Brownian motion of a domain wall and the diffusion constants

Y. Wada* and J. R. Schrieffer
Department of Physics, University of Pennsylvania, Philadelphia, Pennsylvania 19104
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We have studied interactions between a domain wall and phonons in a one-dimensional-model system of a structurally unstable lattice with a double-well local potential and nearest-neighbor coupling. We find that a nonlinear effect in the interacting phonon amplitudes gives rise to a Brownian-like motion of isolated domain walls at low temperatures as well as higher harmonic generation of transmitted and reflected phonons. When there is a domain wall at rest, it was known that the linearized equation of motion has three types of independent solutions: "translation mode," "amplitude oscillation" of the domain wall, and propagating "phonons." In the second-order approximation, these modes interact. An incoming phonon produces a translation of the wall, giving rise to its Brownian motion. The magnitude of the translation is computed together with the amplitude and phase shift of the higher harmonics. We estimate the diffusion constant of walls, using the fluctuation-dissipation theorem and the thermal average over the phonons, to be $D = 0.516\ \omega_0 l^2(k_BT/\mu_0^2\omega_0^2)^2$, where l is the lattice spacing and ω_0 is the frequency of small oscillation of the ion (with mass m) around u_0, a minimum point of an isolated double-well potential.

I. INTRODUCTION

In recent years, considerable progress has been made in the study of nonlinear equations in various fields of physics. Of particular importance are nonlinear equations which admit large-amplitude solitary-wave solutions. The usual perturbation calculations, which postulate small-amplitude deviations, are inadequate to obtain such solutions. One example of solitary-wave solution is the domain wall which was discussed by Krumhansl and one of the present authors (JRS)[1] (hereafter KS). They studied thermodynamics and some dynamic properties of a one-dimensional-model system whose displacement field Hamiltonian is strongly anharmonic, and is representative of those used to study displacive phase transitions. It is the model system of a structurally unstable lattice, having a double-well local potential and nearest-neighbor coupling. A domain-wall excitation is characterized by the following distribution of ions at each lattice point. Over nearly all the semi-infinite region of the left-hand side of the domain wall, the ions are uniformly at the potential minimum of the same side of the lattice point. Nearly all ions on the right-hand side of the wall occupy the minimum of the other side. The transition takes place through a domain wall of a finite thickness. The wall can move with a constant velocity which is less than the velocity c_0 of low-amplitude sound waves (phonons). At low temperature, the thermodynamic function was evaluated in two ways: exactly by the functional integral methods and phenomenologically by regarding both phonons and domain walls as elementary excitations. The agreement of the results of the two evaluations confirmed the idea that phonons and domain-wall excitations play an important role. In addition to this static property, a number of dynamic properties could depend strongly on the presence of domain walls. The dynamic correlation function is one of them. A possible relation between the development of a "central peak" in the dynamic correlation function and the distribution of domain wall was pointed out. It was later shown by Bishop, Domany, and Krumhansl[2] that the appearance of phonons and domain walls as elementary excitations survives the passage from classical to quantum mechanics.

Molecular dynamics computer simulations have been carried out for this problem. Koehler, Bishop, Krumhansl, and Schrieffer[3] showed the motion of the linear chain as a series of snapshots in time for various temperatures. The results showed pronounced domain structure at low temperature—a feature emphasized in the analysis of KS. They further found that there is a phonon dressing of domain walls. Domain-wall potential energy E_{DP}, determined with the help of correlation length, turned out to be smaller than the bare value, estimated by KS, at low temperature. It was also observed that the domain walls do not keep moving freely between collisions with other walls. Rather, isolated walls appear to undergo Brownian-like motion.

Aubry[4] also performed molecular dynamics calculations to obtain the dynamic correlation function of the one-dimensional system. He pointed out the possiblity that the domain walls participate in developing the central peak. Simulations of a two-dimensional system were done by Schneider and Stoll.[5] They found clustering phenomenon to be very important in this case. This clustering phenomenon is equivalent to the appearance of two-dimensional domain structure.

The same model has been investigated by elementary-particle physicists. It is called a ϕ^4 model in one-plus-one dimension. The domain-wall solution describes the Fourier transform of the form factor of an elementary particle. It was shown that,[6] when there is a domain wall at rest, the equation of motion linearized with respect to the deviation from the domain-wall solution has three types of independent solutions: a "translation mode," and "amplitude oscillation" of the domain wall, and propagating "phonons." The translation mode is a Goldstone mode[7] which arises due to the breaking of translation symmetry by the presence of the domain wall. The amplitude-oscillation mode gives rise to a modification of the form of the domain wall. It costs some energy and thus corresponds to an excited state in the language of elementary-particle physics. The phonon modes are the continuum solutions which except in the vicinity of the domain wall resemble the linearized solutions of the original equation in the absence of domain walls. By examining the asymptotic form of the solutions for $x \to \pm\infty$, one finds that the phonons suffer only a phase shift when passing through the domain wall. In this sense, the phonons do not interact with the domain wall. This is the reason why Koehler *et al.*[3] suggested that the observed diffusive wall motion might be a result of effects nonlinear in the phonon amplitudes, as well as possible discrete-lattice effects.

The purpose of this study is to show that the nonlinear effect, in fact, can give rise to the Brownian-like motion of the domain walls. When a wave packet of phonons, with typical frequency ω, is incident on a domain wall, the nonlinear effect generates two harmonics: one with almost vanishing frequency and the other with 2ω. The former excites the translation mode, shifting the domain wall a finite distance. The wall moves as if the effective interaction with the incoming phonon is attractive. Since phonons make collisions with the wall randomly, it behaves as a Brownian particle. The other component with the frequency 2ω is partially transmitted and partially reflected with a phase shift.

The diffusive wall motion is characterized by a diffusion constant. It can be estimated using the fluctuation-dissipation theorem. If we denote the position of the domain wall at time t by $\delta(t)$, the diffusion constant D is given by[8]

$$D = \langle[\delta(t)]^2\rangle/2t, \tag{1.1}$$

for the one-dimensional system. Here the angular brackets mean an average over the distribution of phonons. The time t should be long in comparison with the "mean- free time" of the collisions. Since we are interested only in the lowest order of nonlinear contribution to $\delta(t)$, we may ignore nonlinear terms in the phonon-distribution function which contribute to higher-order corrections to the diffusion constant. This is a good approximation when the number of excited phonons is small at low temperature. The diffusion constant, thus obtained, turns out to be proportional to T^2, indicating that the diffusive wall motion is a second-order effect.

In Sec. II, we review the one-dimensional model of KS, the linearization of the equation of motion when there is a domain wall, and the three types of the solutions. In Sec. III, nonlinear collisions of a phonon with a domain wall are investigated. The shift of the domain wall, the coefficients of transmission and reflection of the higher harmonics and their phase shift are calculated as a function of the wave number of the incoming phonon. In Sec. IV, the statistical mechanics of phonons in the presence of a domain wall is developed. Using the fluctuation-dissipation theorem, it is applied to obtain the diffusion constant. Finally, in Sec. V, we discuss the obtained results and some remaining problems.

II. MODEL AND LINEARIZED SOLUTIONS

The Hamiltonian proposed by KS has a continuum representation

$$H = \int \frac{dx}{l}\left[\frac{p(x)^2}{2m} + \frac{A}{2}u(x)^2 + \frac{B}{4}u(x)^4 + \frac{mc_0^2}{2}\left(\frac{du}{dx}\right)^2\right], \tag{2.1}$$

in the displacive case. Here l is the lattice spacing and x locates an ion with mass m. The fields $u(x)$ and $p(x)$ are the displacement and momentum of the displacing ion at x with respect to some heavy ion or reference lattice. A and B are parameters which characterize the local potential. KS discussed the case of a structurally unstable lattice, taking $A = -|A|$ and $B > 0$. The local potential is a double-well potential with minima at

$$u = \pm u_0 = \pm(|A|/B)^{1/2}. \tag{2.2}$$

The classical equation of motion for the displacement field $u(x)$ which follows from (2.1) is

$$m\partial^2 u/\partial t^2 + Au + Bu^3 - mc_0^2\partial^2 u/\partial x^2 = 0. \tag{2.3}$$

This has a domain-wall solution

$$u = u_0 \tanh[(x - vt)/\sqrt{2}\xi], \tag{2.4}$$

with

$$\xi^2 = m(c_0^2 - v^2)/|A|. \tag{2.5}$$

Suppose a domain wall is located at $x = 0$ and not moving. Deviation from the domain-wall solution would be small at low temperatures. If we put

$$u(x,t)=u_0\tanh(x/\sqrt{2}\xi_0)+\psi(x,t), \tag{2.6}$$

the deviation ψ satisfies the equation

$$\frac{\partial^2\psi}{\partial t^2}-\frac{c_0^2\partial^2\psi}{\partial x^2}+\left[\omega_0^2-\left(\frac{3\omega_0^2}{2}\right)\cosh^2\!\left(\frac{x}{\sqrt{2}\xi_0}\right)\right]\psi=-\left(\frac{B}{m}\right)\left[3u_0\tanh\!\left(\frac{x}{\sqrt{2}\xi_0}\right)\psi^2+\psi^3\right], \tag{2.7}$$

where $\xi_0^2=mc_0^2/|A|$ and $\omega_0^2=2|A|/m$. It has been shown[6] that the eigenvalue problem

$$-c_0^2d^2\varphi/dx^2+[\omega_0^2-(3\omega_0^2/2)\cosh^2(x/\sqrt{2}\xi_0)]\varphi=\omega^2\varphi \tag{2.8}$$

has eigenvalues and eigenfunctions:

$$\omega^2=0,\quad \varphi_0(x)=\cosh^{-2}(x/\sqrt{2}\xi_0), \tag{2.9a}$$

$$\omega^2=\tfrac{3}{4}\omega_0^2,\quad \varphi_1(x)=\sinh\!\left(\frac{x}{\sqrt{2}\xi_0}\right)\cosh^{-2}\!\left(\frac{x}{\sqrt{2}\xi_0}\right), \tag{2.9b}$$

$$\omega^2=\omega_0^2+c_0^2q^2\equiv\omega_q^2,\quad (\omega_q>0), \tag{2.9c}$$

$$\varphi_q(x)=e_{iqx}\left[3\tanh^2\!\left(\frac{x}{\sqrt{2}\xi_0}\right)-3\sqrt{2}iq\xi_0\tanh\!\left(\frac{x}{\sqrt{2}\xi_0}\right)-1-2q^2\xi_0^2\right].$$

These three solutions have simple physical interpretations. When $\varphi_0(x)$ is added to the domain-wall solution, one finds that the sum

$$u_0\tanh(x/\sqrt{2}\,\xi_0)+\beta_0\varphi_0(x)\simeq u_0\tanh(x/\sqrt{2}\xi_0+\beta_0/u_0)$$

corresponds to a domain wall which is translated by an amount $\delta=-\sqrt{2}\xi_0\beta_0/u_0$. Thus the $\omega^2=0$ solution yields the "translation mode" of the domain wall. It is a Goldstone mode[7] which arises due to the breaking of symmetry by the presence of the domain wall. When $\varphi_1(x)$ is added to the domain-wall solution, the wall does not move, but its form undergoes a variation with time. We may call it an "amplitude-oscillation mode" of the domain wall. The third solution $\varphi_q(x)$ constitues the continuum mode. Except in the vicinity of the domain wall, it is a propagating plane wave whose spectrum is identical with that of small oscillations of ions around the bottom of one of the walls in the absence of domain walls. Therefore, these solutions correspond to the "phonons." They are not reflected by the domain wall but suffer only a phase shift $\Delta(q)$,

$$e^{i\Delta(q)}=(2-Q^2-3iQ)/(2-Q^2+3iQ),$$
$$\Delta(q)=2\tan^{-1}[3Q/(Q^2-2)], \tag{2.10}$$

where $Q=\sqrt{2}q\xi_0$.

Because the solutions $\varphi_i(x)$ $(i=0,1,q)$ are eigenfunctions of the self-adjoint eigenvalue problem (2.8), they form a complete set which spans the space of functions of x. The orthogonality relations are

$$\int_{-\infty}^{\infty}\varphi_0^2(x)\,dx=\tfrac{4}{3}\sqrt{2}\xi_0 \tag{2.11a}$$

$$\int_{-\infty}^{\infty}\varphi_1^2(x)\,dx=\tfrac{2}{3}\sqrt{2}\xi_0, \tag{2.11b}$$

$$\int_{-\infty}^{\infty}\varphi_q^*(x)\varphi_{q'}(x)\,dx=2\pi(1+Q^2)(4+Q^2)\delta(q-q'), \tag{2.11c}$$

while the completeness relation has the form

$$\frac{3}{4\sqrt{2}\xi_0}\varphi_0(x)\varphi_0(x')+\frac{3}{2\sqrt{2}\xi_0}\varphi_1(x)\varphi_1(x')+\int_{-\infty}^{\infty}\frac{dq\,\varphi_q(x)\varphi_q^*(x')}{2\pi(1+Q^2)(4+Q^2)}=\delta(x-x'). \tag{2.12}$$

The relations (2.11c) and (2.12) are proved in Appendix A.

Let us suppose that, at time $t=t_0\ll 0$, a wave packet of phonon is at $x\ll 0$ moving in the direction of the domain wall. It gives the initial condition for ψ:

$$\psi(x,t)=\frac{1}{L}\sum_q u_0^2\alpha_q\sin(qx-\omega_qt+\theta_q), \tag{2.13}$$

when $t\simeq t_0$. Here $\omega_q>0$ and α_q is nonvanishing only at $q>0$. L is the length of the system. The quantity α_q gives the amplitude of the incoming phonon which we assume to be small in comparison with unity. Since α_q would be a localized function around a typical wave number $\bar{q}$, the initial form (2.13) can be rewritten

$$\psi(x,t)=\mathrm{Im}\exp[i(\bar{q}x-\bar{\omega}_qt+\bar{\theta}_q)]f(x-v_qt-x_0), \tag{2.14a}$$

where

$$f(x)=\frac{u_0^2}{L}\sum_q\alpha_q\exp[i(q-\bar{q})x], \tag{2.14b}$$

and $\bar{\omega}_q$ and $\bar{\theta}_q$ are the values of ω_q and θ_q at $q=\bar{q}$. The quantity v_q is the group velocity

$$v_q=(d\omega_q/dq)_{q=\bar{q}}=c_0^2\bar{q}/\bar{\omega}_q. \tag{2.15}$$

The quantity x_0 is defined by

$$x_0=-(d\theta_q/dq)_{q=\bar{q}}\,. \tag{2.16}$$

It specifies the initial position of the wave packet at $x_0+v_qt_0$.

The first-order approximation of the equation of motion for ψ (2.7) is

$$\frac{\partial^2\psi_1}{\partial t^2} - \frac{c_0^2\partial^2\psi_1}{\partial x^2} + [\omega_0^2 - \tfrac{3}{2}\omega_0^2\cosh^2(x/\sqrt{2}\xi_0)]\psi_1 = 0. \tag{2.17}$$

We can immediately write down the solution which satisfies the initial condition (2.13)

$$\psi_1(x,t) = \frac{u_0^2}{2iL}\sum_q \{\alpha_q\phi_q(x)\exp[i(-\omega_q t + \theta_q)] - \phi_q^*(x)\exp[i(\omega_q t - \theta_q)]\}, \tag{2.18}$$

where the function ϕ_q is defined by

$$\phi_q(x) = \varphi_q(x)/(2 - Q^2 + 3iQ). \tag{2.19}$$

After transmitting through the domain wall, the function ψ_1 takes the form at $x \gg 0$ and $t \gg 0$

$$\psi_1(x,t) \to \frac{u_0^2}{L}\sum_q \alpha_q \sin[qx - \omega_q t + \theta_q + \Delta(q)]$$
$$= \mathrm{Im}\exp\{i[\bar{q}x - \bar{\omega}_q t + \bar{\theta}_q + \Delta(\bar{q})]\} \times f(x - v_q t - x_0 - \Delta x_1), \tag{2.20}$$

where

$$\Delta x_1 = -\left(\frac{d\Delta(q)}{dq}\right)_{q=\bar{q}} = \frac{6\sqrt{2}\xi_0(2+\bar{Q}^2)}{4+5Q^{-2}+\bar{Q}^4}. \tag{2.21}$$

Here we have used a notation

$$\bar{Q} = \sqrt{2}\,\bar{q}\xi_0. \tag{2.22}$$

The shift Δx_1 is illustrated in Fig. 1.

III. NONLINEAR PROCESSES

When the amplitude of the incident phonon α_q is small in comparison with unity, the deviation from the domain-wall solution can be written in a form of power series in α_q

$$\psi(x,t) = \psi_1(x,t) + \psi_2(x,t) + \cdots, \tag{3.1}$$

where the function ψ_2 is bilinear in α_q's. Substituting into the equation of motion (2.7), we equate the bilinear terms on both sides to obtain

$$\frac{\partial^2\psi_2}{\partial t^2} - c_0^2\frac{\partial^2\psi_2}{\partial x^2} + [\omega_0^2 - \tfrac{3}{2}\omega_0^2\cosh^2(x/\sqrt{2}\xi_0)]\psi_2 = -(3Bu_0/m)\tanh(x/\sqrt{2}\xi_0)\,\psi_1^2. \tag{3.2}$$

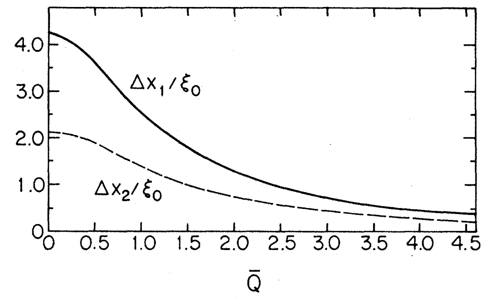

FIG. 1. Shift of the phonon wave packet due to the interaction with a domain wall as a function of the wave number $\bar{q}$. Solid curve is the shift of the incident packet Δx_1 and the dashed curve that of the higher harmonics Δx_2. The abscissa is $\bar{Q} = \sqrt{2}\,\bar{q}\xi_0$.

We expand ψ_2 in terms of the φ_i

$$\psi_2(x,t) = \beta_0(t)\varphi_0(x) + \beta_1(t)\varphi_1(x) + \frac{1}{L}\sum_k \beta_k(t)\varphi_k(x). \tag{3.3}$$

Substitution into (3.2) and use of the orthonormality of the φ's give

$$\frac{d^2\beta_0}{dt^2} = -\frac{9Bu_0}{4\sqrt{2}m\xi_0}\int_{-\infty}^{\infty} dx \tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_0\psi_1^2, \tag{3.4a}$$

$$\frac{d^2\beta_1}{dt^2} + \tfrac{3}{4}\omega_0^2\beta_1 = -\frac{9Bu_0}{2\sqrt{2}m\xi_0}\int_{-\infty}^{\infty} dx \tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_1\psi_1^2, \tag{3.4b}$$

$$\frac{d^2\beta_k}{dt^2} + \omega_k^2\beta_k = -\frac{3Bu_0}{m(1+K^2)(4+K^2)} \times \int_{-\infty}^{\infty} dx \tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_k^*\psi_1^2, \tag{3.4c}$$

where $K = \sqrt{2}k\xi_0$.

These equations should be integrated so that the β's and $d\beta/dt$'s are zero at $t = t_0$, since the initial condition is completely satisfied by ψ_1. Instead of the above condition, we introduce adiabatic hypothesis, taking $t_0 \to -\infty$ and assuming that the nonlinear interaction on the right-hand sides of Eqs. (3.4a)–(3.4c) have gradually increased from zero as if there is an additional factor $\exp \epsilon t$, $\epsilon > 0$. To simplify the integration, we introduce the Fourier transform of ψ_1^2

$$\psi_1^2(x,t) = \int_{-\infty}^{\infty} d\omega\, e^{(-i\omega t)}\chi(x,\omega), \tag{3.5a}$$

$$\chi(x,\omega) = -\frac{u_0^4}{4L^2}\sum_{qq'}\alpha_q\alpha_{q'}\{\delta(\omega - \omega_q - \omega_{q'})\phi_q\phi_{q'}\exp[i(\theta_q + \theta_{q'})] + \delta(\omega + \omega_q + \omega_{q'})\phi_q^*\phi_{q'}^*\exp[-i(\theta_q + \theta_{q'})] - 2\delta(\omega - \omega_q + \omega_{q'})\phi_q\phi_{q'}^*\exp[i(\theta_q - \theta_{q'})]\}. \tag{3.5b}$$

Then, integration of (3.4) gives

$$\beta_0(t)=\frac{9Bu_0}{4\sqrt{2}m\xi_0}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dx\,d\omega\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_0\chi \times\exp[-i\omega t/(\omega+i\epsilon)^2], \quad (3.6a)$$

$$\beta_1(t)=\frac{9Bu_0}{2\sqrt{2}m\xi_0}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dx\,d\omega\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_1\chi \times\exp\{-i\omega t/[(\omega+i\epsilon)^2-\tfrac{3}{4}\omega_0^2]\}, \quad (3.6b)$$

$$\beta_k(t)=3Bu_0/m(1+K^2)(4+K^2) \times\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}dx\,d\omega\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_k^*\chi \times\exp\{-i\omega t/[(\omega+i\epsilon)^2-\omega_k^2]\}. \quad (3.6c)$$

Substituting the expression (3.5b) of χ into (3.6a), we can carry out the ω integration with the help of the δ functions to obtain

$$\beta_0(t)=-\frac{9Bu_0^5}{16\sqrt{2}m\xi_0L^2}\sum_{qq'}\alpha_q\alpha_{q'}\int_{-\infty}^{\infty}dx\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_0(x)\Bigg[\phi_q(x)\phi_{q'}(x)\exp\left(\frac{-i(\omega_q+\omega_{q'})t+i(\theta_q+\theta_{q'})}{(\omega_q+\omega_{q'}+i\epsilon)^2}\right) + \phi_q^*(x)\phi_{q'}^*(x)\exp\left(\frac{i(\omega_q+\omega_{q'})t-i(\theta_q+\theta_{q'})}{(\omega_q+\omega_{q'}-i\epsilon)^2}\right) - 2\phi_q(x)\phi_{q'}^*(x)\exp\left(\frac{i(\omega_q-\omega_{q'})t+i(\theta_q-\theta_{q'})}{(\omega_q-\omega_{q'}+i\epsilon)^2}\right)\Bigg]. \quad (3.7)$$

The integrand of the q and q' integrals is nonsingular except for the last term in the parentheses at $\omega_q=\omega_{q'}$. The contribution of these nonsingular terms corresponds to a forced oscillation of the translation mode by the incident phonon. The frequency $\omega_q+\omega_{q'}$ is not the eigenfrequency of the translation mode. The forced oscillation would relax quickly as soon as the incident wave packet passes. On the other hand, the singularity of the integral does give rise to the generation of the translation mode to which we shall confine our discussions hereafter.

After some calculations, which are given in Appendix B, we can show

$$\int_{-\infty}^{\infty}dx\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_0\varphi_q\varphi_{q'} =\frac{\pi i(Q^2-Q'^2)^2\xi_0[1+(Q^2+Q'^2)/4]}{2\sqrt{2}\sinh[\pi(Q+Q')/2]}. \quad (3.8)$$

where $Q'=\sqrt{2}q'\xi_0$. At the singular point $q'\sim q$, the x integral in (3.7) takes the form

$$\lim_{q'\to q}\int_{-\infty}^{\infty}dx\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_0\phi_q\phi_{q'}^* =\frac{\sqrt{2}i(Q-Q')Q^2\xi_0(2+Q^2)}{4+5Q^2+Q^4}. \quad (3.9)$$

It is important to note that the singularity is not of second order but of first order, since the numerator (3.9) vanishes linearly there. Contribution of the region in the vicinity of the singularity can be evaluated as follows (at $t\gg 0$):

$$\beta_0(t)=\frac{9iBu_0^5}{4\sqrt{2}mL^2}\sum_{qq'}\alpha_q\alpha_{q'}\left(\frac{dq}{d\omega_q}\right)Q^2\xi_0(2+Q^2) \times\exp\left(\frac{-i(\omega_q-\omega_{q'})t+i(\theta_q-\theta_{q'})}{(4+5Q^2+Q^4)(\omega_q-\omega_{q'}+i\epsilon)}\right)$$

$$=\frac{9Bu_0^5}{4\sqrt{2}mL}\sum_q\alpha_q^2\left(\frac{dq}{d\omega_q}\right)^2\frac{Q^2\xi_0(2+Q^2)}{4+5Q^2+Q^2}$$

$$=\frac{9u_0^3}{\sqrt{2}\xi_0L}\sum_q\frac{\alpha_q^2\omega_q^2(2+Q^2)}{\omega_0^2(4+5Q^2+Q^4)}$$

$$=\frac{9u_0^3}{4\sqrt{2}\xi_0L}\sum_q\frac{\alpha_q^2(2+Q^2)}{1+Q^2}. \quad (3.10)$$

The quantity β_0 is related to the shift of the domain wall δ, which is given by

$$\delta=\frac{\sqrt{2}\xi_0\beta_0}{u_0}=-\frac{9u_0^2}{4L}\sum_q\frac{\alpha_q^2(2+Q^2)}{1+Q^2}. \quad (3.11)$$

The domain wall moves in the negative direction by a finite distance. The discussion so far can be reiterated for the case of a phonon coming in from the positive x side of the domain wall. The shift of the wall is again given by (3.11) with the opposite sign. It moves in the positive direction by the same distance. The interaction between the domain wall and the incoming phonon is effectively attractive. The motion of the domain wall should look like a random walk in very low temperature where the phonons collide with the wall in a random way. If

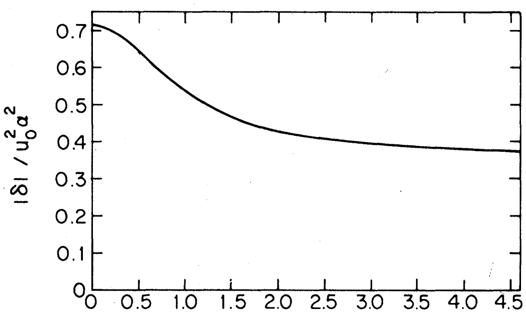

FIG. 2. Magnitude of the translation of the domain wall $|\delta|$ as a function of the wave number of the incident phonon $\bar{q}$. The abscissa is $\bar{Q}=\sqrt{2}\,\bar{q}\xi_0$.

the phonon is almost coherent, we may put

$$\alpha_q^2=\alpha^2\delta(q-\bar{q}). \qquad (3.12)$$

Equation (3.11) then becomes

$$\delta=-(9u_0^2\alpha^2/8\pi)(2+\bar{Q}^2)/(1+\bar{Q}^2), \qquad (3.13)$$

which is shown in Fig. 2.

Substitution of the expression (3.5b) for χ into (3.6b) gives $\beta_1(t)$ which is composed of three terms. One of them involves $\phi_q\phi_{q'}$, another $\phi_q^*\phi_{q'}^*$, and the last $\phi_q\phi_{q'}^*$. The denominator of the first two takes the form $(\omega_q+\omega_{q'}\pm i\epsilon)^2-\frac{3}{4}\omega_0^2$ which does not vanish since $\omega_q\geq\omega_0$. The denominator of the last term $(\omega_q-\omega_{q'}+i\epsilon)^2-\frac{3}{4}\omega_0^2$ does not either, if the incident phonon wave packet has enough coherence so that the distribution of the function α_q is well localized. The wave numbers q and q' should be close to each other in the localized region and $|\omega_q-\omega_{q'}|$ is less than $\frac{1}{2}\sqrt{3}\omega_0$. Therefore, the motion of the amplitude oscillation is the forced oscillation by the incoming phonon, since the integrand of (3.6b) is nonsingular. It would relax very rapidly.

Substituting (3.5b) into (3.6c), we again obtain three terms for $\beta_k(t)$ which involve $\phi_q\phi_{q'}$, $\phi_q^*\phi_{q'}^*$, and $\phi_q\phi_{q'}^*$, respectively. The above argument can be applied to the last term. Contribution by the singularity of the integrand is due to the first two terms which can be written

$$\beta_k(t)=-\frac{3Bu_0^5}{2m(1+K^2)(4+K^2)L^2}\,\mathrm{Re}\sum_{qq'}\alpha_q\omega_{q'}\int_{-\infty}^{\infty}dx\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_k^*\phi_q\phi_{q'}\times\exp\left(\frac{-i(\omega_q+\omega_{q'})t+i(\theta_q+\theta_{q'})}{(\omega_q+\omega_{q'}+i\epsilon)^2-\omega_k^2}\right). \qquad (3.14)$$

We may denote the last term of ψ_2, given by (3.3), by ψ_2^{ph}, since it will be shown to be related to higher harmonics. With the help of (3.14), it takes the form

$$\begin{aligned}\psi_2^{\mathrm{ph}}(x,t)&=\frac{1}{2\pi}\int_{-\infty}^{\infty}dk\,\beta_k(t)\varphi_k(x)\\&=-\frac{3Bu_0^5}{4\pi mL^2}\,\mathrm{Re}\sum_{qq'}i\alpha_q\alpha_{q'}\int_{-\infty}^{\infty}dk\,F(-k,q,q')\varphi_k(x)\\&\quad\times\exp\{-i(\omega_q+\omega_{q'})t+i(\theta_q+\theta_{q'})+\tfrac{1}{2}i[\Delta(q)+\Delta(q')]\}/[(1+K^2)(4+K^2)]^{1/2}\\&\quad\times[(\omega_q+\omega_{q'}+i\epsilon)^2-\omega_k^2],\end{aligned} \qquad (3.15)$$

where $F(k,q,q')$ is defined by

$$F(k,q,q')=\frac{-i\int_{-\infty}^{\infty}dx\,\tanh(x/\sqrt{2}\xi_0)\varphi_k\varphi_q\varphi_{q'}}{[(1+K^2)(4+K^2)(1+Q^2)(4+Q^2)(1+Q'^2)(4+Q'^2)]^{1/2}}. \qquad (3.16)$$

The integration is carried out in the Appendix C to show that $F(k,q,q')$ is real and

$$\begin{aligned}\int_{-\infty}^{\infty}dx\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_k\varphi_q\varphi_{q'}=\sqrt{2}\pi i\xi_0\Big(6(P_3+P_2P_3-P_5)\delta(P)+\frac{P}{\sinh(\pi P/2)}(8+5P_2+\tfrac{5}{4}P_4-\tfrac{1}{8}P_2^2-3PP_3+\tfrac{9}{4}P_2P^2\\-\tfrac{3}{8}P^4+3P_5P-\tfrac{15}{8}P_4P^2-\tfrac{1}{9}P_3^2-\tfrac{8}{3}P_3P_2P\\-\tfrac{1}{9}P_3P^3+\tfrac{17}{16}P_2^2P^2+\tfrac{35}{48}P_2P^4-\tfrac{31}{144}P^6)\Big),\end{aligned} \qquad (3.17a)$$

where P is the principal part and the various quantities are defined by

$$P=Q+Q'+K\ ,\quad P_n=Q^n+Q'^n+K^n\ ,\quad (n=2,3,4,5)\,. \tag{3.17b}$$

Singularities in the k integral of (3.15) are at

$$k=\pm(\kappa+i\epsilon)\ ,\quad \kappa=(1/c_0)\,[(\omega_q+\omega_{q'})^2-\omega_0^2]^{1/2}\,. \tag{3.18}$$

We shall first discuss the transmitted wave at the region with a large positive x. The k integral in (3.15) can be closed by a contour of a large semicircle on the upper half of complex k plane. The residue at the pole $\kappa+i\epsilon$ gives the only contribution to the integral which takes the form

$$\psi_2^{\rm ph}(x,t)\xrightarrow[x\to+\infty]{}-\frac{3Bu_0^5}{4mc_0^2L^2}\times\mathrm{Re}\sum_{qq'}\frac{\alpha_q\alpha_{q'}}{\kappa}F(-\kappa,q,q')\times\exp\{i\kappa x-i(\omega_q+\omega_{q'})t+i(\theta_q+\theta_{q'})+\tfrac{1}{2}i[\Delta(\kappa)+\Delta(q)+\Delta(q')]\}. \tag{3.19}$$

The phase function is expanded at the point $q=q'=\bar q$. The wave number κ can be approximated by

$$\kappa\cong\bar\kappa+(v_q/v_\kappa)(q-\bar q+q'-\bar q), \tag{3.20a}$$

when can be derived with the help of (3.18). Here $\bar\kappa$ and v_κ are defined by

$$\bar\kappa=(1c_0)\left(4\bar\omega_q^2-\omega_0^2\right)^{1/2},\quad v_\kappa=(d\omega_q/dq)_{q=\bar\kappa}\,. \tag{3.20b}$$

The transmitted wave (3.19) finally takes the form

$$\psi_2^{\rm ph}(x,t)_{x\to+\infty}\to t(\bar q)\ \mathrm{Re}\exp\left(i\{\bar\kappa x-2\bar\omega_q t+2\bar\theta_q+[\tfrac{1}{2}\Delta(\bar\kappa)+\Delta(\bar q)]\}\right)\times[f((v_q/v_\kappa)x-v_qt-x_0-\Delta x_2)]^2, \tag{3.21}$$

where

$$t(q)=-(3/4u_0\xi_0^2\bar\kappa)F(-\bar\kappa,\bar q,\bar q), \tag{3.22a}$$

$$\Delta x_2=(\tfrac{1}{2}\Delta x_1)-(v_q/2v_\kappa)[d\Delta(\kappa)/d\kappa]_{\kappa=\bar\kappa}\,. \tag{3.22b}$$

The constant B was replaced by $mc_0^2/u_0^2\xi_0^2$, using (2.2) and a relation below (2.7). After a lengthy calculation, making use of (3.17a) and a relation $\bar K^2=4\bar Q^2+12$, we obtain

$$-i\int_{-\infty}^{\infty}dx\tanh(x/\sqrt{2}\xi_0)\varphi_{\bar\kappa}^*\varphi_{\bar q}^2=-\frac{4\sqrt{2}\pi\xi_0(4+\bar Q^2)^3}{\sinh[\pi(\bar Q-\frac{1}{2}\bar K)]}, \tag{3.23}$$

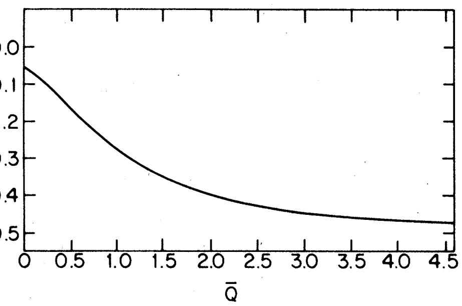

FIG. 3. Amplitude of the transmitted higher harmonics $t(\bar q)$. The abscissa is $\bar Q=\sqrt{2}\,\bar q\xi_0$.

where

$$\bar K=\sqrt{2}\bar\kappa\xi_0. \tag{3.24}$$

The amplitude of the transmitted wave $t(\bar q)$ is found to be

$$t(\bar q)=\frac{3\pi}{u_0\sinh[\pi(\bar Q-\frac{1}{2}\bar K)]}\ \frac{(\bar Q^2+4)^{3/2}}{\bar K(\bar Q^2+1)(4\bar Q^2+13)^{1/2}}\,. \tag{3.25}$$

The function $t(\bar q)$ is illustrated in Fig. 3. The transmitted wave is shifted forward by the amount

$$\Delta x_2=3\sqrt{2}\xi_0[(2+\bar Q^2)/(4+5\bar Q^2+\bar Q^4)+2\bar Q(2+\bar K^2)/\bar K(4+5\bar K^2+\bar K^4)], \tag{3.26}$$

which is shown in Fig. 1.

The reflected wave at the region with a large negative x can be obtained by the k integral in (3.15) with an additional contour of a large semicircle on the lower half of the complex k plane. The residue at the other pole $-\kappa-i\epsilon$ gives the contribution. Iterating the discussion above, we find

$$\psi_2^{\rm ph}(x,t)_{x\to-\infty}\to r(\bar q)\mathrm{Re}\exp\left(i\{-\bar\kappa x-2\bar\omega_qt+2\bar\theta_q+[\tfrac{1}{2}\Delta(\bar\kappa)+\Delta(\bar q)]\}\right).\times[f(-(v_q/v_\kappa)x-v_qt-x_0-\Delta x_2)]^2, \tag{3.27}$$

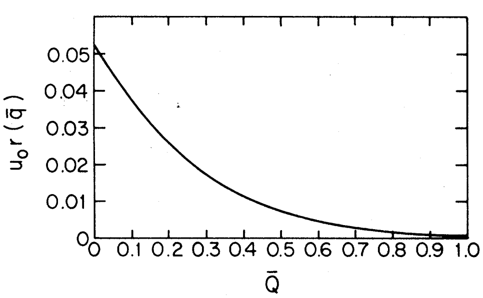

FIG. 4. Amplitude of the reflected higher harmonics $r(\bar q)$. The abscissa is $\bar Q=\sqrt{2}\,\bar q\xi_0$.

with the amplitude of the reflected wave

$$r(\bar{q})=\frac{3\pi}{u_0\sinh[\pi(\bar{Q}+\frac{1}{2}\bar{K})]}\frac{(\bar{Q}^2+4)^{3/2}}{\bar{K}(\bar{Q}^2+1)(4\bar{Q}^2+13)^{1/2}}\ . \tag{3.28}$$

It is illustrated in Fig. 4.

IV. STATISTICAL MECHANICS AND DIFFUSION CONSTANT

We have studied in Sec. III the elementary process of collision between a domain wall and a wave packet of phonon, which is nonlinear in the amplitude of the phonon. It gives rise to a motion of the domain wall. It should be one of the motives of the Brownian-like motion. However, the result of the simulation[3] shows that the wave trains of phonons are so long and overlapping that the concept of a wave packet hardly applies even at the low temperature $\bar{T}=k_BTB/A^2=0.117$. It is necessary to generalize the discussion of the elementary processes to the case that the phonon has an arbitrary distribution.

We are interested in the lowest-order effect of the nonlinear processes, that is, the effect to second order in the phonon amplitude. This means that it is unnecessary to take into account nonlinear effect in the phonon distribution. The latter contributes a term, to the diffusion constant, which is of the same order as that due to higher-order elementary processes. In this sense, our discussion is valid only at low temperature.

The displacement and momentum fields $u(x)$ and $p(x)$ are expanded in terms of the φ_i

$$u(x)=u_0\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)+\left(\frac{3}{4\sqrt{2}\xi_0}\right)^{1/2}q_0\varphi_0(x)+\left(\frac{3}{2\sqrt{2}\xi_0}\right)^{1/2}q_1\varphi_1(x)+\sum_k\frac{q_k\varphi_k(x)}{[2L(1+K^2)(4+K^2)]^{1/2}} \tag{4.1a}$$

$$p(x)=\left(\frac{3}{4\sqrt{2}\xi_0}\right)^{1/2}p_0\varphi_0(x)+\left(\frac{3}{2\sqrt{2}\xi_0}\right)^{1/2}p_1\varphi_1(x)+\sum_k\frac{p_k\varphi_k(x)}{[2L(1+K^2)(4+K^2)]^{1/2}}\ . \tag{4.1b}$$

Since these fields are real, the coefficients satisfy the relations

$$q_0^*=q_0,\quad q_1^*=q_1,\quad q_k^*=q_{-k}\,,$$
$$p_0^*=p_0,\quad p_1^*=p_1,\quad p_k^*=p_{-k}\,. \tag{4.2}$$

Introducing the real and imaginary parts of q_k and p_k by

$$q_k=q_{k1}+iq_{k2}\,,\quad p_k=p_{k1}+ip_{k2}\,,$$

we can show that the transformation of variables in a functional integral

$$(p(x_1),\ldots,p(x_n),u(x_1),\ldots,u(x_n))\to(p_0,p_1,\ldots p_{k1},p_{k2},\ldots q_0,q_1\ldots q_{k1},q_{k2}\ldots)$$

is canonical and

$$\prod_{i=1}^{N}dp(x_i)du(x_i)=(\Delta x)^{-N}dp_0dp_1dq_0dq_1\times\prod_{k>0}dp_{k1}dp_{k2}dq_{k1}dq_{k2}\,. \tag{4.3}$$

The proof of (4.3) is given in Appendix D.

Substitution of (4.1a) and (4.1b) into Hamiltonian (2.1) gives

$$H=-\int\frac{dxA^2}{4lB}+E_{DP}+\frac{1}{2ml}\left(p_0^2+p_1^2+\sum_{k>0}|p_k|^2\right)+\frac{m}{2l}\left(\frac{3\omega_0^2}{4}q_1^2+\sum_{k>0}\omega_k^2|q_k|^2\right), \tag{4.4}$$

where higher-order terms in the q_i are neglected, since the nonlinear effect in the phonon distribution is irrelevant. The constant E_{DP} is a domain wall potential energy introduced by KS. Relation (4.4) is derived in Appendix E.

Corresponding to (2.13), initial condition for the fields, $\psi(x)$ and $p(x)$, at $t=t_0$, can be written

$$\psi(x,t_0)=\left(\frac{3}{2\sqrt{2}\xi_0}\right)^{1/2}q_1\varphi_1(x)+\sum_k\frac{q_k\varphi_k(x)}{[2L(1+K^2)(4+K^2)]^{1/2}}, \tag{4.5a}$$

$$p(x,t_0)=m\dot{\psi}(x,t_0)=\left(\frac{3}{2\sqrt{2}\xi_0}\right)^{1/2}p_1\varphi_1(x)+\sum_k p_k\varphi_k\frac{(x)}{[2L(1+K^2)(4+K^2)]^{1/2}}\,. \tag{4.5b}$$

Distribution of the p_i and q_i is determined by Hamiltonian (4.4). In comparison with (4.1a) and (4.1b), we have chosen that $q_0=p_0=0$ since the domain wall is at the origin and not moving initially.

We can write the first-order solution of (2.17) as

$$\psi_1(x,t)=\left(\frac{3}{2\sqrt{2}\xi_0}\right)^{1/2}\left[a_1\exp\left(\frac{-i\sqrt{3}\omega_0t}{2}\right)+a_1^*\exp\left(\frac{i\sqrt{3}\omega_0t}{2}\right)\right]\varphi_1(x)+\sum_k\frac{[a_k\exp(-i\omega_kt)+a_{-k}^*\exp(i\omega_kt)]\varphi_k(x)}{[2L(1+K^2)(4+K^2)]^{1/2}}, \tag{4.6}$$

since the function ψ_1 is real. The initial conditions (4.5a) and (4.5) are satisfied if we require

$$q_k = a_k + a^*_{-k}\,, \quad p_k = mi\omega_k(a^*_{-k} - a_k)\,, \qquad (4.7)$$
$$q_1 = a_1 + a^*_1\,, \quad p_1 = \tfrac{1}{2}\sqrt{3}mi\omega_0(a^*_1 - a_1)\,.$$

Here were some trivial factors $\exp(\pm i\omega_k t_0)$ and $\exp(\pm\frac{1}{2}i\sqrt{3}\omega_0 t_0)$ which were removed by a proper redefinition of the a_i.

The second-order equation (3.2) is solved making use of the expansion (3.3). The unknown $\beta_0(t)$ satisfies (3.4a) where the function $\psi_{\rm I}$ on the right-hand side is now given by (4.6). Introducing the notations

$$F_0(k,k') = \left[-i\int_{-\infty}^{\infty} dx \tanh\frac{x}{\sqrt{2}\xi_0}\;\varphi_0\varphi_k\varphi_{k'}\right] \times [(1+K^2)(4+K^2)(1+K'^2)(4+K'^2)]^{-1/2}\,, \qquad (4.8a)$$

$$F_{01}(k) = \int_{-\infty}^{\infty} dx \tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_0\varphi_1\varphi_k \times [(1+K^2)(4+K^2)]^{-1/2}\,, \qquad (4.8b)$$

we can rewrite (3.4a),

$$\frac{d^2\beta_0}{dt^2} = -\frac{9c_0^2}{8\sqrt{2}u_0\xi_0^3}\left(\frac{i}{L}\sum_{kk'} F_0(k,k')(a_k e^{-i\omega_k t} + a^*_{-k}e^{i\omega_k t})(a_{k'}e^{-i\omega_{k'}t} + a^*_{-k'}e^{i\omega_{k'}t}) + \left(\frac{6\sqrt{2}}{\xi_0 L}\right)^{1/2}\sum_k F_{01}(k)[a_1 e^{-i\sqrt{3}\omega_0 t/2} + a_1^* e^{i\sqrt{3}\omega_0 t/2}[a_k e^{-i\omega_k t} + a^*_{-k}e^{i\omega_k t}]\right)\,. \qquad (4.9)$$

Use is made of the fact that

$$\int_{-\infty}^{\infty} dx \tanh\frac{x}{\sqrt{2}\xi_0}\;\varphi_0\varphi_1^2 = 0\,. \qquad (4.10)$$

We will again use the adiabatic hypothesis in order to integrate (4.9). If we put

$$\Phi(\omega,t) = \int_{-\infty}^{t} dt_1\int_{-\infty}^{t_1} dt_2\, e^{-i\omega t_2 + \epsilon t_2} = -\frac{\exp(-i\omega t)}{(\omega+i\epsilon)^2}\,, \qquad (4.11)$$

the integration of (4.9) gives

$$\beta_0(t) = -\left(\frac{9c_0^2}{8\sqrt{2}u_0\xi_0^3}\right)\Bigg\{\frac{i}{L}\sum_{kk'} F_0(k,k')[a_k a_{k'}\Phi(\omega_k+\omega_{k'},t) + 2a_k a^*_{-k'}\Phi(\omega_k - \omega_{k'},t) + a^*_{-k}a^*_{-k'}\Phi(\omega_k+\omega_{k'},t)^*]$$
$$+\left(\frac{6\sqrt{2}}{\xi_0 L}\right)^{1/2}\sum_k F_{01}(k)\left[a_1 a_k \Phi\left(\frac{\sqrt{3}\omega_0}{2} + \omega_k t\right) + a_1 a^*_{-k}\Phi\left(\frac{\sqrt{3}\omega_0}{2} - \omega_k, t\right) + a_1^* a_k \Phi\left(\frac{\sqrt{3}\omega_0}{2} - \omega_k, t\right)^*$$
$$+ a_1^* a^*_{-k}\Phi\left(\frac{\sqrt{3}\omega_0}{2} + \omega_k, t\right)^*\right]\Bigg\}. \qquad (4.12)$$

Thermal average of various quantities are easily evaluated with the help of Hamiltonian (4.4). Since $\langle q_k^2\rangle = \langle q_{k1}^2 - q_{k2}^2\rangle = 0$, $\langle p_k^2\rangle = 0$, $\langle |q_k|^2\rangle = 2lk_BT/m\omega_k^2$, and $\langle |p_k|^2\rangle = 2mlk_BT$, the relations in (4.7) lead to

$$\langle a_k a_{k'}\rangle = 0\,, \quad \langle a_k^* a_{k'}\rangle = (lk_BT/m\omega_k^2)\delta_{kk'}\,, \quad \langle a_1^2\rangle = 0\,, \quad \langle a_1^* a_1\rangle = 2lk_BT/3m\omega_0^2. \qquad (4.13)$$

Thermal average of the translation of the domain wall vanishes;

$$\langle\delta(t)\rangle = -\sqrt{2}\xi_0\langle\beta_0(t)\rangle/u_0 = 0\,, \qquad (4.14)$$

since it is the sum of the term $F_0(-k,k)$ which vanishes as (3.8) shows. Fluctuation of the translation $\langle\delta^2(t)\rangle$ turns out to be

$$\langle\delta(t)^2\rangle = \left(\frac{9\omega_0^2 lk_BT}{8mu_0^2 L}\right)^2\sum_{kk'}\left(\frac{F_0(k,k')}{\omega_k\omega_{k'}}\right)^2[|\Phi(\omega_k+\omega_{k'},t)|^2 + |\Phi(\omega_k-\omega_{k'},t)|^2]$$
$$+\frac{1}{\sqrt{2}\xi_0 L}\left(\frac{9\omega_0 lk_BT}{4mu_0^2}\right)^2\sum_k\left(\frac{F_{01}(k)}{\omega_k}\right)^2\left[\left|\Phi\left(\frac{\sqrt{3}\omega_0}{2}+\omega_k,t\right)\right|^2 + \left|\Phi\left(\frac{\sqrt{3}\omega_0}{2}-\omega_k,t\right)\right|^2\right]. \qquad (4.15)$$

As discussed in Sec. I, the diffusive wall motion is characterized by a diffusion constant D. According to the fluctuation-dissipation theorem, the knowledge of the fluctuation $\langle\delta(t)^2\rangle$ gives us the magnitude of the diffusion constant by relation (1.1):

$$D=\langle\delta(t)^2\rangle/2t\,,$$

when t is long in comparison with the mean free time. We are therefore interested in a component of $\langle\delta(t)^2\rangle$ which increases linearly with time. In other words, a component of $\langle\delta(t)^2\rangle$ which diverges linearly with $\epsilon\to 0$ is important. With the help of (4.11), we have

$$|\Phi(\omega,t)|^2=(\omega^2+\epsilon^2)^{-2}\,. \tag{4.16}$$

It is now evident that among the four terms in (4.15) the term with $|\Phi(\omega_k-\omega_{k'},t)|^2$ has a possibility to give such a contribution. It can be transformed as

$$\langle\delta(t)^2\rangle=\left(\frac{9\omega_0^2 lk_BT}{8\sqrt{2}\pi mu_0^2}\right)^2\times\int_0^\infty\int_0^\infty\frac{dk\,dk'\{[F_0(k,k')]^2+[F_0(k,-k')^2\}}{\omega_k^2\omega_{k'}^2[(\omega_k-\omega_{k'})^2+\epsilon^2]^2}\,. \tag{4.17}$$

Since $F_0(k,k')$ vanishes as $(k-k')^2$ at $k\sim k'$, as (3.8) shows, this term in the numerator of the integrand can be neglected. On the other hand, we obtain with the help of (3.8) and (4.8a),

$$F_0(k,-k')=\frac{\sqrt{2}\xi_0(K-K')K^2(2+K^2)}{(1+K^2)(4+K^2)}\,,\quad\text{at } k\sim k'\,. \tag{4.18}$$

Substitution into (4.17) gives

$$\langle\delta(t)^2\rangle=\left(\frac{9\omega_0^2\xi_0^2 lk_BT}{4\sqrt{2}\pi mu_0^2}\right)^2\int_0^\infty dk\frac{K^4(2+K^2)^2}{(1+K^2)^2(4+K^2)^2\omega_k^4(d\omega_k/dk)^3}\int_{-\infty}^\infty d\omega_{k'}\frac{(\omega_{k'}-\omega_k)^2}{[(\omega_{k'}-\omega_k)^2+\epsilon^2]^2}$$
$$=\left(\frac{9lk_BT}{2\sqrt{\pi}mu_0^2}\right)^2\frac{1}{\epsilon}\int_{\omega_0}^\infty\frac{d\omega_k(2\omega_k^2-\omega_0^2)^2}{\omega_k^4(4\omega_k^2-3\omega_0^2)^2}=\frac{81}{4\pi}\omega_0 l^2\left(\frac{k_bT}{mu_0^2\omega_0^2}\right)^2\frac{1}{\epsilon}\int_1^\infty\frac{dx(2x^2-1)^2}{x^4(4x^2-3)^2}\,. \tag{4.19}$$

The definite integral is evaluated to give a constant

$$\int_1^\infty\frac{dx(2x^2-1)^2}{x^4(4x^2-3)^2}=\left(\frac{7}{27\sqrt{3}}\right)\ln(2+\sqrt{3})-\tfrac{1}{27}\simeq 0.160\,.$$

The diffusion constant turns out to be

$$D=\frac{\langle\delta(t)^2\rangle}{2t}=\langle\delta(t)^2\rangle\Big/\left(2\int_{-\infty}^0 dt\,e^{\epsilon t}\right)$$
$$=\tfrac{1}{2}\epsilon\langle\delta(t)^2\rangle$$
$$=0.160\frac{81}{8\pi}\omega_0 l^2\left(\frac{k_BT}{mu_0^2\omega_0^2}\right)^2$$
$$=0.516\omega_0 l^2\left(\frac{k_BT}{mu_0^2\omega_0^2}\right)^2\,. \tag{4.20}$$

It is worth remarking that we have obtained the diffusion constant making use of the same mechanism as the finite translation of the domain wall was derived in the discussion of Sec. III. The singularity of energy denominator is somewhat suppressed by the vanishing numerator. It led to the finite domain-wall translation in Sec. III. It gives in this section the fluctuation of the translation which is proportional to t.

V. DISCUSSION

We have studied interaction between a phonon wave packet and domain wall. The second-order process in the amplitude of the incoming phonon gives rise to a translation of the domain wall, the effective interaction being attractive. The distance of the translation is rather insensitive to the wave number of the phonon. It decreases as the wave number increases. The value at the limit of short wavelength is one half of that of the limit of long wavelength. The order of magnitude of the translation is $|\delta|\sim u_0^2\alpha^2$ as given in (3.13). With the help of (2.13) and (3.12), we can find

$$\int_{-\infty}^\infty\psi_1^2\,dx\simeq\frac{u_0^4\alpha^2}{4\pi}\,, \tag{5.1}$$

which gives

$$|\delta|\sim\int_{-\infty}^\infty\frac{\psi_1^2\,dx}{u_0^2}\,. \tag{5.2}$$

In order to estimate the translation, we may calculate the produce of mean-square deviation of ions and the width of the packet. Its ratio with u_0^2 gives $|\delta|$

The higher harmonic generation is another interesting phenomenon. This does not happen in a situation with no domain walls. It is essential that the wave number of phonons may not be conserved during the generation process because of the presence of the domain wall. Suppose we try to observe the transmitted waves at $x>0$. We will observe two signals. The stronger one is that of the incident phonon. It reaches x at a time $(x-x_0-\Delta x_1)/v_q$ which is earlier by the amount $\Delta x_1/v_q$ than in a system without the domain wall. The weaker signal is due to the higher harmonic. Its "total intensity" $\int_{-\infty}^{\infty}(\psi_2^{\text{ph}})^2\,dx$ is of the order of $\int_{-\infty}^{\infty}\psi_1^4\,dx/u_0^2$ as shown with the help of (3.21), (3.25), and (2.20). It arrives at x when $t=x/v_\kappa-(x_0+\Delta x_2)/v_q$. Since $\Delta x_1>\Delta x_2$, the stronger signal is observed first if the distance x is so close that $x<\bar{K}(\Delta x_1-\Delta x_2)/(\bar{K}-2\bar{Q})$. The weaker signal travels ahead if $x>\bar{K}(\Delta x_1-\Delta x_2)/(\bar{K}-2\bar{Q})$, since its group velocity v_κ is faster than v_q.

We can observe also the reflected wave at $x<0$. In this case, there is only one signal due to the higher harmonic. It arrives at $-|x|$ when $t=|x|/v_\kappa-(x_0+\Delta x_2)/v_q$. The amplitude of the reflected signal will be much reduced compared to that of the transmitted wave as Fig. 4 shows.

It might be rather difficult to observe these phenomena in an actual physical system. One may be able to prepare an ideal quasi-one-dimensional system. But it would be hard to control the configuration of ions so as to form one domain wall. On the other hand, it would be easy to simulate the elementary processes in the molecular-dynamics calculation. It may allow us to evaluate the relative importance of the nonlinear process and the possible discrete-lattice effects in the diffusive-wall motion.

We have next studied interaction between a domain wall and a phonon field with an arbitrary distribution. The probability distribution is given by statistical mechanics in terms of a Hamiltonian which is bilinear in the phonon field when there is a domain wall. Use of the fluctuation-dissipation theorem gives us the diffusion constant at low temperature. It has turned out to be proportional to T^2. This temperature dependence is a result of the nonlinear process. Since the translation of the domain wall is proportional to the square of the phonon field, fluctuation of the translation is given by a quadruplet. Its thermal average by Hamiltonian (4.4) is, therefore, proportional to $(lk_BT)^2$. The ratio between the diffusion constant and $(lk_BT)^2$ has the dimension of $(\text{length})^{-4}\,(\text{time})^3\,(\text{mass})^{-2}$. In our formulation, we have introduced four constants m, A, B, and c_0. They are equivalently described by m, ω_0, ξ_0, and u_0. Thus it is clear that D should be proportional to $\omega_0^{-3}m^{-2}$. In order to understand why the diffusion constant does not depend on the wall thickness ξ_0, we consider the dependence on u_0. It is important to note that the eigenvalue problem (2.8) does not involve u_0 as a parameter. Neither does the Hamiltonian (4.4). Therefore, the first-order solution (4.6) does not depend on u_0. Equation (3.2) shows that the second-order solution is proportional to $Bu_0\propto u_0^{-1}$, leading to the relation $\beta_0(t)\propto u_0^{-1}$. The translation of the wall δ is thus proportional to u_0^{-2}. Finally, the diffusion constant turns out to be inversely proportional to u_0^4. The independence on the wall thickness is characteristic to the second-order nonlinear effect as the temperature dependence which is T^2.

Measurement of the diffusion constant should be more feasible than the elementary process since we do not need an ideal configuration of one domain wall and the constant is related to a dissipation process. The difficulty we have to meet is to obtain a good one-dimensional sample. The temperature and wall thickness dependence of the diffusion constant should be the most interesting properties to be measured. It is also important to obtain quantitative information on the magnitude of the diffusion constant with the help of molecular-dynamics computer simulation. It will clearly show if the nonlinear effect, discussed here, is really the most dominant mechanism which gives rise to the Brownian-like motion of domain walls.

Much remains to be done even when the nonlinear effect would turn out to be the dominant mechanism. Correction due to quantum effects in dynamics and statistics would have to be discussed at low temperature. It would be important to derive a Langevin equation for the motion of domain walls. It would give us information about the random force acting on the domain wall. We should be able to derive the fluctuation-dissipation theorem of the second kind which is a relation between the diffusion constant and fluctuation of the random force. The phonon dressing of domain walls, discovered by the simulation work,[3] should also be an interesting problem. It should have a close relationship with the nonlinear process discussed in this paper.

We would finally like to point out a new feature of our discussions. Unlike the usual Brownian particles, our domain walls and phonons are made of the common constituents—the ions. The difference is only in the manner of motion of the constituents. This situation is more universal in solid-state physics than that corresponding to the usual Brownian particles. Magnetic domain walls and spin waves are another example. One can find other examples in so-called soliton phenomena of various problems. Our work shows a possibility of investigating the interactions between the soliton and its surroundings when both are composed of the same constituents. Namely, we can use "normal modes" when there is a soliton, in which the Goldstone mode plays an important role. It is very likely that the method developed in this work has a wide range of application.

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APPENDIX A: ORTHONORMALITY RELATION (2.11c) AND COMPLETENESS RELATION (2.12)

With the help of the definition of $\varphi_q(x)$, (2.9c), we have

$$\int_{-\infty}^{\infty}\varphi_q^*(x)\varphi_{q'}(x)\,dx=\sqrt{2}\xi_0[9I_p(4)+9PI_p(3)-(3Q^2+3Q'^2-9QQ'+6)I_p(2)+3P(QQ'-1)I_p(1)]$$
$$+2\sqrt{2}\xi_0\int_0^{\infty}dy\,[(Q^2Q'^2-2Q^2-2Q'^2+9QQ'+4)\cos Py+3P(QQ'+2)\sin Py]\,, \tag{A1}$$

where $P=Q'-Q$. We define the quantities $I_p(n)$ by

$$I_p(2n)=2\int_0^{\infty}dy\,\cos Py(\tanh^{2n}y-1)\,,$$
$$I_p(2n+1)=2\int_0^{\infty}dy\,\sin Py(\tanh^{2n+1}y-1)\,. \tag{A2}$$

Integrating by parts, we can obtain a recursion formula

$$I_p(2n)=I_p(2n-2)-2/(2n-1)-[P/(2n-1)]I_p(2n-1)\,,$$
$$I_p(2n+1)=I_p(2n-1)+(P/2n)I_p(2n)\,. \tag{A3}$$

This is solved to give

$$\begin{aligned}
I_p(2)&=-2-PI_p(1)\,,\\
I_p(3)&=-P+(1-\tfrac{1}{2}P^2)I_p(1)\,,\\
I_p(4)&=-\tfrac{8}{3}+\tfrac{1}{3}P^2+(-\tfrac{4}{3}P+\tfrac{1}{6}P^3)I_p(1)\,,\\
I_p(5)&=-\tfrac{5}{3}P+\tfrac{1}{12}P^3+(1-\tfrac{5}{6}P^2+\tfrac{1}{24}P^4)I_p(1)\,,\\
I_p(6)&=-\tfrac{46}{15}+\tfrac{2}{3}P^2-\tfrac{1}{60}P^4\\
&\quad+(-\tfrac{23}{15}P+\tfrac{1}{3}P^3-\tfrac{1}{120}P^5)I_p(1)\,,\\
I_p(7)&=-\tfrac{98}{45}P+\tfrac{7}{36}P^3-\tfrac{1}{360}P^5\\
&\quad+(1-\tfrac{49}{45}P^2+\tfrac{7}{22}P^4-\tfrac{1}{720}P^6)I_p(1)\,.
\end{aligned} \tag{A4}$$

The integral $I_p(1)$ is given by[9]

$$I_p(1)=\frac{2}{P}\left(-1+\int_0^{\infty}dy\,\cos Py\,\mathrm{sech}^2y\right)=-\frac{2}{P}+\frac{\pi}{\sinh(\frac{1}{2}\pi P)}\,. \tag{A5}$$

Substitution of (A5) into (A4) gives

$$\begin{aligned}
I_p(2)&=-P\pi/\sinh(\tfrac{1}{2}\pi P)\,,\\
I_p(3)&=-2/P+(1-\tfrac{1}{2}P^2)\pi/\sinh(\tfrac{1}{2}\pi P)\,,\\
I_p(4)&=(-\tfrac{4}{3}P+\tfrac{1}{6}P^3)\pi/\sinh(\tfrac{1}{2}\pi P)\,,\\
I_p(5)&=-2/P+(1-\tfrac{5}{6}P^2+\tfrac{1}{24}P^4)\pi/\sinh(\tfrac{1}{2}\pi P)\,,\\
I_p(6)&=(-\tfrac{23}{15}P+\tfrac{1}{3}P^3-\tfrac{1}{120}P^5)\pi/\sinh(\tfrac{1}{2}\pi P)\,,\\
I_p(7)&=-2/P+(1-\tfrac{49}{45}P^2-\tfrac{7}{72}P^4\\
&\quad-\tfrac{1}{720}P^6)\pi/\sinh(\tfrac{1}{2}\pi P)\,.
\end{aligned} \tag{A6}$$

The integrals of the trigonometric functions are

$$\int_0^{\infty}dy\,\cos Py=\lim_{\epsilon\to 0+}\int_0^{\infty}dy\,e^{-\epsilon y}\cos Py=\pi\delta(P)\,.$$
$$\int_0^{\infty}dy\,\sin Py=\lim_{\epsilon\to 0+}\int_0^{\infty}dy\,e^{-\epsilon y}\sin Py=\mathrm{P}/P\,, \tag{A7}$$

where P is the principal part.

Substituting (A5)–(A7) into (A1), we find the right-hand side cancels each other except the integral of $\cos Py$ which gives

$$\int_{-\infty}^{\infty}dx\,\varphi_q^*(x)\varphi_{q'}(x)=2\pi(1+Q^2)(4+Q^2)\delta(q-q')\,. \tag{A8}$$

With the help of (2.9c), the third term on the left-hand side of (2.12) can be rewritten

$$\int_{-\infty}^{\infty}\frac{dq\,\varphi_q(x)\varphi_q^*(x')}{2\pi(1+Q^2)(4+Q^2)}=\int_{-\infty}^{\infty}\frac{dq}{2\pi}e^{iq(x-x')}\Bigg[1+(1+Q^2)^{-1}(4+Q^2)^{-1}\Bigg(3iQ^3\left[\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)-\tanh\left(\frac{x'}{\sqrt{2}\xi_0}\right)\right]$$
$$-Q^2\left[3\tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right)+3\tanh^2\left(\frac{x'}{\sqrt{2}\xi_0}\right)-9\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\tanh\left(\frac{x'}{\sqrt{2}\xi_0}\right)+3\right]$$
$$+3iQ\left\{\tanh\left(\frac{x'}{\sqrt{2}\xi_0}\right)\left[3\tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right)-1\right]-\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\left[3\tanh^2\left(\frac{x'}{\sqrt{2}\xi_0}\right)-1\right]\right\}$$
$$+9\tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right)\tanh^2\left(\frac{x'}{\sqrt{2}\xi_0}\right)-3\tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right)-3\tanh^2\left(\frac{x'}{\sqrt{2}\xi_0}\right)-3\Bigg)\Bigg]\,.$$

If $x>x'$, $(x<x')$, the q integral along a large semicircle on the upper (lower) half of the complex q plane can be added to form a closed contour. The poles, at $q=i/\sqrt{2}\xi_0, \sqrt{2}i/\xi_0, (-i/\sqrt{2}\xi_0, -\sqrt{2}i/\xi_0)$ make contribution to give

$$\int_{-\infty}^{\infty}\frac{dq\,\varphi_q(x)\varphi_q^*(x')}{2\pi(1+Q^2)(4+Q^4)}=\delta(x-x')+\frac{3}{2\sqrt{2}\xi_0}\exp\left(-\frac{1}{\sqrt{2}\xi_0}|x-x'|\right)$$
$$\left\{\tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right)\tanh^2\left(\frac{x'}{\sqrt{2}\xi_0}\right)\right.$$
$$\left.-\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\tanh\left(\frac{x'}{\sqrt{2}\xi_0}\right)\pm\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\tanh\left(\frac{x'}{\sqrt{2}\xi_0}\right)\left[\tanh\left(\frac{x'}{\sqrt{2}\xi_0}\right)-\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\right]\right\}$$
$$-\frac{3}{4\sqrt{2}\xi_0}\exp\left(-\frac{\sqrt{2}}{\xi_0}|x-x'|\right)\left\{1+\tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right)\tanh^2\left(\frac{x'}{\sqrt{2}\xi_0}\right)+\tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right)\right.$$
$$+\tanh^2\left(\frac{x'}{\sqrt{2}\xi_0}\right)-4\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\tanh\left(\frac{x'}{\sqrt{2}\xi_0}\right)$$
$$\left.\mp2\left[\tanh\left(\frac{x'}{\sqrt{2}\xi_0}\right)-\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\right]\left[1-\tanh\left(\frac{x}{\sqrt{2}\xi_0}\right)\tanh\left(\frac{x'}{\sqrt{2}\xi_0}\right)\right]\right\}$$
$$=\delta(x-x')-\frac{3}{4\sqrt{2}\xi_0}\varphi_0(x)\varphi_0(x')-\frac{3}{2\sqrt{2}\xi_0}\varphi_1(x)\varphi_1(x').\tag{A9}$$

APPENDIX B: DERIVATION OF EQ. (3.8)

With the help of the definition of $\varphi_q(x)$ (2.9c), we can rewrite the integral (3.8)

$$\int_{-\infty}^{\infty}dx\,\tanh(x/\sqrt{2}\xi_0)\varphi_0\varphi_q\varphi_{q'}=\sqrt{2}\xi_0 i\{P[9I_p(6)-(12+3QQ')I_p(4)+(3+3QQ')I_p(2)]$$
$$-9I_p(7)+(15+3Q^2+3Q'^2+9QQ')I_p(5)$$
$$-(7+4Q^2+4Q'^2+9QQ'+Q^2Q'^2)I_p(3)+(1+Q^2)(1+Q'^2)I_p(1)\},\tag{B1}$$

where $P=Q+Q'$. Substituting (A4) and (A5), we obtain

$$\int_{-\infty}^{\infty}dx\tanh(x/\sqrt{2}\xi_0)\varphi_0\varphi_q\varphi_{q'}=\frac{\pi i(Q^2-Q'^2)^2\xi_0[1+(Q^2+Q'^2)/4]}{2\sqrt{2}\sinh[\pi(Q+Q')/2]}.\tag{B2}$$

APPENDIX C: DERIVATION OF EQ. (3.17a)

Calculation is lengthy but straightforward. We shall write here an intermediate expression for the integral (3.17a)

$$\int_{-\infty}^{\infty}dx\tanh(x/\sqrt{2}\xi_0)\varphi_k\varphi_q\varphi_{q'}=\sqrt{2}\xi_0 i\{27I_p(7)-27I_p(6)+(-27+\tfrac{9}{2}P_2-\tfrac{27}{9}P^2)I_p(5)$$
$$+9(2P-\tfrac{1}{2}P_2P+\tfrac{1}{2}P^3)I_p(4)$$
$$+(9+\tfrac{3}{2}P_2+\tfrac{3}{8}P_2^2+\tfrac{3}{4}P_4+\tfrac{9}{2}P^2-\tfrac{9}{4}P^2P_2+\tfrac{9}{8}P^4)I_p(3)$$
$$+3(-P-P_2P+P_3-\tfrac{1}{2}PP_2^2+P_2P_3+\tfrac{1}{2}P_4P-P_5)I_p(2)$$
$$-[1+P_2+\tfrac{1}{2}P_2^2-\tfrac{1}{2}P_4+\tfrac{1}{6}P^3+\tfrac{1}{2}P_2P-\tfrac{1}{3}P_3)^2]I_p(1)\}$$
$$+2\sqrt{2}\xi_0 i(8+5P_2+\tfrac{5}{4}P_4-\tfrac{1}{8}P_2^2-\tfrac{1}{9}P_3^2-9P^2$$
$$-\tfrac{9}{4}P^2P_2+\tfrac{9}{8}P_4+\tfrac{1}{3}PP_3P_2-\tfrac{1}{9}P_3P^3-\tfrac{1}{4}P_2^2P^2+\tfrac{1}{6}P_2P^4-\tfrac{1}{36}P^6)\int_0^{\infty}dy\sin Py$$
$$+6\sqrt{2}\xi_0 i(P_3+P_2P_3-P_5)\int_0^{\infty}dy\cos Py.$$

APPENDIX D: PROOF OF EQ. (4.3)

We introduce a lattice space in order to carry out the functional integral in a thermal average over the phonons. The length of the system L is divided into N parts by the points $(x_1, x_2, \ldots, x_N)$ which are distributed uniformly with the distance Δx; $L = N\Delta x$. The distance Δx would physically be identical with l, but mathematically we may assume that Δx is independent of l. In this lattice space, the completeness relation (2.12) reads

$$\frac{3\Delta x}{4\sqrt{2}\,\xi_0}\varphi_0(x_i)\varphi_0(x_j)+\frac{3\Delta x}{2\sqrt{3}\,\xi_0}\varphi_1(x_i)\varphi_1(x_j)+\sum_q \frac{\varphi_q(x_i)\varphi_q^*(x_j)}{N(1+Q^2)(4+Q^2)}=\delta_{ij}\,. \tag{D1}$$

Tranformation of integration variables generally gives a relation

$$\prod_{i=1}^{N} dp\,(x_i)du(x_i)=J\begin{pmatrix} p(x_1) & \cdots & p(x_N) \\ P_0P_1 \cdots & p_{k1}p_{k2}\cdots & \end{pmatrix} J\begin{pmatrix} u(x_1) & \cdots & u(x_N) \\ q_0q_1 \cdots & q_{k1}q_{k2} & \cdots \end{pmatrix} \times dp_0dp_1dq_0dq_1 \prod_{k>0} dp_{k1}dp_{k2}dq_{k1}dq_{k2}\,. \tag{D2}$$

Both Jacobians have the same value since the transformation (4.1a) is identical with (4.1b) except for a constant term $u_0\tanh(x)/\sqrt{2}\xi_0)$. It is easy to find that

$$J\begin{pmatrix} u(x_1) & \cdots & u(x_N) \\ q_0q_1 \cdots & q_{k1}q_{k2} & \cdots \end{pmatrix}=$$

$$\begin{matrix} \left(\frac{3}{4\sqrt{2}\,\xi_0}\right)^{1/2}\varphi_0(x_1)\left(\frac{3}{2\sqrt{2}\,\xi_0}\right)^{1/2}\varphi_1(x_1)\cdots & \frac{\mathrm{Re}\varphi_k(x_1)}{\sqrt{L(1+K^2)(2+K^2/2)}} & \frac{-Im\rho_k(x_1)}{\sqrt{L(1+K^2)(2+K^2/2)}} & \cdots \\ \left(\frac{3}{4\sqrt{2}\,\xi_0}\right)^{1/2}\varphi_0(x_2)\left(\frac{3}{2\sqrt{2}\,\xi_0}\right)^{1/2}\varphi_1(x_2)\cdots & \frac{\mathrm{Re}\varphi_k(x_2)}{[L(1+K^2)(2+K^2/2)]^{1/2}} & \frac{-Im\varphi_k(x_2)}{[L(1+K^2)(2+K^2/2)]^{1/2}} & \cdots \\ \vdots \quad \cdots & \vdots & & \cdots \end{matrix}$$

With the help of the completeness relation (D1), we obtain

$$J^2=JJ^{\text{transposed}}=\begin{vmatrix} (\Delta x)^{-1} & 0 & 0 & \cdots \\ 0 & (\Delta x)^{-1} & 0 & \cdots \\ 0 & 0 & (\Delta x)^{-1} & \cdots \\ \vdots & \vdots & \vdots & \cdots \end{vmatrix}=(\Delta x)^{-N}\,. \tag{D3}$$

APPENDIX E: DERIVATION OF EQ. (4.4)

With the help of the expansion of $p(x)$ (4.1b), it is easily seen

$$\int_{-\infty}^{\infty}\frac{dxp(x)^2}{2m}=\frac{1}{2m}\left(p_0^2+p_1^2+\sum_{k>0}|p_k|^2\right), \tag{E1}$$

where the orthogonality relations (2.11a)–(2.11c) are used with

$$2\pi\delta(k-k')=L\delta_{kk'}\,. \tag{E2}$$

Neglecting higher-order terms in the q_i, we can similarly obtain

$$\int_{-\infty}^{\infty} dx\, u(x)^2 = \int_{-\infty}^{\infty} dx \left\{ u_0^2 \tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right) + 2u_0 \tanh\left(\frac{x}{\sqrt{2}\xi_0}\right) \left[\left(\frac{3}{2\sqrt{2}\xi_0}\right)^{1/2} q_1\varphi_1 + \sum_k \frac{q_k\varphi_k}{[2L(1+K^2)(4+K^2)]^{1/2}}\right]\right\} + q_0^2 + q_1^2 + \sum_{k>0} |q_k|^2 , \quad \text{(E3)}$$

$$\int_{-\infty}^{\infty} dx\, u(x)^4 \simeq \int_{-\infty}^{\infty} dx \left\{ u_0^4 \tanh^4\left(\frac{x}{\sqrt{2}\xi_0}\right) + 4u_0^3 \tanh^3\left(\frac{x}{\sqrt{2}\xi_0}\right)\left[\left(\frac{3}{2\sqrt{2}\xi_0}\right)^{1/2} q_1\varphi_1 + \sum_k \frac{q_k\varphi_k}{[2L(1+K^2)(4+K^2)]^{1/2}}\right] + 6u_0^2 \tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right)\left[\left(\frac{3}{4\sqrt{2}\xi_0}\right)^{1/2} q_0\varphi_0 + \left(\frac{3}{2\sqrt{2}\xi_0}\right)^{1/2} q_1\varphi_1 + \sum_k \frac{q_k\varphi_k}{[2L(1+K^2)(4+K^2)]^{1/2}}\right]^2\right\} , \quad \text{(E4)}$$

$$\int_{-\infty}^{\infty} dx \left(\frac{du}{dx}\right)^2 = \int_{-\infty}^{\infty} dx \left\{\left(\frac{u_0^2}{2\xi_0^2}\right) \operatorname{sech}^4\left(\frac{x}{\sqrt{2}\xi_0}\right) + \frac{\sqrt{2}u_0}{\xi_0}\operatorname{sech}^2\left(\frac{x}{\sqrt{2}\xi_0}\right)\left[\left(\frac{3}{2\sqrt{2}\xi_0}\right)^{1/2} \frac{q_1 d\varphi_1}{dx} + \sum_k \frac{q_k d\varphi_k}{[2L(1+K^2)(4+K^2)^{1/2}]}\right] + \left[\left(\frac{3}{4\sqrt{2}\xi_0}\right)^{1/2} \frac{q_0 d\varphi_0}{dx} + \left(\frac{3}{2\sqrt{2}\xi_0}\right)^{1/2} \frac{q_1 d\varphi_1}{dx} + \sum_k \frac{q_k d\varphi_k}{[2L(1+K^2)(4+K^2)]^{1/2}}\right]^2\right\} . \quad \text{(E5)}$$

Substitution of (E3)–(E5) into the Hamiltonian (2.1) shows that the linear terms with respect to q_1 and q_k cancel each other, since

$$(\tfrac{1}{2}A)2u_0 \tanh\left(\frac{x}{\sqrt{2}\xi_0}\right) + (\tfrac{1}{4}B)4u_0^3 \tanh^3\left(\frac{x}{\sqrt{2}\xi_0}\right) - \frac{mc_0^2}{2}\frac{\sqrt{2}u_0}{\xi_0}\frac{d}{dx}\operatorname{sech}^2\left(\frac{x}{\sqrt{2}\xi_0}\right) = 0 , \quad \text{(E6)}$$

where the last term is obtained by a partial integration. The cross terms in the quadratic form also vanish. For example, the $q_0 q_k$ term has a coefficient proportional to

$$(\tfrac{1}{4}B)6u_0^2 \int_{-\infty}^{\infty} dx \tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_0\varphi_k + \frac{mc_0^2}{2}\int_{-\infty}^{\infty} dx \frac{d\varphi_0}{dx}\frac{d\varphi_k}{dx} = \frac{|A|}{2}\left[3\int_{-\infty}^{\infty} dx \tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_0\varphi_k - \xi_0^2\int_{-\infty}^{\infty} dx \frac{d^2\varphi_0}{dx^2}\varphi_k\right] , \quad \text{(E7)}$$

which vanishes with the help of the relation

$$d^2\varphi_0/dx^2 = -\varphi_0/\xi_0^2 + (3\varphi_0/\xi_0^2)\tanh^2(x/2\xi_0) . \quad \text{(E8)}$$

This relation gives the coefficient of q_0^2 term

$$(\tfrac{1}{4}B)6u_0^2 \int_{-\infty}^{\infty} dx \tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_0^2 + \frac{mc_0^2}{2}\int_{-\infty}^{\infty} dx \left(\frac{d\varphi_0}{dx}\right)^2 = \frac{|A|}{2}\int_{-\infty}^{\infty} dx\, \varphi_0^2 = \frac{2\sqrt{2}\xi_0|A|}{3} . \quad \text{(E9)}$$

Similarly, the coefficient of $q_1 q_k$ term is proportional to

$$(\tfrac{1}{4}B)6u_0^2 \int_{-\infty}^{\infty} dx \tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_1\varphi_k + \frac{mc_0^2}{2}\int_{-\infty}^{\infty} dx \frac{d\varphi_1}{dx}\frac{d\varphi_k}{dx} = \frac{|A|}{2}\left[3\int_{-\infty}^{\infty} dx \tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_1\varphi_k - \xi_0^2\int_{-\infty}^{\infty} dx \frac{d^2\varphi_1}{dx^2}\varphi_k\right] , \quad \text{(E10)}$$

which vanishes with the help of the relation

$$d^2\varphi_1/dx^2 = -5\varphi_1/2\xi_0^2 + (3/\xi_0^2)\tanh^2(x/\sqrt{2}\xi_0)\varphi_1 . \quad \text{(E11)}$$

Thus we also have the coefficient of q_1^2 term

$$(\tfrac{1}{4}B)6u_0^2 \int_{-\infty}^{\infty} dx \tanh^2\left(\frac{x}{\sqrt{2}\xi_0}\right)\varphi_1^2 + \frac{mc_0^2}{2}\int_{-\infty}^{\infty} dx \left(\frac{d\varphi_1}{dx}\right)^2 = \tfrac{5}{4}|A|\int_{-\infty}^{\infty} dx\, \varphi_1^2 = \frac{5\xi_0|A|}{3\sqrt{2}} . \quad \text{(E12)}$$

The coefficient of $q_k q_{k'}$ term is proportional to

$$3\int_{-\infty}^{\infty}dx\tanh^2\left(\frac{x}{\sqrt{2}\,\xi_0}\right)\varphi_k\varphi_{k'}+\xi_0^2\int_{-\infty}^{\infty}dx\left(\frac{d\varphi_k}{dx}\right)\left(\frac{d\varphi_{k'}}{dx}\right)$$

$$=\sqrt{2}\,\xi_0\{45I_P(6)+45PI_P(5)-[54+45KK'+18(K^2+K'^2)]I_P(4)-[39P+18PKK'+3(K^3+K'^3)]I_P(3)$$
$$+[21+12(K^2+K'^2)+24KK'+3(K^2+K'^2)KK'+\tfrac{15}{2}K^2K'^2]I_P(2)$$
$$+[12P+3(K^3+K'^3)+6PKK'+\tfrac{3}{2}PK^2K'^2]I_P(1)\}$$
$$+2\sqrt{2}\,\xi_0[12-21KK'-6(K^2+K'^2)+3(K^2+K'^2)KK'+\tfrac{15}{2}K^2K'^2]\int_0^{\infty}dx\cos Px$$
$$+2\sqrt{2}\,\xi_0(18P-12PKK'+\tfrac{3}{2}PK^2K'^2)\int_0^{\infty}dx\sin Px-2\sqrt{2}\,\pi\xi_0[8KK'+2KK'(K^2+K'^2)+\tfrac{1}{2}K^3K'^3]\delta(P)\,, \qquad \text{(E13)}$$

where $P=K+K'$.

Substituting (A5)–(A7) into (E13) and using (E2), we obtain

$$3\int_{-\infty}^{\infty}dx\tanh^2\left(\frac{x}{\sqrt{2}\,\xi_0}\right)\varphi_k\varphi_{k'}+\xi_0^2\int_{-\infty}^{\infty}dx\left(\frac{d\varphi_k}{dx}\right)\left(\frac{d\varphi_{k'}}{dx}\right)=L(12+17K^2+\tfrac{11}{2}K^4+\tfrac{1}{2}K^6)\delta_{k-k'}\,. \qquad \text{(E14)}$$

The constant term in the Hamiltonian is

$$\int_{-\infty}^{\infty}\frac{dx}{l}\left[\tfrac{1}{2}Au_0^2\tanh^2\left(\frac{x}{\sqrt{2}\,\xi_0}\right)+\tfrac{1}{4}Bu_0^4\tanh^4\left(\frac{x}{\sqrt{2}\,\xi_0}\right)+\frac{mc_0^2u_0^2}{4\xi_0^2}\operatorname{sech}^4\left(\frac{x}{\sqrt{2}\,\xi_0}\right)\right]=E_{DP}+\int_{-\infty}^{\infty}\left(\frac{dx}{l}\right)\left(\frac{Au_0^2}{2}\right)+\left(\frac{Bu_0^4}{4}\right)$$
$$=E_{DP}-\int_{-\infty}^{\infty}\frac{dxA^2}{4lB}\,, \qquad \text{(E15)}$$

where E_{DP} is the domain-wall potential energy introduced by KS. Substituting the various relations obtained above into (2.1), we finally find

$$H\simeq-\int_{-\infty}^{\infty}\frac{dxA^2}{4lB}+E_{DP}+\left(\frac{1}{2ml}\right)\left(p_0^2+p_1^2+\sum_{k>0}|p_k|^2\right)$$
$$+\left(\frac{A}{2l}\right)\left(q_0^2+q_1^2+\sum_{k>0}|q_k|^2\right)+\left(\frac{|A|}{2l}\right)q_0^2+\left(\frac{5|A|}{4l}\right)q_1^2+\frac{|A|}{2l}\sum_k\frac{12+17K^2+\frac{11}{2}K^4+\frac{1}{2}K^6}{2(1+K^2)(4+K^2)}|q_k|^2$$
$$=-\int_{-\infty}^{\infty}dx\frac{A^2}{4lB}+E_{DP}+\frac{1}{2ml}\left(p_0^2+p_1^2+\sum_{k>0}|p_k|^2\right)+\left(\frac{m}{2l}\right)\left(\frac{3\omega_0^2}{4}q_1^2+\sum_{k>0}\omega_k^2|q_k|^2\right). \qquad \text{(E16)}$$

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*Permanent address: Department of Physics, University of Tokyo, Tokyo, Japan.

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