# QUANTUM AND CLASSICAL MOTION OF DISLOCATIONS IN A PEIERLS POTENTIAL RELIEF

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A string located in a periodic potential relief and acted on by a constant external force is considered. The probabilities of transition of the string from one potential relief valley to a neighboring one are computed. At low temperatures such transitions are of the quantum tunneling type. The results obtained are used to estimate the velocities of the dislocations.

## 1. INTRODUCTION

As is well known, the motion of dislocations in crystals with high Peierls barriers takes place through the formation and subsequent expansion of double kinks. At high temperatures this phenomenon is due to thermal fluctuations. It is clear that, in principle, at sufficiently low temperatures the thermal fluctuations are replaced by quantum fluctuations, the probability of which is temperature-independent. This circumstance was first pointed out apparently by Weertman[1]. The model he adopted had, however, little in common with the original formulation of the problem.

The simplest model of a dislocation is the so-called string model. Although the properties of this model have been discussed for quite a long time, no systematic computations of the probability of an elementary event of formation of a double kink have thus far been done in the framework of this model The difficulty of this problem lies in the fact that it is necessary to consider the motion of a system with an infinite number of degrees of freedom. We carry out in the present paper such a systematic computation in the framework of the string model, at least in certain limiting cases.

We consider an elastic string in a two-dimensional potential relief $U(y)$ (Fig. 1a) made up of a periodic potential (Peierls potential) and a linear term, $Fy$, due to an external stress $F$. It is assumed that the string is initially at rest at the bottom of one of the relief valleys ($y = 0$) in an equilibrium configuration for $F = 0$. The inclusion of the external force makes this equilibrium configuration metastable. Owing to thermal or quantum fluctuations, the string makes a transition to a neighboring valley $y = b$. The problem is to compute the transition probability per unit time, or the inverse quantity—the transition time. The configuration of the string is described by the function $y(x, t)$, where $x$ is the coordinate along the bottom of the valley, $y$ is the transverse coordinate, and $t$ is the time. The Hamiltonian of the string is written in the usual form:

$$H = T + V,$$
$$T = \frac{\rho}{2}\int\left(\frac{\partial y}{\partial t}\right)^2 dx, \quad V = \int\left[\frac{\varkappa}{2}\left(\frac{\partial y}{\partial x}\right)^2 + U(y)\right]dx. \qquad (1)$$

Here $\rho$ is the linear density and $\varkappa$ is the rigidity of the string. Since we are interested in only the transition between two valleys, we can forget about the existence of all other minima, and consider, instead of the original periodic potential, the potential $U_0(y)$ with two minima shown in Fig. 1b.

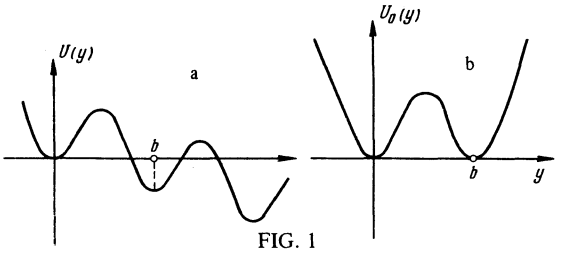

FIG. 1

The problem consists, in principle, in finding the most probable route of transition from the metastable equilibrium configuration $y = 0$ to the stable equilibrium configuration $y = b$. We have in mind a trajectory in a multidimensional space whose points (vectors) represent the configurations of the string $y = y(x)$.

The problem admits of an explicit solution in two limiting cases: low stresses and those close to the Peierls stress. The Peierls stress $F_p$ is defined as the maximum of the derivative $U_0'(y)$. At stresses higher than $F_p$, the maxima and minima in the potential $U(y)$ disappear. In the first case $F \ll F_p$, as is shown in Sec. 2, a narrow steep-walled trough leading from the "point" $y(x) = 0$ through a saddle point to the "point" $y(x) = b$ exists in the potential relief $V$ in the multidimensional space of $y(x)$. Therefore, in both the classical and quantum cases, the transition trajectories of interest lie almost along the bottom of the trough. This makes it possible to reduce the problem to a one-dimensional problem.

Thus, this is yet another case, when the problem of subbarrier tunneling in a multidimensional system admits of an asymptotically exact solution. Our paper is closest in spirit to the paper by Iordanskiĭ and Finkel'shteĭn[2]. Its success was due to the fact that the line of steepest descent turned out in the adopted model to be a straight line (in the multidimensional space). Therefore, the "classical" trajectory coincides in this case with the line of steepest descent. In our case, the "classical" trajectory is close, but not coincident with the line of steepest descent, and it is not a straight line. The situation here is similar to the classical problem with almost separable variables, when the

motion can be considered as slow along one of the coordinates (along the bottom of the trough), and fast along the transverse coordinates. The solution of the quantum problem is analogous in result to I. Lifshitz and Yu. Kagan's work[3] on the quantum production of of the nucleus of a new phase. In our case the role of different phases is played by the sections of the string which are in different valleys. Such an approach to the problem of thermal transition of dislocations was developed in[4,5].

At stresses close to $F_p$, the determination of the classical trajectory reduces to the solution of a standard problem, and this makes it possible to find the dependence on the parameters and estimate the numerical constants. This problem is analogous to the problem of tunneling in a quantum liquid near the lability point[3].

We also solve in the present paper the classical problem of diffusion of the string for small F and for F close to $F_p$. A short report on the results of the work described here was published somewhat earlier[6].

## 2. THE POTENTIAL RELIEF FOR SMALL STRESSES

Let us consider the potential energy V in the space whose points are the functions y(x) describing the configuration of the string. We already know that the potential V has two minima at the points y(x) = 0 and y(x) = b. Between these two minima is the saddle point $y_0(x)$ defined by the equation

$$\delta V / \delta y(x) = 0. \tag{2}$$

Using the expression (1) for V, we reduce the equation for the saddle point to the following form:

$$-\varkappa \partial^2 y_0 / \partial x^2 + U'(y_0) = 0. \tag{3}$$

Equation (3) admits of a simple mechanical analogy in which U plays the role of a potential and x plays the role of time in Newton's equation. The "particle" leaves the top of the potential hump (at $x \to -\infty$), is reflected at the point of closest approach to the second hump, and returns to the initial position at $x \to +\infty$. To such mechanical motion corresponds the form of the kink shown in Fig. 2. At small stresses the heights of the potential humps differ from each other by a small amount Fb. Therefore the "particle" approaches the turning point with a small "velocity" and spends a long "time" there. This corresponds to a large length $l_c$ of the critical double kink which is equal to

$$l_c = \sqrt{\varkappa / U_0''} \ln (bU_0'' / 2F). \tag{4}$$

The formula (4) is valid with a logarithmic accuracy and $U_0''$ is computed at the point y = 0.

Of special interest is the case F = 0. In this case Eq. (3) determines the point of relative minimum of $y_1(x)$, which satisfies the conditions $y_1(x) \to 0$ for $x \to -\infty$, and $y_1(x) \to b$ for $x \to +\infty$. Clearly, $y_1(x)$ depends only on the specific form of the Peierls barrier $U_0(y)$. We shall henceforth assume that $U_0(y)$ is symmetric about the point b/2. Then $y_1(x)$ is antisymmetric about this point. Evidently, at small F and, consequently, large $l_c$, the double kink $y_0(x)$ can behave as if it consisted of two isolated kinks

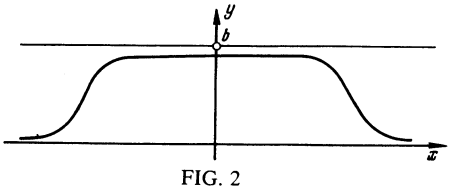

FIG. 2

$$y_0(x) = y_1(x + {}^1/_2 l_c) - y_1(x - {}^1/_2 l_c). \tag{5}$$

Naturally, Eq. (3) is invariant with respect to an arbitrary displacement along the x axis. The magnitude of the potential energy at the saddle point $V_0$ is equal to

$$V_0 = 2V_1 - Fbl_c, \tag{6}$$

where $V_1$ is the energy of an isolated kink. The quantity $V_1$ has been computed by Guyot and Dorn[7] for some concrete forms of the potential.

From the saddle point to the minima runs the trough, which it is natural to define in the following manner. Let y(x, s) be a one-parameter family of vectors that define the bottom of the trough (s is a parameter denoting a point on the bottom of the trough). Then when y changes in the direction perpendicular to the bottom of the trough the potential energy should increase. Let the change in y(x) be equal to $\delta y(x)$. The vector tangential to the bottom of the trough is collinear to $\delta y(x, s)/\partial s$. The condition of orthogonality of $\delta y(x)$ to the tangent vector has the form

$$\int \delta y(x) \frac{\partial y(x, s)}{\partial s} dx = 0. \tag{7}$$

Let us now write down the condition for minimum of the potential energy $V\{y\}$ at the point y(x, s) for displacements satisfying the additional condition (7):

$$\delta V / \delta y - \lambda \partial y / \partial s = 0. \tag{8}$$

This is an equation defining the bottom of the trough. For our concrete choice of V (formula (1)) Eq. (8) takes the form

$$-\varkappa \frac{\partial^2 y}{\partial x^2} + U'(y) - \lambda \frac{\partial y}{\partial s} = 0. \tag{9}$$

Here, $\lambda$ is an arbitrary function of the perpendicular s, which is connected with the possibility of an arbitrary choice of the parameter s itself. We shall assume that at the saddle point s = 0 and $\lambda(0) = 0$, and, moreover, $\lambda$ vanishes at the minimum points.

In the vicinity of the bottom of the trough $V\{y\}$ has the following form:

$$V\{y(x, s) + \delta y\} \approx V(s) + \frac{1}{2} \int \frac{\delta^2 V}{\delta y(x) \delta y(x')} \delta y(x) \delta y(x') dx\, dx'. \tag{10}$$

It is assumed in formula (10) that the displacements $\delta y(x)$ are perpendicular to the bottom of the trough. The separation into coordinates along and perpendicular to the bottom of the trough carried out here makes sense in that one of the motions—along the bottom of the trough—turns out to be slow, whereas the motions perpendicular to the bottom of the trough turn out to be fast. To verify that, let us first consider the vicinity of the saddle point. We have for small s

$$y(x, s) \approx y(x, 0) + \frac{\partial y(x, 0)}{\partial s} s \equiv y_0(x) + \frac{\partial y}{\partial s} s. \tag{11}$$

Substituting (11) into (9) and taking Eq. (3) for $y_0(x)$ into account, we obtain correct to linear terms in s

$$-\varkappa\frac{\partial^2}{\partial x^2}\frac{\partial y}{\partial s}+U''(y_0)\frac{\partial y}{\partial s}-\frac{\partial\lambda}{\partial s}\frac{\partial y}{\partial s}=0. \quad (12)$$

Thus, it turned out that $\partial y/\partial s$ is the solution of the Schrödinger equation with the potential $U_0''(y_0(x))$, and $\partial\lambda/\partial s$ is the eigenvalue.

Differentiating Eq. (3) with respect to x, we easily verify that $\partial y_0/\partial x$ also satisfies the Schrödinger equation with zero eigenvalue

$$-\varkappa\frac{\partial^2}{\partial x^2}\frac{\partial y_0}{\partial x}+U''(y_0)\frac{\partial y_0}{\partial x}=0. \quad (13)$$

This is a different expression of the fact that the Hamiltonian in Eq. (3) is invariant with respect to displacement along the x axis. This remains true in the absence of stresses, and the function $\partial y_1/\partial x$ also satisfies the Schrödinger equation

$$-\varkappa\frac{\partial^2}{\partial x^2}\frac{\partial y_1}{\partial x}+U''(y_1)\frac{\partial y_1}{\partial x}=0. \quad (14)$$

Let us now consider an arbitrary small displacement $\delta y(x)$ relative to the saddle point. The potential energy V near the saddle point can be represented in the quadratic form

$$V\approx V_0+\frac{1}{2}\int\frac{\delta^2V}{\delta y(x)\delta y(x')}\delta y(x)\delta y(x')\,dx\,dx'. \quad (15)$$

The quadratic form can be reduced to the diagonal form by some orthogonal transformation. Its eigenvalues $\mu_n$ and eigenvectors $\varphi_n$ are determined by the equation

$$\int\frac{\delta^2V}{\delta y(x)\delta y(x')}\varphi_n(x')\,dx'=\mu_n\varphi_n(x), \quad (16)$$

or for our concrete choice of V:

$$-\varkappa\partial^2\varphi_n/\partial x^2+U''(y_0)\varphi_n=\mu_n\varphi_n. \quad (17)$$

We already know that this equation has a zero eigenvalue with $\partial y_0/\partial x$ as the corresponding eigenfunction (see formula (13)). We show that this equation has a negative eigenvalue $\mu_0\sim -F$, while all the other eigenvalues are positive and weakly dependent on F.

By comparing Figs. 1b and 2, we can verify that the potential $U''(y_0(x))$ represents two wells separated by the distance $l_c$, as shown in Fig. 3. At infinity and in the space between the wells the potential is equal to the positive quantity $U_0''(0)$. For small F the wells have almost the standard form, which is the form obtained for the single kink $U_0''(y_1)$. It is known that in each of such wells, the lowest level is the $\mu = 0$ level. This level splits into two; to one of them corresponds, as before, $\mu = 0$. We can, however, verify that this level is not the ground level since the wave function corresponding to it is odd and has a node. Whence it follows that to the ground state corresponds the negative level $\mu_0$, whose value is determined by the usual overlap integral:

$$\mu_0\sim-\exp\left\{-\int\sqrt{\varkappa^{-1}U''(y_0(x))}\,dx\right\}\sim-\text{const}\cdot F. \quad (18)$$

All the other eigenvalues are obtained by means of a weak splitting of the discrete and continuous eigenvalues pertaining to one well and, therefore, separated from the ground level by a finite interval $\sim U_0''$.

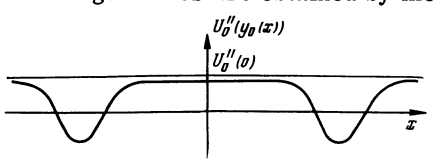

FIG. 3

Only the negative eigenvalue $\mu_0$ can correspond to the direction of steepest descent. Indeed, according to Eq. (8),

$$\lambda(s)=\frac{1}{N}\frac{dV(s)}{ds},\quad N=\int\left(\frac{\partial y}{\partial s}\right)^2dx. \quad (19)$$

The normalization integral N can be made equal to unity by a proper choice of the parameter s. Then $\lambda(s) = \mu_0 s$, and

$$V(s)=V_0+{}^1/_2\mu_0s^2. \quad (20)$$

Let us now consider the nonzero values of s. For $s > 0$ it is clear from physical considerations that $y(x, s)$ has the same form as $y_0(x)$, but the distance $l(s)$ between the single kinks is greater than $l_c$. For $s < 0$ the distance between the kinks decreases. We shall, however, consider only that region in which $l$ is still much larger than the length $l_1$ of a single kink. We can introduce in the whole of this space the parameter $l$—the distance between the kinks—instead of the parameter s. The solution of Eq. (8) can be approximately written in the form

$$y(x, l)=y_1(x+{}^1/_2l)-y_1(x-{}^1/_2l). \quad (21)$$

The tangent to the bottom of the trough is in this approximation

$$\frac{\partial y}{\partial l}=\frac{1}{2}\left[\frac{\partial y_1}{\partial x}\left(x+\frac{l}{2}\right)+\frac{\partial y_1}{\partial x}\left(x-\frac{l}{2}\right)\right]. \quad (22)$$

The diagonalization of the quadratic form (10) at an arbitrary point of the trough leads to the Schrödinger equation of the form (17) in which, however, $U''(y(x, l))$ serves as the potential. Considerations similar to those presented above show that this equation has the eigenvalue $\mu_1 = 0$, to which corresponds the eigenfunction $\partial y(x, l)/\partial x$, which is orthogonal to $\partial y/\partial l$. This solution corresponds, however, to the cyclic coordinate denoting displacement of the double kink as a whole along the x axis. The remaining solutions of the Schrödinger equation correspond to the split nonzero levels of the problem with one well ($F = 0$). Therefore, they are orthogonal to $\partial y/\partial l$ in that approximation in which the formula (22) is true. Thus, we have shown that for $s \neq 0$ the frequencies of the transverse motions do not depend on F and are equal to $\sqrt{aU_0''/m}$ in order of magnitude.

The assertion that the eigenvalues corresponding to the transverse and longitudinal motions are different becomes incorrect for $l$ of the order of the width of a single kink.

Let us compute $V(l)$. To do this we substitute in the expression for $V\{y\}$ (formula (1)) $y(x, l)$ in the form (21). We obtain

$$V(l)=2V_1-Fbl-{}^1/_2b^2\sqrt{U_0''\varkappa}\exp\{-\sqrt{U_0''/\varkappa}l\}. \quad (23)$$

The graph of $V(l)$ is shown in Fig. 4.

The first two terms of Eq. (23) correspond to the macroscopic approach. The first one corresponds to the energy of the boundaries between the phases; the second, to the linear energy of the new phase. In the one-dimensional case a purely macroscopic approach leads to the absurd conclusion that the curve $V(l)$ has

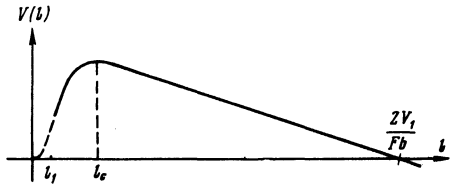


FIG. 4

no maximum, i.e., that no critical dimension exists for a nucleus. The third term in (23) corresponds to a long-range attraction between the single kinks. We can likewise take into account other forms of interaction, e.g., a Coulomb-type attraction between the kinks, an interaction which follows from the theory of elasticity. It leads to the addition of the term $\alpha/l$ to $V(l)$. Such an interaction has been considered in[4,5].

Expression (23) loses meaning at small $l$. If we formally introduce the parameter $l$, for example, as

$$l=\frac{1}{b}\int y(x,s)\,dx, \tag{24}$$

then, as $l \to 0$, $V(l)$ vanishes as well.

Let us note the following circumstance. The equation (9) of the bottom of the trough is a modified time-dependent Ginzburg-Landau equation. The similarity becomes even more striking if we choose $U_0(y)$ in the form of a polynomial of the fourth degree in y and introduce the variable $\tau$ connected with s by the relation $d\tau = ds/\lambda(s)$. In contrast to the usual Ginzburg-Landau equation, if we discard the time derivative, the equation contains a coordinate-independent term F. The analysis of the equation of the bottom of the trough may also be regarded as proof of the fact that the real solution to the modified Ginzburg-Landau equation is of the nature of a double kink.

## 3. TUNNELING PROBABILITY

The transition probability is given by the well-known Feynman formula[8]:

$$w=\Big|\sum \exp\{iS/\hbar\}\Big|^2, \tag{25}$$

where S is the action computed along the trajectories originating from the point y = 0 and ending at the point y = b. The summation is over all the trajectories. In the quasi-classical limit we select from the sum the trajectories along which the action is stationary:

$$\delta S = 0.$$

In this sense the trajectories can be called classical, although no real trajectory of a classical "particle" satisfies the imposed boundary conditions (the law of conservation of energy is violated). In the stationary formulation of the problem we are forced to deal with an imaginary action. We must choose from all the classical trajectories originating from the point y = 0 only that trajectory which gives a minimum imaginary part of the action. Furthermore, instead of the condition y = b at the end point, it is sufficient to require that the energy at the end point of the trajectory be equal to the initial value. After the transition the string will tend to slide down to the position y = b of minimum energy. We shall not consider the energy-transfer mechanism, assuming that the string spends the major part of the time in overcoming the barrier.

Let us consider the classical trajectories in the vicinity of the bottom of the trough. The Hamilton-Jacobi equation has the form

$$\frac{\rho}{2}\int\left(\frac{\delta S}{\delta y(x)}\right)^2 dx + V\{y\} = E. \tag{26}$$

We can locally separate the coordinate $l$ along the bottom from the transverse coordinates $\eta_n$.

Going over to the coordinates $l$ and $\eta$, we obtain

$$\frac{1}{2M}\left(\frac{\partial S}{\partial l}\right)^2+\frac{1}{2m}\sum\left(\frac{\partial S}{\partial \eta_n}\right)^2+V(s)+\sum\frac{\mu_n}{2}\eta_n^2=E. \tag{27}$$

Here, m is the mass of the "atom" ($m = \rho a$). The mass M corresponding to the longitudinal motion can be determined from the expression (1) for the kinetic energy for the longitudinal motion:

$$T=\frac{\rho}{2}\int\left(\frac{\partial y}{\partial l}\right)^2 dx\left(\frac{dl}{dt}\right)^2=\frac{M}{2}\dot{l}^2. \tag{28}$$

We find from (28)

$$M=\rho\int\left(\frac{\partial y}{\partial l}\right)^2 dx. \tag{29}$$

Substituting (21) into (29), we obtain

$$M\approx\frac{\rho}{2}\int\left(\frac{\partial y_1}{\partial x}\right)^2 dx. \tag{30}$$

The mass M corresponding to the longitudinal motion is equal in order of magnitude to

$$M\sim \rho b^2/2l_1 \sim mb/2l_1,$$

where $l_1$ is the length of a single kink.

The variables are approximately separable, so that we can write

$$S=S_0(l)+\sum S_n(\eta_n). \tag{31}$$

we obtain from this in the usual manner the conserved adiabatic invariants $I_n$ for the transverse motions and the equation of the one-dimensional longitudinal motion

$$\frac{1}{2M}\left(\frac{dS_0}{dl}\right)^2+V(l)=E_0. \tag{32}$$

The location of the minimum y = 0 corresponds to $V(l) = 0$ and $dS_0/dl = 0$. Therefore in equation (32) $E_0 = 0$ and

$$S_0=i\int\sqrt{2MV(l)}\,dl. \tag{33}$$

Formula (23) may be used in the integration over $l$. The situation, however, becomes simplified if we take into account the fact that $V(l)$ increases from zero to $2V_1$ in the interval

$$\Delta l\sim l_c\sim\sqrt{\varkappa/U_0''}\ln(bU_0''/F)$$

and then decreases linearly to zero in the interval

$$\Delta l\sim 2V_1/Fb.$$

The important contribution to the integration is given by only the second interval in which we can replace $V(l)$ by the linear function $2V_1 - Fbl$. Whence

$$S_0=i\frac{2}{3}\sqrt{2M}\frac{(2V_1)^{3/2}}{Fb}. \tag{34}$$

The transition probability, apart from a pre-exponential factor, is equal to

$$w\sim\exp\{2iS_0/\hbar\}=\exp\{-{}^{16}/_3 M^{1/2}V_1^{3/2}/\hbar Fb\}. \tag{35}$$

It is characteristic of tunneling that the entire $V(l)$ curve, and not only the vicinity of the saddle point $l_c$, is important for the computation of the probability.

Clearly, quantum tunneling begins to play a significant role below that temperature at which the probability of quantum tunneling is equal to the probability of thermal activation $w_T \sim \exp\{-V_0/T\}$. There exists, however, some temperature range in which a complex process is most probable: first thermal activation occurs with a change E in the energy, followed by tunneling. The probability of such a process is proportional to the product of exponential functions

$$w \sim w_T w_q \sim \exp\left\{-\frac{E}{T}-\frac{2^{5/2}}{3}\frac{M^{1/2}}{\hbar F b}(2V_1-E)^{3/2}\right\}. \quad (36)$$

The most probable value of E is

$$E(T) = 2V_1 - {}^1/_8 F^2 b^2 \hbar^2 / MT^2. \quad (37)$$

It is clear from the expression (37) that tunneling with preliminary activation is realized only at temperatures

$$T > T_0 = {}^1/_4 Fb\hbar / \sqrt{MV_1}. \quad (38)$$

In this temperature range the transition probability is expressible in the following manner:

$$w \sim \exp\left\{-\frac{2V_1}{T}+\frac{1}{24}\frac{\hbar^2F^2b^2}{MT^3}\right\}. \quad (39)$$

Formula (35) is valid at temperatures $T < T_0$, and the transition probability is temperature-independent (with exponential accuracy).

Let us estimate the order of magnitude of $|\ln w|$. To do this we use Guyot and Dorn's calculation[7] for the quantity $V_1$ and determine the orders of magnitude of $\kappa \sim Ga^2$ and $\rho \sim m/a$ (G is the shear modulus):

$$|\ln w| \approx \frac{a}{\hbar}\sqrt{Ga^3m}\frac{F_p}{F}. \quad (40)$$

The factor standing before the ratio $F_p/F$ characterizes the magnitude of the zero-point oscillations. It is clear from this that the quantum effects should be searched for in substances in which the amplitude of the zero-point oscillations is not too small. We must in the first place point out crystals of the inert elements, as well as of hydrogen, deuterium, and methane.

## 4. TUNNELING AT STRESSES CLOSE TO THE PEIERLS STRESS

At stresses F close to $F_p$, the potential relief does not have a pronounce trough, and the classical problem cannot be solved by the method developed in Secs. 2 and 3. In this case we can use the fact that the maximum and minimum of the potential U(y) converge (see Fig. 5), and in the region of y of interest to us the Peierls potential U(y) can be approximated by a cubic polynomial

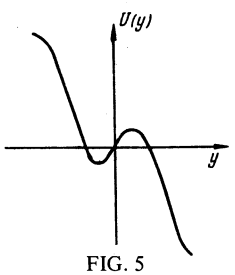

FIG. 5

$$U(y) = \alpha y - \beta y^3, \quad (41)$$

where $\alpha = F_p - F$, $\beta = {}^1/_6|U'''(0)|$ (the derivative is evaluated at the saddle point of $U_0(y)$).

The Hamilton-Jacobi equation has the following form:

$$\int\left[\frac{1}{2\rho}\left(\frac{\delta S}{\delta y}\right)^2+\frac{\kappa}{2}\left(\frac{\partial y}{\partial x}\right)^2+U(y)+\frac{2}{3\sqrt{3}}\frac{\alpha^{3/2}}{\beta^{1/2}}\right]dx = E. \quad (42)$$

In the case under consideration E = 0.

Let us go over to the variables $\sigma$, $\eta$, and $\xi$ connected with S, y, and x by the relations

$$S = i\frac{\alpha}{\beta}\sqrt{\kappa\rho}\,\sigma \equiv iS_0\sigma, \quad y = \sqrt{\frac{\alpha}{\beta}}\eta, \quad x = \frac{\kappa^{1/2}}{\alpha^{1/2}\beta^{1/4}}\xi. \quad (43)$$

In terms of these variables the Hamilton-Jacobi equation (42) takes the standard form:

$$-\frac{1}{2}\int\left(\frac{\delta\sigma}{\delta\eta}\right)^2 d\xi+\int\left[\frac{1}{2}\left(\frac{\partial\eta}{\partial\xi}\right)^2+\eta-\eta^3+\frac{2}{3\sqrt{3}}\right]d\xi = 0. \quad (44)$$

To the optimal classical trajectory corresponds a certain value $\sigma_0$ which does not depend on the parameters. The transition probability is expressed in terms of $\sigma_0$ and the parameters of the problem by the formula

$$w \sim \exp\{-2\sigma_0\alpha\sqrt{\kappa\rho}/\hbar\beta\}. \quad (45)$$

The order of magnitude of $|\ln w|$ can be estimated after finding $\sigma_0$ from the solution of the variational problem. It turns out that $\sigma_0 \leq 5$. Whence

$$|\ln w| \sim 10\frac{a\sqrt{Ga^3m}}{\hbar}\frac{F_p-F}{F}. \quad (46)$$

Let us ascertain how w varies at nonzero temperatures. As in the preceding section, we shall assume that the tunneling is preceded by thermal fluctuation which imparts an energy E to the string. Then the tunneling takes place along the trajectory defined by the Hamilton-Jacobi equation (46) with $E \neq 0$. We may go over to a dimensionless variable $\epsilon$ connected with E by the relation

$$E = E_0\varepsilon = \kappa^{1/2}\alpha^{5/4}\beta^{-3/4}\varepsilon. \quad (47)$$

Equation (42) goes over to (44) with one alteration: on the right hand side of (44) will appear $\epsilon$.

Let us define, as before, the saddle point $\eta_0$ by the condition

$$\frac{1}{E_0}\frac{\delta V}{\delta\eta} = -\frac{\partial^2\eta_0}{\partial\xi^2} - 1 + 3\eta_0^2 = 0. \quad (48)$$

We denote the corresponding value $V_0/E_0 = {}^1/_5 \times 2^{7/2} \times 3^{1/4}$ by $\epsilon_0$.

A schematic plot of the function $\sigma(\epsilon)$ is shown in Fig. 6. As before, the transition probability is defined as the product of the activation and tunneling probabilities

$$w \sim \exp\{-\varepsilon E_0/T - 2S_0\sigma(\varepsilon)/\hbar\}. \quad (49)$$

Minimization of the exponent leads to the equation

$$\sigma'(\varepsilon) = -\hbar E_0/2TS_0. \quad (50)$$

Clearly, the solution of Eq. (50) exists in the temperature range

$$T < T_1 = E_0\hbar/2S_0|\sigma'(\varepsilon_0)|.$$

In computing $\sigma(\epsilon)$ for $\epsilon \to \epsilon_0$ we can restrict ourselves to the quadratic neighborhood of the saddle point. The variables in the classical problem are in this case separable, and the motion along the direction of

steepest descent $\eta_0$, which has an imaginary action, is real. $\sigma(\epsilon)$ is easily computed

$$\sigma(\varepsilon)=\int \sqrt{2[V(\eta_0)-\varepsilon]}\,d\eta_0=\frac{\pi}{\sqrt{|\mu_0|}}(\varepsilon_0-\varepsilon).$$

Whence

$$T_1=\frac{\sqrt{|\mu_0|}\,\hbar E_0}{2\pi S_0}=\frac{1}{\pi}\sqrt{\frac{5}{8}}\,\frac{\hbar}{\sqrt{\rho}}\sqrt[4]{\frac{|U_0'''|}{2}(F_p-F)}.$$

At temperatures $T > T_1$ formula (49) goes over to the usual activation function

$$w \sim \exp\{-\varepsilon_0 E_0/T\}. \quad (51)$$

## 5. TRANSITION PROBABILITY AT HIGH TEMPERATURES

We shall investigate here in greater detail the high-temperature region. In particular, we shall determine the dependence on the stress F of the pre-exponential factor in w for the two limiting cases considered above.

The transition is realized at high temperatures owing to thermal fluctuations of the atoms, which lead to diffusion in the configuration space of the string. If in this case the dimension of the thermal fluctuations (e.g., the phonon wavelength) is much smaller than the characteristic dimensions of the configurations (e.g., the length $l_1$ of a single kink), then we can use the concept of diffusion of a chain of connected atoms.

Let us write down the continuity equation for the distribution function $f(y_i)$

$$\frac{\partial f}{\partial t}+\sum_i\frac{\partial J_i}{\partial y_i}=0, \quad (52)$$

where the $y_i$'s are the coordinates of the atoms of the chain, and the components $J_i$ of the current density are equal to

$$J_i=-D\frac{\partial f}{\partial y_i}-\frac{D}{T}\frac{\partial V}{\partial y_i}f \quad (53)$$

(D is the diffusion coefficient).

To determine the transition probability at small F, we use the data obtained in Sec. 2 on the potential relief. In the vicinity of the bottom of the trough, $V\{y\}$ is made up of V(s) and a quadratic form in the transverse coordinates $\eta_n$:

$$V=V(s)+\frac{1}{2}\sum\mu_n\eta_n^2. \quad (54)$$

The variables in Eq. (52) are separable, and the solution can be obtained in the form

$$f(s,\eta_n,t)=\varphi(s,t)\exp\left\{-\sum\frac{\mu_n}{2T}\eta_n^2\right\}, \quad (55)$$

$\varphi(s, t)$ satisfying the one-dimensional diffusion equation

$$\frac{\partial\varphi}{\partial t}=D\frac{\partial^2\varphi}{\partial s^2}+\frac{D}{T}\frac{\partial}{\partial s}\left(\frac{\partial V}{\partial s}\varphi\right). \quad (56)$$

We shall assume that $f(s, \eta, t)$ goes over to the equilibrium function $Z_0^{-1}\exp\{-E(s,\eta)/T\}$ at sufficiently large negative s ($Z_0$ is a normalization factor).

It is easy in the quasistationary approximation to solve Eq. (56) and find the current density $J_s$:

$$J_s=\frac{D}{Z_0}\exp\left\{-\sum\frac{\mu_n}{2T}\eta_n^2\right\}\Big/\int\exp\left\{\frac{V(s)}{T}\right\}ds. \quad (57)$$

In order to determine the total current, we should integrate over all the transverse coordinates. The integration over $\eta_n$ yields the factor

$$Z_1=\prod_{n=2}^{\infty}\sqrt{2\pi T/a\mu_n}.$$

The ratio $Z_1/Z_0$ can be computed if a specific model of the potential $U_0(y)$ is assumed. The order of magnitude of the ratio can be estimated without recourse to a model: $Z_1/Z_0 \sim aU_0''/T$. It is also necessary to integrate over the coordinate $\eta_1$ corresponding to the translation of the double kink as a whole along the x axis. It is convenient to change simultaneously to integration over x instead of $\eta_1$, and $l$ instead of s in the denominator of (57). Integration over x amounts to multiplication by L, the length of the string. Then the current I is equal to

$$I\sim\frac{DaU_0''}{T}L\Big/\int\exp\left\{\frac{V(l)}{T}\right\}dl. \quad (58)$$

Evaluating the integral with $V(l)$ from (23), we obtain

$$I\sim\frac{Da(U_0'')^{3/2}}{T\varkappa^{1/2}}Le^{-V_0/T}\frac{e^{-\gamma}\gamma^{\gamma}}{\Gamma(\gamma)},\qquad \gamma=\frac{Fb}{T}\sqrt{\frac{\varkappa}{U_0''}}. \quad (59)$$

The probability of production of a double kink is, for small $\gamma$, directly proportional to the stress, as has already been established[4,5],

$$I\sim DU_0''T^{-2}Fa^2Le^{-V_0/T}. \quad (60)$$

At large $\gamma$

$$I\sim\frac{Da^{3/2}(U_0'')^{5/4}}{T^{3/2}\varkappa^{1/4}}F^{1/2}Le^{-V_0/T}. \quad (61)$$

It is sufficient for the derivation of the last result and the computation of the transition probability at even higher stresses to know only the vicinity of the saddle point in the potential relief. The problem of the growth of a nucleating center has been considered by many authors in such a formulation, and the corresponding methods of computation have been well developed (see, for example, Langer[9]).

The expression for the current is obtained in the same way as (53):

$$I=\frac{D}{Z_0}\sqrt{\frac{\mu_1}{2\pi T}}\prod_{n=2}^{\infty}\sqrt{\frac{2\pi T}{\mu_n}}e^{-V_0/T}\mathcal{L},$$

$$\mathcal{L}=L\left\{\int\left(\frac{\partial y_0}{\partial x}\right)^2\frac{dx}{a}\right\}^{1/2}. \quad (62)$$

The factor $\mathcal{L}$ appeared as a result of the integration over the coordinate corresponding to the displacements of the configuration at the saddle point $y_0(x)$ along the x axis. A small shift $\delta x$ in functional space produces a displacement $\delta y = (\partial y_0/\partial x)\delta x$ of absolute magnitude $|\delta y| = (\mathcal{L}/L)\delta x$. Integration over x gives the total length L of the string.

At stresses close to $F_p$, Eq. (17) for the eigenvalues $\mu_n$ can be solved exactly, and this makes it possible to completely determine the pre-exponential factor:

$$I=\frac{5\cdot 3^{11/8}}{2^{3/4}}\frac{DaL}{(2\pi T)^{3/2}}\frac{\beta^{3/8}a^{11/8}}{\varkappa^{1/4}}e^{-V_0/T}. \quad (63)$$

## 6. CONCLUSIONS

The principal results of the paper are as follows. At sufficiently low temperatures the probability for

tunneling of a dislocation to a neighboring valley of the Peierls relief under the action of a stress $F \ll F_p$

$$w \sim \exp\{-{}^{16}/_{3}V_1^{3/2}\sqrt{M}/\hbar Fb\}. \quad (C.1)$$

Here, $V_1$ is the energy of a single kink, M is the effective mass, connected with the linear density $\rho$ of the string and the shape of the single kink $y_1(x)$ by the relation

$$M=\frac{\rho}{2}\int\left(\frac{\partial y_1}{\partial x}\right)^2 dx. \quad (C.2)$$

The indicated dependence is valid at $T < T_0 = Fb\hbar/4\sqrt{MV_1}$.

At $T > T_0$ the tunneling is preceded by thermal fluctuation, and the probability for such a complex process is

$$w \sim \exp\left\{-\frac{2V_1}{T}+\frac{1}{24}\frac{F^2b^2\hbar^2}{MT^3}\right\}. \quad (C.3)$$

For $T \gg T_0$ the formula (C.3) goes over into the well-known activation function.

Another limiting case for which an explicit expression for the tunneling probability has been obtained is for a stress F close to the Peierls stress $F_p$. In this case

$$|\ln w| \approx 2\sigma_0(F_p - F)\sqrt{\varkappa\rho}/\hbar\beta, \quad (C.4)$$

where $\sigma_0$ is a number for which an upper bound has been obtained, $\sigma_0 < 5$. Formula (C.4) is valid for temperatures

$$T \ll T_1 = \sqrt{\frac{5}{8}}\frac{\hbar}{\pi\sqrt{\rho}}\sqrt[4]{\frac{|U_0'''|}{2}(F_p - F)}.$$

As $T \to T_1$ the index of the exponential function smoothly goes over from (C.4) to ${}^1/_5 \times 2^{7/2} \times 3^{1/4} E_0$ (see the formulas (49) and (51)).

It is reasonable to expect the manifestation of the quantum properties of dislocations in crystals in which the zero-point oscillations are not too small.

The pre-exponential factors in the expressions for the transition probabilities at high temperatures have also been found.

The results obtained can be used to compute the velocity of dislocations in the following manner. The quantity which we calculated is actually the probability of formation of a double kink per unit time per unit length. Let us denote it by R. Let v be the velocity of the lateral recession of the kinks. Then, the time t the whole dislocation takes to tunnel to the neighboring valley of the potential relief is equal to

$$t \sim 1/\sqrt{vR}. \quad (C.5)$$

Notice that the logarithm of the dislocation velocity is half as large as ln w, a very important result in the estimation of exponentially small effects.

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