SOME PROBLEMS IN THE DYNAMICS OF CRYSTAL LATTICES AND OF THE THEORY OF ELASTICITY

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Two problems of the dynamics of an infinite crystal are solved in the harmonic approximation: 1) two semi-bounded parts of a crystal possessing at the initial time equal but opposite velocities perpendicular to the interface (collision); 2) external forces act on the atoms of an arbitrary crystal plane. It is shown that the solutions are integrals which are superpositions of plane waves and can be separated into decaying and nondecaying perturbations. The nondecaying perturbations have the form of "step-like" waves and are solutions of the aforementioned problems in the theory of elasticity. The decaying perturbations are a refinement of the macroscopic theory; they move with velocities that differ from the velocity of sound. Perturbations connected with inflection points of the dispersion curves decay least. A connection is noted between the problems considered and similar problems in the theory of frequency filters and iris-loaded waveguides.

INTRODUCTION

In considering certain processes in solids (for example, the propagation of perturbations resulting from the collision of solids, or from the action of external forces on the solid) one restricts oneself to the macroscopic picture provided by the theory of elasticity. However, the theory of elasticity of anisotropic, as well as isotropic, media is only an approximate theory of the mechanical processes in crystals. A more exact (microscopic) picture compared with the theory of elasticity is obtained by the methods of crystal lattice dynamics. The special solutions of the equations of motion of the lattice are harmonic plane waves, and the solutions of specific problems, like those mentioned above, are obtained in the form of a superposition of plane waves. The presence of such solutions makes it possible to show the effect of the entire frequency spectrum on the propagation of perturbations in the crystal. In this connection there appears also the converse possibility of reconstructing the lattice spectrum, or at least some of its features, from the propagation of perturbations in the crystal.

In this paper we shall consider for simplicity the case of a crystal with a simple lattice; however, the generalization of the problems considered to the case of a more complicated lattice presents no difficulties.

1. THREE-DIMENSIONAL CRYSTAL AND LINEAR CHAINS

Let us consider a crystal with a Bravais lattice. Following Born ([1], Sec. 22), we divide the crystal into a system of equidistant crystal planes. Let the basis vectors $\mathbf{a}_1$ and $\mathbf{a}_2$ be located in a crystal plane, and let the vector $\mathbf{a}_3$ connect arbitrary lattice points of two neighboring crystal planes; the origin of the coordinates is on one of the lattice points, two coordinate axes x_1 and x_2 are in the crystal plane, and the x_3 axis is perpendicular to it. Since the radius vector of an arbitrary lattice point is $\mathbf{r}^n = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3$, it is readily seen that n_3 numbers the planes.

The reciprocal lattice vector $\mathbf{b}_3 = \mathbf{a}_1 \times \mathbf{a}_2/(\mathbf{a}_1 \times \mathbf{a}_2)\cdot \mathbf{a}_3$, perpendicular to the crystal planes, can, like the planes themselves, in a certain sense be arbitrarily oriented with respect to the crystal. One sees readily that the set of all the possible orientations of the vector $\mathbf{b}_3$ occupies in the set of all the possible orientations of the wave vector $\mathbf{k}$ a position similar to that of the set of rational numbers with respect to the set of real numbers.

Let us consider plane waves with the wave vector $\mathbf{k} = q\mathbf{b}_3\,(-\pi \le q \le \pi)$, i.e., waves

$$u_i^{\mathbf{n}(s)}(q\mathbf{b}_3) = e_i^{(s)}(q\mathbf{b}_3)\exp[i(qn_3 \pm \omega^{(s)}(q\mathbf{b}_3)t)], \qquad (1.1)$$

where $s = 1, 2, 3$—the number of the spectrum branch. It is readily seen that these lattice motions are characterized by the fact that each crystal plane moves as a whole. From the equations of motion of the crystal

$$M\ddot{u}_i^{\mathbf{n}} = -\sum_{\mathbf{m}j} \Phi_{ij}^{\mathbf{nm}} u_j^{\mathbf{m}}$$

one can separate the equations for such motions:

$$M\ddot{u}_i^{n} = -\sum_{mj} A_{ij}^{nm} u_j^{m}, \qquad A_{ij}^{nm} = \sum_{m_1 m_2} \Phi_{ij}^{\mathbf{nm}}, \qquad (1.2)$$

where $n = n_3$ is no longer a vector, but a scalar. The coefficients A_{ij}^{nm} could be called interplanar force constants. We see that Eqs. (1.2) are equivalent to the equations of motion of some linear (but three-dimensional chain of atoms).

If the direction $\mathbf{b}_3$ is a symmetry axis of the crystal, then $A_{23}^{nm} = A_{13}^{nm} = 0$ and one can separate from Eq. (1.2) equations for longitudinal plane waves with the wave vector $\mathbf{k} = q\mathbf{b}_3$:

$$M\ddot{u}_3^{n} = -\sum_{m} A_{33}^{nm} u_3^{m}. \qquad (1.3)$$

Equations (1.3) are equivalent to the equations of motion of a linear one-dimensional chain of atoms. In our case this is a simple chain, whereas in the case of a complex crystal the chain will be complex (binary, etc.).

It is known that the problem of the propagation of waves in linear chains (one- and three-dimensional) is mathematically equivalent to the problem of the propagation of electromagnetic waves in frequency filters and iris-loaded wave-guides (see, for example, [2]); therefore the results obtained in the following sections may be useful in considering similar problems in the theory of filters and waveguides.

2. SOLUTION OF THE EQUATIONS OF MOTION OF THE LATTICE FOR CERTAIN SIMPLE INITIAL CONDITIONS

We thus chose an arbitrary direction in the crystal, obtained a chain of crystal planes, the equations of motion of these planes (1.2), and the particular solutions of these equations. Here we can go over to the following simple notation:

$$n_3 \to n, \quad \omega^{(s)}(q\mathbf{b}_3) \to \omega^{(s)}(q), \quad \mathbf{e}^{(s)}(q\mathbf{b}_3) \to \mathbf{e}^{(s)}(q),$$

where the functions $\omega^{(s)}(q)$ and $\mathbf{e}^{(s)}(q)$ have the following properties:

$$\omega^{(s)}(q) = \omega^{(s)}(-q), \quad \mathbf{e}^{(s)}(q) = \mathbf{e}^{(s)}(-q) \qquad (2.1)$$

and for $q \to 0$

$$\omega^{(s)}(q) \to 0, \quad \frac{d}{dq}\omega^{(s)}(q) \to c^{(s)}|\mathbf{b}_3| \equiv \frac{c^{(s)}}{a}, \quad \frac{d^2}{dq^2}\omega^{(s)}(q) \to 0. \qquad (2.2)$$

Here $c^{(s)}$ are the three sound velocities for the corresponding direction $\mathbf{b}_3$, and a is the distance between neighboring planes.

Let one of the planes (denoted by l) have at the initial instant a velocity which differs from zero and is directed perpendicular to the plane, then the initial conditions of the problem will be of the form:

$$u_i^n(0) = 0, \qquad (2.3)$$

$$\dot{u}_i^n(0) = \delta_{i3}\delta_{ln}v. \qquad (2.4)$$

From (1.1) we obtain particular solutions satisfying conditions (2.3):

$$u_i^{n(s)}(q, t) = e_i^{(s)}(q)\sin[\omega^{(s)}(q)t]e^{inq}.$$

A solution satisfying simultaneously conditions (2.3) and (2.4) will be sought in the form of a superposition

$$u_i^n(t) = \sum_{(s)} \frac{1}{2\pi}\int_{-\pi}^{\pi} A^{(s)}(q)e_i^{(s)}(q)\sin[\omega^{(s)}(q)t]e^{inq}\,dq. \qquad (2.5)$$

Then

$$\dot{u}_i^n(0) = \frac{1}{2\pi}\int_{-\pi}^{\pi}\left\{\sum_{(s)} A^{(s)}(q)e_i^{(s)}(q)\omega^{(s)}(q)\right\}e^{inq}\,dq. \qquad (2.6)$$

We see that the quantities $\dot{u}_i^n(0)$ are Fourier coefficients of the sums in the integrand of (2.6). Hence and from conditions (2.4) we obtain a system of three linear equations with three unknowns. Solving these, we obtain

$$A^{(s)}(q)\omega^{(s)}(q) = v\Delta^{(s)}(q)e^{-ilq}, \qquad (2.7)$$

where

$$\Delta^{(1)}(q) = \begin{vmatrix} e_1^{(2)} & e_1^{(3)} \\ e_2^{(2)} & e_2^{(3)} \end{vmatrix}, \quad \Delta^{(2)}(q) = \begin{vmatrix} e_1^{(3)} & e_1^{(1)} \\ e_2^{(3)} & e_2^{(1)} \end{vmatrix},$$

$$\Delta^{(3)}(q) = \begin{vmatrix} e_1^{(1)} & e_1^{(2)} \\ e_2^{(1)} & e_2^{(2)} \end{vmatrix}.$$

Here $\det(e_i^{(s)}) = 1$, since we are using polarization vectors normalized to unity. Substituting (2.7) in (2.5) and bearing in mind (2.1), we obtain

$$u_i^n(t) = \sum_{(s)} \frac{v}{\pi}\int_0^{\pi} \frac{\Delta^{(s)}(q)e_i^{(s)}(q)}{\omega^{(s)}(q)} \times \sin[\omega^{(s)}(q)t]\cos(n-l)q\,dq. \qquad (2.8)$$

Equations (1.2) can also be readily solved if at the initial instant one of the planes is displaced from its equilibrium position, or if it has a velocity along one of the coordinate axes. Since Eqs. (1.2) are linear, their solutions can be summed. This makes it possible to obtain a solution of Eqs.

(1.2) for arbitrary initial conditions (nonvanishing initial displacements and velocities).

3. A MODEL OF THE PROBLEM OF THE COLLISION OF TWO SEMI-BOUNDED CRYSTALS

Let us solve Eqs. (1.2) with the initial conditions

$$u_i^n(0) = 0;$$

$$\dot{u}_i^n(0) = -{}^1\!/_2 v\delta_{i3}, \quad n = 1, 2, 3, \ldots; \qquad \dot{u}_i^n(0) = {}^1\!/_2 v\delta_{i3}, \quad n = 0, -1, -2, \ldots \tag{3.1}$$

The problem with such initial conditions is apparently a rather interesting model of the problem of the collision of two semi-bounded crystals, since the latter can sometimes be considered in the rigorous formulation as a problem with initial conditions which differ from conditions (3.1) only close to the plane with n = 0. The relation between the solutions of these problems will be discussed at the end of Sec. 4.

Let us go over from displacements of the planes from their equilibrium conditions to new variables $\sigma_i^n(t)$ which have an analogy in the theory of elasticity:

$$\sigma_i^n(t) = a^{-1}(u_i^n(t) - u_i^{n+1}(t)) \tag{3.2}$$

(a is, as before, the distance between neighboring crystal planes). Starting from the linearity of Eqs. (1.2), it can be shown that the variables $\sigma_i^n(t)$ satisfy the the same Eqs. (1.2) as the variables $u_i^n(t)$. As is readily seen from (3.1) and (3.2), the initial conditions for the variables $\sigma_i^n(t)$ will be the conditions

$$\sigma_i^n(0) = 0, \qquad \dot{\sigma}_i^n(0) = \delta_{i3}\delta_{0n}v/a. \tag{3.3}$$

Bearing in mind (2.2) and comparing conditions (2.3) and (2.4) with (3.3), we obtain from (2.8)

$$\sigma_i^n(t) = \sum_{(s)} I_i^{(s)}(t, n), \tag{3.4}$$

where

$$I_i^{(s)}(t, n) = \int_0^\pi \psi_i^{(s)}(q)\, q^{-1} \sin[\tau^{(s)}\varphi^{(s)}(q)] \cos nq\, dq, \tag{3.5}$$

and

$$\psi_i^{(s)}(q) = \frac{v}{c^{(s)}\pi}\frac{\omega'^{(s)}(0)\,q}{\omega^{(s)}(q)}\Delta^{(s)}(q)\, e_i^{(s)}(q),$$

$$\varphi^{(s)}(q) = \omega^{(s)}(q)/\omega'^{(s)}(0), \qquad \tau^{(s)} = c^{(s)}t/a. \tag{3.6}$$

It can be shown that integrals of the form (3.5) can be separated into decaying and nondecaying perturbations (see the Appendix).

4. COLLISION OF CRYSTALS IN LATTICE DYNAMICS AND IN THE THEORY OF ELASTICITY

Bearing in mind (3.5) and using the results obtained in the Appendix [Eq. (A.9)], we can write the following approximations:

$$I_i^{(s)}(t, n) \approx \begin{cases} (v/2c^{(s)})\Delta^{(s)}(0)\, e_i^{(s)}(0), & c^{(s)}t/a > n \\ 0, & c^{(s)}t/a < n \end{cases}. \tag{4.1}$$

Substituting (4.1) in (3.4), we obtain an approximate solution of the problem of the collision of crystals. This solution is at the same time in all probability the exact solution of this problem in the theory of elasticity. Let us note certain features of this solution:

1. Three nondecaying shock waves with velocities $c^{(1)}$, $c^{(2)}$, and $c^{(3)}$ propagate in both directions along the x_3 axis from the point of collision. A jump-like displacement ("step" function) and a jump-like compression of the lattice take place on the passage of each wave.

2. Since the polarization vectors are mutually orthogonal, the condition $\Delta^{(s)}e_3^{(s)} > 0$ is fulfilled and the compressions will indeed be compressions —there will be no expansions.

3. On the other hand, the displacements will be both along the positive and negative directions of the x_1 and x_2 axes. Indeed, as is readily seen,

$$\sum_{(s)} \Delta^{(s)} e_i^{(s)} = 0 \quad (i = 1, 2), \tag{4.2}$$

and therefore the three terms of this sum cannot simultaneously have the same signs. Thus if we separate in our mind within the crystal an infinite rod with its axis perpendicular to the collision plane, one can see that after the collision this rod will break in each half-space at three points and form four "joints". The lengths of the first three inclined "joints" are determined by the sound velocities $c^{(s)}$. The fourth "joint" which is farthest and extends into infinity, remains along the previous axis. The beginning of the first "joint" will remain in its previous position (point of collision), a fact which one can readily verify by using relation (4.2).

Making use of the results obtained in the Appendix, one can assert that the microscopic picture of the collision of the crystals differs from the macroscopic picture provided by the theory of elasticity by the presence of additional decaying perturbations, among which perturbations of the order of $t^{-1/3}$ or $n^{-1/3}$ are most important. Using the results obtained in the Appendix and the known formulas of the asymptotic methods (see [3]), one can carry out a more specific estimate of the decaying perturbations.

As is seen from (3.4) and (4.1), the solution of the problem depends on the directions of the polarization vectors for various values of the variable q and in particular for $q \to 0$. Let us consider two interesting cases.

A. The direction of the vector $\mathbf{b}_3$ is a symmetry axis of the crystal. In this case one of the polarization vectors becomes longitudinal for all values of the variable q. Therefore, only one of the nine integrals of (3.5), containing decaying and nondecaying longitudinal waves, will differ from zero. In any case, the same solution could be obtained by considering the collision of linear one-dimensional chains with equations of motion (1.3) in the form of an expansion in particular solutions of Eqs. (1.3)—in longitudinal plane waves.

B. For the $\mathbf{b}_3$ direction one of the polarization vectors does not become longitudinal for all values of q, but only for $q \to 0$. Such directions are apparently possible in certain crystals.[4] In this case, although all the integrals do not vanish, only one of them contains a nondecaying wave—a "step-like" compression wave. In transverse displacements of the planes relative to one another the main role will be played by nondecaying perturbations connected with inflection points of the dispersion curves, including also the points $q = 0$.

As has already been noted, the solution of the problem in this section is not an exact solution of the problem of the collision of two semi-bounded crystals. However, as a result of the linearity of Eqs. (1.2), the solution of the second problem is equal to the sum of the solutions of the first problem and of a certain third problem, the initial conditions of which differ from zero only near the plane with $n = 0$. It can be shown that the solution of this third problem contains no nondecaying waves. In some instances the initial conditions of the third problem will depend weakly on the collision velocity, and for a sufficiently large collision velocity the decaying perturbations of the third problem will then be small compared with the same perturbations of the first problem. It is readily seen that in such cases the first problem will be a good approximation of the second.

5. THE MOTION OF CRYSTAL PLANES UNDER THE ACTION OF EXTERNAL FORCES

Let all the atoms of the crystals be located at the initial instant at the lattice points and let their velocities be zero; an equal force perpendicular to the plane begins to act on each atom of the plane with $n = 0$. It is readily seen that we have arrived at the problem of the motion of a chain of planes. We write down the equations of motion and the initial conditions:

$$M\ddot{u}_i^n = -\sum_{mj} A_{ij}^{nm} u_j^m + F(t)\,\delta_{i3}\delta_{0n};$$

$$u_i^n(0) = 0, \quad \dot{u}_i^n(0) = 0. \qquad (5.1)$$

The solution of this problem can be obtained by a known method (see, for example,[5] p. 275) from the solution of the problem considered in Sec. 2. Thus we obtain from (2.8)

$$u_i^n(t) = \sum_{(s)} \int_0^t \frac{F(\tau)}{\pi M} \int_0^\pi \frac{\Delta^{(s)}(q)\, e_i^{(s)}(q)}{\omega^{(s)}(q)} \times \sin\left[(t-\tau)\,\omega^s(q)\right] \cos nq\, dq\, d\tau. \qquad (5.2)$$

We can consider $F(t)$ to be an arbitrary, for instance periodic, function of the time. We shall consider the case when this function is in the form of a square pulse:

$$F(t) = \begin{cases} F, & 0 \leqslant t \leqslant T \\ 0, & t > T \end{cases}. \qquad (5.3)$$

Going over to the same variables $\sigma_i^n(t)$ as in Sec. 3, we obtain for times $t > T$

$$\sigma_i^n(t) = \sum_{(s)} [L_i^{(s)}(t, n) + L_i^{(s)}(t - T, n)], \qquad (5.4)$$

$$L_i^{(s)}(t, n) = \frac{-F_a}{[c^{(s)}]^2 \pi M} \int_0^\pi \frac{2\omega'^{(s)}(0) \sin {}^1\!/_2 q}{\omega^{(s)}(q)} \Delta^{(s)}(q)\, e_i^{(s)}(q) \times \frac{1}{q} \frac{q\omega'^{(s)}(0)}{\omega^{(s)}(q)} \cos\left[\frac{c^{(s)}t}{a} \frac{\omega^{(s)}(q)}{\omega'^{(s)}(0)}\right] \sin\left(n + \frac{1}{2}\right) q\, dq. \qquad (5.5)$$

Here we encounter the problem of analyzing integrals of the form

$$L(\tau, n) = \int_0^\pi \frac{\psi(q)}{q} \cos[\tau\varphi(q)] \sin\left(n + \frac{1}{2}\right) q\, dq. \qquad (5.6)$$

By virtue of simple trigonometric relations this problem is almost identical with the problem of analyzing integrals of the form (A.1). Having obtained the asymptotic expansions of integrals of the form (5.6), we can write

$$L_i^{(s)}(t, n) - L_i^{(s)}(t - T, n) \approx \begin{cases} 0, & (n + {}^1\!/_2)\, a > c^{(s)} t \\ \dfrac{Fa\Delta^{(s)}(0)\, e_i^{(s)}(0)}{[c^{(s)}]^2\, 2M}, & c^{(s)}(t - T) < (n + {}^1\!/_2)\, a < c^{(s)} t. \\ 0, & (n + {}^1\!/_2)\, a < c^{(s)}(t - T) \end{cases} \qquad (5.7)$$

Substituting (5.7) in (5.4), we obtain an approximate solution of our problem which is an exact solution of this problem in the theory of elasticity. It differs from the solution of the collision problem by the presence of two groups of nondecaying waves, separated from one another by a time interval T, the second group canceling the deformation produced by the first, so that the crystal remains undeformed after the passage of both groups. It is readily seen that by using the dynamical method considered here one can solve the purely static problem of unidirectional compression of a crystal (two equal but opposite forces perpendicular to the planes act on two parallel planes of the crystal), and also other static problems.

The decaying perturbations will be of the same form as in the collision problem. It should be noted that decaying perturbations propagating at arbitrarily large velocities occur in the solutions of both problems. This is due to the fact that the equations of motion (1.2) do not take into account the "inertia of the binding energy" ([6], p. 127). However, account of the retardation would not lead to any considerable change in the solutions, since it would affect only perturbations propagating at velocities close to the speed of light, and would limit these to the speed of light. In the solutions which we have obtained perturbations propagating at velocities close to the speed of light are, as can be readily seen from the Appendix, negligible; they are therefore of no interest to us.

In conclusion I express my gratitude to V. A. Zhdanov for discussing the results of this paper.

APPENDIX

DECAYING AND NONDECAYING PERTURBATIONS

Let us consider an integral of the form

$$I(\tau, n) = \int_0 \frac{\psi(q)}{q} \sin[\tau\varphi(q)] \cos nq \, dq;$$
$$0 \leqslant \tau < \infty, \quad n = 0, 1, 2, \ldots \qquad (A.1)$$

Here $\psi(q)$ and $\varphi(q)$ are functions having a sufficient number of continuous derivatives in the interval $[0, \pi]$ and $\psi(0) \neq 0$. Bearing in mind (2.2) and (3.6), we can write

$$\varphi(q) \approx q + \frac{\varphi'''(0)}{3!} q^3 \quad \text{for} \quad q \to 0. \qquad (A.2)$$

We shall consider the cases $\tau \geq n$ and $\tau < n$ separately. Then

$$I(\tau, n) = \begin{cases} {}^1/_2[J^+(\tau, n) + J^-(\tau, n)], & n/\tau \leqslant 1 \\ {}^1/_2[K^+(\tau, n) - K^-(\tau, n)], & n/\tau > 1 \end{cases};$$

$$J^\pm(\tau, n) = \int_0^\pi \frac{\psi(q)}{q} \sin\tau\left[\varphi(q) \pm \frac{n}{\tau} q\right] dq,$$

$$K^\pm(\tau, n) = \int_0^\pi \frac{\psi(q)}{q} \sin n\left[q \pm \frac{\tau}{n}\varphi(q)\right] dq. \qquad (A.3)$$

When $\tau \gg 1$, the integrals $J^\pm$ can be expanded in the large parameter τ, using the stationary-phase method.[3] If $n \gg 1$, one can expand the integrals $K^\pm$ by the stationary-phase method.

Let us consider the integral $J^+(\tau, n)$. In order to apply to it the stationary-phase method directly, we must get rid of the zero in the numerator of the integrand. To this end we replace the integral $J^+(\tau, n)$ by a sum of integrals:

$$J^+(\tau, n) = J_1(\tau, n) + J_2(\tau, n) + J_3(\tau, n);$$

$$J_1(\tau, n) = \int_0^{q^*} \left(\frac{\psi(q)}{q} - \psi(0)\frac{h'(q)}{h(q)}\right) \sin\tau h(q) \, dq,$$

$$J_2(\tau, n) = \int_{q^*}^{\pi} \frac{\psi(q)}{q} \sin\tau h(q) \, dq,$$

$$J_3(\tau, n) = \psi(0) \int_0^{z^*} \frac{\sin z}{z} dz, \qquad (A.4)$$

where $h(q) = \varphi(q) + nq/\tau$, q^* is the stationary point closest to $q = 0\,[h'(q^*) = 0]$, and $z^* = \tau h(q^*)$.

The asymptotic expansion of the integral sine of large positive values of the argument [it is readily seen that $h(q^*) > 0$] is known[7] and therefore

$$J_3(\tau, n) \approx \psi(0)\left\{\frac{\pi}{2} - \frac{\cos z^*}{z^*}\left(1 - \frac{2!}{(z^*)^2} + \frac{4!}{(z^*)^4}\right) - \frac{\sin z^*}{z^*}\left(\frac{1}{z^*} - \frac{3!}{(z^*)^3}\right)\right\}. \qquad (A.5)$$

The stationary-phase method can be applied to the integrals J_1 and J_2. Let us write down the condition of stationarity:

$$h'(q) \equiv \varphi'(q) + n/\tau = 0, \qquad \varphi'(q) = -n/\tau. \qquad (A.6)$$

It follows from (A.6) that for a given dispersion law the position of the stationary points depends only on the ratio n/τ, i.e., each $n/\tau = \alpha = \text{const}$ has its own stationary points. Since only stationary points contribute in the asymptotic expansion, it becomes possible to separate from the integrals J_1 and J_2 the perturbations which appear at the time $\tau = 0$ at the point $n = 0$, and then propagate with a constant velocity αc.

It can be readily shown that if there corresponds to the stationary point q^* a point $k^* = q^*/a$ $(k = |\mathbf{k}|)$ at which the group velocity $\partial\omega(k^*\mathbf{k}_0)/\partial k = w$, then there corresponds to it also a perturbation which propagates along the lattice with a velocity w. It can also be shown that these perturbations are of an oscillatory nature, the oscillation frequency being equal to the frequency at the point of the dispersion curve with which this perturbation is connected.

From the stationarity condition (A.6) it is seen that the stationary points q^* will mainly be first-order stationary points, i.e., $h'(q^*) = 0$, $h''(q^*) \neq 0$, and the perturbations corresponding to them will be of the order of $\tau^{-1/2}$. We note that from the condition $n/\tau \leq 1$ imposed on the integral $J^+(\tau, n)$ it follows that its stationary points can occur on those sections of the interval $[0, \pi]$ where $-1 \leq \varphi'(q) < 0$. Second-order stationary points can appear if inflection points of the dispersion curve $[\varphi''(q^*) = 0]$ exist in these sections. Indeed, in this case the conditions $h'(q^*) = 0$, $h''(q^*) = 0$, and $h'''(q^*) \neq 0$ can be fulfilled. The perturbation corresponding to the point of inflection of the dispersion curve is of the order $\tau^{-1/3}$ and propagates with a velocity equal to the group velocity at this point.

Corresponding to the fact that the integral (A.1) is divided into four integrals, the interval of integration $[0, \pi]$ is divided into four groups of sections. Each integral has its corresponding group of sections where the integral has stationary points of non-zero order. Each point of inflection occurring on the interval $[0, \pi]$ contributes to the asymptotic expansion of one of the integrals a contribution of the order of $\tau^{-1/3}$ or $n^{-1/3}$. It is readily seen from (A.2) that the point $q = 0$ is a point of inflection and contributes to the asymptotic expansion of the integral $J^-(\tau, n)$ a contribution of the order of $\tau^{-1/3}$. The perturbation corresponding to this point will propagate with the speed of sound c.

In view of the fact that the function $\varphi'(q)$ is bounded from above and from below, non-zero stationary points will not exist for all n/τ. Consequently there exists a maximum velocity W characterized by the fact that perturbations propagating with a velocity larger than W are of an order no larger than n^{-1}. The stationary-phase method degenerates in this case into the method of integration by parts—only the boundary points 0 and π contribute to the expansions. As can be readily seen, W cannot be less than the speed of sound c, and we are therefore dealing here only with the integrals $K^{\pm}(\tau, n)$. Thus for $w > W$ the integral (A.1) is equal to the difference between the integrals K^+ and K^- which have the same stationary points.

It can be shown that the summary perturbations propagating with velocities larger than W are of an order no higher than τ/n^2, i.e., the decay depends here on the propagation velocity of the perturbation and increases with increasing velocity. It may be assumed that this estimate is inaccurate and that the perturbations decay even more strongly. We see from (A.5) that the integral $J^+(\tau, n)$ contains, in addition to decaying perturbations of various orders, also a constant; hence we can write down the principal term of the asymptotic expansion:

$$J^+(\tau, n) \approx \psi(0)\pi/2. \tag{A.7}$$

In the same way we can obtain

$$J^-(\tau, n) \approx K^-(\tau, n) \approx K^+(\tau, n) \approx \psi(0)\pi/2. \tag{A.8}$$

Substituting (A.7) and (A.8) in (A.3), we obtain

$$I(\tau, n) \approx \begin{cases} \psi(0)\pi/2, & \tau > n \\ 0; & \tau < n \end{cases}. \tag{A.9}$$

We have thus separated from the integral (A.1) the principal perturbation which does not decay with the displacement.

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