PHYSICAL REVIEW B VOLUME 10, NUMBER 6 15 SEPTEMBER 1974

Elastic waves in a glasslike disordered chain

Ming-Shih Lu, Mark Nelkin, and Masayuki Arita*

School of Applied and Engineering Physics and Materials Science Center, Cornell University, Ithaca, New York 14850

(Received 17 April 1974)

The attenuation of long-wavelength elastic waves is studied in a glasslike harmonic chain. The structural disorder gives rise to a phase incoherence of an initial plane-wave disturbance. In addition the dynamic disorder introduces a phase incoherence and an exponential localization of the normal modes. The phase-incoherence contribution can interfere with the structural disorder since the spring constant is strongly correlated with equilibrium separation. To calculate the attenuation the long-wavelength normal modes must be explicitly constructed. This is done by a slight modification of the state-ratio method of Matsuda and Ishii, and a straightforward extension of this method from the random mass chain to the random spring-constant chain. In the absence of structural disorder, the attenuation of the average displacement is shown to have equal contributions from the phase incoherence and from the localization of the modes. With structural disorder, when the spring constant is a decreasing function of equilibrium separation, the attenuation is decreased by the interference between dynamical and structural phase incoherence. The low-frequency limit of the density of states is also calculated. It is related to the sound speed exactly as in the ordered case.

I. INTRODUCTION

Recent experiments at low temperatures[1] have focused attention on the low-lying vibrational modes of glasses. Although anharmonic mechanisms may have to be invoked to explain some of the results, our extremely limited understanding of the disordered harmonic solid strongly inhibits serious theoretical work on the problem. Long-wavelength elastic waves are observed, but we know very little about how fluctuations modify the plane-wave nature of the associated normal-mode amplitudes. Perhaps there are also a class of fluctuation-dominated low-lying modes which are not wavelike. In two or more dimensions there is little to guide such speculations. In one dimension, however, there is a vast literature on the disordered chain, most of it concerned with a random distribution of masses on a lattice with fixed spring constant. A small part of this literature deals with wave propagation, and the theoretical methods are well enough developed that a detailed understanding of fluctuation effects on the low-lying modes is possible.

Consider first the random mass chain with the mass m_j at the jth site a random variable with mean M and variance $M^2\mu^2$. At low frequencies a perturbation expansion in $(m_j - M)\omega^2$ is natural, and has been carried out by several authors. In particular, Maradudin, Weiss, and Jepsen[2] used many-body perturbation theory, and Chow and Keller[3] used the language of wave propagation in random media. They both calculate the effective propagation constant for the average displacement $\langle u\rangle$. For a chain with spring constant Γ and lattice spacing a, the result to lowest order in ω is

$$k = k_0 + 2i\gamma a^{-1}, \qquad (1.1)$$

where

$$k_0 = (M\omega^2/\Gamma a^2)^{1/2}$$

and

$$\gamma = \frac{1}{8}\frac{M\mu^2\omega^2}{\Gamma}.$$

A more rigorous study of the propagation of low-frequency elastic waves in the random mass chain was carried out by Rubin,[4] and extended by Matsuda and Ishii.[5] Matsuda and Ishii considered the asymptotic behavior of the state ratio $z_j = u_j/u_{j-1}$. They found that

$$|z_j| \to e^{\gamma} \text{ for large } j. \qquad (1.2)$$

The apparent factor-of-2 discrepancy between Eqs. (1.1) and (1.2) was noticed by Chow and Keller,[3] and a correct qualitative description of its origin is given in the introduction to a recent paper by Chow.[6] That there will in general be a difference between the localization distance defined by Eq. (1.2) and the attenuation length for the average Green's function given by Eq. (1.1) has been explained recently by Thouless.[7] The attenuation of the average displacement arises partly from localization and partly from a phase incoherence due to fluctuations. For our extension to the glasslike chain we need to carefully separate these two contributions. We return to this point in detail in Sec. III.

In one dimension, structural disorder of the equilibrium positions does not affect the normal modes. In the absence of dynamic disorder these have a constant phase change from one site to the next. A typical wave-number-dependent experimental quantity such as the displacement-displacement correlation function $\langle uu(k,\omega)\rangle$ will, however, reflect the structural disorder. An initial plane-wave disturbance is a superposition of normal modes of slightly different frequencies, and will thus decay due to phase mixing. In an earlier paper,[8] an example of this phenomenon has been worked out in detail. In Sec. II we extend the long-wavelength limit of Ref. 8 to the case of arbitrary probability distribution for the equilibrium separations. The Lorentzian line shape follows naturally from the application of the central-limit theorem to the probability distribution of the distances between widely separated sites.

In Sec. III we construct the long-wavelength normal-mode amplitudes of the random mass chain. We use a slightly modified version of the state-ratio method of Matsuda and Ishii. The resulting amplitude contains a phase incoherence and an exponential localization. We then consider the calculation of the correlation function $\langle uu(k,\omega)\rangle$. The central-limit theorem can be applied to the phase-incoherence contribution just as in the structural-disorder case of Sec. II. The phase incoherence and localization each contribute half of the line width of $\langle uu(k,\omega)\rangle$. The two contributions together agree with the perturbation calculation of Refs. 2 and 3.

In Sec. IV we consider the chain with fixed mass and random spring constant Γ_j. A straightforward transformation shows that the force in each link obeys the same equation of motion as does the displacement in the random mass case. The only change is that the relevant random variable is now Γ/Γ_j instead of m_j/M. In the low-frequency limit the displacement is simply related to the result of Sec. III for the random mass chain. Again half of the damping for the average displacement comes from phase incoherence and half from the localization of the modes.

In Secs. III and IV we also consider the low-frequency limit of the density of states. Using a result of Schmidt,[9] this is easily calculated in terms of the low-frequency limit of the stationary probability distribution $w(z)$ for the state ratio z. The latter is explicitly given by Matsuda and Ishii. The final result, which is not surprising, is that the sound-wave modes are responsible for all of the zero-frequency contribution. The low-temperature heat capacity in one dimension is thus linear in T, and is given exactly by the Debye value.

In Sec V we consider the glasslike chain in which the equilibrium separation is random, but the spring constant is a given function of equilibrium position. The phase incoherence due to structural and dynamic disorder then interferes. When the spring constant decreases with increasing equilibrium separation, as is physically reasonable, this interference is destructive. A simple illustrative example is worked out.

II. STRUCTURAL DISORDER

Following Ref. 8 we consider the correlation function

$$\phi(k,t)=\frac{M}{Nk_BT}\sum_{l,j}\langle V_l(t)\,V_j(0)\rangle\, e^{-ik(R_l-R_j)}, \qquad (2.1)$$

where R_j is the equilibrium position of the jth atom, and $V_j(t)$ is its velocity at time t. We introduce an orthonormal set of exact normal modes C_j satisfying

$$\sum_{l=1}^{N} C_l^{\nu} C_l^{\nu'*}=\delta_{\nu\nu'}, \quad \sum_{\nu=1}^{N} C_l^{\nu} C_j^{\nu*}=\delta_{lj}. \qquad (2.2)$$

In the dynamically ordered chain, the normal-mode solutions for periodic boundary conditions are

$$C_l^{\nu}=N^{-1/2}e^{2\pi i\nu l/N},$$
$$\omega_\nu^2=\frac{4\Gamma}{M}\sin^2\frac{\pi\nu}{N}, \qquad (2.3)$$
$$\nu=1\cdots N.$$

Expanding in terms of these normal modes we write

$$\phi(k,t)=N^{-1}\sum_{\nu=1}^{N}F(\nu,k)\cos\omega_\nu t, \qquad (2.4)$$

where

$$F(\nu,k)=\sum_{l,j}C_l^{\nu}C_j^{\nu*}e^{-ik(R_l-R_j)}. \qquad (2.5)$$

The Fourier transform $\phi(k,\omega)$ is then given by

$$\phi(k,\omega)=\rho(\omega)\,F(\nu_\omega,k), \qquad (2.6)$$

where $\rho(\omega)$ is the density of states, and ν_ω is the inverse function to ω_ν and gives the mode number as a function of its frequency. We note that ν is restricted to be positive, and we will explicitly consider only positive ω. Since $\phi(k,t)$ in Eq. (2.4) is an even function of time, $\phi(k,\omega)$ is an even function of ω. Since

$$\phi(k,\omega)=\omega^2\langle uu(k,\omega)\rangle,$$

the displacement-displacement correlation function is determined by studying the function $F(\nu,k)$ defined by Eq. (2.5).

The above discussion can be applied directly to the low-lying modes of the dynamically disordered chain. Only Eq. (2.3) is restricted to the dynamically ordered case. We return to this in Sec. III.

To calculate $F(\nu,k)$ for the dynamically ordered chain we substitute Eq. (2.3) into Eq. (2.5) and do the sums over l and j. Changing the summation variables from l and j to $n=l-j$ and j, taking the limit that $N\to\infty$, we obtain

$$F(\nu,k)=\sum_{n=-\infty}^{\infty}e^{2\pi i\nu n/N}\langle e^{-ik\rho_n}\rangle, \qquad (2.7)$$

where $\rho_n=R_{j+n}-R_j$ is the equilibrium separation of nth nearest neighbors, and the averaging is over the probability distribution of ρ_n.

It is essential to distinguish the averaging which appears in Eq. (2.1) from that which appears in Eq. (2.7). In Eq. (2.1) we consider a particular realization of the structural disorder in a very long chain, and average only over the equilibrium dynamical states of the harmonic oscillators to get the desired equilibrium correlation function. In Eq. (2.7) the sum over j averages over the structural disorder. In the absence of long-range order, a sum over j in the limit that $N \to \infty$ is equivalent to an ensemble average.

In Ref. 8 we calculated $F(\nu, k)$ analytically for the case that ρ_n had a Gaussian distribution for all n. In the long-wavelength limit, $\phi(k, \omega)$ had a Lorentzian line shape, and the linewidth behaved in a conventional "hydrodynamic" manner. To see the physical origin of this limiting result, consider the case that ρ_n is the sum of n independent and identically distributed random variables, each with mean a, variance σ^2, and probability distribution $p(\rho)$. For small n we can't make any simplifications unless $p(\rho)$ is Gaussian, but in the limit of large n, the central-limit theorem of probability theory tells us that

$$\langle e^{-ik\rho_n}\rangle = e^{-ikna}\, e^{-|n|k^2\sigma^2/2}. \qquad (2.8)$$

In the limit of small k the sum in Eq. (2.7) will be dominated by large n, so that Eq. (2.8) can be used to calculate the asymptotic long-wavelength behavior. The sum over n then becomes a geometric series, and $F(\nu, k)$ takes on the Lorentzian form

$$F(\nu, k) = f(\epsilon, k) = \frac{k^2\sigma^2}{(\epsilon - ka)^2 + (\frac{1}{2}k^2\sigma^2)^2}, \qquad (2.9)$$

where $\epsilon = 2\pi\nu/N$. The small-k limit thus depends on the dominance of large n, the applicability of the central-limit theorem for large n, and the geometric nature of the resulting series. All of this will remain true in the dynamically disordered case.

III. RANDOM MASS CHAIN

Consider a harmonic chain with nearest-neighbor forces, spring constant Γ, with mass m_j at the jth site. Let m_j be a random variable with mean M and variance $M^2\mu^2$. The masses at each site are assumed independently distributed. We want to calculate the displacement u_n of the nth atom in a normal mode of angular frequency ω. Following Matsuda and Ishii,[5] we introduce the state ratio

$$z_j = u_j/u_{j-1} \qquad (3.1)$$

and calculate the displacement u_n from

$$u_n = u_0 \prod_{j=1}^{n} z_j. \qquad (3.2)$$

The equation of motion for the displacements can be written as a recursion relation for the state ratios:

$$z_{j+1} = 2 - \epsilon^2 \alpha_j - z_j^{-1}, \qquad (3.3)$$

where $\alpha_j = m_j/M$, and $\epsilon^2 = M\omega^2/\Gamma$.

First we review the principal results of Matsuda and Ishii.[5] They look for a stationary probability distribution for the state ratio z. It is more convenient to transform variables from z to ϕ, where

$$z = \cos(\phi + \lambda)/\cos\phi = \cos\lambda - \sin\lambda\tan\phi, \qquad (3.4)$$

$$\epsilon^2 = 2(1 - \cos\lambda), \qquad (3.5)$$

and ϕ is defined in the interval $-\frac{1}{2}\pi < \phi < \frac{1}{2}\pi$. In the ordered case $z_n = \cos n\lambda/\cos(n-1)\lambda$. The corresponding stationary probability distribution $F(\phi)$ is uniform in ϕ. In the disordered case Matsuda and Ishii express $F(\phi)$ as a power series in ϵ:

$$F(\phi) = F_0(\phi) + \epsilon F_1(\phi) + \epsilon^2 F_2(\phi) + \cdots \qquad (3.6)$$

and find that

$$\frac{dF_1}{d\phi} = -(2\pi)^{-1}\mu^2(\cos 4\phi + \cos 2\phi). \qquad (3.7)$$

Of principal interest is

$$\gamma = \langle \ln|z|\rangle = \int_{-\pi/2}^{\pi/2} F(\phi)\ln|z(\phi)|\,d\phi, \qquad (3.8)$$

which is given to lowest order in ϵ by

$$\gamma = \tfrac{1}{8}\mu^2\epsilon^2. \qquad (3.9)$$

From the Matsuda-Ishii result we can easily calculate the low-frequency limit of the density of states. Counting the number of nodes, Schmidt[9] showed that

$$M(\omega^2) = \int_{-\infty}^{0} w(z, \omega^2)\,dz, \qquad (3.10)$$

where $M(\omega^2)$ is the total number of states with frequency less than ω, and $w(z)$ is the stationary probability distribution of the state ratio z. (Schmidt's z is our z^{-1}, but this does not affect the counting argument.) We note that

$$w(z) = F(\phi)\frac{d\phi}{dz}$$

and use Eqs. (3.6) and (3.7) for $F(\phi)$. The final result is

$$\frac{dM}{d\omega} = (2/\pi)(\omega_0^2 - \omega^2)^{-1/2}(1 - A\mu^2\epsilon^4 + \cdots), \qquad (3.11)$$

where $\omega_0^2 = 4\Gamma/M$.

Thus the only change from the ordered chain at low frequencies is that the mass m is replaced by the average mass M. This is also the correct prescription for calculating the sound speed and the macroscopic compressibility. The Debye theory relating the low-temperature heat capacity to the elastic properties is thus unmodified by mass disorder in one dimension.

In this paper our principal objective is a more detailed study of the amplitudes of the low-lying normal modes. We find it convenient to introduce a complex state ratio $\tilde{z}_j$ and to define a new variable ζ_j by

$$\tilde{z}_j = e^{i\lambda(1+\zeta_j)}. \tag{3.12}$$

In the ordered case $\zeta_j = 0$. Substituting Eq. (3.12) into Eq. (3.3) and expanding to order ϵ^2 we have

$$(\zeta_{j+1} - \zeta_j) + i\epsilon(\zeta_{j+1} + \zeta_j) = i\epsilon(\alpha_j - 1) - \tfrac{1}{2}i\epsilon(\zeta_{j+1}^2 + \zeta_j^2). \tag{3.13}$$

Summing Eq. (3.13) from $j=1$ to $j=n$, neglecting end effects for large n, and using Eq. (3.2) we have

$$u_n = u_0 \exp\left(in\epsilon + \tfrac{1}{2}i\epsilon\sum_{j=1}^{n}(\alpha_j - 1) - \tfrac{1}{2}i\epsilon\sum_{j=1}^{n}\zeta_j^2 + O(\epsilon^3)\right). \tag{3.14}$$

In the limit of large n the random variable $\frac{1}{2}\epsilon\sum_{j=1}^{n}(\alpha_j - 1)$ is normally distributed with mean zero and variance $\frac{1}{4}n\epsilon^2\mu^2$. It remains to calculate the contribution from

$$Q_n = \sum_{j=1}^{n} \zeta_j^2$$

from an appropriate approximate solution to Eq. (3.13). The leading term in Q_n is of order $n\epsilon$ and can be calculated by dropping the quadratic terms in Eq. (3.13). The linearized equation has the solution

$$\zeta_{j+1}^{(1)} = \frac{i\epsilon}{1+i\epsilon}(\beta_j + y\beta_{j-1} + y^2\beta_{j-2} + \cdots), \tag{3.15}$$

where $y = (1-i\epsilon)/(1+i\epsilon)$ and $\beta_j = \alpha_j - 1$.

The average value of $Q_n^{(1)}$ is obtained by squaring Eq. (3.15), summing over j, and noting that

$$\langle\beta_j\beta_k\rangle = \mu^2\zeta_{jk}.$$

The result is

$$\langle Q_n^{(1)}\rangle = \left(\frac{i\epsilon}{1+i\epsilon}\right)^2 n\mu^2 \sum_{j=0}^{n} y^{2j} \approx \tfrac{1}{4}in\epsilon\mu^2. \tag{3.16}$$

Fluctuations in Q_n will be important only to higher order in ϵ. Substituting Eq. (3.16) into Eq. (3.2) we finally obtain

$$u_n = u_0 \exp\left(in\epsilon + \tfrac{1}{2}i\epsilon\sum_{j=1}^{n}\beta_j + \tfrac{1}{8}n\epsilon^2\mu^2 + O(\epsilon^3)\right). \tag{3.17}$$

The exponential growth in Eq. (3.9) is in agreement with that calculated by Matsuda and Ishii.[5] In addition we have the phase incoherence from the term in $\sum_{j=1}^{n}\beta_j$ which is essential in reconciling the Matsuda-Ishii result with perturbation-theory calculations. We should note that neither in Ref. 5 nor here has the possible buildup of fluctuations in u_n been carefully studied. In our paper it is the replacement of Q_n by its average value $\langle Q_n^{(1)}\rangle$ calculated from the linearized equations which deserves more careful study. In Ref. 5 the question is avoided by considering only $\langle\ln|z|\rangle$. Even though the various z_j are strongly correlated, we can still write

$$\langle\ln|u_n|\rangle = \ln u_0 + \sum_{j=1}^{n}\langle\ln|z_j|\rangle \approx n\gamma.$$

For other statistical properties of the u_n the fact that the z_j are identically but not independently distributed will be of importance.

The solution (3.17) that we have constructed grows with increasing n. Matsuda and Ishii have shown that an appropriate choice of boundary conditions allows one to construct a localized solution from the growing solution. Thus a solution localized around $n=0$ will have the form

$$u_n = u_0 \exp\left(in\epsilon + \tfrac{1}{2}i\epsilon\sum_{j=1}^{n}\beta_j - \tfrac{1}{8}|n|\epsilon^2\mu^2\right). \tag{3.18}$$

The quantity of interest for our correlation function calculation, Eq. (2.5), is $C_{j+n}^{\nu}C_j^{\nu*}$. When appropriately normalized this then becomes

$$C_{j+n}^{\nu}C_j^{\nu*} = N^{-1}\exp\left(in\epsilon + \tfrac{1}{2}i\epsilon\sum_{k=j}^{j+n}\beta_k - \tfrac{1}{8}|n|\epsilon^2\mu^2\right). \tag{3.19}$$

The transformation from Eq. (3.17) to Eq. (3.19) is not as rigorous as we would like, but it is the only physically sensible one. The correlation function of interest then becomes

$$F(\nu, k) = \sum_{j=1}^{N}\sum_{n} C_{j+n}^{\nu}C_j^{\nu*}e^{-inka} \tag{3.20}$$

when structural disorder is neglected. We then carry out the average over the arbitrarily chosen localization center j. This is equivalent to an ensemble average, and depends only on the probability distribution of the random variable $\sum\beta_k$. Since the β_k are independently and identically distributed with mean zero and variance μ^2 this average can be calculated for large n using the central-limit theorem. The final results, in the limit of infinite N, is given by

$$f(\epsilon, k) = \sum_{n=-\infty}^{\infty} e^{-in(\epsilon-ka)}e^{-|n|\epsilon^2\mu^2/4}. \tag{3.21}$$

Equation (3.21) is only applicable for small ϵ where the series is dominated by large n. Only in this limit can we replace the mode index ν by the dimensionless frequency ϵ. At arbitrary frequency there will not be a well-defined normal-mode amplitude for each frequency. We note that the attenuation in the nth term has equal contributions from two sources. The first is the localization of the normal modes, and the second is a phase incoherence associated with the β_j. The two contributions together agree with the attenuation of the average Green's function as calculated from perturbation theory.[2,3] In the presence of structural disorder the contribution from phase incoherence can interfere with the structural disorder, but the localization contribution is unchanged. This will be considered explicitly in Sec. V. That both contributions should be present was pointed out in a more general context by Thouless.[7] The backward scattering of the unperturbed waves by the randomness determines the localization, while the forward scattering gives a phase incoherence which also contributes to the attenuation of the average Green's function. Thouless's discussion remains relevant for strong disorder in the limit of low frequency where the scattering by the disorder is weak.

Finally we carry out the sum in Eq. (3.21) to obtain

$$f(\epsilon, k)=\frac{\epsilon^2\mu^2}{(\epsilon-ka)^2+(\frac{1}{4}\epsilon^2\mu^2)^2}\,. \tag{3.22}$$

Recalling that $\epsilon^2=M\omega^2/\Gamma$, Eq. (3.22) gives a sound wave peak at $\omega^2=c^2k^2$, with $c^2=\Gamma a^2/M$. This agrees with the sound speed calculated from the macroscopic compressibility, and with the low-frequency limit of the density of states. The damping due to mass disorder in the long-wavelength limit is very similar to that due to structural disorder calculated in Ref. 8 and in Eq. (2.9) of this paper.

IV. RANDOM SPRING-CONSTANT CHAIN

Consider a harmonic chain with fixed mass M and random spring constant Γ_l coupling site l to site $l-1$. For a uniform compression, the force in each link is the same, and the compression of each spring is inversely proportional to its spring constant. The longitudinal sound speed is thus given by

$$c^2=\Gamma a^2/M,$$

with the effective spring constant Γ defined by

$$\Gamma^{-1}=N^{-1}\sum_{j=1}^{N}\Gamma_j^{-1}\,. \tag{4.1}$$

The equation of motion for the state ratios is

$$-M\omega^2=\Gamma_{l+1}(z_{l+1}-1)-\Gamma_l(1-z_l^{-1}). \tag{4.2}$$

The expansion corresponding to Eq. (3.13) is somewhat more complicated, and is obtained by defining a new variable δ_l through

$$z_l=e^{i\lambda(\zeta_l+\delta_l)}, \tag{4.3}$$

where

$$\zeta_l=\Gamma/\Gamma_l. \tag{4.4}$$

Substituting Eq. (4.3) into Eq. (4.2) and expanding to order ϵ^2, we have

$$\delta_{l+1}(\zeta_{l+1}^{-1}+i\epsilon)-\delta_l(\zeta_l^{-1}-i\epsilon)$$
$$=-\tfrac{1}{2}i\epsilon(\zeta_l+\zeta_{l+1}-2)-\tfrac{1}{2}i\epsilon(\zeta_{l+1}^{-1}\delta_{l+1}^2+\zeta_l^{-1}\delta_l^2). \tag{4.5}$$

Equation (4.5) is analogous to Eq. (3.13), and it can be solved approximately by the same procedures which led from Eq. (3.13) to Eq. (3.17). The algebra is more complicated, but the final result is very similar. The displacement u_n is given by

$$u_n=u_0\exp\left(in\epsilon+\tfrac{1}{2}i\epsilon\sum_{j=1}^{n}\eta_l+\tfrac{1}{8}n\epsilon^2\tau^2+O(\epsilon^3)\right), \tag{4.6}$$

where

$$\eta_l=(\Gamma/\Gamma_l)-1=\zeta_l-1 \tag{4.7}$$

is a random variable with mean zero and variance τ^2. The problem is thus equivalent to the random mass chain with the random variable η_l of Eq. (4.7) replacing the random variable $\beta_l=m_l/M-1$.

This result could have been anticipated more directly. Introduce the new dependent variable.

$$F_l=\Gamma_l(u_l-u_{l-1}). \tag{4.8}$$

The equation of motion for F_l is

$$-\epsilon^2(\Gamma/\Gamma_l)F_l=F_{l+1}-2F_l+F_{l+1}\,, \tag{4.9}$$

which is the same as the random mass equation of motion for u_l except that m_l/M is replaced by Γ/Γ_l. Equation (4.8) can be rewritten

$$F_l=\Gamma_l u_l(1-z_l^{-1})\approx-i\epsilon\Gamma_l u_l(\Gamma/\Gamma_l+\delta_l).$$

The large fluctuations from site to site are extracted in the term Γ/Γ_l. The remaining term δ_l is of order ϵ. At long wavelengths both F_l and u_l must vary slowly from site to site, and we have

$$F_l\approx-i\epsilon\Gamma u_l.$$

Thus the solution for F_l using the results of Sec. III is directly applicable to the displacement in the random spring-constant case, as verified by direct calculation.

The arguments leading from Eq. (4.6) to a calculation of the displacement-displacement correlation function are identical to those leading from Eq. (3.17) to Eq. (3.22). The result corresponding to Eq. (3.19) is

$$C_{j+n}^{\nu}C_j^{\nu *}=N^{-1}\exp\left(in\epsilon+\tfrac{1}{2}i\epsilon\sum_{k=j}^{j+n}\eta_k-\tfrac{1}{8}|n|\epsilon^2\tau^2\right). \tag{4.10}$$

When structural and dynamic disorder are both present, we must start from Eq. (4.10). This is considered in Sec. V.

The calculation of the density of states is unchanged from Sec. III. The transformation (4.8) from displacement u_l to force F_l is linear. The counting of normal modes is the same for both choices of dependent variable. Since the F_l obey the same equation studied in Sec. III the result is the same. Again the Debye theory is correct. The only caution is that the effective spring constant appropriate to both elastic properties and low-temperature heat capacity is given by Eq. (4.1). This simple transformation of the random spring problem into the random mass problem holds only in one dimension. In more than one dimension even the correct sound speed is unknown in the random spring case.

V. GLASSLIKE CHAIN

If both the spring constant and equilibrium separation are disordered we must combine the effects considered in Secs. II and IV. Substituting Eq. (4.10) into Eq. (2.5), and proceeding as we did to obtain Eq. (2.7) we find

$$F(\nu, k)=\sum_{n=-\infty}^{\infty} e^{in\epsilon}\, e^{-|n|\epsilon^2\tau^2/8}\langle e^{-ik\rho_n}\, e^{i\epsilon\phi_n}\rangle, \tag{5.1}$$

where the random variable ρ_n was defined in Sec. II, and the random variable

$$\phi_n = 1/2\sum_{l=1}^{n}\eta_l \tag{5.2}$$

is normally distributed with mean zero and variance $\frac{1}{4}n\tau^2$. The problem is trivial if the spring constant and equilibrium separation are independently distributed. We then have

$$\langle e^{-ik\rho_n}\, e^{i\epsilon\phi_n}\rangle = \langle e^{-ik\rho_n}\rangle\langle e^{i\epsilon\phi_n}\rangle$$

and the final result is a Lorentzian line shape as in Eq. (3.22) with the only change being that

$$\mu^2 \to \tau^2 + 2(\sigma/a)^2.$$

Of more physical interest is the case that the spring constant is a given function of the equilibrium separation. Then ρ_n is still a normally distributed random variable with mean na and variance $n\sigma^2$, but ϕ_n is a given function of ρ_n. To illustrate the point consider the simplest case where

$$\Gamma/\Gamma_l = 1 + Ca^{-1}(R_{l+1}-R_l-a). \tag{5.3}$$

A positive value of C corresponds to the physically plausible case in which the spring constant decreases with increasing equilibrium separation. Equation (5.3) can be written

$$\phi_n = \tfrac{1}{2}Ca^{-1}(\rho_n - na). \tag{5.4}$$

In particular the variance of Γ/Γ_l becomes

$$\tau^2 = (C\sigma/a)^2 \tag{5.5}$$

and

$$\langle e^{-ik\rho_n}\, e^{i\epsilon\phi_n}\rangle = e^{-ikna}\, e^{-|n|\theta}, \tag{5.6}$$

where

$$\theta = \tfrac{1}{2}(\sigma/a)^2(ka - \tfrac{1}{2}\epsilon C)^2. \tag{5.7}$$

In the Brillouin peak we can replace ϵ by ka so that

$$\theta \approx \tfrac{1}{2}(k\sigma)^2(1+\tfrac{1}{4}C^2 - C). \tag{5.8}$$

The first term in Eq. (5.8) gives the structural damping of Sec. II. The second term gives the phase-incoherence contribution to the dynamical damping of Sec. IV. The third term gives the destructive interference between them. The physical origin of this destructive interference is easily understood. Consider an equilibrium separation less than the mean value. The spring constant will be increased. This more nearly matches the phase change in a plane wave which will be reduced when the separation is less than average. Thus a plane wave more nearly matches a single normal mode, and the damping is reduced. In particular when $C=2$ the damping due to phase incoherence can be eliminated entirely. The damping due to the localization will, however, still remain. The final result, combining Eqs. (5.1), and (5.6) is

$$f(\epsilon, k) = \frac{\epsilon^2\psi^2}{(\epsilon - ka)^2 + (\frac{1}{4}\epsilon^2\psi^2)^2},$$

where

$$\psi^2 = \tfrac{1}{2}\tau^2 + 2(\sigma/a)^2(1-\tfrac{1}{2}C)^2 = \tau^2(1-2C^{-1}+2C^{-2}).$$

In summary we have extended the discussion of wave propagation in a disordered chain to include the combined effects of structural and dynamic disorder and the correlations between them. To do this we had to distinguish the dynamical effects of phase incoherence from those of normal-mode localization. The main physical point is that fluctuations in one dimension can contribute subtle effects to the attenuation of long-wavelength sound modes, but they can not change the dominant low-frequency behavior. We have used, however, much of the arsenal of special one-dimensional tricks. None of our conclusions can be extended to three-dimensional systems of direct physical interest.

ACKNOWLEDGMENT

This work was supported by the National Science Foundation through the Materials Science Center at Cornell University.

*Permanent address: Department of Nuclear Engineering, Kyoto University, Kyoto, Japan.

[1]R. C. Zeller and R. O. Pohl, Phys. Rev. B 4, 2029 (1971).

[2]A. A. Maradudin, G. H. Weiss, and D. W. Jepsen, J. Math. Phys. 2, 349 (1961).

[3]P. L. Chow and J. B. Keller, J. Math. Phys. 13, 1404 (1972).
[4]R. J. Rubin, J. Math. Phys. 9, 2252 (1968); 11, 1857 (1970).
[5]H. Matsuda and K. Ishii, Progr. Theor. Phys. Suppl. 45, 56 (1970).
[6]P. L. Chow, J. Math. Phys. 14, 1364 (1973).
[7]D. J. Thouless, J. Phys. C 6, L49 (1973).
[8]K. Kim and M. Nelkin, Phys. Rev. B 7, 2762 (1973).
[9]H. Schmidt, Phys. Rev. 105, 425 (1957).