Localization of the phonon modes in a disordered elastic chain

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It is shown that all the normal phonon modes in a disordered harmonic elastic chain are localized. Their localization length $l(\omega)$ is frequency dependent, and tends to infinity as $\omega \to 0$. Investigation of the evolution of the kinetic-energy fluctuation indicates the absence of diffusional behavior. Allowance for the anharmonicity leads to a finite lifetime for the localized vibrations. In the case of an anomalously large variance of the random parameters of the model, the localization of the eigenfunctions is the cause of the variation of the exponents of the frequency dependences of the wavelength, the density of states, and the localization length.

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1. INTRODUCTION

The phenomenon whereby the eigenfunctions in one-dimensional disordered systems are localized has apparently a general character. At present we already understand quite well the characteristics of the Mott localization of an electron in a one-dimensional conductor in the presence of some random potential due to impurities, structural defects, etc.[1-9] The correct mathematical description of the electron localization was first given by Berezinskiĭ in Ref. 2, where he also derived the frequency dependence of the conductivity $\sigma(\omega) \propto \omega^2 \ln^2 \omega$. Further improvement of the method allowed a number of new results to be obtained.[3-9] At the same time, it should be noted that the methods of Refs. 2–5 have thus far been applied exclusively to the electron-localization problem. This is primarily explained by the fact that one-dimensional conductors are a system under intensive study at present and possesses a number of unusual and interesting physical properties, some of which are directly connected with electron localization. There is, however, a considerable general-physics interest in the localization of the eigenstates in systems such as disordered spin and elastic chains.

In the present paper we dwell on the problem of phonon-mode localization in a disordered elastic chain. It turns out that, in the harmonic approximation, i.e., when the phonon–phonon interaction is neglected, each of the modes is localized over a distance of length $l(\omega)$ that depends on the frequency ω of the mode in question, and tends to infinity as $\omega \to 0$. The localization length $l(\omega)$ turns out in this case to be of the order of the mean free path of a phonon on the defects if the latter distance is computed with the aid of the conventional kinetic theory. Thus, diffusive spreading of the thermal fluctuations along the entire chain does not occur when the anharmonicity is neglected. Allowance for the three-phonon anharmonicity leads to the possibility of the decay of a localized phonon into two other phonons with great localization lengths, or of the absorption of the phonon in question by a phonon with a smaller localization length. Consequently, the concept of localization has meaning for fairly "dirty" chains and only for those modes for which the mean free time on the defects $\tau(\omega) = l(\omega)/u$ (here u is the speed of sound) is shorter than the lifetime $\tau^A(\omega, T)$ determined by the phonon–phonon interaction. But this limitation turns out to be fairly weak.

Let us note that no light is cast on the important role of eigenfunction localization in a number of recent papers[10-13] in which a model essentially equivalent to the elastic-harmonic-chain model is intensively investigated. On the other hand, although the assertion that the phonon modes in disordered chains are localized has been repeatedly made in the literature (see, for example, Refs. 14–16), a complete investigation of the behavior of the normal modes, as well as the anomalies of the kinetic properties, has apparently not yet been carried out. We shall show (see also Ref. 17) how this problem reduces to the problem of electron localization,[2-5] and find as a result the frequency dependence of the localization length $l(\omega)$ in those cases in which it exceeds the phonon wavelength $\lambda(\omega)$.

2. FORMULATION OF THE PROBLEM AND THE DERIVATION OF THE BASIC EQUATIONS

The Hamiltonian corresponding to a disordered elastic chain has, in the nearest-neighbor approximation, the form

$$H = \sum_{n=1}^{N} m_n (\dot{u}_n)^2 + \sum_{n=0}^{N} W_{n+1/2}(u_{n+1} - u_n), \tag{1}$$

where m_n is the mass of the nth atom, u_n is the displacement of this atom from the equilibrium position (the ends of the chain are considered to be fixed: $u_0 = u_{N+1} = 0$), and $W_{n+1/2}(x)$ is the potential energy corresponding to the coupling between the atoms n and $n+1$. It is natural to assume that $W_{n+1/2}(x)$ changes by an amount of the order of the melting temperature T_m when x changes by an amount of the order of the lattice constant a. Retaining in (1) at low temperatures $T \ll T_m$ at which $u_n \ll a$, only the terms quadratic in the displacements, we obtain the Hamiltonian of the elastic chain in the harmonic approximation:

$$H_0 = \sum_{n=1}^{N} m_n (\dot{u}_n)^2 + \frac{1}{2} \sum_{n=0}^{N} (u_{n+1} - u_n)^2 \gamma_{n+1/2}. \tag{2}$$

The next term of the expansion (1) in powers of the displacements corresponds to the three-phonon anharmonicity:

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$$H_3=\frac{1}{3!}\sum_{n=0}^{N}(u_{n+1}-u_n)^3A_{n+1/2}. \tag{3}$$

Let us note the orders of magnitude of the quantities $\gamma_{n+1/2}$ and $A_{n+1/2}$ used in (2) and (3):

$$\gamma_{n+1/2}=\frac{\partial^2W_{n+1/2}}{\partial x^2}\Big|_{x=0}\sim\frac{T_m}{a^2}, \tag{4}$$

$$A_{n+1/2}=\frac{\partial^3W_{n+1/2}}{\partial x^3}\Big|_{x=0}\sim\frac{T_m}{a^3}. \tag{4'}$$

We shall investigate the phonon-mode-localization problem within the framework of the harmonic approximation (2) without allowance for the phonon–phonon interactions. Next, using (3) as a perturbation, we shall estimate the lifetime $\tau^A(\omega,T)$ of the localized phonon as a function of its frequency ω and of the temperature T.

From (2) we obtain the following system of equations of motion:

$$m_n\ddot{u}_n=\gamma_{n+1/2}(u_{n+1}-u_n)-\gamma_{n-1/2}(u_n-u_{n-1}). \tag{5}$$

The model described by the system (5) has been investigated in the literature for quite a long time now, starting from Dyson's well-known paper.[18] But most of the investigations were devoted to the elucidation of the spectral properties of disordered chains (see Refs. 16 and 18–21). As to the localization of the phonon modes, it was inferred from the exponential increase of the displacements u_n with distance from one edge into the interior of the chain.[14-16] In this case no boundary condition was fixed at the other edge of the chain. It should be noted that a very important property of the normal modes of the system (5) is lost in such a formulation. Indeed, the localization of the normal modes indicates that the exponential increase of the displacements u_n should give way somewhere in the interior of the chain to an exponential decrease. This subtle problem has not yet been investigated within the framework of the model (5) for the elastic harmonic chain.

Let us perform the standard expansion of the displacements $u_n(t)$ in terms of the normal modes of the system:

$$u_n(t)=\sum_{\nu=1}^{N}u_n^{\nu}\frac{1}{(2\omega_\nu)^{1/2}}[b_\nu^{+}\exp(i\omega_\nu t)+b_\nu\exp(-i\omega_\nu t)]. \tag{6}$$

Here the u_n^ν and ω_ν are the eigenvectors and eigenvalues corresponding to the system of equations

$$-\omega_\nu^2u_n^\nu=\frac{\gamma_{n+1/2}}{m_n}(u_{n+1}^\nu-u_n^\nu)-\frac{\gamma_{n-1/2}}{m_n}(u_n^\nu-u_{n-1}^\nu) \tag{7}$$

with the boundary conditions

$$u_0^\nu=u_{N+1}^\nu=0. \tag{8}$$

The relations (7) and (8) constitute an eigenvalue problem for, generally speaking, a nonsymmetric $N\times N$ matrix. Therefore, the eigenvectors u_n^ν will not be orthogonal. We can, following Dyson,[18] go over to the new variables $\psi_n=m_n^{1/2}u_n^\nu$. Then the system of equations (7) assumes the form

$$-\omega_\nu^2\psi_n^\nu=\frac{\gamma_{n+1/2}}{(m_{n+1}m_n)^{1/2}}\psi_{n+1}^\nu-\frac{\gamma_{n+1/2}+\gamma_{n-1/2}}{m_n}\psi_n^\nu+\frac{\gamma_{n-1/2}}{(m_nm_{n-1})^{1/2}}\psi_{n-1}^\nu,$$

which now corresponds to a symmetric matrix. Thus, the set ψ_n^ν is a complete system of orthonormal eigenvectors:

$$\sum_{n=1}^{N}\psi_n^\nu\psi_n^\mu=\sum_{n=1}^{N}m_nu_n^\nu u_n^\mu=\delta_{\nu\mu}, \tag{9}$$

$$\sum_{\nu=1}^{N}\psi_n^\nu\psi_k^\nu=\sum_{\nu=1}^{N}m_n^{1/2}u_n^\nu m_k^{1/2}u_k^\nu=\delta_{nk}. \tag{9'}$$

But it will be more convenient for us to deal with the old variables u_n^ν and the equations (6)–(9), since in the low-frequency limit $\omega\to0$ the variables u_n^ν, in contrast to the ψ_n^ν, are slowly varying functions of the site number n, which allows the passage to the continuous limit.

As usual, in order to quantize the vibrations of the harmonic chain (5), we must regard b_ν^+ and b_ν from (6) as creation and annihilation operators for one vibration quantum with frequency ω_ν. The commutation relations $[b_\nu,b_\mu^+]=\delta_{\nu\mu}$ corresponding to the Bose particles lead to the usual quantum-mechanical commutation rules for the displacement operators $u_n(t)$, which are determined with the aid of (6), and the momentum operators $p_n(t)=m_n\partial u_n(t)/\partial t:[p_n,u_k]=-i\delta_{nk}$. To perform the averaging $(\langle\,\rangle_T)$ of some operator over the thermodynamic ensemble at a given temperature T, we must first express the operator in terms of the Bose operators b_ν^+ and b_ν. A certain set of the operators $b_\nu^+b_\nu$ can be averaged in standard fashion, e.g.,

$$\langle b_\nu^+b_\mu\rangle_T=\delta_{\nu\mu}N(\omega_\nu)=\delta_{\nu\mu}[\exp(\omega_\nu/T)-1]^{-1},$$

where $N(\omega_\nu)$ is the average number of phonons in the normal mode at the temperature T. Thus, the mean thermodynamic value of the kinetic-energy operator

$$K_n(t)=p_n^2(t)/2m_n$$

for the nth atom of the lattice is given by the relation

$$\langle K_n(t)\rangle_T=\overline{K}_n=\frac{1}{2}\int_0^\infty d\omega\left(N(\omega)+\frac{1}{2}\right)\omega\left[\sum_\nu\delta(\omega-\omega_\nu)m_n(u_n^\nu)^2\right]. \tag{10}$$

The expression in square brackets in (10) is the density of states per unit energy interval at the nth lattice site for a given distribution of the random parameters m_n and $\gamma_{n+1/2}$ of the model (5). Averaging $(\langle\,\rangle_U)$ over this distribution, we obtain the mean value of the density of states:

$$\nu(\omega)=\left\langle\sum_\nu\delta(\omega-\omega_\nu)m_n(u_n^\nu)^2\right\rangle_U\equiv\frac{1}{N}\left\langle\sum_\nu\delta(\omega-\omega_\nu)\right\rangle_U. \tag{11}$$

Here the second equality is easily obtained by summing (11) over n with allowance for the normalization (9). The kinetic energy of the whole chain

$$\sum_{n=1}^{N}\overline{K}_n=\frac{1}{2}\sum_\nu\omega_\nu\left(N(\omega_\nu)+\frac{1}{2}\right)$$

is, as it should, equal to one half the total energy.

Let us now introduce the simplest retarded kinetic-energy-fluctuation correlator:

$$F(n-n_0,t)=\langle\langle(K_n(t)-\overline{K}_n)(K_{n_0}(0)-\overline{K}_{n_0})\rangle_T\rangle_U. \tag{12}$$

If the correlator (12) does not tend to zero as $t\to\infty$, this means that the kinetic-energy fluctuation is not spread over the whole length of the chain in an infinite time. In other words, we do not have the usual diffusional be-

havior in this case. Performing the thermodynamic averaging in (12), we obtain the following expression at $t=\infty$:

$$F(n-n_0,\infty)=\frac{1}{4}\int_0^\infty d\omega N(\omega)[N(\omega)+1]\omega^2 F_\omega(n-n_0), \tag{13}$$

where the mean quantity

$$F_\omega(n-n_0)=\left\langle \sum_\nu \delta(\omega-\omega_\nu) m_n (u_n^\nu)^2 m_{n_0}(u_{n_0}^\nu)^2 \right\rangle_U \tag{14}$$

describes the localization of the normal modes with frequency ω. Indeed, the mean quantity (14) for the nonlocalized states will contain the factor $1/N$ (as a result of the normalization of the eigenfunctions to the whole length of the chain), and will tend to zero as $N\to\infty$. On the other hand, for the localized states we should obtain

$$F_\omega(n-n_0)\propto l^{-1}\exp(-|n-n_0|a/l),$$

since the localized normal modes are normalized to the localization length l. Thus, the absence of diffusive spreading of the kinetic-energy fluctuation is connected with the localization of the phonon modes, the distance $l(\omega)$ over which they are localized being determined by the asymptotic form of the mean (14) for $n-n_0\to\infty$. Let us note here that the conclusion of Bernasconi *et al.*[10-13] that diffusion, which leads to (5), occurs in the system was drawn on the basis of an investigation of correlator $\langle u_n(t)u_n(0)\rangle$ simpler than (12) and corresponding to a single-particle Green function. But it is well known that the single-particle Green function carries information about the spectrum and its damping, but is insensitive to the localization of the eigenfunctions. This characteristic manifests itself also in the equality (11), from which it can be seen that the localization has no effect on the density of states.

For the computation of the asymptotic behavior of the correlator (14), it is quite useful to go over from (7) to another system of equations into which the disorderings of the masses m_n and of the elastic constants $\gamma_{n+1/2}$ enter in a symmetric fashion. This will allow us to find the solution when both types of disorder are present togehter. Thus far, the cases in which the harmonic chain (5) contains only one of the two possible types of disorder, i.e., in which either the m_n or the $\gamma_{n+1/2}$ are constant, have been investigated in detail.[10-11,19-21] In Dyson's paper[18] the density of states

$$\nu(\omega\to 0)\propto\omega^{-1}\ln^{-3}\omega$$

is obtained in another quite specific case, namely, when the only independent random quantity is some combination of the m_n and $\gamma_{n+1/2}$. As a result, the parameters m_n and $\gamma_{n+1/2}$ turn out to be correlated in a complicated nonlocal fashion. In fact, this Dyson case corresponds in the tight-binding approximation to a half-filled electronic band, when the values of the overlap integrals are random quantities (cf. Refs. 22–24).

Let us introduce additional variables defined at the half-integer points of the lattice:

$$v_{n+1/2}=\omega^{-1}\langle m\rangle^{-1/2}\langle 1/\gamma\rangle^{1/2}\gamma_{n+1/2}(u_{n+1}-u_n).$$

Now the system of equations (7) can be rewritten in the form

$$u_{n+1}-u_n=(E+EV_{n+1/2})v_{n+1/2}, \tag{15}$$
$$v_{n+1/2}-v_{n-1/2}=-(E+EU_n)u_n,$$

where we have used the following dimensionless designations:

$$E=\omega\langle m\rangle^{1/2}\langle 1/\gamma\rangle^{1/2}, \tag{16}$$
$$U_n=(m_n-\langle m\rangle)/\langle m\rangle, \tag{17}$$
$$V_{n+1/2}=(1/\gamma_{n+1/2}-\langle 1/\gamma\rangle)/\langle 1/\gamma\rangle. \tag{18}$$

The boundary conditions at the points 0 and $N+1$ are, as before, the conditions (8).

The system (15) is of the form of the Dirac equations on a lattice. If, as $\omega\to 0$, we go over in (15) to the continuous limit, then we obtain for the spinor $\hat{u}=\begin{bmatrix}u\\ v\end{bmatrix}$ an equation of the Dirac type:

$$\left\{\left[E+\frac{1}{2}E(U+V)\right]\hat{e}+\frac{1}{2}E(U-V)\hat{\sigma}_z+i\hat{\sigma}_y a\frac{\partial}{\partial x}\right\}\hat{u}=0, \tag{15'}$$

where $\hat{\sigma}_x$ and $\hat{\sigma}_y$ are Pauli matrices. In (15'), $U(x)$ and $V(x)$ describe the random distributions of the masses and elastic constants in accordance with (17) and (18):

$$U(x)=\sum_n U_n a\delta(x-an), \tag{17'}$$

$$V(x)=\sum_n V_{n+1/2}a\delta(x-an-a/2). \tag{18'}$$

Let us point out one important characteristic of the Eqs. (15) and (15'). The functions U and V, which describe the disorder in the elastic chain, enter in (15) and (15') multiplied by the dimensionless frequency E from (16). Thus, in the low-frequency limit the disorder (17), (18) becomes less and less effective in terms of phonon scattering as ω tends to zero. This observation bears a direct relation to the frequency dependence of the cross section for Rayleigh scattering of a wave by a point defect.

3. COMPUTATION OF THE DENSITY OF STATES AND THE LOCALIZATION LENGTH

In this section we consider the density of states (11) and the asymptotic behavior of the correlator (14) for the harmonic chain described by the system of equations (15). We shall assume the magnitude of the disorder to be bounded from above, i.e., that

$$|U_n|,\ |V_{n+1/2}|\leqslant\bar{U} \tag{19}$$

and consider only those phonon modes for which the scattering by one defect of strength $\bar{U}$ is characterized by some smallness parameter:

$$E(1-E^2/4)^{-1/2}\bar{U}\ll 1. \tag{20}$$

The exact meaning of the last limitation will be given a little later.

Let us now turn to the solution of the system of equations (15), or, in the long-wave limit $E\ll 1$, to Eq. (15'). Let us begin with the case of a regular elastic chain ($U_n=V_{n+1/2}=0$), when the solution to the system (15) is obvious:

$$\begin{bmatrix}u_n\\ v_{n+1/2}\end{bmatrix}=R\begin{bmatrix}\sin(\varphi+kn)\\ \cos(\varphi+kn+k/2)\end{bmatrix}, \tag{21}$$

where the amplitude R and the phase φ are constants,

determined respectively by the normalization (9) and one of the boundary conditions (8). The second boundary condition in (8) fixes the quantization rule for the wave vector $k=a/\lambda$, which is connected with the frequency E by the relation

$$E=2\sin(k/2), \quad 0<k<\pi. \tag{22}$$

To obtain the solution to Eq. (15′) from (21) and (22), we need only go in (21) to the continuous limit and expand (22) in powers of $k \ll 1$.

We shall seek the solution to the system (15) with a nonzero disorder in the same form (21), (22) as for the regular chain. To do this, we have to assume that φ and R undergo jumps at the points n and $n+\frac{1}{2}$ every time U_n and $V_{n+1/2}$ are not equal to zero. Let us, for definiteness, consider an isolated defect at the point n_0, i.e., the case in which $U_{n_0} \neq 0$, while all the remaining U_n and the $V_{n+1/2}$ in the equations (15) are equal to zero. To the left and right of the defect we have the solution (21) with the parameters R^L, φ^L, and R^R, φ^R. Let us introduce at the exact location of the defect the parameter values

$$R_{n_0}=\tfrac{1}{2}(R^R+R^L), \quad \varphi_{n_0}=\tfrac{1}{2}(\varphi^R+\varphi^L),$$

and let us also define the magnitudes of the corresponding jumps as

$$(\Delta R)_{n_0}=R^R-R^L, \quad (\Delta\varphi)_{n_0}=\varphi^R-\varphi^L.$$

Knowing the solution (21) to the left of the defect, we can easily express the values of R^R and φ^R in terms of R^L, φ^L, and U_{n_0} with the aid of the equations (15). Similarly, we can determine the R_n, φ_n and $(\Delta R)_n$, $(\Delta\varphi)_n$ at each point of the general disordered elastic chain. Below we shall be concerned with those phonon modes for which the phase and amplitude jumps are small, i.e., for which $(\Delta\varphi)_n \ll 1$ and $(\Delta R)_n/R_n \ll 1$, which situation is guaranteed by the inequality (20). Up to terms of second order in the parameter (20) we have

$$(\Delta\varphi)_n=\tfrac{1}{2}E(1-E^2/4)^{-1/2}U_n[1-\cos(2\varphi_n+2kn)], \tag{23}$$

$$(\Delta R)_n/R_n=-\tfrac{1}{2}E(1-E^2/4)^{-1/2}U_n\sin(2\varphi_n+2kn), \tag{24}$$

$$(\Delta\varphi)_{n+1/2}=\tfrac{1}{2}E(1-E^2/4)^{-1/2}V_{n+1/2}[1+\cos(2\varphi_n+2kn+k)], \tag{23′}$$

$$(\Delta R)_{n+1/2}/R_{n+1/2}=\tfrac{1}{2}E(1-E^2/4)^{-1/2}V_{n+1/2}\sin(2\varphi_n+2kn+k). \tag{24′}$$

The random phase jumps (23), (23′) lead to a change in the quantization rules for the wave vector k, and, generally speaking, modify the behavior of the density of phonon states (11). At the same time, the amplitude jumps (24), (24′) alter the character of the normalization of the normal modes, and cause the localization of these modes.

It turned out that the relations (24) and (23) correspond totally to the analogous formulas obtained in the theory of electron localization in a one-dimensional disordered conducting chain.[2,5] In this theory the phase and amplitude of the electron wave function $\psi=R\sin(\varphi+kx)$ undergo jumps at each point where there is a short-range impurity potential. The characteristics of the impurity potential that are responsible for forward and backward scattering can be chosen so as to obtain (23) and (24), or (23′) and (24′). In Ref. 5 it is shown how to find the probability distribution functions for the random values of the phase, the amplitude, the normalization, etc., using the expressions for the phase and amplitude jumps. In this case the Markov process is constructed essentially under the assumption that the impurity-potential distribution has a localized character. With the aid of the indicated probability distribution functions it is possible to investigate the behavior of the averages corresponding to the density of states, the localization, the frequency dependence of the conductivity, etc. Thus, the expressions (23) and (24) enable us to compute the density of states (11), and determine the asymptotic behavior of the correlator (14).

It should be noted that the umklapp processes are quite important in the vicinity of the points of strong commensurability, where the wave vector k is close to 0, π, or $\pi/2$. This manifests itself in the fact that it is no longer possible to separate in (23) and (24) the fast coordinate dependence due to the wave vector k and the slow dependence that results from the phase and amplitude jumps. As a result, the density of states and the localization of the eigenfunctions acquire characteristic properties.[18,22-24] We, however, limit ourselves here to the case (the simplest one) of the incommensurate wave vector

$$k, \pi-k, |k-\pi/2| \gg E^2(1-E^2/4)^{-1}(\langle U^2\rangle+\langle V^2\rangle), \tag{25}$$

when the umklapp processes can be neglected.

Taking all the foregoing into account, we obtain the following asymptotic expression in the region (20), (25) for the correlator (14) at $|n-n_0| \gg l/a$ (cf. Ref. 3):

$$F_\omega(n-n_0)\to\nu(\omega)\frac{\pi^{1/2}}{64}\frac{[l(\omega)/a]^{1/2}}{|n-n_0|^{1/2}}\exp\left(-\frac{a|n-n_0|}{l(\omega)}\right) \tag{26}$$

where the density of phonon states $\nu(\omega)$ has the form

$$\nu(\omega)=\pi^{-1}\langle m\rangle^{1/2}\langle 1/\gamma\rangle^{1/2}(1-\tfrac{1}{4}\langle m\rangle\langle 1/\gamma\rangle\omega^2)^{-1/2}. \tag{27}$$

The specific form of the formula for the localization length $l(\omega)$ depends essentially on the character of the correlation between the m_n and $\gamma_{n+1/2}$ distributions. Thus, in the case of independent mass and elastic-constant distributions we have

$$l(\omega)=16aE^{-2}(1-E^2/4)/(\langle U^2\rangle+\langle V^2\rangle). \tag{28}$$

Let us now consider one correlated-distribution case in which the elastic constant of the coupling of two atoms is determined by the masses of these atoms through the relation

$$V_{n+1/2}=\tfrac{1}{2}(U_{n+1}+U_n). \tag{29}$$

Then, as can be seen from Eq. (15′), there occurs in the long-wave limit a strong cancellation in the term with $\hat{\sigma}_z$, which is responsible for the localization. Let us, using (29), rewrite the relations (23), (23′) and (24), (24′) in the form of total phase and amplitude jumps:

$$(\Delta\varphi)_n=E(1-E^2/4)^{-1/2}[1-\tfrac{1}{4}E^2\cos(2\varphi_n+2kn)], \tag{23″}$$

$$(\Delta R)_n/R_n=-\tfrac{1}{4}E^2(1-E^2/4)^{-1/2}\sin(2\varphi_n+2kn). \tag{24″}$$

From this it follows that the case (29) corresponds in the low-frequency limit to anomalously weak backward

scattering. Since only the backward scattering leads to localization, the expression

$$l(\omega)=64aE^{-6}(1-E^2/4)/\langle U^2\rangle, \qquad (28')$$

which follows from (23″), (24″), exhibits a much stronger low-frequency singularity [$l(\omega\to 0)\propto\omega^{-6}$] than the $l(\omega\to 0)\propto\omega^{-2}$ singularity exhibited in the case of the uncorrelated distributions. Notice that as $\omega\to 0$ the localization length in both (28) and (28′) increases more rapidly than the characteristic wavelength $\lambda(\omega\to 0)=a/E$.

Let us recall that the results (26)–(28) were obtained within the framework of the limitations (20) and (25). Under these conditions the density of states (27) turns out to be the same as for a regular elastic chain with parameters $m_0=\langle m\rangle$ and $\gamma_0=\langle 1/\gamma\rangle^{-1}$. This result has been obtained in many papers[21,10-13] in the low-frequency limit $\omega\to 0$ and under the condition $\gamma_{n+1/2}=\text{const}$ or $m_n=\text{const}$. On the other hand, numerical calculations[19,20] show that $\nu(\omega)$ begins to differ markedly from (27) near the point $E=2$, which corresponds to the upper limit of the spectrum of the regular chain. At even higher frequencies, the shape of $\nu(\omega)$ is characterized by a number of sharp peaks and dips. This can be due to the fact that, according to (23) and (24), as $E\to 2$, scattering on any defect becomes anomalously strong, i.e., the inequality (20) is violated. As a result, the localization length (28) or (28′) assumes a value of the order of the lattice constant, and the density of states is determined by clusters containing a small number of atoms, as is assumed in Ref. 19.

Let us also note, in connection with the phonon-mode localization, the results[15,16] of the investigation of the rate of exponential growth of the solution $u_n(\omega)\propto\exp[\alpha(\omega)n]$ corresponding to Eq. (7) with boundary conditions at one end of the chain. It has already been noted above that the distinguishing features of the eigenfunctions are lost in this simplest approach to the localization problem. We give the expression obtained in Ref. 15 (see also Ref. 16) for $\alpha(\omega)$ for an elastic chain with random masses $m_n(\gamma_{n+1/2}=\text{const})$ in the limit of low frequencies:

$$\alpha^{-1}(\omega\to 0)=8E^{-2}/\langle U^2\rangle,$$

which agrees with (28) if we leave out a factor of 4. The relation between $\alpha^{-1}(\omega)$ and $l(\omega)$ naturally turns out here to be the same as in the theory of electron localization (see, for example, Ref. 25 for a review).

4. THE LIFETIME OF THE LOCALIZED VIBRATION

Thus far, we have discussed the character of the localization of the normal modes within the framework of the harmonic approximation (2), (5). It is clear that anharmonicity leads to the possibility of decay or coalescence of the localized phonons. With a view to finding the condition of applicability of the above results, we shall now estimate the lifetime of the localized vibration as a function of the frequency and the temperature. To begin with, let us note that, without allowance for the anharmonicity, the correlator $F(n-n_0,t)$ of the kinetic-energy fluctuations contains the time-independent contribution (13). This is due to the fact that the mean square fluctuation

$$\langle b_\nu^+ b_\nu b_\nu^+ b_\nu\rangle_T-\langle b_\nu^+ b_\nu\rangle_T^2=N_\nu(N_\nu+1) \qquad (30)$$

of the occupation number for the νth state [see the formula (13)] does not vanish in time, since the phonon–phonon interaction is neglected. Now we shall seek the lifetime τ_ν^A of the fluctuation (30), using the three-phonon anharmonicity (3) as the perturbation. In other words, τ_ν^A is the time required for the establishment of thermal equilibrium at the level ν. On the other hand, this level ν is characterized by its localization length l_ν and mean free time $\tau_\nu=l_\nu/u$. Thus, to speak of localization as applied to the given level ν makes sense only when $\tau_\nu<\tau_\nu^A$. As the value characterizing τ_ν. we can take the averaged time $\tau(\omega)=l(\omega)/u$, which we find in the case of independent m_n and $\gamma_{n+1/2}$ distributions from (28):

$$\frac{1}{\tau(\omega)}=\frac{\tilde\omega}{8}\frac{\omega^2}{\tilde\omega^2-\omega^2}(\langle U^2\rangle+\langle V^2\rangle)\ll\omega, \qquad (31)$$

where $\tilde\omega=2\langle m\rangle^{-1/2}\langle 1/\gamma\rangle^{-1/2}$ is the upper limit of the spectrum of a regular chain with parameters $m_0=\langle m\rangle$ and $\gamma_0=\langle 1/\gamma\rangle^{-1}$. The inequality in (31) follows from (25).

We now proceed to compute τ_ν^A. Using the expansion in terms of the eigenfunctions u_n^ν of the problem (7), (8), we represent the Hamiltonian $H=H_0+H_3$ in the form

$$H_0=\sum_\nu\omega_\nu(b_\nu^+b_\nu+{}^1/_2), \qquad (2')$$

$$H_3=\frac{1}{3!}\sum_{\nu\mu\rho}A^{\nu\mu\rho}(b_\nu^++b_\nu)(b_\mu^++b_\mu)(b_\rho^++b_\rho), \qquad (3')$$

where

$$A^{\nu\mu\rho}=(8\omega_\nu\omega_\mu\omega_\rho)^{-1/2}\sum_{n=0}^{N}A_{n+1/2}(u_{n+1}^\nu-u_n^\nu)(u_{n+1}^\mu-u_n^\mu)(u_{n+1}^\rho-u_n^\rho). \qquad (32)$$

Perturbation theory in terms of H_3 allows us to determine the probability for decay of the phonon ν into two other phonons. Thus, we find the time $\tau_\nu^{A\,\mathrm{I}}$:

$$1/\tau_\nu^{A\,\mathrm{I}}=2\pi\sum_{\mu\rho}(N_\mu+N_\rho+1)|\langle\mu\rho|H_3|\nu\rangle|^2\delta(\omega_\nu-\omega_\mu-\omega_\rho). \qquad (33)$$

Another process that makes a contribution to the damping of the occupation-number fluctuation (30) is the coalescence of the given phonon ν with some phonon μ, as a result of which a phonon ρ appears. The corresponding time, which we denote by $\tau_\nu^{A\,\mathrm{II}}$, is given, similarly to (33), by the first nonvanishing term of the perturbation theory in terms of H_3:

$$\frac{1}{\tau_\nu^{A\,\mathrm{II}}}=2\pi\sum_{\mu\rho}(N_\mu-N_\rho)|\langle\rho|H_3|\nu\mu\rangle|^2\delta(\omega_\rho-\omega_\nu-\omega_\mu). \qquad (34)$$

The sum of the expressions (33) and (34) gives the reciprocal lifetime $1/\tau_\nu^A$ of the fluctuation (30).

Notice that, for a regular chain, the expression (32) contains the law of quasimomentum conservation in the three-phonon interaction. This, together with the energy conservation law in (33), (34), prohibits three-phonon processes in our case of nondecaying spectrum (22). Phonon scattering by the defects generally speaking removes this prohibition. We shall, for simplicity, consider the acoustic-phonon case, in which the energy-

conservation law coincides, on account of the linearity of the spectrum, with the law of conservation of the wave vector k from (22). More precisely, we shall assume that the corrections from the nonlinearity of the spectrum are smaller than the corrections due to the scattering on the defects:

$$\omega^3/\bar{\omega}^2 < 1/\tau(\omega). \tag{35}$$

Let us, using (3'), rewrite (33) in the form

$$\frac{1}{\tau^{AI}} = 2\pi \int_0^{\omega} d\xi (N(\xi)+N(\omega_\nu-\xi)+1) \left[\sum_{\mu\rho} \delta(\xi-\omega_\mu)\delta(\omega_\nu-\xi-\omega_\rho)(A^{\nu\mu\rho})^2 \right]. \tag{33'}$$

Let us now estimate the expression standing in the square brackets in (33'). First, let us point out that the localization of all the three phonons ν, μ, and ρ can be regarded as statistically independent. The point is that, as the theory of electron localization shows,[2-5] the averagings over the random-potential realizations of the quantities corresponding to the two states ν and μ are statistically independent if $|\varepsilon_\nu - \varepsilon_\mu| \gg 1/\tau$, where τ is the mean free time in the localized state. In our case, as can be seen from (33'), the difference between the frequencies of any two of the phonons ν, μ, and ρ is, in order of magnitude, equal to ω, which, according to the inequality (31), is much higher than $1/\tau(\omega)$. Further, we can eliminate from the expression (32) the fast dependence on the lattice-site number, and go over from the sum to an integral as follows:

$$A^{\nu\mu\rho} \propto \int dx R^\nu R^\mu R^\rho \cos(\varphi_\nu - \varphi_\mu - \varphi_\rho),$$

where we have used under the cosine sign the energy-conservation law in (33) and the linearity of the acoustic spectrum, i.e., the condition (35). To estimate the quantity $A^{\nu\mu\rho}$, let us note that it is nonzero (i.e., not exponentially small) only for those phonon triplets ν, μ, and ρ whose localization regions overlap. Then the integration over the coordinate in $A^{\nu\mu\rho}$ is performed largely within the limits of the smallest of the three localization lengths. Taking account of the foregoing, as well as the normalization (9) of the eigenfunctions and the orders of magnitude of the quantities (4) and (4'), we obtain

$$\left[\sum_{\mu\rho} \delta(\xi-\omega_\mu)\delta(\omega_\nu-\xi-\omega_\rho)(A^{\nu\mu\rho})^2 \right] \sim \frac{\omega\xi(\omega-\xi)}{\bar{\omega}^2 T_m} \frac{l(\omega)}{a}.$$

Thus, for $1/\tau_\nu^{AI}$ we obtain from (33') the estimate

$$1/\tau^{AI}(\omega, T) \sim \begin{cases} \omega > T: & \omega^2/T_m(\langle U^2\rangle + \langle V^2\rangle) \\ \omega < T: & T\omega/T_m(\langle U^2\rangle + \langle V^2\rangle) \end{cases}. \tag{36}$$

Similar arguments in the case of $1/\tau_\nu^{AII}$ lead to the estimate

$$1/\tau^{AII}(\omega, T) \sim \begin{cases} \omega > T: & T^2/T_m(\langle U^2\rangle + \langle V^2\rangle) \\ \omega < T: & T\omega/T_m(\langle U^2\rangle + \langle V^2\rangle) \end{cases}. \tag{37}$$

Comparing (36) and (37), we arrive at the conclusion that $\tau^A \sim \tau_\nu^{AI}$.

The condition of applicability of the localization concept to phonons of frequency ω at a temperature T is, as has already been noted, the inequality $\tau(\omega) < \tau^A(\omega, T)$. Therefore, first, it is necessary that the chain be more disordered than anharmonic, i.e., that

$$\langle U^2\rangle + \langle V^2\rangle > (\bar{\omega}/T_m)^{1/2}. \tag{38}$$

Second, after (38) has been met, the localization concept has meaning at the given temperature T for not too low-lying vibrations, i.e., for those vibrations whose frequencies satisfy the condition

$$\omega > T \frac{\bar{\omega}/T_m}{(\langle U^2\rangle + \langle V^2\rangle)^{1/2}}. \tag{39}$$

The inequalities (38) and (39) can, naturally, be quite weak for sufficiently dirty elastic chains.

5. SOME GENERALIZATIONS OF THE RESULTS FOR THE HARMONIC CHAIN

In applications (see Refs. 10–13) it is sometimes necessary to investigate a model of the harmonic-chain type (2),(5), in which the random parameters fluctuate so strongly that some of the averages in the formulas (25)–(28) become infinite. Therefore, the indicated results concerning the behavior of the density of states $\nu(\omega)$, the wavelength $\lambda(\omega)$, and the localization length $l(\omega)$ are inapplicable in this anomalous case. The point is that such a large spread in the values of the parameters $\gamma_{n+1/2}$ and m_n indicates that there exist at some points of the chain arbitrarily strong scatterers for which the conditions (19) and (20) are violated. It is, however, possible to avoid this difficulty by introducing in some way truncated random-parameter distribution functions.

Let us assume that the $\gamma_{n+1/2}$ and m_n distributions for the model (5) are independent, and let us denote the corresponding probability distribution functions by $W_1(\gamma)$ and $W_2(m)$. If, moreover, we assume that the averages $\langle 1/\gamma\rangle$ and $\langle m\rangle$ are finite, then we can go over to the dimensionless variables (16)–(18), and derive for them probability distribution functions $P_1(V)$ and $P_2(U)$. Since these functions allow the occurrence of scatterers with arbitrarily great strength, the inequality (19) is, generally speaking, violated for any finite $\tilde{U}$. But we can introduce the truncated distribution functions:

$$\tilde{P}_{1(2)}(U, \tilde{U}) = P_{1(2)}(U)\theta(\tilde{U}-U) + \delta(U-\tilde{U}) \int_{\tilde{U}}^{\infty} dU P_{1(2)}(U), \tag{40}$$

for which the condition (19) is fulfilled. The $V_{n+1/2}$ and U_n distributions given by the functions (40) differ from the initial distributions in that all the scatterers with strength $V_{n+1/2} > \tilde{U}$ or $U_n > \tilde{U}$ are replaced with scatterers with strength $\tilde{U}$. It is easy to compute the mean distance between these adjusted scatterers:

$$L(\tilde{U}) = a \Big/ \int_{\tilde{U}}^{\infty} dU\,[P_1(U) + P_2(U)]. \tag{41}$$

The operational procedure in the present case is now clear. Let us first fix the cutoff parameter $\tilde{U}$. All the results obtained by us are applicable in the case of the truncated functions (40), i.e., we can find the density of states $\tilde{\nu}(\omega, \tilde{U})$, the wavelength $\tilde{\lambda}(\omega, \tilde{U})$, and the localization length $\tilde{l}(\omega, \tilde{U})$ for those phonon modes which satisfy the condition (20). If now the found characteristic lengths $\tilde{\lambda}(\omega, \tilde{U})$ and $\tilde{l}(\omega, \tilde{U})$ turn out to be smaller than the distance $L(\tilde{U})$ from (41), then the procedure is self-consistent. This method was proposed by Alexander and Bernasconi.[11]

We can make further progress if we notice that the localization length $l(\omega)$ is essentially a cutoff parameter for the distribution function $W(\gamma, m)$. Indeed, the phonon mode, localized over the distance $l(\omega)$, is insensitive to those details of the distribution function which manifest themselves at distances greater than $l(\omega)$. In other words, as long as $L(\tilde{U}) \gg l(\omega)$ we have the relations

$$l(\omega, \tilde{U}) = l(\omega), \quad \bar{\nu}(\omega, \tilde{U}) = \nu(\omega)$$

etc., which are valid to first order in the parameter $l(\omega)/L(\tilde{U})$. Consequently, the characteristic cutoff parameter $\tilde{U}(\omega)$ is determined by the localization length at the given frequency:

$$L(\tilde{U}(\omega)) \sim l(\omega) \sim l(\omega, \tilde{U}(\omega)). \tag{42}$$

Using (40)–(42), we can easily find the frequency dependences $\nu(\omega \to 0)$, $\lambda(\omega \to 0)$, and $l(\omega \to 0)$ corresponding to the various types of distribution functions $P_1(V)$ and $P_2(U)$. In the case in which the average $\langle 1/\gamma \rangle$ or $\langle m \rangle$ is infinite, the described truncation procedure should be applied to the function $W_1(\gamma)$ or $W_2(m)$.

In conclusion, let us consider as an example the case of the anomalous $\gamma_{n+1/2}$ distribution described by the following distribution function: $W(\gamma \to 0) \propto \gamma^{\alpha}$. When $\alpha > 1$, the averages $\langle 1/\gamma \rangle$ and $\langle 1/\gamma^2 \rangle$ are finite, and the results (27) and (28) remain valid. In the range $0 < \alpha < 1$, we have $\langle 1/\gamma \rangle < \infty$, but $\langle 1/\gamma^2 \rangle = \infty$. Using the truncation procedure (40)–(42), we find that the frequency dependence of the localization length changes in this region: $l(\omega \to 0) \sim a(\omega/\tilde{\omega})^{-1-\alpha}$, whereas the wavelength $\lambda = a(2\omega/\tilde{\omega})^{-1}$ and the density of states (27) remain unchanged. Finally, for the even stronger anomaly in the region $-1 < \alpha < 0$, where $\langle 1/\gamma \rangle = \infty$, we have $l(\omega \to 0) \sim \lambda(\omega \to 0) \sim a(\omega/\tilde{\omega})^{-(1+\alpha)/(1+\alpha/2)}$ and $\nu(\omega \to 0) \propto \omega^{\alpha/(2+\alpha)}$, which agree with the results obtained in Ref. 11. Let us also note that exactly the same answers are obtained in the case of the anomalous mass distribution:

$$W_2(m \to \infty) \propto m^{-2-\alpha}.$$

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[1]N. F. Mott and W. D. Twose, Adv. Phys. **10**, 107 (1961).
[2]V. L. Berezinskiĭ, Zh. Eksp. Teor. Fiz. **65**, 1251 (1973) [Sov. Phys. JETP **38**, 620 (1974)].
[3]A. A. Gogolin, V. I. Mel'nikov, and É. I. Rashba, Zh. Eksp. Teor. Fiz. **69**, 327 (1975) [Sov. Phys. JETP **42**, 168 (1975)].
[4]A. A. Abrikosov and I. A. Ryzhkin, Adv. Phys. **27**, 147 (1978).
[5]V. L. Berezinskiĭ and L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **77**, 2498 (1979) [Sov. Phys. JETP **50**, 1209 (1979)].
[6]V. L. Berezinskiĭ and L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **78**, 812 (1980) [Sov. Phys. JETP **51**, 409 (1980)].
[7]L. P. Gor'kov, O. N. Dorokhov, and F. V. Prigara, Solid State Commun. **37**, 869 (1981).
[8]V. L. Berezinskii, L. P. Gor'kov, and O. N. Dorokhov, Solid State Commun. **37**, 61 (1981).
[9]O. N. Dorokhov, S. I. Matveenko, and F. V. Prigara, Fiz. Nizk. Temp. **7**, 738 (1981) [Sov. J. Low Temp. Phys. **7**, 360 (1981)].
[10]J. Bernasconi, S. Alexander, and R. Orbach, Phys. Rev. Lett. **41**, 185 (1978).
[11]S. Alexander and J. Bernasconi, J. Phys. C **12**, L1 (1979).
[12]J. Bernasconi, W. R. Schneider, and W. Wyss, Z. Phys. B **37**, 175 (1980).
[13]S. Alexander, J. Bernasconi, W. R. Schneider, and R. Orbach, Rev. Mod. Phys. **53**, 175 (1981).
[14]P. Dean, Proc. Phys. Soc. London **84**, 727 (1964).
[15]H. Matsuda, T. Migata, and K. Ishii, J. Phys. Soc. Jpn. Suppl. **26**, 40 (1969).
[16]K. Ishii, Prog. Theor. Phys. Suppl. **53**, 77 (1973).
[17]O. N. Dorokhov, Solid State Commun. **41**, 431 (1982).
[18]F. J. Dyson, Phys. Rev. **92**, 1331 (1953).
[19]P. Dean, Proc. R. Soc. London Ser. A **260**, 263 (1961).
[20]R. L. Agacy, Proc. Phys. Soc. London **83**, 591 (1964).
[21]S. A. Gradeskul and L. A. Pastur, Teor. Mat. Fiz. **23**, 132 (1975).
[22]L. P. Gor'kov and O. N. Dorokhov, Solid State Commun. **20**, 789 (1976); **21**, 7 (1977).
[23]A. A. Gogolin and V. I. Mel'nikov, Zh. Eksp. Teor. Fiz. **73**, 706 (1977) [Sov. Phys. JETP **46**, 369 (1977)].
[24]L. P. Gor'kov and O. N. Dorokhov, Fiz. Nizk. Temp. **4**, 332 (1978) [Sov. J. Low Temp. Phys. **4**, 160 (1978)].
[25]T. N. Antsygina, L. A. Pastur, and V. A. Slyusarev, Fiz. Nizk. Temp. **7**, 5 (1981) [Sov. J. Low Temp. Phys. **7**, 1 (1981)].

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