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TO THE THEORY OF TYPE-I SUPERCONDUCTORS SURFACE TENSION AND TWINNING-PLANE-SUPERCONDUCTIVITY

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1. Introduction

Twinning-plane-superconductivity (TPS) is a new interesting type of two-dimensional superconductivity[1]. At temperatures higher than the bulk critical temperature T_c near the twinning plane (TP) there arises a narrow superconducting layer observed via its own diamagnetic moment. Bicrystals are cut in cylindrical form, and the axis of the cylinder lies in the TP. The magnetic moment is measured by a SQID and special attention is paid to compensate the fluctuational diamagnetism of the bulk metal. Experimental methods are described in [2]. For external magnetic fields H parallel to the TP, the superconducting layer is homogeneous and for obtaining such thermodynamical characteristics as the temperature dependence of the critical magnetic field $H_s(T)$ of the type-I TPS, the diamagnetic moment per unit TP area $M(T,H)$, therm-capacity C it is necessary to study the properties of the flat superconducting-normal phase boundary. The TPS critical temperature T_s is very close to the bulk one. For tin [3] for example

$$(T_s - T_c)/T_c = 0.04\,K/3.72\,K.$$

Because of this proximity it is possible to describe TPS in the framework of the Ginsburg-Landau (GL)[4,5] theory. Really, the numerical calculations[6] in the framework of this mean-field theory are in good agreement with the experimental data for tin [3]. The tin metal is a type-I superconductor with the GL parameter $\varkappa_{Sn}=0.13$, and this small parameter can be used for obtaining analytical results in the TPS theory.

As is known since the pioneering GL work[4], the precision of $\varkappa=0$ approximation for surface tension α is comparably small. A correction arises to α which is proportional to the square root of $\varkappa$. This correction is connected with the energy of the superconducting--normal phase boundary. The boundary has a thickness of order of $\varkappa^{1/2}\xi(T)$, where $\xi(T)$ is the temperature-dependent correlation radius [5] (the GL coherence length). Except for the TPS case such phase boundaries arise in a mixed superconducting state of type-I superconductors. The $\varkappa = 0$ approximation neglects the thickness and the energy of these phase boundaries. Analytical result for the TPS phase diagram is in poor agreement with the experiment[3]. It is of methodical interest whether that correction to the surface tension is the same correction ΔG which is necessary for the TPS Gibbs free energy $G(T,H)$. This universal correction is obtained in this paper by solving the universal GL[4] equations for the phase boundary. Energy of the phase boundary is nonanalytical in the small GL parameter $\varkappa$. This energy is proportional to $\varkappa^{1/2}$ and thus its consideration is essential practically for all type-I superconductors. Subsequent corrections to α contain $\varkappa^{3/2}$ and higher powers. Their calculation is only of academical interest even with a contemporary experimental precision.

The aim of this paper is to obtain explicit formulae for the surface tension of type-I superconductors and TPS free energy as functions of the GL parameter $\varkappa$.

2. Model

The TP contains a crystalline-distingushed layer of atoms embedded in the bulk metal. Irrespective of a specific microscopical mechanism of TPS (it can be connected with the change of the phonon spectrum of TP atoms or with the appearance of the two-dimensional electrons confined by TP) in the framework of the GL theory, the influence of TP is taken into account by adding appropriate boundary conditions to GL equations. For describing surface problems (see the well-known text-book [7]) we use the boundary condition for order parameter

$$d\Psi/dZ\big|_{Z=0} = \Psi/\lambda, \tag{1}$$

where λ is the extrapolation length, and Z is the Cartesian coordinate perpendicular to the layer (TP in our case). This boundary condition describes the jump of the gauge-invariant logarithmical derivative of superconducting order parameter on TP. The boundary condition (1) is equivalent to adding a new δ-like term[8] to the Gibbs-free-energy GL-functional [5]

$$G(T,H)=\int dV\Big\{|(-i\hbar\nabla - e^*A/c)\Psi|^2/2m^* + a|\Psi|^2 + b|\Psi|^4/2$$
$$+(\mathrm{rot}A-H)^2/8\pi - (\hbar/m^*\lambda)\,\delta(Z)|\Psi|^2\Big\}, \tag{2}$$

where $e^* = 2e$, m^* are the charge and mass of the Cooper pair, c is the light velocity, $\hbar$ is the Planck constant, A is the vector potential, b is the temperature-independent interaction constant for the order parameter, and a depends on the temperature by the rule $a = \mathrm{const}\,(T-T_c)$. The parameter a tends to zero at the bulk transition critical temperature. Integration in (2) is performed throughout the whole volume of the superconductor.

For external magnetic fields H parallel to the TP we will use the gauge[5]

$$B_y(z) \equiv (\mathrm{rot}\,A)_y = dA_x/dz, \quad A_y = A_z = 0,$$

$$B_y(z = \pm\infty) = H_y .$$

Recall connections [5] between the parameters of functional (2) and the correlation radius $\xi(T)$, thermodynamical critical field $H_c(T)$, equilibrium value of order parameter Ψ_0 , the Ginsburg number Gi, GL parameter $\varkappa$ and the London screening depth δ :

$$\hbar^2/2m^*\xi^2(T) = |a|, \quad H_c^2(T)/8\pi = a^2/2b, \quad \Psi_0^2 = |a|/b,$$

$$Gi^{1/2} = 8\pi\varkappa^2(e^2/\hbar c)\{T_c/[e^2/\xi(T=0)]\},$$

$$\varkappa = m^* c\, b^{1/2}/(2\pi)^{1/2}|e^*|\hbar, \quad \delta^{-2} = 4\pi e^{*2}\Psi_0^2/m^* c^2. \tag{3}$$

Let us introduce, following[6], useful for TPS theory variables:

$$t = (T-T_c)/(T_s-T_c), \quad H_s = H_c(t=-1), \quad \xi_s = \xi(t=-1),$$

$$h = |H_y|/H_s, \quad \rho_s = H_s^2/8\pi, \quad G_s = \xi_s \rho_s, \quad \Psi_s = \Psi_0(t=-1)$$

$$x = z/\xi_s, \quad A(x) = A_x(z)/H_s\xi_s, \quad \theta(x) = \Psi(z)/\Psi_s . \tag{4}$$

Near to T_s , when the order parameter is small, the compatibility of the solution of the linearised GL equation

with the boundary condition (1) gives the equality

$$\xi_s = \lambda .$$

The last of the parameters of functional (2), the fundamental for TPS length λ , can be determined with the help of this equality. The same coherence length is determined by the known equality [7]

$$\xi(T=0) = (\Phi_0/2\pi T_c)^{1/2}(-dH_{c2}/dT)^{-1/2}\Big|_{T_c},$$

where $\Phi_0 = 2\pi\hbar c/e^*$ is the magnetic fluxion, H_{c2} is the supercooling field. The GL parameter is obtained by the equation

$$\varkappa = H_{c2}/2^{1/2}H_c\Big|_{T=T_c-0} .$$

In the case of a parallel to TP external magnetic field there arises effectively one dimensional problem. In new variables we obtain for the TPS-free-energy (per unit area) functional

$$G = G_s\int_{-\infty}^{+\infty} dx\big[2(d\theta/dx)^2 + (A\theta/\varkappa)^2 + 2t\theta^2 + \theta^4 - 4\delta(x)\theta^2 + (dA/dx - h)^2\big]. \tag{5}$$

Before calculating the corrections to G and α in power series of $\varkappa$, in the next section we describe the basic term, the case of the extreme type-I superconductor with $\varkappa = 0$.

3. The $\varkappa = 0$ approximation

The Ginsburg-Landau equations are the Euler equations for the free energy functional (5)

$$(\delta G/\delta\theta)/2G_s = -2\,d^2\theta/dx^2 + (A/\varkappa)^2\theta + 2t\theta^2 - 4\delta(x)\theta + 2\theta^3 = 0, \tag{6a}$$

$$(\delta G/\delta A)/2G_s = -d^2A/dx^2 + (\theta/\varkappa)^2 A = 0. \tag{6b}$$

These equations have (for $x \neq 0$) a first integral

$$\sigma_{zz} = \rho_s\big[2(d\theta/dx)^2 + (dA/dx)^2 - 2t\theta^2 - \theta^4 - (A\theta/\varkappa)^2\big] = \rho_s h^2 = H_y^2/8\pi = \mathrm{const}. \tag{7}$$

It is the conserving zz component of the strain tensor. If formally we replace in (5) $dx \leftarrow g(x)dx$, the strain tensor can be obtained as a variational derivative with respect to the metric (the Lame coefficient $g(x)$ in this case)

$$\sigma_{zz} = -\delta G/\delta g\Big|_{g=1} .$$

The case of the extreme type-I superconductor $\varkappa = 0$ corresponds to the full Meissner effect. The equations (6) can have solutions only if $\theta A = 0$. I.e. $A = 0$ in the superconducting domain where $\theta \neq 0$, and vice versa, $\theta = 0$ in the normal domain where the magnetic field penetrates and $A \neq 0$. With the help of this condition the distribution of order parameter can be easily expressed in elliptical integrals. Sequentially, replace in (7), from the obtained equality express

$$|dx|/2^{1/2} = |d\theta|/(\theta^4 + 2t\theta^2 + h^2)^{1/2},$$

$$|d\theta/dx|/2^{1/2} = (\theta^4 + 2t\theta^2 + h^2)^{1/2}, \tag{8}$$

and substitute them into (5). Thus we obtain for the free energy in this approximation

$$G^{(0)} = 2G_S\left[2^{3/2}\int_0^{\theta_{TP}}(\theta^4 + 2t\theta^2 + h^2)^{1/2} - 2\theta_{TP}^2\right]. \tag{9}$$

Multiplier 2 accounts for the two sides of TP. The last term in brackets (arising from the δ -term in (5)) describes the interaction of the order parameter with TP. The maximal value of order parameter on the TP

$$\theta_{TP}^2 = (1-t) + \left[(1-t)^2 - h^2\right]^{1/2},$$

is obtained by solving the quadratic equation for θ^2 . This equation is derived from (7) where $(d\theta/dx)^2$ is replaced by θ^2 using the boundary condition on the TP and the full Meissner effect condition $A = 0$. Integration of (8) gives for the distribution of order parameter and full thickness of the superconducting layer 2L the formulae

$$|x| = 2^{1/2}\int_{\theta(x)}^{\theta_{TP}} d\theta/(\theta^4 + 2t\theta^2 + h^2)^{1/2} < L, \tag{10}$$

$$2L = 2^{3/2}\int_0^{\theta_{TP}} d\theta/(\theta^4 + 2t\theta^2 + h^2)^{1/2}.$$

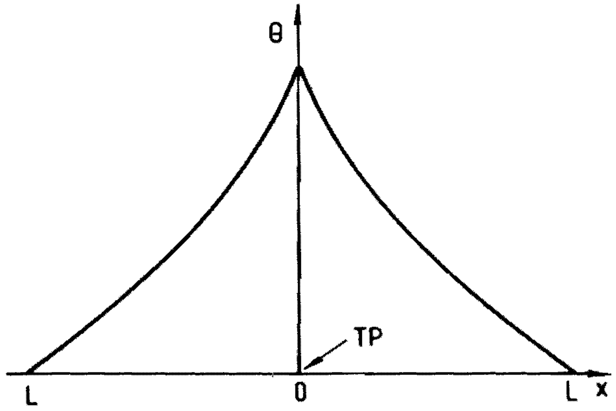

Fig. 1. The dimensionless order parameter as a function of $x =$ (distance to the TP) / (extrapolation length λ).

In fig. 1 shown is the solution to eq., $\theta(x)$, (10) for $t = 0$ $(T = T_c)$ and h near to the critical TPS field H_S at this temperature. Outside of the superconducting layer the magnetic field is equal to the external magnetic field

$$A(x) = \begin{cases} h(x-L), & x > L \\ 0, & -L < x < L \\ h(x+L), & x < -L. \end{cases} \tag{11}$$

For comparison and test, the known GL result for the surface tension can be obtained formally from formula (9) for the TPS free energy, if: 1) we omit the first multiplier 2, 2) omit the last term in brackets, 3) replace θ_{TP}^2 by the equilibrium bulk value of order parameter $\theta_B^2 = (-t)$, 4) replace the external magnetic field h by the thermodynamic critical field for the bulk metal $h_B = (-t)$, 5) perform an elementary integration. In this way, for α we obtain [4,5]

$$\alpha^{(0)} = 2^{5/2} G_S (-t)^{3/2}/3 = 1.89\,\xi(T) H_c^2(T)/8\pi. \tag{12}$$

But the surface tension contains a correction proportional to which is comparable with the basic term (12) practically for all type-I superconductors. Calculation of this correction is expounded in the next section.

4. The $\varkappa^{1/2}$ correction

Let us now investigate the distribution of the order parameter and the vector-potential near the superconducting-normal phase boundary. Solution of the GL equations (6) in this region, must be smoothly on the solutions (10,11) obtained in the $\varkappa=0$ approximation.

To obtain just the correction to the free energy, it is necessary near the boundary to substitute the solution of GL equations into functinnal (5), and to subtract from the obtained result the functional (5) value when into it as trial functions the $\varkappa=0$ solutions (10,11) are inserted.

Using $\varkappa$ as a small parameter is not possible when $\varkappa$ is the multiplier of the second derivative as in GL equations (6). Let us now introduce the variables

$$\tau = C_1(x-L), \quad \bar{\Psi} = 2^{1/2}\theta/B_1, \quad \bar{A} = A/B_1, \tag{13}$$

where

$$A_1 = 2^{1/4}\varkappa^{1/2}h^{3/2}, \quad B_1 = 2^{1/4}(\varkappa h)^{1/2}, \quad C_1 = 2^{-1/4}(h/\varkappa)^{1/2}.$$

In these variables the free energy functional (5) takes the form

$$G = A_1 G_S \int_{-\infty}^{+\infty} d\tau \Big[(d\bar{\Psi}/d\tau)^2 + (dA/d\tau - 1)^2 + \bar{A}^2\bar{\Psi}^2 + 2^{1/2} t(\varkappa/h)^2\bar{\Psi}^2 + (\varkappa h)^2\bar{\Psi}^4 + 2^{1/4}(\varkappa/h)^{1/2}\bar{\Psi}^2\delta(t - C_1 L)\Big]. \tag{14}$$

The coefficient A_1 already contains the first correction to G which is proportional to $\varkappa^{1/2}$. Therefore in the first approximation we will neglect in (14) all $\varkappa$-depending terms. In this approximation the free energy dependence on the temperature t and magnetic field h disappears. Also disappears the influence of the twinning plane on the phase boundary. In this manner we obtain the universal phase boundary functional

$$G = A_1 G_S \int_{-\infty}^{+\infty} d\tau \Big[(d\bar{\Psi}/d\tau)^2 + (d\bar{A}/d\tau - 1)^2 + \bar{A}^2\bar{\Psi}^2 \Big]. \tag{15}$$

The variation of (15) leads to the universal GL equations

$$d^2\bar{\Psi}/d\tau^2 = \bar{A}^2\bar{\Psi}, \quad d^2\bar{A}/d\tau = \bar{\Psi}^2\bar{A} \tag{16}$$

which should be solved numerically only once [4]. The boundary conditions will be obtained from the conditions of smooth joining with the solutions (10,11). Identifying (as $\varkappa\to 0$) the points $x = L+0$ and $\tau = +\infty$, we find

$$\bar{\Psi}(\infty) = 0, \quad d\bar{A}/d\tau\big|_{\tau=\infty} = 1. \tag{17a}$$

The first equation describes the disappearance of the superconducting order parameter just behind the phase boundary. The second one, simply fixes the external magnetic field value in the new variables (13). Analogical identification of the points $x = L - 0$ and $\tau = -\infty$ gives

$$d\bar{\Psi}/d\tau\big|_{\tau=-\infty} = -1, \quad \bar{A}(-\infty) = 0. \tag{17b}$$

The first equation gives the value of $\theta(x)$ derivative (10) in new variables, and the second one expresses the Meissner effect. Symmetry of the equations (16) and boundary conditions (17) leads to the expression of the order parameter through the vector-potential

$$\bar{\Psi}(\tau) = \bar{A}(-\tau) \tag{18}$$

and a simpler universal equation for the dimensionless vector-potential

$$d^2\bar{A}/d\tau^2 = \bar{A}^2(-\tau)\bar{A}(\tau). \tag{19}$$

The solution of this universal equation is shown in fig. 2. The equations (16) have an integral analogous to (7)

$$(d\bar{\Psi}/d\tau)^2 + (d\bar{A}/d\tau)^2 - \bar{A}^2\bar{\Psi}^2 = 1. \tag{20}$$

Let us express the $\bar{A}^2\bar{\Psi}^2$ from the above equation and substitute it into (15)

$$G = 2A_1 G_S \int_{-\infty}^{+\infty} d\tau \Big[(d\bar{\Psi}/d\tau)(d\bar{\Psi}/d\tau + 1) - (d\bar{A}/d\tau)(d\bar{A}/d\tau - 1) - d\bar{\Psi}/d\tau \Big].$$

The last term in brackets vanishes when from the functional of solutions of (16) we subtract the functional of the trial functions (10, 11). We take the $\bar{\Psi}$ from (18), substitute it into the above functional and obtain for the searched free-energy correction

$$\Delta G = -B^* \varkappa^{1/2} h^{3/2}, \tag{21}$$

here

$$\bar{B} = d\bar{A}/d\tau,$$

$$B^* = 2^{9/4} \int_{-\infty}^{+\infty} d\tau (1 - \bar{B})\bar{B} = 2.06.$$

The last equality is obtained by the numerical solution of (19). The simplest numerical method for solving the universal equation

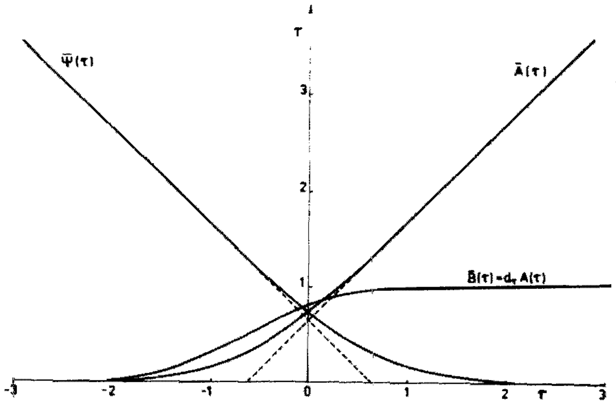

Fig. 2. The structure of the phase boundary between the superconducting and the normal phase. There is shown the dimensionless order parameter $\bar{\Psi}$, vector-potential $\bar{A}$, and magnetic field $\bar{B}$, as functions of the dimensionless distance to the phase boundary τ. Mention that the tunnelling of the superconducting order parameter in the normal phase and penetration of the vector-potential into the superconducting phase are symmetrical.

(19) consists of the following steps: the discretisation

$$(d^2\bar{A}/d\tau^2)_i = (\bar{A}_{i-1} - 2\bar{A}_i + A_{i+1})/d^2,$$

where

$$i = -N, \dots, +N, \qquad N \gg 1, \quad d \ll 1, \quad Nd \gg 1.$$

The choice for the initial approximation of a solution-like function, for example, for the $\varkappa = 0$ case,

$$\bar{A}_i = \begin{cases} 0, & i = -N, \dots, 0 \\ id, & i = 1, \dots, N \end{cases} .$$

Fixing of the boundary condition in the beginning of every iteration

$$\bar{A}_{-N} \leftarrow 0, \qquad \bar{A}_N \leftarrow \bar{A}_{N-1} + d$$

In cycle performing the appropriations

$$\bar{A}_i \leftarrow (\bar{A}_{i-1} + \bar{A}_{i+1})/(2 + d^2 \bar{A}_{-i}^2).$$

The index i sequentially runs over the values:

$$i = N-1, N-2, \dots, 2,$$

and after that in the backward direction

$$i = 2, 3, \dots, N-1.$$

Calculate the value of the integral (21) after a sufficient number of iterations.

Finally we obtain for the TPS free energy

$$G_{TPS} = 2(\xi_s H_s^2/8\pi)\Big[2^{3/2}\int_0^{\theta_{TP}} (\theta^4 + 2t\theta^2 + h^2)^{1/2} d\theta - \theta_{TP}^2 - B^* \varkappa^{1/2} h^{3/2} + O(\varkappa^{3/2})\Big]. \tag{22}$$

The phase diagram obtained by solving the equation $G_{TPS}(t, h) = 0$ is shown in fig. 3 (let us mention that for a normal metal $G = 0$).

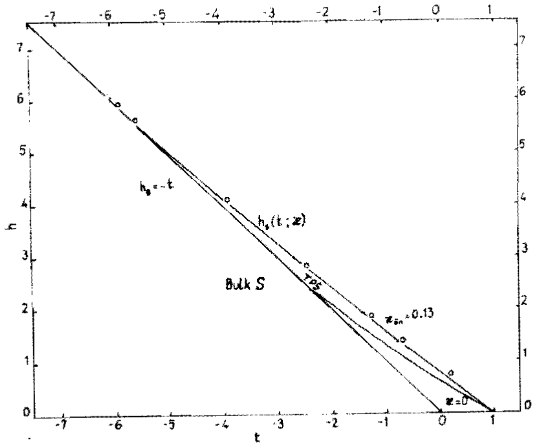

Fig. 3. Critical magnetical fields $h_s(t;\varkappa)$ (in dimensionless units) for type-I TPS. Experimental points are from paper [3]. There is shown the $\varkappa = 0$ case and bulk critical field $h_B(t) = -t$.

This phase diagram is identical with the experimental data [3] and the results of the numerical calculations by the finite-element method [6]. The diamagnetic moment (per unit TP area) can be easily obtained from (22) by ordinary differentiation

$$M = -(\partial G/\partial H)_T = -(\xi_s H_s/4\pi)\Big[2^{3/2}\int_0^{\theta_{TP}} d\theta/(\theta^4 + 2t\theta^2 + h^2)^{1/2} - 3B^*(\varkappa h)^{1/2} + O(\varkappa^{3/2})\Big]. \tag{23}$$

In the zero magnetic field the thermocapacity does not depend on the fundamental for TPS constant λ

$$C(T) = (4/T_c)(H_c^2(T=0)/8\pi)\,\xi(T) \propto 1/t^{1/2}.$$

This result is valid when $\xi(T)$ is much smaller than the specimen size, and of course when $T_c < T < T_{s1}$.

The next correction to the surface energy can be obtained when in the integrand in (14) the term linear in $\varkappa$ is taken into account. Thus we obtain for the surface tension:

$$\alpha(T) = (\xi(T) H_c^2(T)/8\pi)\left[A^* - \varkappa^{1/2}(B^* + \varkappa C^* + O(\varkappa^2))\right]. \qquad (24)$$

A formula useful for interpolation aims can be obtained if the coefficient $C^* = 0.26$ is determined by the well-known condition [5]

$$\alpha(\varkappa = 2^{-1/2}) = 0.$$

The dependence $\alpha(\varkappa)$ is shown in fig. 4.

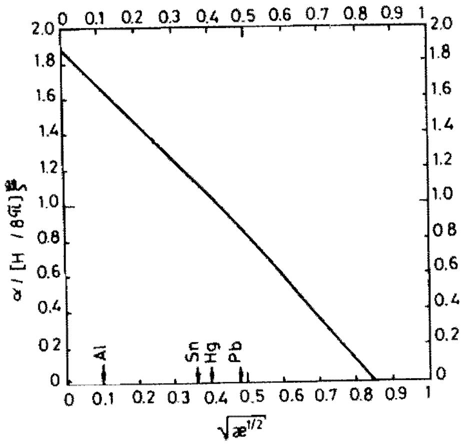

Fig. 4. The surface tension as a function of the GL parameter. Mention the satisfactory accuracy even only the first correction is proportional to the $\varkappa^{1/2}$.

5. Discussion

Historically, the theory of the surface tension is the first problem solved in the framework of the GL theory, it is an object of the classical GL paper [4]. Exact measurements of the TPS phase diagram [3] give a possibility of checking the theory with a per cent precision. Effects of nonlocality, the crystal anisotropy, and uncertainty in $\varkappa$ are effects of the same few per cent.

With the help of the solution of the universal equation it is possible to write the distribution of the magnetic field near the phase boundary as follows:

$$B_y(z) = H_y \bar{B}(z/w),$$

where w is the width of the phase boundary. For $H_y = H_c(T)$

$$w = \xi_s / C = 2^{1/4} \varkappa^{1/2} \xi(T).$$

The universal GL equations (16) are now better known as an Euclidian version of the Yang-Mills equations. These equations and similar ones are often used in the theory of dynamical systems [9-11]. If we associate the τ variable with the time, $\bar{\Psi}$ and $\bar{A}$ with coordinates, the solution of universal GL equations is an instanton connected with the color change. The constant B^* is proportional to the classical action of the instanton, and the G in (15) is the functional of action. The term $U = -\bar{\Psi}^2 \bar{A}^2$ in the integrand (15) has the meaning of a potential energy of a fictitious particle moving in the ($\bar{\Psi}$, $\bar{A}$) plane.

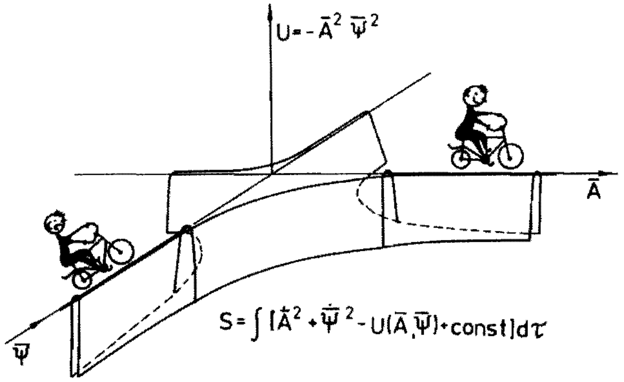

Fig. 5. The mechanical model for the universal GL equations (16) (see the text).

In fig. 5 shown is the trajectory of this particle in ($\bar{\Psi}$, $\bar{A}$, U) variables. The strong instability of the solution is obvious. By numerical calculations of domain walls, the indicated instability is removed if we take into account simultaneously both the boundary conditions at $\tau = \pm\infty$. The numerical method used in this paper for solving the universal equation of the phase boundary is realized on a pocket computer; while the numerical finite-element methods for solving the GL equation require nontrivial and difficult-to-reproduce calculations [6].

The $\varkappa=0$ TPS case is discussed in paper [8], but the phase diagram in this paper is incorrect. The exact solution presented in this paper does not satisfy the differential equation. Wrong is also in this paper the formula for the critical temperature of a TP superlattice. The correct phase diagram (for $\varkappa=0$ case) is given graphically in paper [3], but there is not given the derivation of the system of equations from which it is obtained.

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Мишонов Т.М. E17-88-413

К теории поверхностного натяжения сверхпроводников первого рода и сверхпроводимости плоскости двойникования

Найдена поправка к поверхностному натяжению сверхпроводников первого рода, которая пропорциональна квадратным корням параметра Гинзбурга - Ландау κ . Эта поправка является существенной для получения фазовой диаграммы и других термодинамических переменных для узкого сверхпроводящего слоя вблизи плоскости двойникования в некоторых металлах.

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To the Theory of Type-I Superconductors Surface Tension and Twinning-Plane-Superconductivity

A correction is found to the surface tension in type-I superconductors which is proportional to the square root of the Ginsburg - Landau parameter κ . This correction is essential for obtaining the phase diagram and other thermodynamical variables of the narrow superconducting layer arising near the twinning plane in some metals.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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