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RESPONSE OF AN ANHARMONIC CRYSTAL TO A LOCALIZED INITIAL IMPETUS

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There is much interest in the time dependence of the atomic displacements in a crystal after an initial impetus because of the need to examine the interactions of an atomic-particle beam with a solid surface, which includes nonstationary deformation after localized action of impact type. There are several papers dealing with the response of crystals to external shocks or with discussion of the physical effects associated with the response function [1-4]. Nearly all theoretical papers on this topic employ the harmonic approximation. The role of slight anharmonicity has been discussed in [5].

However, most of the physical processes involved here are based on levels of initial excitation such that one cannot assume that anharmonic effects are small or unimportant. Therefore, major interest attaches to proper incorporation of the nonlinearity in the interaction. Numerical calculations, although useful, are only partial in character and cannot completely replace analytical consideration designed to elucidate the general features. Here we present a certain class of solutions for the displacements in a decidedly nonlinear structure.

We take a structure with a power-law dependence for the potential energy on the relative displacements, which under certain conditions given below allows one to determine the main features in the process. We give the following form to the equations of dynamics for a one-dimensional atomic chain with interaction between nearest neighbors:

$$d^2x_n/dt^2 = \alpha\{(x_{n-1} - x_n)^{2p+1} - (x_n - x_{n+1})^{2p+1}\}, \tag{1}$$

where x_n is the displacement of an atom, which is assigned subscript n, relative to its equilibrium position, while p is an integer that is not zero (subject to certain reservations, the constructions given below can be extended to the case of arbitrary nonnegative value of p). Equation (1) does not contain a linear component. This feature of the force interaction occurs for example in the transverse component of the vibrations in a rectilinear atomic chain, where the lowest order in the dependence of the forces on the displacements corresponds to the third degree. Also, the role of the linear component may be secondary for other structures with vibrations of large scale. Of course, incorporation of the components linear in the displacements would extend the range of real objects that correspond qualitatively to (1), but in that case one does not obtain clear final formulas. On the other hand, solutions in the form of long-wave solitons that can be derived are of other interest, but the purposes differ from those of this study. Therefore, we take (1) as the starting point.

The continuum approximation for (1) gives

$$\frac{\partial^2 x}{\partial t^2} = \alpha \frac{\partial}{\partial n}\left(\frac{\partial x}{\partial n}\right)^{2p+1}. \tag{2}$$

Considerations of scale invariance for (2) suggest that it is desirable to seek the solutions in the form

$$x(n,\ t) = f(\xi), \quad \xi = nt^{-1/(p+1)}. \tag{3}$$

Substitution of (3) into (2) reduces the latter to an ordinary differential equation:

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$$\frac{p+2}{(p+1)^2}\,\xi\,\frac{df}{d\xi}+\frac{\xi^2}{(p+1)^2}\,\frac{d^2f}{d\xi^2}=\alpha\,\frac{d}{d\xi}\left(\frac{df}{d\xi}\right)^{2p+1}. \tag{4}$$

We multiply (4) by

$$|df/d\xi|^{-p/(p+2)},$$

to reduce it to an equation in first-order total differentials for the modulus of the derivative of f with respect to ξ, which gives

$$y^{2p}=B\xi^2-C_1y^{-2(p+2)},\quad y=|df/d\xi|,\quad B=1/[\alpha(2p+1)], \tag{5}$$

where C_1 is an arbitrary constant.

Equation (5) is an algebraic equation in the expression $y^{2/(p+2)}$ of degree $(p+1)^2$, from which one gets an explicit expression for y and consequently also for f.

Equation (5) defines a certain set of forms for the displacement developing in time and space. For definiteness we consider the form that corresponds qualitatively to concepts on the course of the process after a localized impetus and also to analysis of the solutions for the corresponding linear cases.

In the region of positive values of ξ and C_1, the $y=y(\xi)$ dependence given by (5) has two branches, whose asymptotic forms for $\xi\to\infty$ are $\xi^{1/p}$, $\xi^{-(p+2)}$, and the region of existence of the solutions is bounded by the condition

$$\xi>\xi_0,\quad \xi_0^2=\frac{1}{B}\left(y_0^{2p}+C_1y_0^{-\frac{2}{p+2}}\right),\quad y_0=\left[\frac{C_1}{p(p+2)}\right]^{\frac{p+2}{2(p+1)^2}}.$$

The solution determining the absence of displacements at small times and at large distances from the point $n=0$ corresponds to the branch decaying for $\xi\to\infty$. Therefore, the distribution of the displacements in the peripheral region of space is defined by

$$x(n,t)\approx-(p+1)\left(\frac{C_1}{B}\right)^{(p+2)\,2}\frac{t}{n^{p+1}}-\frac{p+2}{2C_1(2p^2+5p+3)}\left(\frac{C_1}{B}\right)^{(2p^2+5p+4)/2}\frac{t^{(2p^2+5p+4)/(p+1)}}{n^{2p^2+5p+3}}. \tag{6}$$

Equation (6) is only approximate because one cannot solve the algebraic equation of high degree (5) exactly. Of course, one can write more accurate formulas for the displacement law quantitatively. However, incorporation of the latter terms in (6) is significant only for the immediate neighborhood of the boundary $\xi=\xi_0$ and does not alter the qualitative picture of the distribution.

Expression (6) for $t\to0$ gives zero everywhere apart from the region $n\to0$, which means that the relationship corresponds to the development of nonstationary displacements after an initial localized displacement at $n=0$. The boundary of the region where the distribution of (6) applies moves in space with speed

$$v=[\xi_0/(p+1)]\,t^{-p/(p+1)}. \tag{7}$$

Formula (7) defines the scale of the propagation speed for the bunch of displacements, i.e., it can be considered as the analog of the speed of sound. It should be noted that although the case $p=0$ requires certain reservations within the framework of this treatment, the value of v calculated for this case from (7) coincides with the speed of sound in the literal meaning of that concept.

The energy flux at point n at time t is defined in this approach by

$$j=\frac{\alpha}{p+1}\,\frac{n}{t^{(p+3)/(p+1)}}\,y(\xi)^{2p+2}. \tag{8}$$

We see from (5)-(7) that the basic scale characteristics are dependent on C_1, which was introduced as an arbitrary constant. Physically, this quantity is determined by the level of the initial excitation and can be calculated for example from (8) for some nominal initial value of j. A reduction in C_1 implies a reduction in the scale of the displacements and the velocity v.

In the region $\xi<\xi_1$ ($\xi_1\geqslant\xi_0$), the displacement distribution is determined by (5) also, where however the arbitrary constant is to be taken as negative. The choice of this constant and of constants ξ_1 is determined by the requirement for continuity in the energy and momentum fluxes at the boundary $\xi = \xi_1$ in a coordinate system where this boundary is at rest.

On passing from the functions y to the displacements x, it becomes possible to vary a further arbitrary constant for the internal zone of the distribution, so clearly the distribution can always be made continuous. Discontinuities in the derivatives of the functions at the boundary between the internal and external zones should not cause surprise, since this feature is directly related to the essence of our view on the nature of this boundary as a certain front of shock-wave type corresponding to a traveling kink in the displacement distribution.

One can see that the distribution of the displacements in this nonlinear structure differs from that occurring in the linear case, where a perturbation will propagate without distortion at a constant speed. In the structure considered here, the motion of the displacement bunch slows down, while the profile of the distribution flattens out, while retaining the characteristic scale of the displacements defined by $f(\xi_1)$.

In a nonlinear medium, the displacements may also occur in such a way that the maximum displacement at all times corresponds to $n = 0$, while the asymptotic behavior for $t \to \infty$ of all the atoms corresponds to displacement of the structure as a whole by the displacement occurring at $n = 0$. This form does not have an analog in a continuous linear structure, but it is similar to a considerable extent to the atomic displacements occurring in a discrete linear chain.

Note that these constructions do not require that there should be a fixed boundary ξ_1 between the peripheral and central zones. Also, we can speak of a displacement distribution containing several kink points in $f(\xi)$ and including possibly parts where $f = \text{const}$. The structure may also be nonconservative and correspond for example to continuous energy input at $n = 0$. The values of ξ corresponding to the boundaries of the parts are determined by the conservation laws. The realization of any particular form of the process is determined by the conditions of the initial excitation.

The most important conclusion from this study is the prediction that a shock front exists in the propagation of the displacements, which in some forms corresponds to maximal nonstationary stresses in the structure, and this evidently is responsible for the production of defects on shock loading of a solid and also for the shock strength.

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