]). Let us introduce a set of generalized coherent states [27]

\[ |\vec{n}\rangle = \exp\{i\theta(\vec{n} \times \hat{z})\hat{S}\}|m = S\rangle \]  

(19)

parameterized by the unit vector $\vec{n}(\theta, \varphi)$. Here $\hat{z}$ is a unit vector pointing along the $z$ axis, and $|m\rangle$ denotes a spin-$S$ state with $S^z = m$. They form a non-orthogonal ‘overcomplete’ basis so that the following property, usually called a resolution of unity, holds:

\[ \int \mathcal{D}\vec{n} |\vec{n}\rangle\langle\vec{n}| = 1, \]  

(20)

another useful property is that quantum average of $\hat{S}$ on those coherent states is the same as of classical vector of length $S$:

\[ \langle\vec{n}|\hat{S}|\vec{n}\rangle = S\vec{n}. \]

In case of $S=1/2$ those coherent states have a very simple form and are general single-spin wavefunctions:

\[ |\vec{n}\rangle = \cos(\theta/2)|\uparrow\rangle + \sin(\theta/2)e^{i\varphi}|\downarrow\rangle. \]

We again start from the formula for propagator (1) which is essentially a definition of the effective Lagrangian. Slicing the time interval $[0; t_0]$ into infinitely small pieces $\Delta t = t_0/N$, and successively using the identity (20), one can rewrite this propagator in $\vec{n}$-representation as

\[
P_{AB} = \lim_{N \to \infty} \int d\vec{n}_0 d\vec{n}_1 \cdots d\vec{n}_N \langle A|\vec{n}_0\rangle\langle\vec{n}_N|B\rangle \times \prod_{k=0}^{N-1} \langle\vec{n}_k|e^{-i\hat{H}\Delta t/\hbar}|\vec{n}_{k+1}\rangle. \]  

(21)
Passing to the function $\vec{n}(t)$ of the continuum variable $t$, one ends up with the coherent state path integral (1) where the action $A$ is determined by the effective Lagrangian

$$L_{\text{eff}} = \frac{1}{2} \hbar \left\{ \langle \partial_t \vec{n} | \vec{n} \rangle - \langle \vec{n} | \partial_t \vec{n} \rangle \right\} - \langle \vec{n} | \hat{H} | \vec{n} \rangle .$$  

(22)

It can be shown that the dynamical part of this Lagrangian has the form

$$\hbar S (1 - \cos \theta) \frac{d\varphi}{dt};$$  

(23)

for arbitrary $S$ this calculation requires some algebra, but for the simplest case $S = \frac{1}{2}$ it is straightforward. The expression (23) is nothing but the Berry phase \cite{28} for adiabatic motion of a single spin.

It should be remarked that the presence of the full derivative term $\hbar S (d\varphi/dt)$ is rather nontrivial and allows one to capture subtle differences between integer and half-integer spins, as we will see below. For example, consider a single spin $S$ in some crystal-field potential, with the effective Hamiltonian

$$\hat{H} = KS^2_z - K' S^2_x,$$

(24)

where $K, K' > 0$ and the easy-plane anisotropy $K$ is much stronger than the in-plane anisotropy $K'$. The Lagrangian is

$$L = \hbar S (1 - \cos \theta) \frac{d\varphi}{dt} - KS^2 \cos^2 \theta - K' S^2 \sin^2 \theta \cos^2 \varphi .$$

(25)

There are two equivalent classical minima of the potential at $\theta = \frac{\pi}{2}$, $\varphi = 0$ and $\theta = \frac{\pi}{2}$, $\varphi = \pi$. Paths with $\theta \approx \pi/2$ make the main contribution into the tunneling amplitude, so that we can approximately set $\theta = \frac{\pi}{2} + \vartheta$, $\vartheta \ll 1$, and expand in $\vartheta$ up to quadratic terms in the Lagrangian; in the term proportional to $\vartheta^2$ the $K'$ contribution may be neglected as small comparing to the contribution of $K$. After that, the “slave” variable $\vartheta$ can be excluded from the Lagrangian (“integrated out” of the path integral) because the corresponding equation of motion $\delta L/\delta \vartheta = 0$ allows to express $\vartheta$ through $\varphi$ explicitly:

$$\vartheta = - \frac{\hbar}{2KS} \frac{d\varphi}{dt} .$$

(26)

Substituting this solution into the original Lagrangian (25), one obtains the effective Lagrangian depending on $\varphi$ only:

$$L_{\text{eff}} = \hbar S \frac{d\varphi}{dt} + \frac{\hbar^2}{4K} \left( \frac{d\varphi}{dt} \right)^2 + K' S^2 \cos^2 \varphi .$$

(27)

We see that we end up with the Lagrangian of a particle on a circle from the previous section, with the topological term $\gamma = \hbar S$. For each path
where \( \varphi \) changes from 0 to \( \pi \) there is a corresponding antiinstanton path with \( \varphi \) changing from 0 to \( -\pi \), and those paths contribute to the tunneling amplitude with phase factors \( e^{i\pi S} \) and \( e^{-i\pi S} \). For half-integer \( S \) those contributions precisely cancel each other, making the tunneling impossible. This is exactly in line with the well-known Kramers theorem, which states that in absence of external magnetic field all energy levels of a system with half-integer total spin should be twofold degenerate. One can also straightforwardly check that for a single spin in magnetic field, i.e., for \( \vec{H} = g\mu_B H \vec{S}_z \), the correct energy levels can be obtained only with the full derivative term taken into account.

Now we are prepared enough, finally, to consider the problem of tunneling in a small ferromagnetic particle consisting of \( N \) spin-\( S \) spins. If we assume that ferromagnetic exchange interaction is so strong that we may consider all spins as having the same direction, then we come to the “giant spin” model where the entire particle is described as a quantum-mechanical (“zero-dimensional”) system with only two degrees of freedom \( \theta \) and \( \varphi \). In fact, we should postulate that in our path integral, when integrating over the coherent state configurations \( \prod_{i=1}^{N} \otimes |\vec{n}_i\rangle \), the main contribution comes from the subspace with all \( N \) vectors \( \vec{n}_i \) replaced by the same vector \( \vec{n}(\theta, \varphi) \), and we take into account only configurations from this subspace. Assuming that the crystal-field anisotropy has the form (24), we come to essentially the same effective Lagrangian (27), and the only difference is that Eq. (27) should now be multiplied by the total number of spins \( N \). The tunnel splitting of the ground state level, according to Eq. (18), is given by

\[
\Delta E = C(NS^3)^{1/2}(KK')^{1/4} |\cos(\pi NS)| \exp \left\{ -NS(2K'/K)^{1/2} \right\}, \tag{28}
\]

where \( C \) is a numerical constant of the order of 1. A remarkable property of the result (28) is that presence of a large number \( N \) in the exponent can be to some extent compensated by smallness of the ratio \( K'/K \). However, when the in-plane anisotropy \( K' \to 0 \), the splitting vanishes (this reflects the fact that in uniaxial case tunneling is impossible because of the conservation of the corresponding projection of the total spin; the same is true for \( K \to 0 \)). Another remarkable feature is that for half-integer \( S \) the finite splitting can be observed only in particles with even number of spins \( N \); since in any statistical ensemble \( N \) fluctuates a bit, this roughly means that only one half of all particles gives nonzero contribution.

Statistical fluctuations of \( N \) have another, more painful consequence: since \( N \) stays in the exponent, even small fluctuations of the total number of spins in the particle lead to large fluctuations of the splitting. Moreover, since \( N \) scales as the third power of the linear size \( L \), small fluctuations of \( L \) will be considerably enhanced in \( N \). This may be crucial if one tries to detect the splitting by means of some resonance technique: the initially weak signal
would be even more weakened by the strong broadening of the resonance peak. Actually, many factors can prevent one from observing the tunneling resonance, e.g., relaxation, temperature effects, etc. Here we will not at all touch the problem of relaxation because of its complexity; instead of that we refer the interested reader to the review [29]. Taking into account the finite temperature effects is also nontrivial, particularly because it requires changing the procedure of taking averages in the path integral: statistical averages should be taken simultaneously with quantum-mechanical ones. Roughly (and without taking into account the temperature dependence of relaxation mechanisms) the effects of finite temperature can be estimated with the help of the concept of a characteristic temperature \( T_c \) below which the effects of quantum tunneling prevail over thermal transitions. Rough estimate for \( T_c \) is obtained from the comparison of the relative strength of two exponential factors: thermal exponent \( e^{-\Delta U/T} \) and tunneling exponent \( e^{-A_0/\hbar} \), where \( \Delta U \) is the height of barrier separating two equivalent states and \( A_0 \) is the corresponding instanton action, then \( T_c = (\hbar \Delta U/A_0) \). It is easy to see that for the ferromagnetic particle problem considered above

\[
T_{FM} = S(KK'/2)^{1/2},
\]

i.e. the temperature of crossover from classical to quantum transitions is in this case rather small since it is determined by weak (relativistic) anisotropy interaction constants; for typical anisotropy values \( T_{FM} \) is about 0.1 K.

4. Quantum Tunneling in a Small Antiferromagnetic Particle

4.1. CONTINUUM FIELD MODEL OF ANTIFERROMAGNET

The problem of continuum field description of antiferromagnet (AFM) is more complicated but also much more interesting than a similar problem for ferromagnet. Antiferromagnet contains at least two different “sublattices” whose magnetizations compensate each other in the equilibrium state. Thus, when choosing the coherent state wavefunction in the form \( |\Psi\rangle = \Pi_i |\vec{n}_i\rangle \) as described above, one cannot any more consider \( n_i \) as a “smooth” function of the lattice site \( i \). Let us adopt the simplest two-sublattice model which, despite the fact that it may be inadequate for a specific material, still allows one to demonstrate the essential physics of antiferromagnetism. We assume that there are two equivalent sublattices with magnetizations \( \vec{M}_1(\vec{r}) \) and \( \vec{M}_2(\vec{r}) \). \( |\vec{M}_1| = |\vec{M}_2| = M_0 \). Then, when passing to the continuum limit, one has to introduce smooth fields \( \vec{m} = (\vec{M}_1 + \vec{M}_2)/2M_0 \) and \( \vec{l} = (\vec{M}_1 - \vec{M}_2)/2M_0 \) describing net magnetization and sublattice magnetization, respectively. They satisfy the constraints

\(^1\)Subsection 4.2.2 was written together with Vadim Kireev.
\[ \vec{m}\vec{l} = 0, \vec{m}^2 + \vec{l}^2 = 1, \text{ and we further assume that} |\vec{m}| \ll |\vec{l}|. \] The energy of AFM \( W = \langle \hat{H} \rangle \) then can be expressed as a functional of \( \vec{m} \) and \( \vec{l} \):

\[
W[\vec{m}, \vec{l}] = M_0^2 \int dV \left\{ \frac{1}{2} \delta \vec{m}^2 + \frac{1}{2} \alpha (\nabla \vec{l})^2 + w_a(\vec{l}) - g M_0 (\vec{m} \cdot \vec{H}) \right\}.
\]

(30)

Here the phenomenological constants \( \delta \) and \( \alpha \) describe homogeneous and inhomogeneous exchange, respectively, \( \vec{H} \) is the external magnetic field, \( g \) is the Lande factor, the function \( w_a \) describes the energy of magnetic anisotropy, and we use the notation \((\nabla \vec{l})^2 = \sum_i (\partial \vec{l}/\partial x_i)^2\). The magnitude of sublattice magnetization \( M_0 = g \mu_B S/v_0 \), where \( \mu_B \) is the Bohr magneton, \( S \) is the spin of a magnetic ion, and \( v_0 \) is the volume of the magnetic elementary cell.

As we learned from the previous section, the correct Lagrangian, suitable for the quantum-mechanical treatment, has the form

\[
L = \sum_i \hbar S \left\{ (1 - \cos \theta_{1i}) \frac{d\varphi_{1i}}{dt} + (1 - \cos \theta_{2i}) \frac{d\varphi_{2i}}{dt} \right\} - W[\vec{m}, \vec{l}],
\]

(31)

where the angular variables \((\theta_{1i}, \varphi_{1i})\) and \((\theta_{2i}, \varphi_{2i})\) determine the unit vectors describing the orientation of spins in first and second sublattice, respectively. Note that we have kept intact the summation sign in the dynamical part of (31): the reason is that the explicit expression for the Berry phase in the continuum limit strongly depends on the details of the magnetic elementary cell structure (which dictates the correct definition of \( \vec{m} \) and \( \vec{l} \) and the procedure of passing to the continuum limit).

Under the assumption that \( |\vec{m}| \ll |\vec{l}| \), the magnetization \( \vec{m} \) can be excluded from the Lagrangian (31), and one obtains the effective Lagrangian depending only on \( \vec{l} \); after that step \( \vec{l} \) can be regarded as a unit vector, \( \vec{l}^2 = 1 \).

For example, in the simplest case of an antiferromagnet with only two (equivalent) atoms in elementary magnetic cell the dynamic part of the Lagrangian (31) can be written as

\[
\int dV 2 \hbar S \vec{m} \cdot (\vec{l} \times \partial \vec{l}/\partial t),
\]

(32)

and the density of the effective Lagrangian takes the form

\[
\mathcal{L} = M_0^2 \left\{ \frac{\alpha}{2c^2} \left( \frac{\partial \vec{l}}{\partial t} \right)^2 - \frac{\alpha}{2} (\nabla \vec{l})^2 - \tilde{w}_a(\vec{l}) \right\} + \frac{4}{\gamma \delta} \vec{H} \cdot \left( \vec{l} \times \frac{\partial \vec{l}}{\partial t} \right),
\]

(33)

where \( \tilde{w}_a \) is the anisotropy energy renormalized by the magnetic field,

\[
\tilde{w}_a = w_a + \frac{2}{\delta M_0^2} (\vec{l} \cdot \vec{H})^2,
\]

(34)
γ = gμB/h is the gyromagnetic ratio, and 
c = \frac{1}{2}γM_0(αδ)^{1/2} is the limiting
velocity of spin waves. Using general phenomenological arguments, one can
show [30] that in case of arbitrary collinear antiferromagnet the Lagrangian
should have the form similar to (33).

Other, more complicated interactions can be present in Eq. (30). In
some AFM materials (which are, strictly speaking, weak ferromagnets) the
so-called Dzyaloshinskii-Moriya (DM) interaction is possible. It can be de-
scribed by including the term D_{ik}m_i l_k under the integration sign in into
(30), where D_{ik} is some tensor (which is not necessarily symmetric or anti-
symmetric). The origin of the DM interaction is rather nontrivial, and there
is a number of “selection rules” excluding the possibility of its existence,
particularly the DM interaction cannot exist (i) if there is an inversion cen-
ter interchanging sublattices; (ii) if there is a translation which interchanges
sublattices, i.e. if the magnetic elementary cell is larger than the elementary
cell of the original crystal lattice. It can be shown [31] that presence of the
DM interaction can be taken into account by the substitution

$$\vec{H} \mapsto \tilde{\vec{H}} = \vec{H} - \frac{1}{2}M_0 \vec{D}$$

in the Lagrangian (33), where the components of vector \(\vec{D}\) are defined as
\(D_i = D_{ik}l_k\).

If there exists a sublattice-interchanging inversion center, another in-
variant may be present in (30), namely \(μ_i(\vec{m} \cdot ∂\vec{l}/∂x_i)\) (here \(μ_i\) are certain
exchange constants). It is very important for the physics of AFM in one
dimension, as we will see later.

4.2. SPIN TUNNELING IN ANTIFERROMAGNETIC NANOPARTICLE

In case of a small particle one can consider \(\vec{m}\) and \(\vec{l}\) as being uniform
throughout the particle, i.e. as not having any space dependence. Then,
the Lagrangian (33) takes the form

$$L = \frac{hN_S}{\gamma H_e} \left\{ \dot{θ}^2 + \sin^2 θ \dot{ϕ}^2 + 2γθ \left( \tilde{H}_y \cos ϕ - \tilde{H}_x \sin ϕ \right) 
+ 2γϕ \left[ \tilde{H}_z \sin^2 θ - \sin θ \cos θ (\tilde{H}_y \sin ϕ + \tilde{H}_x \cos ϕ) \right] \right\} - M_0^2 \tilde{ω}_a,$$

where \(N\) is the total number of magnetic elementary cells in the particle,
\(H_e = δM_0/2\) is the exchange field, the dot denotes differentiation with
respect to time, and we used angular variables for the vector \(\vec{l}\),

$$l_z = \cos θ, \quad l_x + il_y = \sin θ e^{iϕ}.$$

There is another possible effect, typical only for antiferromagnetic particles:
due to the boundary (surface) effects, the number of spins in two sublattices
can differ from each other. In that case the Lagrangian (36) will contain the additional term
\[ \hbar \nu S (1 - \cos \theta) \dot{\varphi}, \]
which is essentially the Berry phase of \( \nu \) non-compensated spins. Such a sublattice decompensation in fact should be present in any ensemble of nanoparticles, so that \( \nu \) has certain statistical variation.

The full Lagrangian (36) is rather complicated, and for the sake of clarity we will consider separately the effects of field and DM interaction.

4.2.1. Tunneling in presence of external magnetic field
Consider a small AFM particle with easy-axis anisotropy
\[ w_a = \frac{1}{2} \beta (l_y^2 + l_z^2) \]
in external magnetic field \( H \) perpendicular to the easy axis. Then the Euclidean action takes the form
\[
A_{\text{eucl}} = -\frac{\hbar NS}{\gamma H_e} \int d\tau \left\{ \left( \frac{d\theta}{d\tau} \right)^2 + \sin^2 \theta \left( \frac{d\varphi}{d\tau} \right)^2 + 2i\gamma H \sin^2 \theta \frac{d\varphi}{d\tau} + \omega_0^2 \left[ \sin^2 \theta \sin^2 \varphi + (1 + \gamma^2 H^2/\omega_0^2) \cos^2 \theta \right] \right\} + i\hbar \nu S \int d\tau (1 - \cos \theta) \frac{d\varphi}{d\tau},
\]
where \( \tau \) is the imaginary time, and \( \omega_0 = \frac{1}{2} \gamma M_0 (\delta \beta)^{1/2} \) is the characteristic magnon frequency (\( \hbar \omega_0 \) is the magnon gap).

There are two equivalent states \( A \) and \( B \) with opposite direction of \( \vec{l} \) along the easy axis \( Ox \), and obviously the most preferable instanton path is given by \( \theta = \pi/2, \varphi = \varphi(\tau) \). The instanton solution for \( \varphi \) is the same as in case of particle on a circle, and one-instanton action is
\[
\frac{A_0}{\hbar} = \frac{NS}{\gamma H_e} (4\omega_0 \pm 2\pi i\gamma H) \pm i\pi \nu S, \quad (39)
\]
where \( \pm \) signs correspond to instantons and antiinstantons. Thus, the tunneling amplitude \( P_{AB} \) is proportional to
\[
\left( \frac{4NS\omega_0}{\gamma H_e} \right)^{1/2} \exp \left\{ -\frac{4NS\omega_0}{\gamma H_e} \right\} \cos \{ \pi \nu S + 2\pi NS(H/H_e) \}, \quad (40)
\]
and the corresponding magnitude of tunneling level splitting (proportional to \( |P_{AB}| \)) oscillates with the period \( \Delta H = (H_e/2NS) \) when changing the
external field. This period $\Delta H$ may be rather small, for typical values of the exchange field $H_e \sim 10^6$ Oe and the number of spins in the particle $N \sim 10^3 \div 10^4$ one obtains $\Delta H \sim 10^2 \div 10^3$ Oe. The effects of this type were studied in [32, 33].

The result (40) illustrates also another remarkable feature: in any experiment probing the response of the ensemble of AFM nanoparticles at each $H$ there must be only one possible value of splitting (i.e., only one peak in the low-frequency response) when the spin of magnetic ions $S$ is integer; but if $S$ is half-integer then, since in any ensemble $\nu$ arbitrarily takes even and odd values, for approximately one half of all particles the phase of cosine in (40) is shifted by $\pi/2$, and there should be \textit{two} peaks at each $H$.

It is worthwhile to note that the real part of the one-instanton action, which enters the exponent in (40), is proportional to $(K/J)^{1/2}$ (where $J$ and $K$ are the exchange and anisotropy constants) while the corresponding quantity for ferromagnet, according to (28), does not contain the exchange constant and is determined by the rhombicity $(K'/K)^{1/2}$. One may conclude that tunneling in AFM particles is more easy than in FM; indeed, the characteristic crossover temperature below which quantum effects dominate over thermal ones, for antiferromagnets is

$$T_{AFM} \propto S(KJ)^{1/2},$$

which is much greater than for ferromagnets [cf. Eq.(29)]; typically $T_{AFM}$ is about $1 \div 3$ K.

4.2.2. \textit{Tunneling in presence of the DM interaction}

Consider the same small AFM particle from the previous subsection, but imagine that the DM interaction in its simplest form is present, with the energy given by

$$w_d = d(m_y l_z - m_z l_y).$$

Then the DM interaction leads to the contribution into the Lagrangian (36) of the form

$$\Delta L_d = \frac{\hbar N S}{\gamma H_e} \cdot 2H_D \frac{d}{dt}(\sin \theta \cos \varphi),$$

where $H_D = dM_0$ is the so-called Dzyaloshinskii field. This term will contribute to the imaginary part of the Euclidean action (38), and as a result the cosine in (40) will be modified as

$$\cos \{\pi \nu S + 2\pi NS(H/H_e) + 4NS(H_D/H_e)\}.$$

Thus, presence of the DM interaction alone also leads to effective change of the Berry phase and lifts the degeneracy for odd $\nu$ and half-integer $S$. 
5. Spin Tunneling in Topological Magnetic Nanostructures

As we mentioned before, one of the most difficult experimental tasks when trying to detect the resonance on tunnel-split levels in small particles is to prepare the ensemble of particles with very sharp size distribution: even small fluctuations of size lead to large fluctuations of the tunneling probability since they contribute to the power of exponent. Preparing such an ensemble requires high technologies and involves considerable difficulties. One may think about some other, “natural” type of magnetic nanostructures to observe spin tunneling phenomena in. One nice solution, which have actually been used in experiment, is to use biologically produced nanoparticles [14].

Another possible way, proposed in [17, 18, 20], is to use topologically nontrivial magnetic structures: kinks in quasi-1D materials, vortices and disclinations in 2D, etc. Such objects have required mesoscopic scale (e.g., the thickness of a domain wall is usually about 100 lattice constants) and, since their shape is determined by the material constants, they are identical to a high extent (up to a possible inhomogeneity of the sample).

Here we consider several possible scenarios of tunneling in topological nanostructures and show that their use has a number of advantages.

5.1. Tunneling in a Kink of 1D Antiferromagnet

Consider a one-dimensional two-sublattice antiferromagnet with rhombic anisotropy described by the Hamiltonian

\[ \hat{H} = J \sum_i \vec{S}_i \cdot \vec{S}_{i+1} + \sum_i [K_1(S^z_i)^2 + K_2(S^y_i)^2], \]

(45)

where \( i \) labels sites of the spin chain with the lattice constant \( a \), \( K_1 > K_2 > 0 \) are the anisotropy constants (so that \( Oz \) is the difficult axis and \( Ox \) is the easy axis), and \( J \) is the exchange constant. For passing to the continuum field description one may introduce vectors \( \vec{m} \) and \( \vec{l} \) as \( \vec{m}_k = (\vec{n}_{2k+1} + \vec{n}_{2k})/2 \) and \( \vec{l}_k = (\vec{n}_{2k+1} - \vec{n}_{2k})/2 \), where \( \vec{n} \) are the unit vectors describing the direction of spins (the parameters of the corresponding coherent states, see the discussion in Sect. 4.1) above. These fields live on the lattice with the double spacing \( 2a \), and it is easy to see that the energy functional \( W = \langle \hat{H} \rangle \) contains the term \( \vec{m} \cdot \partial_x \vec{l} \). Using the equation \( \delta L/\delta \vec{m} = 0 \), one may express \( \vec{m} \) through \( \vec{l} \) and its derivatives and exclude it from the Lagrangian. The effective Lagrangian takes the following form:

\[ L_{\text{eff}} = \int \frac{dx}{2a} \left\{ \frac{\hbar^2}{4J} (\partial_x \vec{l})^2 - JS^2 a^2 (\partial_x \vec{l})^2 - K_1 S^2 l_z^2 - K_2 S^2 l_y^2 \right\} + L_{\text{top}} \]

(46)

\( ^2 \)Subsection 5.2 was written together with Vadim Kireev.
which represents a \((1+1)\)-dimensional nonlinear \(\sigma\)-model with the so-called topological term

\[
L_{\text{top}} = \frac{1}{2} \hbar S \int dx \mathbf{l} \cdot (\partial_x \mathbf{l} \times \partial_t \mathbf{l}).
\]  

(47)

It is easy to trace the origin of this term: because of presence of \(\mathbf{m} \cdot \partial_x \mathbf{l}\) in the energy, the expression for \(\mathbf{m}\) contains \(\partial_x \mathbf{l}\) which after the substitution into the Berry phase \((23)\) yields the topological term. In agreement with general phenomenological result \((33)\), the Lagrangian \((46)\) is Lorentz-invariant, with the limiting velocity \(c = 2Ja/\hbar\).

A stable kink solution corresponds to rotation of vector \(\mathbf{l}\) in the easy plane \((xy)\):

\[
l_x = \sigma' \tanh(x/\Delta), \quad l_y = \frac{\sigma}{\cosh(x/\Delta)}, \quad l_z = 0,
\]

(48)

where \(\Delta = a(J/K_2)^{1/2}\) is the characteristic kink thickness, and the quantities \(\sigma\) and \(\sigma'\) may take the values \(\pm 1\). The topological charge of the kink \(\sigma'\) is determined by the boundary conditions and cannot change in any thermal or tunneling processes. The situation is different with the quantity \(\sigma\) which determines the sign of \(\mathbf{l}\) projection onto the “intermediate” axis \(O_y\). Two states with \(\sigma = \pm 1\) are energetically equivalent; change of \(\sigma\) is not forbidden by any conservation laws and describes the reorientation of the macroscopic number of spins \(N \sim \Delta/a \gg 1\) “inside” a kink, typically \(N \sim 70 \div 100\).

Again, tunneling between the kink states with \(\sigma = \pm 1\) can be studied using the instanton formalism. In contrast to the case of a nanoparticle, here the tunneling between two inhomogeneous states takes place, so that nontrivial space-time instantons come into play. The instanton solution \(\mathbf{l}_0(x, \tau)\) is now two-dimensional and has the following properties (see Fig. 2):

\[
\begin{align*}
l_x &\to \pm \sigma' \quad \text{at } x \to \pm \infty \\
l_y &\to \mp \sigma \quad \text{at } x = 0, \tau \to \pm \infty \\
l_z &= p = \pm 1 \quad \text{at } x = 0, \tau = 0.
\end{align*}
\]

(49)

Along any closed contour around the instanton center in the Euclidean plane vector \(\mathbf{l}\) rotates through the angle \(2\pi \nu\) in the easy plane \((xy)\), where \(\nu = \sigma \sigma' = \pm 1\). Thus, the instanton configuration has the properties of a magnetic vortex and is characterized by two topological charges \([34, 35]\): vorticity \(\nu\) and polarization \(p\). The instanton solution satisfies the equations

\[
\begin{align*}
\vec{\nabla}^2 \theta + \sin \theta \cos \theta [(1 + \rho \sin^2 \varphi)/\Delta^2 - (\vec{\nabla} \varphi)^2] &= 0, \\
\vec{\nabla} \cdot (\sin^2 \theta \vec{\nabla} \varphi) - (\rho/\Delta^2) \sin^2 \theta \sin \varphi \cos \varphi &= 0.
\end{align*}
\]

(50)
Figure 2. The structure of instanton solution for the problem of tunneling in a kink of a 1D antiferromagnet. Arrows and circles denote projections of vector $\vec{l}$ on the easy plane ($xy$) and on the difficult axis $Oz$, respectively. Vector $\vec{l}$ forms the angle of about $45^\circ$ with the easy axis $Ox$ on thin solid curves, and with the difficult axis $Oz$ on the circle (the circle radius is approximately $r_0$).

where we have introduced the angular variables $l_y + il_z = \sin \theta e^{i\varphi}, l_x = \cos \theta$, $\rho = (K_1 - K_2)/K_2$ is the rhombicity parameter, and $\vec{\nabla} = (\partial/\partial x_1, \partial/\partial x_2)$ is the Euclidean gradient, $(x_1, x_2) \equiv (x, c\tau)$.

Several important properties of the instanton can be obtained without using the explicit form of the solution. First of all, note that this instanton has two zero modes which correspond to shifting the position of its centre along the direction of $\tau$ and $x$ axes, respectively. The physical meaning of the first mode is the same as for 1D instanton, and the second mode corresponds to moving the kink center in real space (the kink position in infinite 1D magnet is not fixed in our continuum model); however, if the kink center is fixed due to some effects (e.g., because of pinning on the lattice, or by boundary conditions), so that the eigenfrequency of its oscillations is comparable with the characteristic magnon frequency, then only one zero-frequency mode is present.

The Euclidean action $A_{\text{eucl}}$ can be represented in the form

$$A_{\text{eucl}} = \frac{1}{2} S\bar{h}F + i2\pi S\bar{h}Q,$$

where
\[ F = \frac{1}{2} \int d^2x \left[ (\nabla^2 \theta)^2 + \sin^2 \theta (\nabla^2 \varphi)^2 + \frac{1}{\Delta^2} \cos^2 \theta (1 + \rho \sin^2 \varphi) \right] \]
\[ Q = \frac{1}{4\pi} \int d^2x \varepsilon_{\alpha\beta} \sin \theta \partial_\alpha \theta \partial_\beta \varphi. \]  

Imaginary part of the Euclidean action is in this case completely determined by the topological term \( L_{\text{top}} \). The word “topological” becomes now clear, because \( Q \) is the homotopical index of mapping of the \((x_1, x_2)\) plane onto the sphere \( l^2 = 1 \) (the Pontryagin index, or the winding number). For uniform boundary conditions at infinity in the \((x_1, x_2)\) plane \( Q \) can take only integer values, but in our case \( Q = -p \nu/2 = \pm \frac{1}{2} \) is half-integer, which is typical for vortices (see, e.g., [34, 35]). For a kink with given \( \sigma' \) there are two instanton solutions with the same vorticity \( \nu \) and different polarizations \( p \). Thus, the tunneling amplitude is proportional to \( \cos(\pi S) \) and vanishes when the spin \( S \) of magnetic ions is half-integer. However, the degeneracy can be lifted in presence of external magnetic field or the DM interaction, as we will see below.

We are not able to construct the exact solution of Eqs. (50), but the estimate of the tunneling amplitude in various limiting cases can be obtained from approximate arguments. For \( \rho \ll 1 \) the characteristic space scale of \( \varphi \) variation \( \Delta/\sqrt{\rho} \) is much greater than the kink thickness \( \Delta \), and the problem can be mapped to one with a finite number of degrees of freedom (one may introduce the variable \( \phi \) having the meaning of the angle of deviation out of the easy plane “inside a kink”, so that the instanton solution can be seeked in the form \( \phi = \phi(\tau) \)), then it is easy to obtain [36]

\[ F \simeq 4\rho^{1/2} \quad \text{at} \quad \rho \ll 1. \]  

In the opposite limiting case \( \rho \gg 1 \) one again has two different length scales: the kink thickness \( \Delta \) and the “core” radius \( r_0 = \Delta(K_2/K_1)^{1/2}, r_0 \ll \Delta \). For \( r \ll \Delta \) all interactions except the exchange one can be neglected, and one may use the “isotropic” vortex solution

\[ \theta = \theta_0(r), \quad \varphi = \nu \chi, \quad \nu = \pm 1, \]
\[ \frac{d^2\theta_0}{dr^2} + \left( \frac{1}{\Delta^2} - \frac{\nu^2}{r^2} \right) + \sin \theta_0 \cos \theta_0 = 0, \]  

where \( r = (x_1^2 + x_2^2)^{1/2}, \chi = \arctan(x_2/x_1) \) are polar coordinates in the \((x_1, x_2)\) plane. For \( r \gg r_0 \), i.e., far outside the core, one can approximately assume that

\[ \theta = \frac{\pi}{2}, \quad \nabla^2 \varphi = \frac{\rho}{2\Delta^2} \sin 2\varphi. \]  

Within a wide range of \( r \) (for \( r_0 \ll r \ll \Delta \)) the solutions (53) and (54) can be regarded as coinciding, and the integrand in \( F \) is proportional to \( 1/r^2 \).
Then, one may divide the integration domain into two parts: $r < R$ and $r > R$, where $R$ is arbitrary in between $r_0$ and $\Delta$. For $r < R$ the solution (53) may be used, yielding $F_{r<R} = \pi \ln(\zeta R/r_0)$ with $\zeta \simeq 4.2$ [37]. For $r > R$, one can use a simple trial function approximately satisfying (54), e.g.,

$$\cos \varphi = \frac{x_2}{r} \frac{1}{\cosh(x/\Delta)}; \quad \sin \varphi = \frac{x_1}{r} \frac{1}{\cosh(x/\Delta)},$$

which yields $F_{r>R} = \pi \ln(\zeta' \Delta/R)$ with $\zeta' \simeq 0.1$. Summing up the two contributions, we obtain

$$F \simeq \pi \ln(0.42\Delta/r_0) \quad \text{at} \quad \rho \gg 1. \quad (56)$$

The tunnel splitting of the “ground state” level of the kink

$$\Gamma \propto \hbar \omega_l \left( FS/2 \right)^{n/2} e^{-FS/2} |\Phi|,$$

where $\omega_l = 2S(JK_2\rho)^{1/2}$ is the frequency of the out-of-plane magnon localized at the kink, $\Phi$ is the factor determined by the imaginary part of the Euclidean action [in the simplest model $\Phi = \cos(\pi S)$], and $n$ is the number of zero modes which can be equal to 1 or 2 depending on whether the kink position is fixed, see above. It is easy to estimate the crossover temperature for the problem of tunneling in a kink, comparing the exponent in (57) with $e^{-U_0/T}$, where $U_0 \simeq 2S^2(\sqrt{JK_1} - \sqrt{JK_2})$ is the barrier height; for $\rho \gg 1$ (i.e., $K_1 \gg K_2$) and $n = 1$ one obtains

$$T_k \propto \frac{S(JK_1)^{1/2}}{\ln(K_1/K_2)}, \quad (58)$$

which is only logarithmically smaller than the corresponding temperature for a particle (41).

Let us discuss now the behavior of the imaginary part of the Euclidean action in case of deviations from the simplest model (45) for which the tunneling is prohibited for half-integer $S$. The most simple observation is that in a spin chain with alternated exchange interaction, when along the chain the strength of exchange constant alternates as $J_1J_2J_1J_2 \cdots$, the topological term (47) acquires additional factor $J_1/J_2$ (see, e.g., [38, 39]), which leads to $\Phi = \cos(\pi SJ_1/J_2)$ and allows tunneling for half-integer $S$. Another way to lift the degeneracy at half-integer $S$ is to “switch on” the DM interaction or external magnetic field.

Consider the same model (45) with the addition of a magnetic field $\vec{H}$ applied in the easy plane ($xy$). Presence of the field leads to the additional
contribution to the imaginary part of $A_{\text{eucl}}$

$$A_{\text{eucl}} \mapsto A_{\text{eucl}} + i\hbar Q' ,$$

$$Q' = \frac{2S}{a} \frac{H}{H_e} \int \vec{n} \cdot \left( \vec{l} \times \frac{\partial \vec{l}}{\partial x_2} \right) d^2x , \quad (59)$$

where $\vec{n} \equiv \vec{H}/H$. The mixed product in (59) can be rewritten in angular variables as

$$- \sin \theta \cos \theta \left( n_x \cos \varphi + n_y \sin \varphi \right) \frac{\partial \varphi}{\partial x_2} + \left( n_y \cos \varphi - n_x \sin \varphi \right) \frac{\partial \theta}{\partial x_2} .$$

One may note that $\sin \theta$ and $\theta$ significantly differ from zero only in the vortex core, and thus the isotropic vortex solution (53) may be used for the calculation of $Q'$. After integration we obtain

$$Q' = 2S \frac{H}{H_e} \frac{\Delta}{a} p(An_x + \nu Bn_y) ,$$

$$A = \int_0^{\infty} (dr/\Delta) \sin \theta_0 \cos \theta_0 , \quad B = \int_0^{\infty} (dr/\Delta) r(d\theta_0/dr) , \quad (60)$$

where $p$ and $\nu$, as earlier, denote the polarization and vorticity of the instanton solution, and $A, B$ are numerical constants (recall that, according to (53), the isotropic solution $\theta_0$ may depend only on $r/\Delta$). After performing the summation in $p, \nu$, and with the account taken of the contribution $Q$ coming from the topological term, the factor $\Phi$ in (57) will be modified as

$$\Phi \mapsto \Phi_H = \cos \left( 2ASn_x H \frac{\Delta}{H_e} a \right) \cos \left( \pi S + 2BSn_y H \frac{\Delta}{H_e} a \right) , \quad (61)$$

which means that for the given geometry only the field component perpendicular to the easy axis lifts the degeneracy existing for half-integer $S$. Similarly to the case of a small AFM particle, the tunneling amplitude is an oscillating function of the external magnetic field $H$, but here the situation is more complicated because the period of oscillations depends on the field orientation.

5.2. TUNNELING IN ANTIFERROMAGNETIC RINGS WITH ODD NUMBER OF SPINS

Another example of a magnetic nanostructure is a ring formed by magnetic atoms; such rings may occur in a dislocation core of a 2D crystal as shown in Fig. 3, and the characteristic feature of this object is that the number of atoms in the ring is odd. Here we consider only antiferromagnetic rings. In terms of the vector $\vec{l}$ such a ring is a spin disclination. Let us assume that
the magnetic anisotropy is of the easy-plane type, and all spins lie in the $(xy)$ plane,

$$S_i = (-1)^i (\vec{e}_x \cos \varphi_i + \vec{e}_y \sin \varphi_i),$$

where $\vec{e}_{x,y}$ are the unit vectors along $x, y$. Then there are two energetically equivalent states of the ring, with $\varphi_i = \chi_i/2$ and $\varphi_i = -\chi_i/2$, where $\chi_i$ is the azimuthal coordinate of the $i$-th spin (let us assume that the ring is a circle of radius $R$). It is possible to construct the instanton solution which links the two states; in terms of $\vec{l}$ it can be written as

$$l_x = \cos \frac{\chi}{2}, \quad l_y = \sin \frac{\chi}{2} \cos \psi, \quad l_z = \sin \frac{\chi}{2} \sin \psi,$$

$$\cos \psi = \pm \tanh(\omega_0 \tau), \quad \omega_0 \simeq \frac{1}{2} \gamma M_0 (\beta \delta)^{1/2}.$$

Calculation shows [22] that the tunneling amplitude is proportional to

$$\cos(\pi S) \exp\{-\pi S R/\Delta\}, \quad \Delta = (\alpha/\beta)^{1/2}, \quad (62)$$

i.e., the probability of tunneling is sufficiently large if the radius of the ring is smaller than the characteristic thickness of the domain wall $\Delta$ (usually $\Delta \sim 100\text{Å}$). Again, the tunneling is suppressed for half-integer $S$, and this can be changed with the help of external magnetic field. More detailed analysis [22] shows that the field $\vec{H}$ should be applied in the easy plane in order to lift the degeneracy, then the cosine in (62) will change into

$$\cos \left( \pi S + \pi S \frac{H \cdot R}{4H_c a} \right),$$
where $a$ is of the order of the lattice constant. For weak fields the above expression describes just the Zeeman splitting of the ground state level of a ring (recall that due to the odd number of spins the ring always has an uncompensated total spin if $S$ is half-integer).

5.3. TUNNELING IN A MAGNETIC VORTEX OF 2D ANTIFERROMAGNET

One more example of a magnetic topologically nontrivial structure is magnetic vortex in quasi-2D easy-plane antiferromagnet. Consider the system described by the Hamiltonian

$$
\hat{H} = J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j + K \sum_i (S^z_i)^2
$$

where $K > 0$ is the anisotropy constant, and $Oz$ is the difficult axis. In terms of the angular variables for the antiferromagnetism vector, $l_z = \cos \theta$, $l_x + il_y = \sin \theta e^{i\varphi}$, a vortex corresponds to the solution

$$
\theta = \theta_0^\pm (r), \quad \varphi = \nu \chi + \varphi_0,
$$

$$
\theta_0^\pm (\infty) = \pi/2, \quad \theta_0^+ (0) = 0, \quad \theta_0^- (0) = \pi,
$$

where $\theta_0$ satisfies the equation from the second line of Eq. (54), $x + iy = re^{i\chi}$, and the solutions $\theta_0^+$ and $\theta_0^-$ have the same vorticity $\nu$ but different polarizations $p = \cos \theta(0) = \pm 1$. The vortex states with $p = \pm 1$ are energetically equivalent, and the transition between them corresponds to reorientation of a macroscopic number of spins $N \sim (\Delta/a)^2$, where $\Delta = a(K/4J)^{1/2}$ is the characteristic radius of the vortex core and $a$ is the lattice constant. It is worthwhile to remark that such a transition would be forbidden in ferromagnet because of the conservation of the $z$-projection of the total spin $S^z$.

The instanton solution $\vec{l}(x, y, \tau)$ linking two vortex configurations $\theta_0^\pm$ with $\nu = 1$ when the imaginary time $\tau$ changes from $-\infty$ to $+\infty$ is schematically shown in Fig. 4. In the 3D Euclidean space $(x, y, \tau)$ it describes a topological configuration of the hedgehog type and has a singularity at the origin. Such a singularity means that in a small space region around the origin (roughly within the distance of about $a$) one has to take into account the change of magnitude of the sublattice magnetization: the length of the vector $\vec{l}$ has to change so that $|\vec{l}(0,0,0)| = 0$. In this case there are four zero modes, three of them correspond to translations along $x$, $y$, $\tau$, and the fourth one corresponds to changing the $\varphi_0$ angle. If the position and structure of the vortex are fixed by some additional interactions, only one zero mode is left.
At $\tau \to \pm \infty$ one has $p = -1$ and $p = +1$ vortices, respectively. The sphere near the origin corresponds to the region where a hedgehog-type solution is adequate.

The Euclidean action derived from the Lagrangian of the $\sigma$-model has the following form

$$A_E = JS^2 \int d\tau \int d^2x \left\{ \frac{1}{c^2} \left( \frac{\partial \vec{l}}{\partial \tau} \right)^2 + (\vec{\nabla} \vec{l})^2 - (\vec{\nabla} \vec{l}(0))^2 + \frac{1}{\Delta^2} (l_z^2 - (l_z^0)^2) \right\},$$

(66)

where $\vec{l}(0)$ describes the vortex solution (64) and $c$ denotes the limiting velocity $c = 2JSa/h$. Away from the singularity (for $\rho \gg a$, $\rho \equiv (c^2 \tau^2 + \ldots$
The condition $l^2 = 1$ holds, and the equations for $\theta, \varphi$ become

\begin{align*}
\vec{\nabla}^2 \theta + \sin \theta \cos \theta [1/\Delta^2 - (\vec{\nabla} \varphi)^2] &= 0, \\
\vec{\nabla} \cdot (\sin^2 \theta \vec{\nabla} \varphi) &= 0.
\end{align*}

(67)

In the region $a \ll \rho \ll \Delta$ this system has an exact centrally symmetric solution of the hedgehog type:

$$
\cos \theta = \frac{c \tau}{\rho}, \quad \tan \varphi = \frac{y}{x}.
$$

(68)

It can be shown that the contribution of the singularity itself is small and can be neglected. Dividing the integration domain into two regions $\rho < R$ and $\rho > R$, where $R \ll \Delta$, one can see that the contribution of the region of small distances $\rho < R$ to the Euclidean action is given by

$$
A_E[\rho < R] = 4\pi (JS^2/c)R.
$$

(69)

For estimating the contribution of the “large” distance region we use a variational procedure with the trial function of the form

$$
\theta(x, y, \tau) = \pi/2 + F(c\tau)[\pi/2 - \theta_0^{(+)}(r)],
$$

(70)

where $F(c\tau)$ is a “smeared step function”: $F \to \pm 1$ as $\tau \to \pm \infty$ and the derivative of $F$ is nonzero in the region of the thickness $\Delta_1$ around $\tau = 0$. A simple estimate shows that the resulting contribution of the region $\rho > R$ is described by

$$
A_E[\rho > R] = (2\pi JS^2/c)[\xi_1 \Delta_1 \ln(\Delta/R) + \xi_2 \Delta_1 + \xi_3 \Delta^2/\Delta_1],
$$

(71)

where $\xi_{1,2,3}$ are numerical constants of the order of unity. Summing up (69) and (71) and minimizing $A_E$ with respect to $\Delta_1$ and $R$, we find $\Delta_1 \sim R \sim \Delta$. Thus, the total one-instanton Euclidean action may be estimated as

$$
A_0 = 2\pi \xi JS^2 \Delta/c = \xi \pi \hbar S \Delta /a,
$$

(72)

where $\xi \sim 1$.

Demanding that the tunneling exponent is not too large, e.g., $A_0 < 20 \div 30$, we see that for $S = 5/2$ this means $\Delta/a < 3 \div 4$, which is rather tight; the continuum field approach we used here formally requires $\Delta \gg a$, but in practice it is still applicable for $\Delta/a \sim 2 \div 3$ [40]. The crossover temperature $T_c \sim S(JK)^{1/2}$ is not small since it is proportional to $\sqrt{J}$.

### 6. Summary, and What is left under the carpet.

Let us mention briefly the problems which are closely related to the topic of this paper but were left out of discussion, and also those problems which are not clear at present, to our opinion.
First of all we would like to remark that we did not touch at all microscopic essentially quantum effects in magnets, e.g., predicted by Haldane destruction of (quasi)long-range order in 1D antiferromagnets with integer spin $S$ caused by quantum fluctuations. Effects of quantum interference are also important for this phenomenon, and its existence is determined by the presence of topological term in the Lagrangian of antiferromagnet (see, e.g., the reviews [34, 39]). For small $S$ and weak anisotropy the ground state of 1D antiferromagnetic system can differ drastically from its classical prototype; e.g., the ground state of a $S = 1$ AFM ring is not sensitive to whether the number of spins is odd or even and is always unique, and the ground state of a $S = \frac{1}{2}$ AFM ring with odd number of spins is fourfold degenerate [22].

We also did not consider the contribution of tunneling-generated internal soliton modes to the thermodynamics and response functions of 1D antiferromagnets, which can lead to interesting effects (see [36, 35, 19, 41]).

Another problem which was ignored in our consideration is the role of relaxation and thermal fluctuations of different origin. Even at low temperature the interaction of spins with other crystal subsystems (lattice, nuclear spins, etc.) may be very important, see [42, 43, 44]. It is clear that stochastic influence on the dynamics of magnetization from thermal fluctuations leads to decoherence and suppresses coherent tunneling. Description of this fundamental problem in any detail goes far beyond the scope of the present lecture, and we refer the reader to the review by Caldeira and Leggett [29].

One more problem which is unclear from our point of view is a justification of considering all spins in a small particle as moving coherently (a “giant spin” approximation usually used in treating the MQT problems and also adopted in the present paper). In fact, the only justification of this approximation is energetical: if the particle size is much smaller than the characteristic domain wall thickness, any inhomogeneous perturbation costs much energy. On the other hand, for the Hamiltonian (24) neither $S^2$ nor $\hat{S}^z$ are good quantum numbers, which means presence of magnons (deviations from collinear order) in the ground state.

Our lecture was devoted first of all to the fundamental aspects of MQT considered as a beautiful physical phenomenon which is rather difficult to observe. But technological development can lead to the situation when this phenomenon will become practically important. The present tendency of increasing the density of recording in the development of information storage devices means decrease of the elementary magnetic scale corresponding to one bit of information, and one may expect that quantum effects will determine the “natural limit” of miniaturization in future.
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