CERTAIN EFFECTS OF A NONLOCAL NATURE IN A CHAIN INVOLVING LONG-RANGE INTERACTION IN AN ELASTIC MEDIUM

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Recently considerable developments have taken place in the nonlocal theory of an elastic medium [1, 3], which is closely related to the theory of the crystal lattice. It is accordingly of particular interest to study the effects of nonlocalized interactions within the framework of an extremely simple model, that of a chain involving long-range forces between its constituents. In this paper we shall present some new results achieved in this direction. In Section 1 we consider the structure of the fundamental solution to the equation of motion of the chain. We shall show that this is determined by the distribution of the roots of the elastic-energy operator in the complex plane of wave numbers, the number of significant roots coinciding with the number of interacting neighbors. We shall give the Green's functions for an unlimited chain and also for the main boundary problems associated with a half chain. For chains with local defects, we shall construct an algorithm for finding the Green's functions in terms of the Green's function of an ideal chain.

The mathematical apparatus so developed will be used in Section 2 in order to study the question of the static elastic interaction of defects in an external field. We shall show that the corresponding energy is nonzero when it is not simply the nearest neighbors which interact with each other in the chain. The dependence of the energy on the distance between the defects bears a nonmonotonic character. The interaction in question may accordingly serve as one of the mechanisms governing the formation of stable complexes of defects when these approach one another within a distance of the order of the radius of the long-range forces of interaction. In conclusion, we shall consider the interaction of a defect with a boundary in an external field.

1. The equation of motion of a nonuniform chain, considered in the harmonic approximation, takes the form [4]

$$\rho(n)\ddot{u}(n,t)+\sum_{n'}\Phi(n,n')\,u(n',t)=q(n,t)$$

Here u and q are the displacements and external forces, depending on the coordinate n and the time t; $\rho(n)$ is the mass of the atom with number n; $\Phi(n, n')$ is the kernel of the elastic-energy operator Φ satisfying the conditions

$$\Phi(n,n')=\Phi(n',n),\qquad \sum_{n'}\Phi(n,n')=0 \tag{1.1}$$

It thus follows that $\Phi(n, n')$ may be expressed in the form

$$\Phi(n,n')=\psi(n)\delta(n-n')-\Psi(n,n'),\qquad \psi(n)=\sum_{n'}\Psi(n,n')$$

where $\Psi(n, n')$ may be interpreted as the rigidity of the effective elastic coupling between the atoms with numbers n and n'. In certain cases, it is more convenient to use $\Psi(n, n')$ rather than $\Phi(n, n')$, in particular when considering boundary problems [5]. We consider that the number of interacting neighbors N is finite, i.e., $\Psi(n, n')=0$ if $|n-n'|>N$.

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In addition to functions of n and t, we shall also consider the Fourier transforms of these, for which we retain the same notation, but with arguments k and ω. For example [2],

$$u(k, \omega) = \sum_n \int dt u(n, t) e^{i(kn-\omega t)}$$

in which k belongs to the segment $|k| \leq \pi$.

If the chain is uniform, then

$$\rho(n) = \rho_0, \quad \Phi(n, n') = \Phi_0(n - n'), \quad \Psi(n, n') = \Psi_0(n - n')$$

and the equation of motion in the (k, ω) representation takes the form

$$\Phi_0(k, \omega)\, u(k, \omega) \equiv [-\omega^2 \rho_0 + \Phi_0(k)]\, u(k, \omega) = q(k, \omega) \tag{1.2}$$

where

$$\Phi_0(k) = 2 \sum_{n=1}^{N} \Psi_0(n)(1 - \cos kn) \tag{1.3}$$

In view of the periodicity of Φ_0 (k), the latter is completely determined by specifying k in the $|\mathrm{Re}\, k| \leq \pi$ band of the complex plane, with identical corresponding boundary points, so that the permissible range of k is the complex cylinder K.

Let us consider the properties of Φ_0 (k) for $k \in K$. We may suppose, for simplicity, that the effective elastic couplings are stable, i.e., $\Psi_0(n) \geq 0$. Then for $k \in K$ function $\Phi_0(k)$ has no roots on the real and imaginary axes, apart from the twofold root $k_0 = 0$. It follows from the frequency and realness of Φ_0 (k) that, if k_m is a zero of Φ_0 (k), then so are $\bar{k}_m$, $-k_m$, $-\bar{k}_m$.

According to (1.3), the function Φ_0 (k) will be a polynomial in cos k of degree N; one of the zeros of this polynomial will be $\cos k_0 = 1$. The reciprocal function $G_0(k) = \Phi_0^{-1}(k)$ will be the Fourier transform of the static Green's function for the unbounded chain. This function may be expanded into very simple fractions:

$$G_0(k) = \frac{1}{2c_0(1 - \cos k)} - \sum_{m=1}^{N-1} \frac{\sin k_m}{\Phi_0'(k_m)(\cos k - \cos k_m)} \quad (\mathrm{Im}\, k_m > 0)$$

$$c_0 = \sum_{n=1}^{N} n^2 \Psi_0(n)$$

where c_0 has the sense of the elastic modulus in the long-wave approximation.

An analogous expansion occurs for the dynamic Green's function:

$$G_0(k, \omega) = \Phi_0^{-1}(k, \omega) = -\sum_{m=0}^{N-1} \frac{\sin k_m(\omega)}{\Phi_0'(k_m(\omega))(\cos k - \cos k_m(\omega))} \quad (\mathrm{Im}\, k_m(\omega) \geq 0)$$

where $k_m(\omega)$ are the roots of Φ_0 (k, ω).

This formula is written down on the assumption that the roots $k_m(\omega)$ are simple. The generalization to the case of multiple roots, which arises, for example, in relation to frequencies corresponding to the extrema on the dispersion curve, is quite obvious.

In the (n, ω) representation we may write

$$G_0(n, \omega) = \sum_{m=0}^{N-1} \frac{ie^{ik_m(\omega)|n|}}{\Phi_0'(k_m(\omega))} \qquad (\mathrm{Im}\, k_m(\omega) \geq 0) \tag{1.4}$$

In the static case we have

$$G_0(n) = -\frac{|n|}{2c_0} + \sum_{m=1}^{N-1} \frac{ie^{ik_m|n|}}{\Phi_0'(k_m)} \qquad (\mathrm{Im}\, k_m > 0) \tag{1.5}$$

For the interaction of two neighbors, in particular, the last expression takes the form

$$G_0(n) = \frac{1}{2c_0}\left[-|n| + \frac{e^{ik_1|n|}}{2\sqrt{\alpha(1+\alpha)}}\right] \tag{1.6}$$

$$e^{ik_1} = -(\sqrt{1+\alpha} - \sqrt{\alpha})^2, \quad \alpha = \frac{\Psi_0(1)}{4\Psi_0(2)} \tag{1.7}$$

The fundamental solution of Eq. (1.2) is obtained by adding to (1.4) the general solution of the corresponding homogeneous equations:

$$\sum_{m=0}^{N-1} [\alpha_m e^{ik_m(\omega)n} + \beta_m e^{-ik_m(\omega)n}] \qquad (\operatorname{Im} k_m(\omega) \geqslant 0)$$

Here α_m, β_m are arbitrary constants. We see from this that the structure of the fundamental solution is completely determined by the distribution of the roots Φ_0 (k, ω) situated in the complex cylinder K.

In considering boundary conditions, it is convenient to use the Green's functions of these problems, which may be obtained from the fundamental solution by appropriately choosing the constants α_m and β_m so as to satisfy the corresponding boundary conditions. A formulation for boundary problems having forces (or displacements) specified in the boundary region may be derived from the conditions under consideration in the intermediate region between chains comprising atoms of different types by letting the elastic couplings characterizing the interaction between the chains tend to zero. The corresponding boundary region is clearly determined by the radius of the long-range forces of interaction. This type of problem formulation was considered earlier [5] for the case of a continuous elastic medium involving long-range interaction.

Omitting some simple but rather cumbersome calculations analogous to those of the earlier paper [5], we shall now give the expressions representing the static Green's functions for a right-handed half chain with interaction between two neighbors.

For a problem with forces specified in the boundary region

$$G_0(n, n') = -\frac{1}{2c_0}\left[|n-n'| + n + n' - \frac{e^{ik_1|n-n'|} + e^{ik_1(n+n')}}{2\sqrt{\alpha(1+\alpha)}}\right] \quad (n, n' \geqslant 0) \tag{1.8}$$

This function satisfies the homogeneous force conditions in the boundary region n = 0, 1.

Correspondingly, for a problem with displacements specified at the boundary we obtain (n, n' $\geq$ 0)

$$G_0(n, n') = -\frac{1}{2c_0}\left[|n-n'| - (n+n') + \frac{e^{ik_1(n+n')} - e^{ik_1(n-n')}}{2\sqrt{\alpha(1+\alpha)}} + \frac{(1-e^{ik_1n})(1-e^{ik_1n'})}{1+\alpha-\sqrt{\alpha(1+\alpha)}}\right] \tag{1.9}$$

It is easy to verify that the following homogeneous boundary conditions are satisfied:

$$G_0(0, n') = G_0(1, n') = 0 \quad (n' \geqslant 0)$$

Let us now turn to the construction of the Green's function for a chain containing local defects, for simplicity confining attention to the static case. The method of construction will be analogous to that set out earlier [6]. Let us use V (n) to denote the characteristic function of the region V containing N_V points, the interaction between which is described by means of "distorted" elastic couplings. The kernel of the elastic-energy operator Φ may be expressed in the form

$$\Phi(n, n') = \Phi_0(n - n') + \Phi_V(n, n')$$

where Φ_V (n, n') characterizes the defects, so that Φ_V(n, n') $\neq$ 0 solely for n, n' $\in$ V. Clearly Φ_V (n, n') satisfies conditions of type (1.1).

The equation for the Green's function G (n, n') in operator form may be written as follows:

$$\Phi_0 G + \Phi_V G = I$$

where I is the unitary operator.

The application of operators G_0 and $\Phi_V G_0$ successively to both sides gives

$$G = G_0 - G_0\Phi_V G \tag{1.10}$$

$$A_V G \equiv [\Phi_V + \Phi_V G_0 \Phi_V] G = \Phi_V G_0 \tag{1.11}$$

The operator A_V satisfies conditions of type (1.1) and hence (generally speaking) has no reciprocal. However, in a special class of functions f_V (n) concentrated in the region V and satisfying the condition

$$\sum_n f_V(n) = 0$$

a reciprocal operator exists and may be determined from

$$A_V A_V^{-1} = A_V^{-1} A_V = I_V$$

where I_V is the projection operator for the function space in question. The kernel of this takes the form

$$I_V(n, n') = V(n)\bar{V}(n')[\delta(n - n') - N_v^{-1}]$$

where δ (n−n') is the Kronecker delta.

Applying the operator A_V^{-1} to both sides of (1.11) and substituting the result in the right-hand side of (1.10), we obtain

$$G = G_0 + G_0 P_V G_0 \tag{1.12}$$

$$P_V = -\Phi_V A_V^{-1} \Phi_V = -[\Phi_V^{-1} + I_V G_0 I_V]^{-1} \tag{1.13}$$

The reciprocal operators here introduced are to be understood in the foregoing sense.

We emphasize that in these relations G_0 may be not only the Green's function of an unlimited chain but also the Green's function of any bounded problem. The formulas in question will provide an expression for the Green's function of the corresponding boundary problem in the case of a chain containing defects. The validity of the corresponding homogeneous boundary conditions for G follows directly from the form of Eq. (1.12).

Let us consider, for example, a chain in which there is one defect atom with number m. Let us suppose that only the couplings between the defect and its nearest neighbors are distorted, so that

$$\Psi(m, m-1) = \Psi(m, m+1) = \Psi_0(1) + \psi$$

After corresponding calculations, we find the expressions for the nonzero elements of the matrix P_V (n, n') (n, n' = m−1, m, m+1):

$$P_V(n, n') = \frac{1}{a_1 a_3 - a_2^2} \begin{Vmatrix} a_1 & -a_1 + a_2 & -a_2 \\ -a_1 + a_2 & a_1 - 2a_2 + a_3 & a_2 - a_3 \\ -a_2 & a_2 - a_3 & a_3 \end{Vmatrix} \tag{1.14}$$

$$a_1 = \psi^{-1} + \Delta_{-1} G_0(m, m)\Delta_{-1}, \quad a_2 = \Delta_{-1} G_0(m, m)\Delta_1,$$
$$a_3 = \varphi^{-1} + \Delta_1 G_0(m, m)\Delta_1 \tag{1.15}$$

where Δ_1 denotes the operation of the first difference, applied, depending on the disposition of the sign, to the first or second argument of G_0 (m, m), for example,

$$\Delta_{-1} G_0(m, m)\Delta_1 = [G_0(m, m) - G_0(m+1, m)]\Delta_1$$
$$= G_0(m, m) - G_0(m, m-1) - G_0(m+1, m) + G_0(m+1, m-1)$$

2. As indicated earlier [4, 6], Green's functions constitute an extremely convenient apparatus for studying the elastic interaction energy of defects in an external field. Let us first consider an unlimited chain with a force q acting upon it. The energy may be written in the form

$$\Phi = \sum_n q(n) u(n) = \sum_{n,n'} q(n) G(n, n') q(n') \tag{2.1}$$

Let us use u_0 (n) to denote the displacements of an ideal chain corresponding to the forces q (n) and Φ_0 to denote its energy. Substituting (1.12) in the latter expression, we obtain

$$\Phi = \Phi_0 + \Phi^*, \quad \Phi^* = \sum_{n,n' \in V} u_0(n) P_V(n, n') u_0(n') \tag{2.2}$$

where Φ^* may be interpreted as the interaction energy of defects with the field u_0.

Let us consider an extremely simple example illustrating the interaction of defects with a field of uniform deformation u_0 (n) = n. Let the atoms with numbers 0, 1 and m, m+1 be connected by defective couplings with characteristics $\Psi = \Psi_0(1) + \psi$. Calculation of the energy Φ^* for such defects leads to the following expression:

$$\Phi^* = -\frac{2}{\psi^{-1} + g(0) + g(m)}, \quad g(m) = \Delta_2 G_0(m) = \Delta_1 \Delta_{-1} G_0(m) \tag{2.3}$$

For a chain involving the interaction of two neighbors we obtain the following from (1.6) and (1.7):

$$g(m)=\frac{(-1)^m}{c_0}\frac{\sqrt{1+\alpha}}{\sqrt{\alpha}}\left(\sqrt{1+\alpha}-\sqrt{\alpha}\right)^{2|m|}$$

This is an alternating function of m, vanishing as $m\to\infty$. Thereupon Φ^* tends to a limiting value

$$\Phi_\infty^*=-\frac{2}{\psi^{-1}+g(0)}$$

corresponding to twice the interaction energy of an isolated defective coupling with the field u_0. The difference $\Phi^*-\Phi_\infty{}^*$ may be interpreted as the interaction energy of the defective couplings with each other in a field of homogeneous (uniform) deformation. This energy is proportional to g (m) and is hence a nonmonotonic function of m. It is easy to show that this result remains valid even for a chain with interaction involving a large number of neighbors. On the other hand, if the interaction between second neighbors may be neglected ($\alpha\to\infty$), then g (m)$\to$ 0 and $\Phi^*-\Phi_\infty{}^*\to 0$.

An analogous effect takes place in the interaction of two defect atoms with distorted couplings between each atom and its nearest neighbors. These couplings are characterized by the same parameter ψ as in the foregoing discussion. Calculation of the corresponding energy Φ^* for the field u_0 (n) =n gives the expression

$$\Phi^*=-\frac{2\left[2\psi^{-1}+\Delta_2(g(0)-g(m))\right]}{(\psi^{-1}+g(0)+g(m-1))(\psi^{-1}+g(0)+g(m+1))-(g(1)+g(m))^2} \tag{2.4}$$

where m is the distance between the defect atoms.

The nonmonotonic character of the relationship between the interaction energy of such defects and the distance between them means that the interaction in question may constitute one of the mechanisms underlying the formation of stable complexes of defects when these approach one another within a distance of the order of the long-range radius of interaction. It should be noted that the absence of interaction between defects in a chain without long-range forces is a one-dimensional effect. In a lattice the defects interact with each other in the presence of an external field, the corresponding energy falling off with increasing distance between the defects in accordance with a power law. When long-range forces of interaction are "connected in," alternating and exponentially attenuating terms are added, and these may cause substantial changes in energy at distances of the order of the long-range interaction radius.

Let us now turn to the question of the interaction of a defect with a boundary. If the forces are specified in the boundary region, Eq. (2.1) for the energy of the chain remains valid, if G is the Green's function of the particular boundary problem. From this follows the validity of (2.2) for Φ^*, where in (1.13) we must substitute the corresponding Green's function G_0 for P_V.

Let us consider, by way of an illustration, a semiinfinite chain with interaction between two neighbors, in which there is one defect atom of the type mentioned in the foregoing. Let the chain be subjected to uniform deformation at infinity (u (n) ~n as $n\to\infty$), while a corresponding balancing force is applied at the starting point of the chain. By using (1.8), we may readily find the displacements in the defect-free chain:

$$u_0(n)=n-\frac{e^{ik_1 m}}{2\sqrt{\alpha(1+\alpha)}}\qquad (n\geqslant 0)$$

Substituting into the second part of Eq. (2.2) and using (1.14), (1.15), and (1.8), we obtain

$$\Phi^*=\frac{b_1+b_2e^{ik_1 m}+b_3e^{2ik_1 m}}{b_4+b_5e^{2ik_1 m}}$$

$$b_1=\frac{2}{\psi}+\frac{2}{c_0}\frac{\sqrt{1+\alpha}}{\sqrt{\alpha}}(1+e^{ik_1}),\quad b_2=-4\left[\frac{1}{\psi}+\frac{2(1+\alpha)}{c_0}\left(\frac{\sqrt{1+\alpha}}{\sqrt{\alpha}}-1\right)\right]$$

$$b_3=2\left[\frac{1+\alpha}{\alpha\psi}+\frac{2(1+\alpha)}{c_0}\left(\frac{\sqrt{1+\alpha}}{\sqrt{\alpha}}+\frac{1}{\alpha}\right)\right],$$

$$b_4=\left(\frac{1}{\psi}+\frac{1}{c_0}\frac{\sqrt{1+\alpha}}{\sqrt{\alpha}}\right)^2-\frac{1+\alpha}{\alpha c_0^2}e^{2ik_1},\ b_5=\frac{2}{c_0}\frac{\sqrt{1+\alpha}}{\sqrt{\alpha}}\left(\frac{1+2\alpha}{\psi}-\frac{2(1+\alpha)}{c_0}\right)$$

Here $m\geq 1$ is the distance of the defect from the start of the chain. It may be shown that the difference $\Phi^*(m)-\Phi^*(\infty)$, which in the present case is to be interpreted as the interaction energy of the defect with the boundary, is a nonmonotonic function of m. An analogous effect takes place in the case of the rigid fitting of the boundary region, when u_0 (n) takes the form

$$u_0(n) = n - \frac{1 - e^{ik_1 n}}{1 - e^{ik_1}} \qquad (n \geqslant 0)$$

In calculating u_0, we use the Green's function (1.9). The calculation of Φ^* may be effected by means of the procedure employed earlier in the first boundary problem, but using (1.9) instead of (1.8). We accordingly obtain

$$\Phi^* = \frac{c_1 + c_2 e^{ik_1 m} + c_3 e^{2ik_1 m}}{c_4 + c_5 e^{2ik_1 m}} \qquad (m \geqslant 1)$$

$$c_1 = b_1, \qquad c_2 = -2\left[\frac{1 + e^{-ik_1}}{\psi} - \frac{4(1+\alpha)}{c_0}\right]$$

$$c_3 = -2\left[\frac{1+2\alpha}{\psi} e^{-ik_1} + \frac{2(1+\alpha)}{c_0}\left(\frac{\sqrt{1+\alpha}}{\sqrt{\alpha}^2} + 1\right)\right], \qquad c_4 = b_4$$

$$c_5 = \frac{2e^{-ik_1}}{c_0} \frac{\sqrt{1+\alpha}}{\sqrt{\alpha}}\left[\frac{1+2\alpha}{\psi} + \frac{2(1+\alpha)}{c_0}\right]$$

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