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Dynamics of anharmonic lattices: Solitons and the central-peak problem in one dimension

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The properties of a model classical Hamiltonian describing one-dimensional anharmonic lattices is studied by a new approach. The Hamiltonian represents particles sitting on one or the other side of a double-well potential and interacting with each other through harmonic forces. The model can describe order-disorder or displacive phase transitions. We look for solutions of the equations of motion of the form $\Psi(x,t)=\Sigma_i \Psi_l^i(x,t)\Psi_{nl}^i(x,t)$, where $\Psi_l^i(x,t)$ is the ith harmonic solution of the linear problem and obtain differential equations for the functions $\Psi_{nl}^i(x,t)$ with the assumption that Ψ_{nl}^i vary slowly compared with Ψ_l^i. The solutions for $\Psi_{nl}^i(x,t)$ are shown to be solitons, which are stationary traveling pulses whose properties have been extensively studied recently. The physical interpretation of solitons seems to be in terms of moving domains and dislocations, which transfer particles from one side of the well to the other during their passage. The energy of the solitons is calculated in terms of their amplitude and their velocity. The effect on the dynamic structure factor of the new solutions is considered. Solitons lead to a frequency width of the phonon and also give a quasielastic peak—the "central peak." The height and width of the central peak and of the phonons depend on the density of the solitons thermally excited and their velocity distribution. The spatial and temporal correlations due to the solitons increase exponentially with decreasing temperature and start becoming important about a temperature which is just the mean-field transition temperature of the conventional theory. In an appendix we study another anharmonic problem by similar methods.

I. INTRODUCTION

Debye's[1] classic paper in 1914 laid the foundation for most of the developments in our understanding of anharmonic (nonlinear) lattices. The basic principle of solution has remained the same: One uses as a basis set the solution of the harmonic (linear) lattice, and treats the nonlinearity in perturbation theory. In quantum-mechanical theory, the solution of the harmonic lattice yields a set of quasiparticles—the phonons. The phonons are labeled by the momentum k and polarization λ. The anharmonicity is expressible as interaction among the phonons. These interactions are treated in perturbation theory and lead to a shift in the energy of the phonons and to a finite lifetime for them. In modern theory, the solution is expressed in terms of the dynamic structure factor $S(\vec{k},\omega)$, which gives the probability distribution of energies at which the lattice can absorb energy at a wave vector $\vec{k}$.

With anharmonic perturbation theory, many of the properties of solids such as thermal expansion, thermal conductivity, sound attenuation, etc., are qualitatively and often quantitatively understood. Generalizations of the same basic theory lead to understanding of even very anharmonic solids like those of the isotopes of helium.

The microscopic theory of the stability of crystal structures and of their phase transformation from one to another structure is also based on anharmonic perturbation theory.[2,3] The question of the stability of a structure against a perturbation at a wave vector $\vec{k}$ is put in terms of the restoring force at that wave vector. When, as a function of temperature or pressure, the restoring force goes to zero, the crystal deforms and acquires the periodicity represented by $\vec{k}$. Equivalently one may calculate the phonon frequency $\omega(\vec{k})$. When $\omega(\vec{k})$ tends to zero as a function of temperature or pressure owing to the energy shifts arising from anharmonicity, the lattice tends to be unstable and the phonon is said to be soft.

In recent years, neutron scattering[4-6] has revealed that a structural phase transition is often accompanied, in addition to the soft phonon mode, by a quasielastic mode ($\omega\simeq 0$). This mode has commonly been termed the "central peak" of the structure factor $S(\vec{k},\omega)$. As the temperature is lowered towards the phase transition the central peak grows in intensity at the expense of the soft mode. While with anharmonic perturbation theory, the soft phonon mode is well understood, the central peak has remained a puzzling feature. One of the approaches[7] taken towards understanding the central peak draws its inspiration from liquids,[8] where such peaks always occur, and are due to the interaction between adiabatic and isothermal vibration modes or due to the interaction of collective phonon modes with internal modes of the molecules. The predictions of this approach do not agree with several features of the experimental results. Another reason[5,9] proposed is that the central peak arises simply from the elastic momentum-independent scattering from the defects in the crystals, the strains around which increase as the phase transition is approached.

It is suspected that as the phase transition is approached the amplitude of vibration of atoms becomes so large that anharmonic perturbation theory may well not be valid. With this view some numerical studies[10,11] of one- and two-dimensional anharmonic lattices have been performed. These numerical studies indicate that at least in one and two dimensions, the central-peak phenomenon is in principle an intrinsic dynamical property. The properties of the central peak obtained are, however, quite different from those observed in real materials. To clarify the situation, it is of considerable interest to study the problem of anharmonic lattices by analytic methods which are not the conventional anharmonic perturbation theory. Such an approach is possible now, at least for a one-dimensional lattice, because of the great strides taken recently in the solutions of (one space and one time dimensional) dispersive nonlinear partial differential equations.[12]

Actually, some of these partial differential equations pertain directly to the classical one-dimensional anharmonic lattice problem. The one-dimensional anharmonic string (lattice) was first studied numerically by Fermi, Pasta, and Ulam[13] with a view to understanding the process of approach to thermal equilibrium following the excitation of a given mode. In fact, it was observed that thermal equilibrium is not achieved and that the energy returned periodically in the initial mode with a period related to the nonlinearity. Further numerical studies were carried out by Zabusky and Kruskal,[14] who also showed that the one-dimensional dispersive string problem could be cast in the form of the solution to the Kortweg–de Vries (KdV) equation, first studied in connection with water waves in shallow channels. The class of equations of which KdV is one has been studied extensively[12,15] by mathematicians in recent years and has some remarkable properties. Any initial perturbation can be shown to break up into a series of stationary traveling pulses which pass through each other without distorting. These pulses have been referred to as solitons.

Tappert and Varma[16] showed that in a real three-dimensional lattice, under certain conditions, the KdV equation is realized. Further, it was shown that an envelope or modulation of plane waves in a one-dimensional anharmonic lattice obeys another nonlinear equation which has recently been well studied—and named the nonlinear Schrödinger equation, which is familiar to physicists as the time-dependent Landau-Ginzburg equation. This equation also has solitons (envelope solitons) under certain conditions as solutions. The solitons were actually observed in heat-pulse experiments in NaF at low temperatures by Narayanamurti and Varma.[17]

Several problems arise in applying the knowledge of the solution of the nonlinear equations to statistical physics. One is that the solutions to the nonlinear equations are radically different in nature from the solution to the linear problem. The former are generally localized (although moving) while the latter are plane waves. One wishes to retain the linear solutions, about which so much is understood, while studying the properties of the new solutions, and understand the relative role of the two as the nonlinearity is altered. We accomplish this by first setting up the differential equation for particle motion for the given Hamiltonian. After finding the solution of this equation we expand the differential equation about it and look for solutions which are sum of the products of the ith harmonic of the linear part of the problem $\Psi_l^{(i)}(x,t)$ and another function $\Psi_{nl}^{(i)}(x,t)$:

$$\Psi(x,t)=\sum_i \Psi_l^{(i)}(x,t)\Psi_{nl}^{(i)}(x,t)\,. \qquad (1)$$

Inserting solutions of the form (1) into the differential equation, we obtain a differential equation that $\Psi_{nl}^{(i)}(x,t)$ must satisfy with appropriate boundary conditions.

Another problem arises because the solutions of these differential equations (solitons) are solutions to boundary-value problems. In trying to make an equilibrium statistical-mechanical theory for them we simply characterize a given soliton by its energy and assume that their density is simply given in terms of their energy and temperature just as for any other excitation.

The model Hamiltonian we study represents each particle sitting in one or another of the minimums of a double-well potential and interacting with each other with harmonic force constants. In conventional theory this model describes ferroelectric phase transformations at which all the particles sit either on the left or the right minimum of the double-well potential. With appropriate choice of parameters, either order-disorder or displacive transformations can be described by this model. We shall call this the double-well problem. In the Appendix we study the properties of another anharmonic Hamiltonian by similar methods.

It turns out that the nonlinear equations we derive have been used in solid-state-physics applications before in the theory of ferromagnetic domain walls by Döring[18] and others, and in the theory of crystalline dislocations by Köchendorfer and Seeger.[19] Actually physical description of our solutions is very much in terms of dislocations and domain walls. While this paper was being written, we learned that some work on this problem has been done by Krumhansl and Schrieffer.[20] The nonlinear solutions of their paper correspond only to our first approximation, Eq. (9) below, to which they simply add the plane wave solutions. Models similar to those discussed in this paper have also been considered in the context of quantum field theory: See, e.g., Ref. 21.

II. DOUBLE-WELL PROBLEM

We consider the following classical Hamiltonian

$$H=\sum_i\left(\frac{m}{2}\dot{y}_i^2+\frac{A_2}{2}y_i^2+\frac{A_4}{4}y_i^4+\frac{mc^2}{2L^2}(y_{i+1}-y_i)^2\right), \tag{2}$$

where y_i is the displacement of the particle at the ith double-well site. The particles have a mean separation L. $A_2<0$ and $A_4>0$ define the single-particle double wells with minima at

$$y_0\equiv\pm(|A_2|/A_4)^{1/2}. \tag{3}$$

The particles interact with each other through harmonic springs with force constants of magnitude mc^2/L^2.

The behavior of the system depends on the ratio

$$\Phi=mc^2/A_2y_0^2, \tag{4}$$

which measures the strength of the interparticle springs to the height of the single-particle potential barrier. For $\Phi\ll1$, the problem reduces to an Ising model with coupling constant proportional to mc^2. This would give rise to an order-disorder transition, which in mean-field theory would occur at $T\sim mc^2$. For $\Phi\gg1$, we have the case of a displacive phase transition with a mean-field transition temperature

$$T_{\rm MF}\sim[(A_2y_0^2)(mc^2)]^{1/2}. \tag{5}$$

In this limit a continuum model is quite appropriate. Accordingly we use the substitution

$$y_{i+1}-y_i\simeq Ly_x,$$

where subscript denotes partial derivatives and obtain from (1) the classical continuum Hamiltonian

$$H=\frac{1}{L}\int dx\left(\frac{m}{2}y_t^2+\frac{mc^2}{2}y_x^2+\frac{A_2}{2}y^2+\frac{A_4}{4}y^4\right). \tag{6}$$

The equation of motion following from (6) is (with $m=1$)

$$y_{tt}-c^2y_{xx}+A_2y+A_4y^3=0. \tag{7}$$

In the linear limit, the dispersion is given by

$$\omega^2(k)=c^2k^2-2A_2. \tag{8}$$

Equation (7) is the special case of an equation which has been misnamed the sine-Gordon equation,

$$\Psi_{tt}-c^2\Psi_{xx}+\sin\Psi=0. \tag{7a}$$

This equation has been extensively analyzed[22] and exact solutions have recently been obtained.[23] Solutions take the form of traveling "kinks," which (in the traveling frame) are constant everywhere except in a small region where they change sign, and of traveling "breathers," which are zero everywhere except in a small region. Both the "kinks" and the "breathers" are solitons. The kinks and breathers are also solutions of (7). Equation (7) can, of course, be trivally solved by looking for stationary solutions in the variable

$$\xi=x-vt.$$

In terms of ξ, equation (7) becomes

$$(c^2-v^2)y_{\xi\xi}=A_2y+A_4y^3,$$

which can be solved as an elliptic integral,

$$\xi=(c^2-v^2)^{1/2}\int_{\bar{y}}^{y}dy'(A_0+A_2y'^2+A_4/2y'^4)^{-1/2}, \tag{9}$$

where A_0 and $\bar{y}$ are constants to be determined by the boundary conditions.

We focus on two kinds of solutions of (7) with obvious boundary conditions:

$$y(\xi)=y_0\operatorname{sech}(\xi/\sqrt{2}\,\xi_0) \tag{10}$$

and

$$y(\xi)=y_0\tanh(\xi/\sqrt{2}\,\xi_0), \tag{11}$$

where

$$\xi_0=[m(c^2-v^2)/A_4y_0^2]^{1/2}. \tag{12}$$

Exact solutions[23] of Eq. (7a) have revealed that it is one of the class of equations in which any given initial perturbation breaks up into a number of solitons [of the type (11) and (12)] which retain their velocity and shape as they pass through each other. The same can be shown to be true of (7). We can therefore write down as the *first solution* of Eq. (7),

$$y(x,t)=y_1(x,t)=\sum_i y_1(\xi_i), \tag{13}$$

where

$$\xi_i=x-x_i-v_i(t-t_i),$$

where y_1 is of the form (10) or (11), and x_i, t_i are the birthplace, birthtime, and velocity of the ith soliton.

The solution of the type (10) has all the particles far to the left of $\xi = 0$ in the left well and all the particles far to the right of $\xi = 0$ in the right well. It may be likened to a moving domain wall. The solution (11) has particles both to the right and to the left of $\xi = 0$ in one side of the double well and those in the vicinity of $\xi = 0$ on the other side. The statistical distribution of particles on the left or the right well is then determined by the density of excitations of the type (10) and (11) present in the system as will be discussed in detail later.

Since Eq. (7) is a nonlinear equation, it can have many solutions besides those we have so far discussed. In particular, small oscillations of "phonon" nature must be present. We now wish to discuss other solutions as perturbations over (13). If one linearizes the equation of motion about solutions of the type (13) for the sine-Gordon equation, one obtains the remarkable fact[22,23] the solitons present reflectionless potentials to the plane waves. The same *is not true* for Eq. (7). Here we do not pursue this problem. Instead we wish to consider the effect of the nonlinearities on the phononlike solutions. We do this by considering the modulation of the linear solutions of Eq. (7). Numerical studies of modulation envelopes of an equation related to (7) have been performed by Tappert and Hardin[24] and soliton behavior for the envelopes was observed.

We wish to consider the solutions of (7) about the first-order solutions (13). To do this we make the approximation of replacing (10) by a step function and (11) by a rectangular function. In other words, we approximate (10) and (11) by $\pm(x-vt)|y_0|$, where $\pm$ is a function of $(x-vt)$. We now introduce

$$\epsilon w = y - y_0 , \tag{14}$$

where ϵ is a small parameter, and expand (7) around y_0. The distribution of y_0 is determined by the first solution of (7), i.e., by the "kinks" and "breathers." $w(x,t)$ satisfies

$$w_{tt} - c^2 w_{xx} - 2A_2 w + 3\epsilon A_4 y_0 w^2 + A_4 \epsilon^2 w^3 = 0 . \tag{15}$$

We look for solutions of (15) which go to the phonons in the linear limit

$$w(x,t) = \varphi^{(1)}(X,T) e^{i(k_0 x - \omega_0 t)} + \text{c.c.} + \epsilon[\varphi^{(0)}(X,T) + \varphi^{(2)}(X,T) e^{2i(k_0 x - \omega_0 t)} + \text{c.c.}] + \cdots . \tag{16}$$

It is assumed that the variation in $\varphi^{(i)}(X,T)$ occurs on a time and space scale slow compared to that in the phonon part. Accordingly we introduce

$$T = \epsilon t, \quad X = \epsilon x .$$

Equation (15) then becomes

$$w_{tt} - c^2 w_{xx} - 2A_2 w + 3\epsilon A_4 y_0 w^2 + \epsilon^2 A_4 w^3 + \epsilon^2 w_{TT} - c^2\epsilon^2 w_{XX} + 2\epsilon w_{tT} - 2c^2 \epsilon w_{xX} = 0 . \tag{17}$$

Inserting (16) in (17) and equating dc, first-harmonic, and second-harmonic terms, we get, respectively,

$$\epsilon(-2A_2\varphi^{(0)} + 3A_4 y_0 |\varphi^{(1)}|^2) + O(\epsilon^2) = 0 , \tag{18}$$

$$(-\omega_0^2 + c^2k_0^2 - 2A_2)\varphi^{(1)} + \epsilon(-2i\omega_0\varphi_T^{(1)} + 2ik_0c^2\varphi_X^{(1)}) + \epsilon^2(A_4|\varphi^{(1)}|^2\varphi^{(1)} + \varphi_{TT}^{(1)} - c^2\varphi_{XX}^{(1)} + 3A_4 y_0 \varphi^{(2)}\varphi^{(1)*}) + O(\epsilon^3) = 0 , \tag{19}$$

and

$$\epsilon(-4\omega_0^2 + 4c^2k_0^2 - 2A_2)\varphi^{(2)} + 3\epsilon A_4 y_0 \varphi^{(1)2} + O(\epsilon^2) = 0 . \tag{20}$$

Using the linear dispersion given by (8) in (20),

$$\varphi^{(2)} = -\tfrac{1}{2}(A_4 y_0/A_2)\varphi^{(1)2} . \tag{21}$$

Using (8) in (19) and introducing new scales

$$z = X - v_g T,$$

$$v_g = \frac{d\omega}{dk},$$

$$s = \epsilon T ,$$

we get on keeping terms to lowest order in ϵ

$$i\varphi_s^{(1)} + (\bar{C}^2/2\omega_0)\varphi_{zz}^{(1)} - \tfrac{5}{4}A_4|\varphi^{(1)}|^2\varphi^{(1)} = 0 , \tag{22}$$

where

$$\bar{C}^2 = C^2 - v_g^2 .$$

From (19) we also get

$$\varphi^{(0)} = +\tfrac{3}{2}(A_4/A_2) y_0 |\varphi^{(1)}|^2 . \tag{23}$$

The solution for the displacement can therefore be written as

$$y = y_1(x,t) \pm (x,t)\tfrac{3}{2}(A_4/A_2)|y_0|\,|\varphi^{(1)}|^2 + \varphi^{(1)}(X,T)e^{i(kx-\omega t)} + \text{c.c.} + \cdots . \tag{24}$$

Equation (24) represents our solution to the double-well problem, where we have explicitly displayed the "dc" and the "first-harmonic" solution to the problem. We now study Eq. (22) for the modulation envelope.

III. BEHAVIOR OF ENVELOPE SOLUTIONS

Consider the equation

$$i\varphi_\tau + p\varphi_{\xi\xi} + q|\varphi|^2\varphi = 0\,, \tag{25}$$

which is the same as Eq. (22) of Sec. II. The solution of Eq. (25) depends in an important way on the sign of pq. For the double-well problem pq is negative; for the other problem we will discuss, it can have either sign, but the phase transition is favored with a negative sign.

For $pq<0$, one family of stable solutions of (25) consists of plane waves. Other stable solutions can be obtained by noting that for $pq<0$, Eq. (25) can be reduced back to the KdV equation. This can be accomplished by following the procedure of Taniuti and Yajima[25] and introducing functions ρ and σ through

$$\varphi = \rho^{1/2}\exp\left(i\int \sigma d\xi/2p\right). \tag{26}$$

Substituting (26) in (25) and separating the real and imaginary parts, one gets[25]

$$\rho_\tau + (\rho\sigma)_\xi = 0\,, \tag{27}$$

$$\sigma_\tau + \sigma\sigma_\xi = 2pq\rho_\xi + p^2[\rho^{-1/2}(\rho^{-1/2}\rho_\xi)_\xi]_\xi\,. \tag{28}$$

Now we introduce a small parameter μ and write

$$\rho = \rho_0 + \mu\rho_1 + \mu^2\rho_2 + \cdots\,, \tag{29}$$

$$\sigma = \sigma_0 + \mu\sigma_1 + \mu^2\sigma_2 + \cdots\,, \tag{30}$$

and also introduce new scales

$$\xi' = \mu^{1/2}(\xi - \gamma\tau)\,, \tag{31}$$

$$\tau' = \mu^{3/2}\tau\,. \tag{32}$$

Substituting (29)–(32) in (27) and (28) and carrying on the asymptotic analysis, we get that

$$\gamma = \sigma_0 + (2|pq|\rho_0)^{1/2}, \tag{33}$$

$$\rho_1(\xi',\tau') = -(2|pq|/\rho_0)^{-1/2}\sigma_1(\xi',\tau')\,, \tag{34}$$

and σ_1 obeys the Kortweg–de Vries equation

$$\sigma_{1\tau'} + \sigma_1\sigma_{1\xi'} + \delta^2\sigma_{1\xi'\xi'\xi'} = 0\,, \tag{35}$$

where

$$\delta^2 = \frac{p^2}{\rho_0}\left(\frac{2|pq|}{\rho_0}\right)^{-1/2}. \tag{36}$$

The stationary solution of Eq. (35) are solitons:

$$\sigma_1 = A\,\mathrm{sech}^2[(\xi' - C\tau')/\Delta]\,, \tag{37}$$

with $C=A/3$ and $\Delta^2 = 12\delta^2/A$.

Exact solutions of (35) have also been obtained.[26,27] From our point of view, the important result is that given an initial condition, the solution breaks up into a definite number of stationary pulses of the shape (37) characterized by the amplitude A (and velocity C and width Δ), which pass through each other without any change in their parameters, so that unless the solitons overlap we can write the solution as

$$\sigma(\xi,\tau) = \sum_i \sigma_i[\xi - \xi_i - C_i(t-t_i)]\,, \tag{38}$$

where σ_i is as in (37) and ξ_i, t_i are arbitrary space-time points. Since ρ_1 is proportional to σ_1, φ also behaves as in (38). We thus conclude that the envelope solutions for the double-well problems are solitons. Since in what we will do next, we make use of only the general properties of the solution, we do not go back here to the physical variables and rewrite expression for $\varphi^{(1)}$ in terms of them. At the end of Sec. VI we shall express the characteristic parameters Δ and C in terms of the parameters entering the Hamiltonian.

For $pq>0$, plane waves are subject to modulational instability. This case has been treated before.[16] The exact solution has recently been found by Zakharov and Shabat.[28]

IV. PHYSICAL DESCRIPTION OF SOLUTIONS

The solution of the problem is given by Eq. (24). The "dc" part of the solution consists of two parts: $y_1(x,t)$ given by Eq. (13) and $\varphi^{(0)}(X,T)$ given by Eq. (23). $y_1(x,t)$ has the properties of a number of moving domain walls and moving dislocations, whereas $\varphi^{(0)}(X,T)$ has the properties of a moving dislocation or of moving vacancy-interstitial pairs. Other differences between the two types of dislocations are (i) $y_1(x,t)$ can have an arbitrary velocity (the distribution of velocities is to be determined by temperature as discussed in Sec. V), whereas $\varphi^{(0)}(X,T)$ has for its minimum velocity, the group velocity of the phonon we are considering or more generally, the average group velocity of the packet of phonons excited at a given temperature. We may generally expect most of the former to move slower than the latter; (ii) the latter are always rarefactive, as may be deduced from the negative sign in Eq. (34)—they may generally be called antisolitons. The former may be both solitons and antisolitons.

In Sec. V we will characterize these nonlinear solutions by their energy and obtain their density and distribution in velocity at any temperature simply in terms of the energy as for any other excitation. At very high temperatures their density will be of order unity (normalized to the density of particles) and the particles will therefore be randomly in the left or right of their double wells and flipping at a random rate. As the temperature is decreased the density of solitons decreases, and ordered regions of particles to the left or right double well emerge. These regions will be moving randomly to the left or right, however. At very low temperature the motion of $y_1(X, T)$ will lead to uniform motion of domains, but the motion of $\varphi^{(0)}(X, T)$ at the much larger thermal group velocity will still flip particles from left to right and restore them back to left (or vice versa) around the point $X - v_g T = 0$. Its effect on the slowly moving domain wall will be to spoil the uniform motion and Brownian-like motion will result. (Such behavior has recently been seen in numerical simulation experiments by Koehler *et al.*) As $T \to 0$, the density of the solutions approaches 0 and the ordering of the whole lattice results. We will show in Sec. V that the temperature at which the correlation among the positions of the particles first begins to appear is just the mean-field transition temperature of the conventional theory.

The random hopping of the particles from left to the right under the influence of solitons will, of course, yield a central peak in the structure factor. Its intensity and width will be determined by the statistics of the solitons as discussed in Sec. V.

Now we turn to the physical nature of the "ac" part of the solution in (24). From Eqs. (26), (34), and (37), we can conclude that the effect of the envelope is to provide a phase shift and an amplitude change to the "phonon" at the position $X - v_g T = 0$. Since this happens randomly the phonon will acquire a width.

V. FREQUENCY SPECTRUM AND THERMODYNAMICS

In contrast to Sec. II–IV, where we rigorously demonstrated that the envelopes of the linear solutions to the anharmonic problems we are considering are solitons, this section is somewhat heuristic and relies on the physical features of the solution discussed in Sec. IV. We hope to take up the more precise development of this section at a later data.

With several solitons present the "dc" and first-harmonic displacement of an atom in the double-well problems can be written

$$y(x, t) = f(x, t) + g(x, t) e^{i(k_0 x - \omega_0 t)} . \qquad (39)$$

In turn $f(x, t)$ and $g(x, t)$ can be written as

$$f(x, t) = \sum_i f[x - x_i - v_i(t - t_i)] , \qquad (40)$$

$$g(x, t) = \sum_i g[x - x_i - v_i(t - t_i)] , \qquad (41)$$

where x_i and t_i are the starting position and starting time of the solitons.

We are interested in calculating

$$S(k, \omega) = \langle y(x, t) y(x', t') \rangle_{(k, \omega)} = S_1(k, \omega) + S_2(k, \omega) , \qquad (42)$$

where

$$S_1(k, \omega) = \langle f(x, t) f(x', t') \rangle_{(k, \omega)} \qquad (43)$$

and

$$S_2(k, \omega) = \langle g(x, t) g(x', t') e^{i(k_0 x' - \omega_0 t')} \rangle_{(k, \omega)} , \qquad (44)$$

and by $\langle\,\rangle_{(k, \omega)}$ we mean the Fourier transform of the quantity in the angular brackets. First consider $S_1(k, \omega)$. Noting that the Fourier transform of $p(x - vt)$ is of the form $\delta(\omega - kv)\tilde{p}(k)$, where $\tilde{p}(k)$ is the transform of $p(x)$, it is straightforward to derive that

$$S_1(k, \omega) = P_v(\omega/k) P_x(k) P_T(\omega) |\tilde{f}(k)|^2 , \qquad (45)$$

where $P_x(k)$ is the Fourier transform of the probability $P_x(x)$ describing the distribution of distances between solitons in space and $P_T(\omega)$ is the Fourier transform of the probability distribution $P_T(t)$ describing the time distribution of solitons at a point, and $P_v(v)$ is the probability distribution of velocity of solitons. Since the solitons are noninteracting, the distribution functions $P_T(t)$ and $P_X(x)$ have the Poisson form:

$$P_T(t) = (1/\tau_0) e^{-t/\tau_0} , \qquad (46)$$

where τ_0 is the mean time for solitons crossing a given point,

$$P(\omega) = \tau_0 / (1 + \omega^2 \tau_0^2) , \qquad (47)$$

and we get a central peak of width τ_0^{-1} and intensity proportional to τ_0. $P_x(k)$ will of course have the same form as $P_T(\omega)$ since we are dealing with stationary traveling waves. $\tilde{f}(k)$ is a function peaked around $k = 0$ and of width proportional to the inverse soliton width. A remaining problem is to evaluate τ_0. Before proceeding with evaluation of τ_0, we note that $S_2(k, \omega)$ can be easily evaluated, using the convolution theorem, to be

$$S_2(k, \omega) = y_0^2 |\tilde{g}(k - k_0)|^2 P_x(k - k_0) P_T(\omega - \omega_0) \times P_v[(\omega - \omega_0)/(k - k_0)] , \qquad (48)$$

where y_0 is the amplitude of the mode of wave vector k_0. Thus we see that the phonon under consideration develops a width in frequency proportional to τ_0^{-1} due to the random modulation effect of the solitons.

To calculate the energy of the solitons, we simply insert the soliton solution in the appropriate Hamiltonian (6) and integrate to get the energy. If we characterize the soliton solution by Eq. (10) or (11)

$$y = y_m \operatorname{sech}[(x - vt)/x_0], \tag{49a}$$

$$y = y_m \tanh[(x - vt)/x_0], \tag{49b}$$

the energy is

$$E = \frac{\beta_1}{L}\frac{m y_m^2}{x_0} v^2 + \frac{\beta_2}{L} A_2 y_m^2 x_0, \tag{50}$$

where β_1, β_2 are numerical constants of order unity. The energy of the envelope soliton for $\varphi^{(1)}(x,t)$ is also given by Eq. (50) since it can be written as (49a). As discussed earlier, however, its velocity is not arbitrary.

Having obtained the energy of solitons in terms of their velocity v and amplitude y_0 we can do thermodynamical calculations by introducing the partition function

$$Z = \operatorname{Tr} e^{-E(y_m, v)/kT}. \tag{51}$$

From (51) we could calculate the free energy, entropy, and density of solitons excited at any temperature. This step is on somewhat shaky grounds, since all the methods of deriving solitons have been "nonequilibrium" methods. We persist nevertheless to calculate τ_0 with this approach.

From (51) we note that the density of solitons with velocity v is $N(v) \sim e^{-M^* v^2/kT}$, where M^* is the effective mass of a soliton. The average velocity $\langle v \rangle$ of solitons is therefore given by

$$\langle v \rangle = (kT/M^*)^{1/2}. \tag{52}$$

τ_0, the average time for solitons to cross a given point, is then given dimensionally by

$$\tau_0 = 1/\rho\langle v \rangle = \rho^{-1}(M^*/kT)^{1/2}, \tag{53}$$

where ρ is the average density of solitons per unit length.

Using (51) and integrating over the velocity, we see that

$$\rho \sim e^{-E_0/kT}, \tag{54}$$

where E_0 is the "potential energy" of the solitons, i.e., the second term in Eq. (50) for the energy of a soliton in the double-well problem. We therefore see from (53) and (45)–(48) that correlations, both *spatial and temporal*, increase exponentially with temperature and the characteristic temperature below which they become important is E_0/k.

At this point it is useful to express y_m and x_0, which determine E_0 in terms of the parameters entering the Hamiltonian. For $y_1(x,t)$, the first solution of the nonlinear equation, the amplitude y_m is restricted to be y_0, as seen in Eqs. (10)–(12), and the width for $v \ll c$ is

$$x_0 = \sqrt{2}\, y_0 \Phi^{1/2} \text{ for } y_1(x,t), \tag{55}$$

where Φ is given by Eq. (4). For $\varphi^{(0)}(x,t)$ and $\varphi^{(1)}(x,t)$ we find from Eq. (37) that on identifying the parameters p and q of Eq. (25) with those in Eq. (22)

$$x_0 \equiv \Delta = \left(\frac{12}{2^{1/2}}\right)^{1/2} y_0 \Phi^{1/2}\left(\frac{2|A_2|/m}{c^2k^2 + 2|A_2|/m}\right)^{1/2}, \tag{56}$$

which for long wavelength ($k \to 0$) reduces to $(12/2^{1/2})^{1/2} y_0 \Phi^{1/2}$. Thus to within numerical factors of order unity the width of the envelope solitons is the same as the solitons of the first-order solution.

Φ measures the ratio of the strength of the harmonic coupling among the particles to the strength of the double-well potential barrier. For $\Phi \ll 1$, we have the order-disorder problem; for $\Phi \gg 1$, we have the displacive problem. Actually our method of solution in which we keep only the low-order harmonics (i.e., assume nonlinear terms small compared to the linear terms) has the implicit assumption that $\Phi \gg 1$, and, therefore, is applicable only for the displacive case. The width of the solitons, Eqs. (55) and (56), then is much larger than the interparticle separation, which is consistent with our starting point, to wit, a continuum model. The energy E_0 for the double-well problem is given by using (56) in the second term of (50),

$$E_0 \sim (A_2 y_m^2 m c^2)^{1/2}. \tag{57}$$

Now it can easily be shown that the mean-field transition temperature for the displacive case is given also by Eq. (57). Our result then is that the correlations begin to be important from about the mean-field transition temperature, as would indeed be expected.

We also write down the mass and velocity of the solitons for the double-well problem,

$$M^* \simeq m(y_0/L)(A_2 y_m^2/mc^2)^{1/2}, \tag{58}$$

and from Eqs. (37) and (33), the velocity of the envelope solitons is

$$v \equiv c = v_g + c(y_p/y_0), \tag{59}$$

where y_p is the phonon amplitude. The velocity is thus effectively equal to the group velocity of the phonon. An extension of the techniques used here to the case of envelope of an incoherent collection of phonons can be made to show that in that case v will be given by the average group velocity of the phonons.

VI. DISCUSSION

In Secs. II and III, we have shown quite rigorously that the solution to the double-well problem can be expressed in terms of the solitons and a modulation of the solutions of the linearized problem by solitons. We have physically interpreted these stationary traveling pulses as moving dislocations and moving domain walls. In Sec. V we have roughly estimated their energy and quite heuristically calculated their effect on the vibrational spectrum. We have found that these pulses lead to a central peak in $S(k, \omega)$ as well as "phonon" damping. In an appendix we will show that the same general properties of the solutions are true for another one-dimensional anharmonic Hamiltonian. We suspect that for any anharmonic and dispersive one-dimensional problem, solitons are a significant part of the solution.

We have used asymptotic scaling methods in Secs. II and III and in the appendix to obtain our results. The scaling methods perform the following functions: stretch the scale of time with respect to space, stretch the space-time scale of one solution with respect to another, and order solutions with respect to decreasing amplitude. Numerical solutions[14,22,24] of similar partial differential equations have revealed that the solutions obtained by asymptotic scaling methods are correct even for amplitudes of solutions that are comparable in successive order. In other words, the first two functions of the scaling methods are much more relevant that the third, and we may trust our solutions for envelopes even at large amplitudes. One of the shortcomings of the development in this paper is that we started with well-defined phonons and derived their modulation envelope due to the nonlinearities, but did not go back and see how the phonons get modified by interaction with the solitons. Presumably, if we do so we will find additional damping of the phonons.

Does this development have any relevance to phenomena observed in real three-dimensional lattices? At present we cannot answer this question definitively one way or the other, but are inclined to be pessimistic. In one dimension solitons occur for arbitrarily small displacements in a nonlinear lattice. We guess that in two or three dimensions, one must exceed a critical displacement before dislocations and domains can occur. Also, in two and three dimensions stable solutions of the dislocation or domain-wall form occur only for very special choices of nonlinearity and dispersion. In one dimension, dislocations and domains are point objects and behave as particles; in two or three dimensions they are lines or planes and probably do not have a simple relation between their energy and their velocity. The general phenomenon of domain formation of course occurs in most three-dimensional (structural) transitions and on general grounds movement of domain walls is much easier near a phase transition. However, we do not expect that in two and three dimensions domains and dislocations have any solitonlike property. Moreover, in one and two dimensions domains and dislocations are thermodynamic objects (with energy proportional to the size of the system) while this is not true in three dimensions. We expect that in real three-dimensional structural transitions the growth and dynamics of domains and dislocations is determined by defects.

One can look at our solutions for the one-dimensional lattice in a rather amusing way. Landau[29] showed the absence of phase transition in a one-dimensional system by arguing that by subdividing the system into domains, the entropy gain more than compensates the energy loss but it has not been shown how this division into subdomains comes about. The solutions obtained here—the solitons—are merely the dynamical objects which subdivide the system into such domains and it is satisfying to generate solutions which have been postulated on equilibrium statistical-mechanical grounds.

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APPENDIX: ANOTHER ANHARMONIC LATTICE PROBLEM

Here we consider the classical Hamiltonian of a linear chain of particles with lattice constants h. In terms of y_i, the displacement from equilibrium of the ith particle,

$$H=\sum_i \tfrac{1}{2} m\dot{y}_i^2+a_2(y_{i+1}-y_i)^2+a_3(y_{i+1}-y_i)^3 + a_4(y_{i+1}-y_i)^4 . \qquad \text{(A1)}$$

To generate a differential equation for the motion, we write

$$y_{i\pm 1}=y\pm hy_x+(\tfrac{1}{2}h^2)y_{xx}\pm(\tfrac{1}{6}h^3)y_{xxx} + (\tfrac{1}{24}h^4)y_{xxxx}+\cdots . \qquad \text{(A2)}$$

The equation of motion is then given by

$$y_{tt}=c^2[y_{xx}(1+\delta p y_x+q y_x^2)+h^2 y_{xxxx}] , \qquad \text{(A3)}$$

where the subscripts indicate partical derivatives, and $c^2=a_2 h_2/m$, $\delta p=a_3 h/a_2$, and $q=a_4 h/a_2$. δ is a small parameter which serves to make the cubic nonlinearity small compared to the quartic. Since we will be dealing with Eq. (A3) rather than the difference equations arising from (A1), our results will be meaningful only for phenomena occuring over a spatial scale large compared to h. In (A3) we have gone beyond the continuum approximation, since the (linear) dispersion is given by

$$\omega^2(k)=c^2k^2(1-h^2k^2)\ . \qquad \text{(A4)}$$

Equation (A4) has been reexpressed in the form of the KdV equation earlier[14,19,30] by other methods. We present the multiple-scaling method required to do so here. We wish to study waves traveling to the right and therefore expand Eq. (A3) along the characteristic $x-ct$. Introducing

$$\xi=\epsilon^a(x-ct),\ \ \tau=\epsilon^b ct/h,\ \ y/h=\delta v\ , \qquad \text{(A5)}$$

and substituting

$$\frac{\partial}{\partial x}=\frac{\epsilon^a}{h}\frac{\partial}{\partial\xi},$$
$$\frac{\partial}{\partial t}=\frac{\epsilon^{a+b}c}{h}\frac{\partial}{\partial\tau}-\frac{\epsilon^a c}{h}\frac{\partial}{\partial\xi} \qquad \text{(A6)}$$

in (A3), we get

$$\epsilon^{2b}v_{\tau\tau}-2\epsilon^b v_{\xi\tau}=\delta p\epsilon^{a+1}v_{\xi\xi}v_\xi+\delta^2 q\epsilon^{2a}v_{\xi\xi}v_\xi + \tfrac{1}{12}\epsilon^{2a}v_{\xi\xi\xi\xi}\ . \qquad \text{(A7)}$$

[Note that in (A3), we have assumed the cubic anharmonicity to be small. Similar results can be derived without this assumption with a slightly different scaling.]

As in Tappert and Varma,[16] we are interested in high-frequency solutions (relatively strong dispersion). Accordingly, we choose $a=1$, $b=3$ in (A7) and obtain after one integration

$$\omega_\tau+(p\delta\omega+q^2\omega^2)\omega_\xi+\tfrac{1}{3}\omega_{\xi\xi\xi}=O(\epsilon^2)\ , \qquad \text{(A8)}$$

where $\omega=v_\xi$. This is the famous (modified) KdV equation (with $q=0$, it is the KdV equation).

Exact solutions of the KdV equation have been recently obtained[26,27] by the inverse scattering method. Any given initial perturbation breaks up into a number of solitons, which retain their velocity and shape as they pass through each other. A most remarkable development[26] is the result that for an initial perturbation $V(x,0)$, the number of solitons given by the KdV equation is equal to the number of bound states of the eigenvalue equation

$$\left(-\frac{d^2}{dx^2}+V(x,0)\right)\Psi(x)=\lambda_n\Psi(x)\ . \qquad \text{(A9)}$$

Further the amplitude of the solitons is simply $2\lambda_n$ and their velocity is equal to $-4\lambda_n$.

Interesting as these results are, they do not seem directly applicable to the statistical physics of our problem since they have nothing to do with the solution to the linear problem—the phonons. (We shall continue to use the word phonon, though strictly speaking it is applicable only to the quantum-mechanical problem.) As discussed in Sec. I, we resolve this difficulty by looking for solutions of the form

$$w=\Psi^{(1)}(\xi',\tau')e^{i(k_0\xi-\omega_0\tau)}+\text{c.c.} + \delta[\Psi^{(0)}(\xi',\tau')+\Psi^{(2)}(\xi',\tau')e^{2i(k_0\xi-\omega_0\tau)}+\text{c.c.}] + O(\delta^2)\ . \qquad \text{(A10)}$$

Here k_0 is the wave vector and ω_0 the energy of the vibration of the linear problem that we wish to specially study, and $\Psi^{(1)}$ is a modulation of the linear solution. An equation for $\Psi^{(1)}$ has been given by Tappert and Varma[16] following the methods of Taniuti and Yajima[25] and others. For completeness we present the derivation here. The basic assumption is that $\Psi^{(1)}(\xi',\tau')$ varies in a slower fashion than $e^{i(k_0\xi-\omega_0\tau)}$. Accordingly we introduce

$$\tau'=\delta\tau,\ \ \xi'=\delta\xi\ .$$

Equation (A8) now becomes

$$\omega+\tfrac{1}{2}(p\delta\omega+q\delta^2\omega^2)+\tfrac{1}{24}\omega_{\xi\xi\xi}+\delta\omega_{\tau'}+\tfrac{1}{2}\delta(p\delta\omega+q\delta^2\omega)\omega_{\xi'} + \tfrac{1}{8}\omega_{\xi\xi\xi'}+\tfrac{1}{8}\delta^2\omega_{\xi\xi'\xi'}+\tfrac{1}{24}\delta^3\omega_{\xi'\xi'\xi'}=0\ . \qquad \text{(A11)}$$

Inserting (A10) in (A11) and equating the coefficient of the dc term, the first harmonic, and the second harmonic, we get, respectively,

$$\delta^2(\Psi^{(0)}_{\tau'}+\tfrac{1}{2}p\,|\Psi^{(1)}|^2_{\xi'})+O(\delta^3)=0\ , \qquad \text{(A12)}$$

$$-i(\omega_0+\tfrac{1}{2}k_0^3)\Psi^{(1)}+\delta(\Psi^{(1)}_{\tau'}-\tfrac{3}{2}k_0^2\Psi^{(1)}_{\xi'})+\delta^2[\tfrac{3}{2}ik_0\Psi^{(1)}_{\xi'\xi'}+\tfrac{1}{4}p(2ik_0\Psi^{(0)}\Psi^{(1)}+2ik_0\Psi^{(2)}\Psi^{(1)*}) + \tfrac{1}{6}q(3ik_0{\Psi^{(1)}}^2\Psi^{(1)*})]+O(\delta^3)=0\ , \qquad \text{(A13)}$$

and

$$\delta[-i(2\omega_0+4k_0^3)\Psi^{(2)}+\tfrac{1}{2}p(ik_0\Psi^{(1)2})]+O(\delta^2)=0\ . \qquad \text{(A14)}$$

From (A12), we see that the linear dispersion in the frame of reference in which ξ and τ are defined as

$$\omega_0=-\tfrac{1}{2}k_0^3\ ,$$

which is merely a reexpression of (A4). We now move with the group velocity $v_g=d\omega/dk=-\frac{3}{2}k_0^2$ by

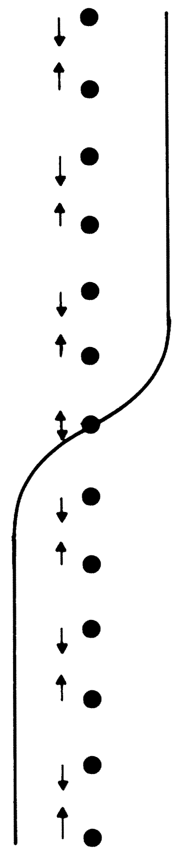

FIG. 1. Illustrating phase difference between particles on one side of a soliton compared to the other for the "dimerization mode" of a linear lattice.

introducing new variables

$$z=\xi'+\tfrac{3}{2}k^2\tau' \ , \quad s=\delta\tau' \ .$$

Then Eq. (A12) yields

$$\Psi^{(0)}=-(p/3k_0^2)\,|\Psi^{(1)}|^2 \ , \qquad \text{(A15)}$$

and Eq. (A14) yields

$$\Psi^{(2)}=-(p/6k_0^2)\Psi^{(1)2} \ . \qquad \text{(A16)}$$

Using (A15) and (A16), Eq. (A13) becomes

$$i\Psi_s^{(1)}=\tfrac{3}{2}k_0\Psi_{zz}^{(1)}+\tfrac{1}{2}k_0(q-p^2/6k_0^2)\,|\Psi^{(1)}|^2\Psi^{(1)} \ . \qquad \text{(A17)}$$

From (A10) the dc and first-harmonic strain are given by

$$\omega=-(p/3k^2)\,|\Psi^{(1)}|^2+(\Psi^{(1)}e^{i(k_0\xi-\omega_0\tau)}+\text{c.c.}) \ . \qquad \text{(A18)}$$

Equation (A17) for the present problem has exactly the same form as Eq. (25) in Sec. III, and its solutions are given by Eqs. (26) and (38).

The important points to note here are that ω is a strain rather than a displacement and that there is no first-order nonlinear "dc" solution in the present problem. If the results are expressed in terms of displacement the soliton solution leads to a phase shift (and change in amplitude) of the phonon. This phase shift for a zone boundary phonon is illustrated in Fig. 1, where particles on one side of the soliton are oscillating out of phase with respect to the other. Again solitons may be interepreted as domains and dislocations.

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