<u>Original Research Article</u>

Fluctuational Dynamics of Extended Systems: Activation-Tunnel Frontier

ABSTRACT

The dynamics of systems in barrier structures is determined by the rate of fluctuation decay of metastable states in a potential relief. The nature of the decay undergoes a qualitative change with variation of temperature. As the temperature decreases, thermal fluctuations freeze out and are replaced by quantum ones, which leads to a kind of phase transition in dynamics. The transition temperature depends on the degree of metastability and can be controlled by an external load. This dependence is calculated for an extended nanosystem in an inclined periodic relief of the "washboard" type in a wide range of load changes, which generalizes the previously known results and can serve as a phase diagram of various dynamics mechanisms.

Keywords: Dynamics of extended systems; metastable states; slip phase; activation-tunneling transition; collective coordinates.

1. INTRODUCTION

The dynamics of extended quasi-one-dimensional objects of various nature is currently being actively studied both experimentally and theoretically [1]. Popular examples are the motion of charge-density waves, the phenomenon of phase slip in Josephson junctions or superconducting nanowires (see, for example, [2,3]). Similar features are also observed in the dynamics of domain boundaries [4] or dislocation movement in the crystal relief [5]. For systems of recording and storing information in barrier structures of spintronics, the issues of switching and stability of states in minima of the potential relief are important [6]. The fundamental characteristic in the low-temperature physics is the boundary that separates the temperature regions of classical thermally activated and quantum mechanical dynamics of systems [7].

Of considerable interest for applications is the reaction of an extended system located in a flat bistable or periodic potential relief to the impact of an external load making the relief valleys nonequivalent. The position of such the system in a minimum of the potential relief disturbed by the load becomes a metastable state, since, overcoming the barrier by means of thermal or quantum fluctuations, the object can move to neighboring energetically preferred minima.

According to the accepted concepts, the evolution of a sufficiently extended system is carried out by the formation of local nuclei of a new state, their expansion and merging. The kinetics of this process is often described in terms of the formation and movement of nucleus boundaries, which are domain walls or kink-solitons (hereinafter referred to as kinks) [4].

With regard to Josephson junctions, the terms fluxon or anti-fluxon are sometimes used instead of kink or anti-kink.

The dynamics of domain walls or kinks is well studied for relatively low loads, at which they can be considered as weakly perturbed quasiparticles characterized by a single degree of freedom – the position of the kink as a whole [8]. The situation is more complicated when the load increases, leading to deformation of the kinks, which reveals their internal degrees of freedom. In this case, the possibility of one-dimensional description is lost and it is necessary to use more complete representations of the configuration space of systems. The purpose of this work is to describe the dynamics of extended metastable systems in a wider range of loads, for which an effective method of collective coordinates will be applied, including an additional degree of freedom – the width of the domain wall that can change. The foundations of this approach were laid in [9, 10].

2. ENERGY RELIEF IN MANYDIMENTIONAL SPACE

Local overcoming barriers by an extended system occurs with a distortion of its configuration, and to describe this process, one needs to know the energetics of the configuration space. The archetypal model used to describe the switching of states of various quasi-one-dimensional systems is the elastic string model. The energy of a string located in a flat potential relief U_0 (y) under the action of an external force f is described by the expression

$$E\{y(x,t)\}=\int_{-\infty}^{\infty} dx\{\frac{\rho}{2}(\frac{\partial y}{\partial t})^2+\frac{\kappa}{2}(\frac{\partial y}{\partial x})^2+U_0(y)-fy(x,t)\}\ . \qquad (1)$$

Here $y(x,t)$ is the string configuration, x is the coordinate along the valleys of the potential $U_0(y)$, which has several minima corresponding to the metastable states of the system, κ is the string stiffness, ρ is the mass density per unit length. The role of the external force in different systems is played by different physical quantities. For example, in the dynamics of charge density waves this is an electric field, in superconductors it is the flowing current or the magnetic field, and at dislocations movement, it is the mechanical stress. The harmonic sine-Gordon potential is often considered as $U_0(y)$ [11]

$$U_0(y) = \frac{U_m}{2}[1-\cos(\frac{2\pi}{h}y)]\ . \qquad (2)$$

Here h is the period of the potential. The derivation of the sine-Gordon model, the physical meaning, and values of its parameters for various systems are given in [11]. For materials in which quantum tunneling effects are observed, the typical parameter values are such that the characteristic energy $h(\kappa U_m)^{1/2}$ is of the order of magnitude 10^{-3} -10^{-2} eV, the characteristic quantum temperature $T_q=(\hbar/\kappa h)\ (U_M/\rho)^{1/2}$~1-10 K.

In the presence of an external driving force f metastable states of the system in minima of $U_0(y)$ have a finite lifetime. The decay time of metastable states is determined by the height of the barriers in the configuration space, and is calculated using expression (1).
We will measure y in units of h, x in $d_0 = h(\kappa/U_m)^{1/2}$, and time t in units of $h(\rho/U_m)^{1/2}$. The energy of a string with potential (2) takes the form

$$E\{y(x,t)\}=\int_{-\infty}^{\infty} dx\{\frac{1}{2}(\frac{\partial y}{\partial t})^2+\frac{1}{2}(\frac{\partial y}{\partial x})^2+U_0(y)-fy(x,t)\}\ , \qquad (3)$$

where the variables are dimensionless: $E \to E/h\sqrt{\kappa U_m}$, $f\to fh/U_m$,. Let the string initially be at the minimum of the potential $U_0(y)$-fy corresponding to y_0 = arcsin(f/π). Next, we count $y(x)$

from y_0 and renormalize the potential U_0(y)-fy so that the minimum will correspond to zero energy $U(y) \to U(y) = U_0(y) - fy - U_0(y_0) + fy_0 = \frac{1}{2}\{[1-(f/\pi)^2]^{1/2}[1-\cos(2\pi y)] + (f/2\pi)\sin(2\pi y)\} - fy$, here y is counted from 0.

The main task is to describe the process of formation of a new state nucleus corresponding to the easiest path to overcome the barrier. We will search this path by the variational method, using a trial function to describe the configuration of the string, which depends on 2 parameters: d and x_0

$$y(x) = y_0 + \frac{\exp[(x+x_0)/d]}{\{1+\exp[(x-x_0)/d]\}\{1+\exp[(x+x_0)/d]\}} = y_0 + \frac{e\exp(x/d)}{[1+(e+1/e)\exp(x/d)+\exp(2x/d)]}. \quad (4)$$

Here and below, $e = \exp(x_0/d)$. The physical meaning of the parameters becomes clear in the limit $x_0 \to \infty$, when

$$y(x,t) \to y_0 + \frac{1}{1+\exp[(x-x_0)/d)]} - \frac{1}{1+\exp[(x+x_0)/d)]},$$

which looks like a kink-antikink pair (see Fig. 1). In this case, $x_0/2$ corresponds to the distance between the kinks, and d to the width of the kink. Taking into account this interpretation, for the sake of convenience, we will call x_0 the longitudinal coordinate, and d - the transverse one. The variables x_0 and d can be time dependent. For small or negative x_0, corresponding to small deviations of the string from the initial position, the clear meaning of the variables is lost, and x_0, d are considered only as variational parameters. The chosen trial function (4) makes it possible to describe a wide spectrum of intermediate states from small sub-barrier fluctuations to fully formed nuclei behind the barrier.

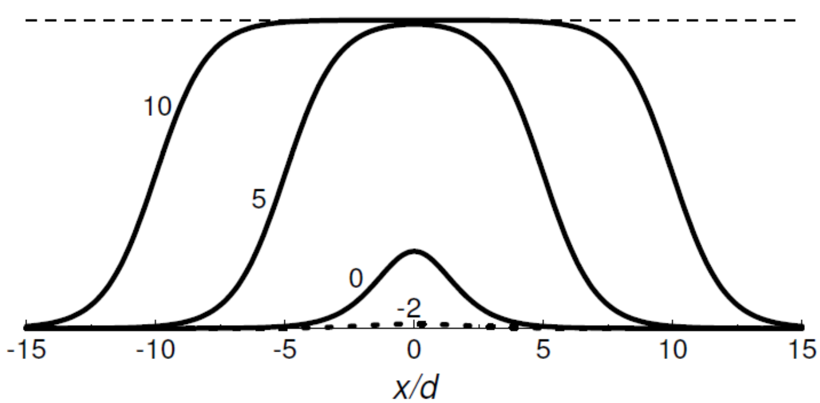

Fig.1. The form of the trial function $y(x)$-y_0 for different values of the parameter x_0/d, indicated by numbers at the curves. The dotted line shows the trial function with a negative value of the parameter x_0/d=-2. The dashed line corresponds to the minimum of potential relief.

We substitute trial function (4) into energy functional (3) to obtain the two-dimensional potential relief $E(x_0,d)$. Changing the scale of the integration variable and replacing the variable x_0 by e, we represent $E(e,d)$ in the form

$$E(e,d) = \frac{e^2}{2d} I_1 + \frac{d}{2}\{[1-(f/\pi)^2]^{1/2} I_2 - f[2eI_3 - (1/\pi)I_{22}]\}. \quad (5)$$

Here I_1, I_2, I_{22} and I_3 are functions of the single variable e, represented by integrals, for some of which it is possible to obtain analytical expressions, while the rest must be calculated numerically:

$$I_1=\int_{-\infty}^{\infty} dx \frac{\exp(2x)[1-\exp(2x)]^2}{[1+(e+1/e)\exp(x)+\exp(2x)]^4} = \frac{1}{e^2}\left(\frac{e^2}{e^2-1}\right)^2\left\{\frac{1}{3}+\frac{4e^2}{(e^2-1)^2}-4\frac{e^4+e^2}{(e^2-1)^3}\ln(e)\right. \quad (6)$$

At $e\to\infty$ $I_1 \to \frac{1}{e^2}\{\frac{1}{3}-(4/e^2)[\ln(e)-7/6]\}$.

$$I_2=\int_{-\infty}^{\infty} dx\{1-\cos[2\pi e\frac{\exp(x)}{1+(e+1/e)\exp(x)+\exp(2x)}]\} . \quad (7)$$

At $e\to\infty$ $I_2\approx -4\mathrm{ci}(2\pi)+4\gamma+4\ln(2\pi)+\{8\pi^2[\mathrm{ci}(2\pi)-\gamma-\ln(2\pi/e)+1]-4\pi\mathrm{si}(2\pi)\}/e^2$, ci($2\pi$) and si($2\pi$) are the values of the integral cosine and integral sine at the argument 2π, γ= 0.5772…- Euler's constant.

$$I_{22}=\int_{-\infty}^{\infty} dx\sin[2\pi e\frac{\exp(x)}{1+(e+1/e)\exp(x)+\exp(2x)}] . \quad (8)$$

At $e\to\infty$ $I_{22}\approx 4\pi[\mathrm{ci}(2\pi)-\gamma-\ln(2\pi/e)+2\pi\mathrm{si}(2\pi)]/e^2 -(8/9)\pi^3/e^3$.

$$I_3=\int_{-\infty}^{\infty} dx\frac{\exp(x)}{1+(e+1/e)\exp(x)+\exp(2x)} = \frac{1}{\sqrt{e^2-4}}\ln\frac{e+\sqrt{e^2-4}}{e-\sqrt{e^2-4}} . \quad (9)$$

At $e\to\infty$ $I_3\approx (2/e)\ln(e)(1+1/e^2)$.

In order to find the optimal way to overcome the barrier, we find the minimum $E(e,d)$ in (5) with respect to d

$$\frac{\partial E}{\partial d} = -\frac{1}{2d^2}e^2 I_1 + \frac{1}{2}\{[1-(f/\pi)^2]^{1/2}I_2-f[2eI_3-(1/\pi)I_{22}]\}=0.$$

Whence the optimal d is

$$d=\left[\frac{e^2 I_1}{[1-(f/\pi)^2]^{1/2}I_2-f[2eI_3-(1/\pi)I_{22}]}\right]^{1/2}. \quad (10)$$

Substituting this value into $E(e,d)$ (5), we find the change of energy along the e coordinate trough the valley of the two-dimensional relief

$$E_v(e)=e\{I_1[(1-(f/\pi)^2)^{1/2}I_2-f(2eI_3-(1/\pi)I_{22})]\}^{1/2}. \quad (11)$$

This line will be called the valley bottom of the potential (two-dimensional) relief. When the longitudinal coordinate changes along the valley, the maximum energy E_M is encountered. From the point of view of the two-dimensional relief, this point corresponds to a pass or "saddle" with a decrease in energy when moving away from it along one coordinate e and an increase in energy along the other d. Figure 2 illustrates the two dimensional potential relief for the driving force f=1 by depicting lines of constant energy and the valley bottom line leading to the pass point in the relief. Note that E_M plays the role of activation energy in the thermally fluctuation formation of the nucleus of the new state of the system.

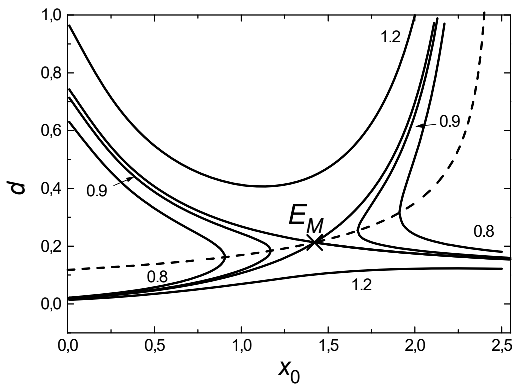

Fig. 2. Two-dimensional potential relief at the driving force f=1. Solid lines correspond to the constant energy levels with the values indicated by numbers near them, the dashed line represents the bottom of the potential relief valley. The cross marks the position of the barrier maximum E_M = 0.93389.

For a demonstration of the effectiveness of the collective coordinate method used, in Fig. 3 the obtained dependence of the energy E_M on the driving force f is compared with the dependence calculated numerically in frame of the full multidimensional approach.

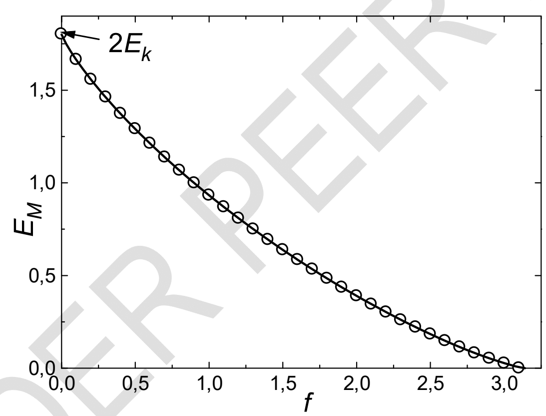

Fig. 3. Dependence of the energy E_M of the formation of the new state nucleus on the driving force f, obtained using two collective coordinates (circles). The solid line shows the result of numerical calculation of this dependence with the full multidimensional approach.

The method that takes into account a few, in the simplest version, two collective coordinates, makes it possible to find the dependence of the quantum tunneling rate on the driving force in a wide range of its changes.

3. QUANTUM MECHANISM OF DECAY OF THE METASTABLE STATE OF AN EXTENDED SYSTEM

In the semiclassical approximation with exponential accuracy, the probability of quantum-mechanical overcoming the barrier is given by the expression

$$\Gamma \approx \exp(-S/\hbar), \tag{12}$$

where S is the action calculated along the trajectory of the sub-barrier transition. Substitute trial function (4) into (14), assuming x0 and d to be time dependent

$$y(x,t)= y_1+ \frac{\exp[(x+x_0(t))/d(t)]}{1+\{\exp[x_0(t)/d(t)]+\exp[-x_0(t)/d(t)]\}\exp[x/d(t)]+\exp[2x/d(t)]}.$$

The kinetic energy takes the form

$$T_k= \frac{e^2}{2d} I_{kx}\dot{x}_0^2 + \frac{e^2}{2d} I_{kd}\dot{d}^{\,2} + \frac{e^2}{d} I_{kxd}\dot{x}_0\,\dot{d}\,, \tag{13}$$

where

$$I_{kx}= \int_{-\infty}^{\infty} dx\exp(2x)\frac{[1+\exp(2x)+2e_{-}\exp(x)]^2}{[1+(e+1/e)\exp(x)+\exp(2x)]^4} =$$

$$\frac{1}{3}\frac{e^2}{(e^2-1)^2} - \frac{8e^4+12e^2}{(e^2-1)^4} + \frac{4e^6+28e^4+8e^2}{(e^2-1)^5}\ln(e), \tag{14}$$

$$I_{kd}= \int_{-\infty}^{\infty} dx\exp(2x)\frac{\{(x_0/d)[1+2\exp(x)/e+\exp(2x)]+x[1-\exp(2x)]\}^2}{[1+(e+1/e)\exp(x)+\exp(2x)]^4}, \tag{15}$$

$$I_{kxd}= \int_{-\infty}^{\infty} dx\exp(2x)\frac{\{(x_0/d)[1+2\exp(x)/e+\exp(2x)]+x[1-\exp(2x)]\}[1+2\exp(x)/e+\exp(2x)]}{[1+(e+1/e)\exp(x)+\exp(2x)]^4}, \tag{16}$$

Euclidean Lagrangian (with inverted potential) $L=T_k+E(x_0,d)$ makes it possible to calculate the action $S=\int Ldt$ by solving the system of two Euler-Lagrange equations in the standard way.

4. ACTIVATED-TUNNELING MODE

At a finite temperature, both quantum and thermal fluctuations contribute to overcoming the barrier. Often, the temperature boundary between the determining influence of one or the other is found simply by equating the probabilities of thermal activated and tunnel overcoming the barrier. However, this approach is inaccurate not only quantitatively, but also qualitatively, since it obscures the physical picture of what is happening. In fact, at a temperature other than absolute zero, an intermediate combined process is possible: tunneling not from the ground, but from the thermally excited state of the system. The probability of such a combined process is mainly determined by some optimal energy preceding tunneling which, as a rule, increases with increasing temperature. The transition temperature is considered to be the one at which the preactivation energy is compared with the barrier height E_M and above which the process has the character of classical thermal activation.

Consider sub-barrier motion with preliminary activation for some energy E. The height of the barrier for subsequent tunneling in this case decreases by the value E, and the action is a decreasing function $S(E)$ of the pre-activation energy. The transition probability is equal to the product of the activation probability with the energy E, given by the Boltzmann factor exp(-E/kT), and the probability of a tunnel transition trough the barrier lowered by E, which is $\exp\{E/kT) - S(E)/\hbar\}$. The optimal preactivation energy corresponds to the maximum exponent over E and is found from the equation

$$\frac{d}{dE}[E/kT+S(E)/\hbar]=1/kT+\frac{1}{\hbar}\frac{dS}{dE}=0. \qquad (17)$$

The maximum possible solution of this equation at the preactivation energy equal to the barrier height $E = E_M$ corresponds to the transition temperature from the classical thermally activated overcoming of the barrier to its overcoming with the participation of the quantum tunneling.

5. TEMPERATURE OF TRANSITION BETWEEN MODES OF OVERCOMING THE BARRIER

To study the transition with decreasing temperature from the classical activated jump over the barrier to overcoming the barrier with the participation of the quantum mechanical tunneling, it is necessary to study the dynamics of the system near the maximum of the potential relief E_M. Let us expand the expressions for the potential and kinetic energies by small deviations near the saddle point x_M and d_M: $x_0 \approx x_M+x$, $d \approx d_M+\delta$. The potential energy will take the form

$$E(x_0,d) \approx E_M+\frac{1}{2}\frac{\partial^2 E}{\partial e^2}(e-e_M)^2+\frac{\partial^2 E}{\partial e \partial d}(e-e_M)\delta+\frac{1}{2}\frac{\partial^2 E}{\partial d^2}\delta^2 \approx E_M+\frac{1}{2}K_x x^2+K_{xd}x\delta+\frac{1}{2}K_d\delta^2. \qquad (18)$$

Here

$$K_x=\frac{1}{d_M}\left(I_1+2e_M\frac{dI_1}{de}+\frac{e_M^2}{2}\frac{d^2I_1}{de^2}\right)+\frac{d_M}{2}\left\{[1-(f/\pi)^2]^{1/2}\frac{d^2I_2}{de^2}-f\left[4\frac{dI_3}{de}+2e_M\frac{d^2I_3}{de^2}-(1/\pi)\frac{d^2I_{22}}{de^2}\right]\right\}e_M^2, \qquad (19)$$

$$K_{xd}=\left\{-\frac{e_M}{d_M^2}I_1-\frac{e_M^2}{2d_M^2}\frac{dI_1}{de}+\frac{1}{2}\left\{[1-(f/\pi)^2]^{1/2}\frac{dI_2}{de}-f\left[2I_3+2e_M\frac{dI_3}{de}-(1/\pi)\frac{dI_{22}}{de}\right]\right\}\right\}e_M, \qquad (20)$$

$$K_d=\frac{e_M^2}{d_M^3}I_1. \qquad (21)$$

The M index marks that all parameters are taken at their values at the maximum of the barrier. The kinetic energy will be given by the quadratic form

$$T_k=\frac{1}{2}M_x\dot{x}^2+M_{xd}\dot{x}\dot{\delta}+\frac{1}{2}M_d\dot{\delta}^2. \qquad (22)$$

Here the components of the anisotropic mass are

$$M_x=2\left\{\frac{I_{kxM}}{2I_{1M}}E_M+\frac{I_{kdM}}{2I_{1M}}\frac{e_M^4}{E_M}\left(2I_{1M}+e_M\frac{dI_{1M}}{de}\right)^2+\frac{I_{kxdM}}{I_{1M}}e_M^2\left(2I_{1M}+e_M\frac{dI_{1M}}{de}\right)\right\}, \qquad (23)$$

$$M_{xd}=\left\{\frac{I_{kdM}}{I_{1M}}\left(2I_{1M}+e_M\frac{dI_{1M}}{de}\right)+\frac{I_{kxdM}}{I_{1M}}E_M\right\}, \qquad (24)$$

$$M_d=\frac{I_{kdM}}{I_{1M}}E_M. \qquad (25)$$

Potential relief (18) near the maximum has the form of a saddle (see Fig. 2) with negative curvature along one direction (pass) y_s and positive curvature along the other y_t, transverse to the pass. The optimal trajectory to overcome the barrier corresponds to movement along the pass direction without excitation of the transverse mode. Minimizing the potential energy (18), for example, with respect to δ, we find that along the pass $\delta=-(K_{xd}/K_d)x$. Substituting this relationship into the potential and kinetic energies (18) and (22), we find that the movement in the saddle direction is described by the Euler-Lagrange equation

$$\ddot{y}_s=-\omega^2 y_s, \qquad (26)$$

where $\omega=\{-(K_x-K_{xd}^2/K_d)/[M_x+M_d(K_{xd}/K_d)^2-2M_{xd}K_{xd}/K_d]\}^{1/2}$.

The action for such a movement is easily calculated. Integration of equation (26) gives

$$\frac{1}{2}\,\dot{y}_s{}^2= -\frac{1}{2}\,\omega^2 y_s{}^2+\text{const.} \qquad (27)$$

The initial conditions correspond to a start with zero velocity $\dot{y}_s=0$ from the boundary of the classically allowed region $y_s= -y_0$ with the given preactivation energy $\frac{1}{2}\,\omega^2 y_0{}^2=E_M-E_{cl}=\Delta E$.

Hence const=$\Delta E=\frac{1}{2}\,\omega^2 y_0{}^2$, and equation (27) takes the form

$$\frac{1}{2}\,\dot{y}_s{}^2= \frac{1}{2}\,\omega^2(y_0{}^2- y_s{}^2). \qquad (28)$$

The action for motion during the half-period π/ω, calculated using equation (28), is

$$\frac{1}{2}\,S=\int_0^{\pi/\omega} dt(\frac{1}{2}\dot{y}_s{}^2+\Delta E-\frac{1}{2}\omega^2 y_s{}^2) = \omega\int_{-y_0}^{y_0} dy(y_0^2-y^2)^{1/2} = \frac{\pi}{2}\,(2\Delta E)/\omega. \qquad (29)$$

The solution to the equation for the preactivation energy (17) exists only for $T_q/T>$ min$|dS/dE|=2\pi/\omega$ in accordance with the known results [12,13] for the second-order phase transition. Thus, the temperature at which the tunnel contribution appears is

$$T_c=\omega|/2\pi=\frac{1}{2^{3/2}\pi}\,\{-(K_x-K_{xd}{}^2/K_d)/[M_x+M_d(K_{xd}/K_d)^2-2M_{xd}K_{xd}/K_d]\}^{1/2}. \qquad (30)$$

The result of the dependence of the transition temperature on the driving force f, calculated using this expression, is shown in Fig. 4. The presented picture can serve as a phase diagram of regions with different mechanisms of dynamics of extended quasi-one-dimensional systems. The inset shows the section of such a diagram for an Sn nanowire measured in [14], which demonstrates a qualitative similarity with the initial section of the theoretical curve. As an example, we indicate quantitative parameters similar to those found for numerous other materials [3]: nanowire diameter is 20 nm ≈(1/10)ξ, ξ is the coherence length of bulk tin, T_{c0}≈4.1 K is the superconducting transition temperature, I_c^{up}≈17 μA is the critical current of the wire at the lowest temperature of the experiment, 0.47 K, I_{c0}≈9.5 μA is the current of the transition to individual phase slip at the same temperature.

In this paper, the transition with decreasing temperature from the classical thermally activated mechanism of motion of an extended system through potential barriers to motion involving quantum mechanical tunneling is studied. The transition boundary can be controlled by an external load, so the main goal was a more complete calculation of the transition temperature dependence on the load than it was done before. Previously, such a transition was studied, in particular, in [15], and for the region of low values of the driving force f, the dependence of the transition temperature T_c was found $T_c\propto f^{1/2}$. Earlier in [12], it was established that for any extended (not only harmonic) potential relief, with the driving force approaching the critical value f_c, the transition temperature behaves like $T_c\propto (f_c-f)^{1/4}$. In these two cases, the scope of manifestation of quantum effects is rather limited. In the present paper, we calculated the dependence of the transition temperature T_c on the external load in the whole range of its variation, including the region in which T_c significantly increases with increasing load. This fact justifies the expansion of the scope of manifestation of low-temperature quantum effects in the dynamics of extended systems of various nature accessible to experimental observation.

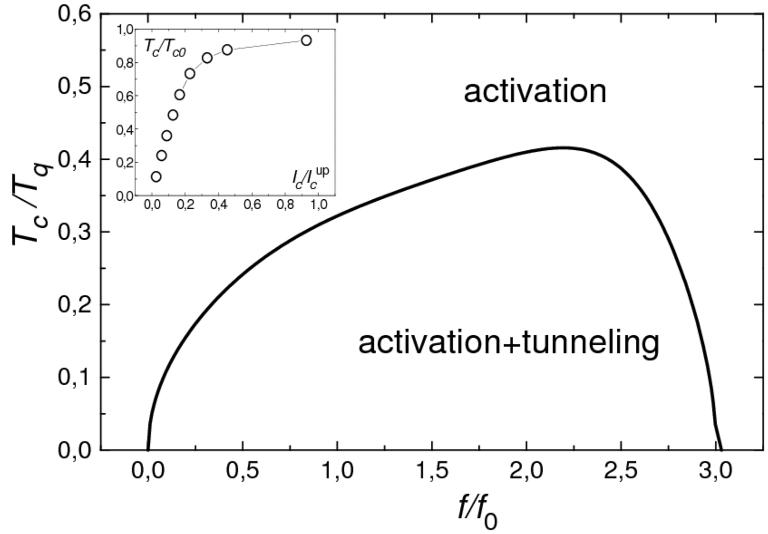

Fig. 4. Dependence on the driving force the temperature of the change of regimes between classical thermal activation and activation-tunneling overcoming of barriers [$f_0=U_M/h$, $T_q=(\hbar/kh)(U_M/\rho)^{1/2}$]. The inset shows the experimentally observed boundary between two modes in a Sn nanowire, one of which corresponds to multiple phase slip events due to thermal activation, and the second corresponds to individual phase slip due to quantum tunneling according to the reconstructed data from [14].

6. CONCLUSION

When current-carrying superconducting nanowires are used as single-photon detectors [3], an increase in the current flowing in them leads to an increase in their sensitivity. At the same time, a corresponding lowering of the barrier for escape from the metastable state increases the probability of fluctuational detector response due to background processes of phase slip and the formation of so-called “dark spots”. To find a compromise, the phase diagram of various mechanisms of the decay of metastable states of quasi-one-dimensional nanosystems calculated in this work can be useful.

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