Absence of sound in one-dimensional disordered crystals

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A one-dimensional crystal is considered, of which one half is ordered (masses and coupling constants constant) and the other disordered. For the case in which the distribution of masses in the disordered part is Markoffian, a simple proof is given that sound moving from the ordered side is completely reflected.

There is very extensive literature devoted to the localization of oscillations in one-dimensional disordered crystals and to the resulting absence of thermal conductivity (for a review of the literature see[1]). The oscillations of such a crystal are described by the simple system of equations (the elastic constant is included in m_n)

$$m_n\frac{d^2u_n}{dt^2}+2u_n-u_{n-1}-u_{n+1}=0, \tag{1}$$

where n is the number of the atom and u_n is the displacement of atom n; atom n in general has some random mass m_n.

We consider hereafter oscillations with frequency ω. Equation (1) can then be written in the alternative form

$$\begin{pmatrix} u_{n+1} \\ u_n \end{pmatrix} = \hat{T}_n \begin{pmatrix} u_n \\ u_{n-1} \end{pmatrix},$$

where the transition matrix $\hat{T}_n$ is

$$\hat{T}_n=\begin{pmatrix} 2-m_n\omega^2 & -1 \\ 1 & 0 \end{pmatrix}. \tag{2}$$

It is quite obvious that the transition from any pair of neighboring atoms to the next is accomplished by a product of random (because of the arbitrariness of m_n) matrices $\hat{T}_n$. Both an individual matrix $\hat{T}_n$ and their product belong to the group SL(2, R), in which each matrix is real and has a determinant equal to unity. The inference about the localization of oscillations in such a random lattice is connected with the general properties of this group (use is made of Furstenberg's theorem[2]), and as a result the proof becomes very complicated. We give below what seems to us a much simpler proof of the absence of acoustic oscillations in a random crystal; the proof is based on quite well known properties of stochastic matrices (see, for example,[3]).

We consider a lattice constructed as follows. Atoms with $n \le 0$ from a regular lattice (for simplicity, $m_n = 1$ in this region). The masses of atoms with $1 \le n \le N$ are random, and for $n > N$ again $m_n = 1$. We shall seek a solution of the system of equations (1) in the following form:

$$u_n=e^{ikn}+Re^{-ikn}, \quad n\le 0, \qquad u_n=De^{ikn}, \quad n>N. \tag{3}$$

Here k is the dimensionless wave vector, connected with the frequency ω by the relation $\omega = 2|\sin(k/2)|$, and the quantities R and D obviously have the meaning of coefficients of reflection and transmission. If we introduce new variables $x_n = u_n/u_{n-1}$, then (1) takes the form

$$x_{n+1}=2-m_n\omega^2-1/x_n. \tag{4}$$

From equation (1) for n = 1, 0 we have

$$(2-\omega^2)u_0-u_{-1}=u_1, \quad (2-\omega^2)u_{-1}-u_{-2}=u_0;$$

by using the condition (3), we get at once

$$2-\omega^2=e^{ik}+e^{-ik}, \quad |R|=\left|\frac{x_1-e^{ik}}{x_1-e^{-ik}}\right|. \tag{5}$$

We shall now suppose that the distribution of masses on this atom is independent of the distribution of masses on the other atoms (that is, the process is Markoffian). We now introduce the distribution function $f_n(x)$ of the values of x for the nth atom,

$$f_n(x)=\langle\delta(x_n-x)\rangle,$$

where the averaging is over the values of mass. It follows from (4) that

$$f_n(x)=\langle\delta[(2-m_n\omega^2-x_{n+1})^{-1}-x]\rangle=\frac{1}{x^2}\int\rho(m)f_{n+1}\left(2-m\omega^2-\frac{1}{x}\right)dm. \tag{6}$$

where $\rho(m)$ is the normalized distribution function of the masses by hypothesis independent of the number n.

If we introduce the function

$$K(x,y)=\frac{1}{x^2}\int\rho(m)\delta\left(2-m\omega^2-\frac{1}{x}-y\right)dm,$$

then (6) takes the form

$$f_n(x)=\int K(x,y)f_{n+1}(y)dy. \tag{7}$$

We note that in accordance with (3), $x_{N+2} = e^{ik}$; that is,

$$f_{N+2}(x)=\delta(e^{ik}-x).$$

The kernel K(x, y) of (7) is stochastic; that is,

$$K(x,y)\ge 0, \quad \int K(x,y)dx=1.$$

Then according to general theorems relating to Markoffian processes, we get for $N\to\infty$ a solution f(x) independent of n and of the initial distribution and satisfying the equation

$$f(x)=\int K(x,y)f(y)dy, \quad \int f(x)dx=1.$$

For quite general distribution $\rho(m)$ it is unique and, what is most important, determinate for real x (the kernel K is here supposed to be regular[3]).

Obviously the coefficient $|R|$ averaged over x_1 is

$$\langle|R|\rangle=\int\left|\frac{x-e^{ik}}{x-e^{-ik}}\right|f(x)dx=1.$$

Thus we have shown that complete reflection occurs at the interface between the ordered and disordered lattices (though of course there is some depth of penetration). We remark here that the result $|R| = 1$ carries over completely to the quantum case of reflection of an electron from a random system of impurities (the role of the ratio x_n is played by the logarithmic derivative z_n).

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[3]F. R. Gantmakher, Teoriya matrits (Theory of Matrices) Gostekhizdat, 1954. (Translation, Chelsea, 1960).

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