The Activation Energy of Domain Walls

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The activation energies of various domain walls are discussed. For the estimation of the activation energy of the thick domain wall, the method of the contour integral is adopted. The ferroelectric domain wall energy and Pierls energy of a double sine-Gordon dislocation are analytically calculated.

§1 Introduction

The problems of domain walls have attracted much attention in the relationship with solitons, discommensurations in the incommensurate phases, dislocations, ferroelectrics and so on.[1-4] The purpose of the present paper is to show a very simple method for estimation of the activation energy in the various systems.

Usually, a model system is represented by the following energy density

$$f(x)=\frac{1}{2}\left(\frac{d\phi}{dx}\right)^2+K^2V(\phi) \tag{1}$$

where K^2 is a parameter characterizing strength of potential. In (1), ϕ is a physical quantity which specifies the state and depends on x. Polarization P, is such a parameter in the ferroelectrics. Potential $V(\phi)$ is an even function with respect to ϕ. The ordinary procedure for finding the most stable configuration of the potential is to solve the Euler-Lagrange equation

$$\frac{d^2\phi}{dx^2}-K^2\frac{\partial V(\phi)}{\partial\phi}=0. \tag{2}$$

As the result, we obtain a kink solution

$$\phi=\phi(x) \tag{3}$$

with the boundary condition

$$\phi(x)\to\pm\infty \quad as \quad x\to\pm\infty. \tag{4}$$

The total energy of the wall is given as

$$F=\int_{-\infty}^{\infty}f(x)\,dx. \tag{5}$$

In the field of ferroelectricity, the system is sometimes called the ϕ^4−system for the second order phase transitions and ϕ^6−system for the first order phase transition, respectively. In this paper, we discuss these problems in detail.[5,6]

§2 Kink Energy of the Thick Domain Walls

Let us take the energy density as

$$f(x)=\frac{1}{2}\left(\frac{d\phi}{dx}\right)^2+\frac{K^2}{2}(1-\phi^2)^2. \tag{6}$$

This model is applicable to domain walls in double minimum potential. By solving the Euler equation (2), we get the solution

$$\phi=\tanh Kx. \tag{7}$$

The energy density and the wall energy are given as

$$f(x)=K^2\mathrm{sech}^4Kx, \tag{8}$$

and

$$F=\int_{-\infty}^{\infty}f(x)\,dx=\frac{4}{3}K^2. \tag{9}$$

When the wall is thin, the continuous model is no more valid. In such case we have to adopt a discrete model, in which the difference and the sum must be used instead of the derivative and the integral. Thus, the wall energy becomes

$$F=a\Sigma f(x), \tag{10}$$

where $x=na$, and the equation govering the structure of wall is given as

$$\phi_{n+1}-2\phi_n+\phi_{n-1}-a^2K^2\phi_n(1-\phi_n^2)=0. \tag{11}$$

The eq. (11) should be solved under the boundary conditions

$$\phi_n=\pm1 \quad for \quad n\to\pm\infty. \tag{12}$$

There are two types of the kink solutions (Fig. 1), which satisfy the above conditions:

$$\phi_{-n}=-\phi_n \quad \text{(the odd type)} \tag{13}$$

and

$$\phi_{-n}=-\phi_{n+1} \quad \text{(the even type)}. \tag{14}$$

In the odd type kink, the center of it is locate

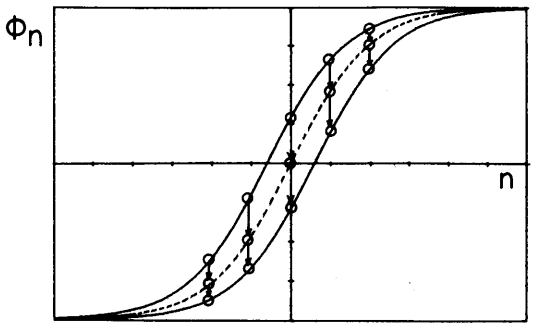

Fig. 1 The structure of a domain wall. Solid lines and dotted line show stable and unstable walls, respectively.

on the lattice site, while in the even type kink, the center is at the midst of two lattice sites.
The difference of these two kinks is called the pinning energy or the Peierls energy. Cahn has already calculated such activation energy, making use of the Poisson sum formula.
The wall energy can be written as

$$\Delta F = a\Sigma f(na) - a\Sigma f(na+\frac{a}{2}). \tag{15}$$

For the simplicity of following calculation, one of the sum can be approximated by the integral, and then

$$\Delta F = a\Sigma f(na) - \int_{-\infty}^{\infty} f(x)\mathrm{d}x. \tag{16}$$

This is equivalent to the errors caused due to approximation of the integration by the summation. On the basis of the Cauchy integral representation of the function, as adopted by Takahashi and Mori,[7] ΔF can be expressed as

$$\Delta F = -\frac{1}{2\mathrm{i}} \oint_c f(z)[\cot \frac{\pi}{a}z + \mathrm{i}]\mathrm{d}z, \tag{17}$$

where the contour c has to surround the real axis. The integration (17) is calculated by the steepest descent method, or by contour integration.
The calculated result for the activation energy is given by

$$\Delta F \sim K(\frac{1}{Ka})^3 \mathrm{e}^{-(\pi^2/aK)} \cdot 4\pi^4. \tag{18}$$

§ 3 Domain Walls in the Ferroelectrics (ϕ^6-model)

Let us take the polarization p for the parameter ϕ, which governs the structure of the wall, and then the free energy density is[4,5]

$$f = \frac{\alpha}{2}p^2 + \frac{\beta}{4}p^4 + \frac{\gamma}{6}p^6 + \frac{\kappa}{2}(\frac{\mathrm{d}p}{\mathrm{d}x})^2. \tag{19}$$

The total free energy is given by (5), and by solving the Euler equation

$$\kappa\frac{\mathrm{d}^2p}{\mathrm{d}x^2} - (\alpha p + \beta p^3 + \gamma p^5) = 0, \tag{20}$$

with the boundary condition that

$$p \to \pm p_0 \quad \text{for} \quad x \to \pm\infty. \tag{21}$$

After calculations we obtain the spatial variation of p as (Fig. 2)

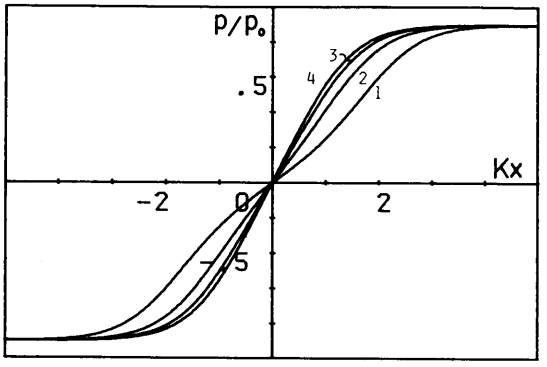

Fig. 2 The spatial variation of p. Curves 1, 2, 3 and 4 correspond to a=. 225, 0.15, 0 and .25, respectively.

$$p(x) = p_0\sqrt{\frac{1-4a}{3(1-2a)-2(1-a)\tanh^2 Kx}}\tanh Kx, \tag{22}$$

where

$$K = \sqrt{\frac{\beta^2}{2\kappa\gamma}(1-a)(1-2a)},$$

$$p_0 = -\frac{\beta}{\gamma}(1-a), \quad a = \frac{1}{2}\left(1-\sqrt{1-\frac{4\alpha\gamma}{\beta^2}}\right) \leqq \frac{1}{4}. \tag{23}$$

The wall energy is given by

$$F_w = \int_{-\infty}^{\infty}(f - f_0)\mathrm{d}x, \tag{24}$$

where

$$f_0 = \frac{\alpha}{2}p_0^2 + \frac{\beta}{4}p_0^4 + \frac{\gamma}{6}p_0^6. \tag{25}$$

The integrand $f - f_0$ can be obtained as

$$f - f_0 \tilde{=} \frac{\mathrm{sech}^4 Kx}{[3(1-2a)-2(1-a)\tanh^2 Kx]^3}, \tag{26}$$

which shows the distribution of free energy density in a domain wall.

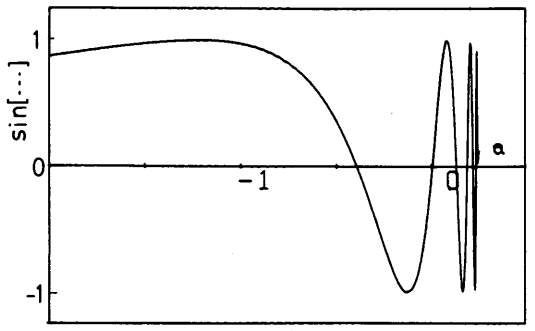

Fig. 3 The temperature dependence of the sinus term of eq. (27).

The activation energy is calculated by contour integral, then we obtain (Fig. 3),

$$\Delta F \sim (\frac{\pi}{Ka})^2 \sin[\frac{2\pi}{Kd}\tanh^{-1}\sqrt{\frac{2(1-a)}{3(1-2a)}}]e^{-\pi^2/Kd}. \quad (27)$$

Because of the factor $e^{-\pi^2/Kd}$, which comes from the y_0 (at poles $z=\pm x_0+iy_0$), ΔF is quite small. The sinusoidal term as a pre-exponential factor which comes from the situation that poles are not located on the imaginary axis, *i.e.*, $x\neq 0$. As a result, ΔF is an oscillating function of temperature.

§4 Double-Sine-Gordon Equation

The calcutation of the activation energy of the dislocation, the Peierls energy is one of the central problem. Among various dislocation models, the one proposed by Frenkel-Kontorova is most famous. As is well known, the equilibrium state of the Frenkel-Kontorova model is obtained by solving the sine-Gordon equation.

Now we solve the double sine-Gordon equation.[6] Let us take the total energy density as

$$f(x)=\frac{\kappa}{2}(\frac{d\phi}{dx})^2+a(1+\cos\phi)+b(1-\cos 2\phi). \quad (28)$$

In this case, the Euler-equation is

$$\kappa\frac{d^2\phi}{dx^2}=-a\sin\phi+2b\sin 2\phi, \quad (29)$$

which is a well known double sine-Gordon equation.

We obtain a so-called kink solution as (Fig. 4)

$$\phi=\cos^{-1}[\frac{2(a+4b)}{a\cosh^2 Kx+4b}-1], \quad (30)$$

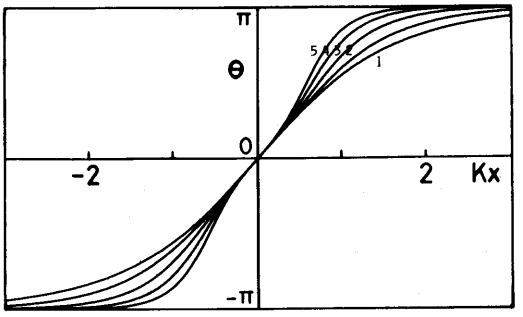

Fig. 4 The kink solution of the double sine-Gordon equation. Curves 1, 2, 3, 4 and 5 correspond to the value of b equal to 0, 0.25, .75, 1.5 and 2.5, respectively. $a=1$.

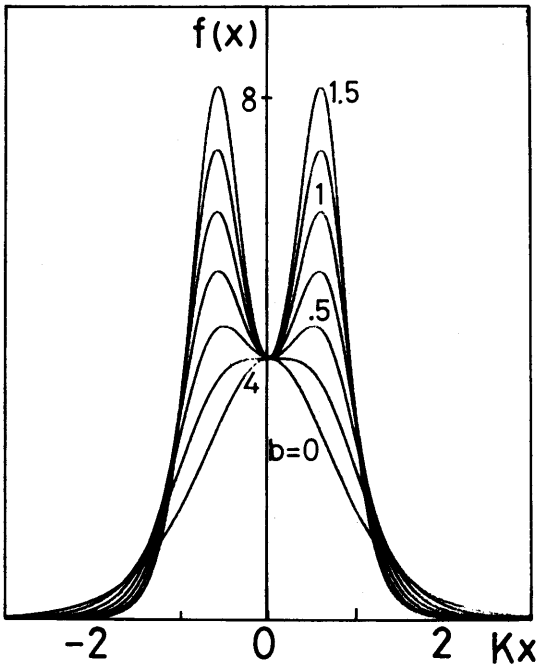

Fig. 5 Energy density vs x given by eq. (32).

where

$$K=\sqrt{a+4b}, \quad (31)$$

which is a measure of the dislocation width.

The total energy is obtained by the integration of the energy density (Fig. 5),

$$f(x)=4a(a+4b)^2(\frac{\cosh Kx}{a\cosh^2 Kx+4b})^2, \quad (32)$$

and

$$F=4\sqrt{a}\left\{\sqrt{1+\frac{4b}{a}}-\frac{1}{2}\sqrt{\frac{a}{4b}}\ln\left|\frac{1-\sqrt{1+\frac{a}{4b}}}{1+\sqrt{1+\frac{a}{4b}}}\right|\right\}. \quad (33)$$

The Pierls energy is the energy required to move a dislocation by one lattice unit and further. The activation energy is calculated by the contour integral

$$F=\frac{1}{2\mathrm{i}}\oint_c\left[\frac{1}{2}\left(\cot\frac{\pi(z-\delta)}{d}+\cot\frac{\pi(z+\delta)}{d}\right)-\cot\frac{\pi z}{d}\right]f(z)\mathrm{d}z, \quad (34)$$

where δ is the displacement from the lattice site, and $f(z)$ is given by the relation

$$f(x)=\frac{1}{2\pi\mathrm{i}}\oint_c\frac{f(z)}{z-x}\mathrm{d}z. \quad (35)$$

The poles of $f(z)$ are located at

$$z_m=\pm x_0\pm\mathrm{i}y_m, \quad (36)$$

where

$$Kx_0=\ln\left(\sqrt{\frac{4b}{a}+1}-\sqrt{\frac{4b}{a}}\right),$$
$$Ky_m=\frac{\pi}{2}+m\pi. \quad (37)$$

As the contribution to ΔF from the poles closest to the real axis ($m=0$) is most dominant, then we obtain

$$|\Delta F|\sim\frac{8\pi^2}{d}|g_1\exp(-\pi^2/Kd)+g_2\exp(-2\pi^2/Kd)|, \quad (38)$$

where

$$g_1\sim\cos\frac{2\pi x_0}{d}\left(\cos\frac{2\pi\delta}{d}-1\right)$$

and

$$g_2\sim 2\cos\frac{4\pi x_0}{d}\left(\cos\frac{4\pi\delta}{d}-1\right). \quad (39)$$

§ 5 Summary

In the present paper, the activation energies are calculated by the contour integral. The result will shed light on the domain wall problems in the system undergoing structural phase transitions. The calculated energy showed that ΔF was a periodic function with the period of the lattice d in the double sine-Gordon system. In the case of ϕ^6−system, ΔF was an oscillating function of temperature (oscillating violently in the close vicinity of the transition temperature). This situation is derived from the fact that at some temperature the odd type domain has a lower energy, while at another temperature the other type of domains is more stable. The even type of domain is always stable in ϕ^4−system.

The wall problems of the improper ferroelectrics are also solved by the double-sine-Gordon equation. [6]

By adding the kinetic energy term, we are able to discuss the two-headed solitons or the extended solitons.

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