Localization of Normal Modes and Energy Transport in the Disordered Harmonic Chain*)

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The feature of normal modes in one-dimensional isotopically disordered harmonic chain is investigated. It is proved for any frequency that the simultaneous difference equations for the displacement u_n of the n-th atom, $(-\infty<n<\infty)$, has a solution in which u_n grows exponentially with n with probability 1. In the low frequency limit the rate of exponential growth γ is explicitly calculated. A necessary and sufficient condition is obtained for there to exist a localized solution such that $\lim_{n\to\pm\infty} u_n=0$. It is proved that any infinite disordered chain, except those with measure 0, can be made to have an exponentially localized solution for any ω by modifying the mass of one atom m_0 to a suitable real value as a function of ω. From this it does not logically follow that almost all normal modes of any given large but finite sample chain are localized in such a way as occurred in the above modified infinite chain. However, the theoretical estimate of the nature of normal modes and energy transport based on the above mentioned value of γ, agrees well with the result of computer experiments. As a by-product of our investigation, the exact expression of the thermal conductivity due to the Kubo formula for the isotopically disordered harmonic chain is obtained in a closed form.

§1. Introduction

The feature of the normal frequency distribution in disordered harmonic systems has rather been clarified. Since Dean's pioneering work[2] by the computer experiment revealed more or less unexpected feature of the disordered harmonic systems, theoretical investigations have been successfully worked out for its interpretation.[3)~5)] Various conditions for the existence of band gaps in disordered systems have been proposed, which are reviewed by Hori in this supplement.[6)~8)] It is theoretically justified for the one-dimensional system that the coarse-grained frequency distribution can in principle be obtained to one's desired accuracy, for instance, by the suitable ensemble average of periodic systems, because of the existence of 'effective distance' for the coarse-grained quantity.[9)] Although to the authors' knowledge no theoretical justification exists for this procedure in higher dimensional systems, comparisons of various approximative calculations with the results of computer experiments seem to indicate that no serious fundamental difficulty exists so long as one is concerned with the coarse-grained frequency spectrum rather

*) This paper includes a part of the study the outline of which was read by T. Miyata and the present authors at the 1968 International Conference on Statistical Mechanics held in Kyoto, and was published in its proceedings.[1)]

than the exact spectrum itself.[10),11)] Indeed, for the physical quantity such as specific heat associated only with the frequency distribution, it does not matter whether the exact spectrum is discrete or continuous.

On the other hand, for the transport phenomena the feature of eigenfunctions is of vital importance. As Halperin has shown,[4)] if the eigenfunction of the Hamiltonian for an electron is suitably localized in space, then the system should have no static conductivity.

In 1958, Anderson[12)] pointed out the absence of spin diffusion in certain random lattices. This property is just the one that the disordered system should exhibit if its energy eigenfunction of an electron is suitably localized in space. In 1961, Mott and Twose[13)] conjectured that essentially all the energy eigenfunctions in an infinitely long one-dimensional random potential are localized in space. Makinson and Roberts[14)] gave some further support to this proposition with arguments that wave functions must be localized at least in the neighborhood of any energy gap.

Borland[15)] considered the wave function of an electron satisfying the one-dimensional Schrödinger equation with random potential. He proved in the high energy limit that the envelope of the wave function grows exponentially with the distance from one end at which the boundary conditions for the wave function are given. From this he inferred that the eigenfunctions for such systems are localized in space in the sense that the envelope of such a function decays on average in an exponential manner on either side of some region. Here we note that his proof for the localization is still unsatisfactory, because it is restricted to high energy limit, apart from the logical gap between the exponential growth and the exponential localization of the eigenfunction of a very large but finite system. We show in this paper that the former restriction can utterly be removed by invoking the powerful theorem due to Furstenberg[16)] concerning the limits of products of noncommuting random variables. Although we have not yet succeeded to completely surmount the latter logical gap, we shall clarify the relation between the exponential growth of the wave function and the existence of the localized solution for the wave equation in an infinite system. The localization of eigenfunctions of the finite system and the existence of the localized solution in an infinite system still may not be equivalent, although they are supposed to be closely correlated. Therefore we shall refer this identification of the behavior of the infinite system and the finite but very large system as IF-assumption.

The similar problem exists for the isotopically disordered harmonic chain. In 1962, Rosenstock and McGill[17)] calculated the normal modes of some isotopic chains containing not more than 16 atoms. They inferred from it that the normal modes for the disordered chain may not be essentially different from those of the regular chain. This was soon objected by Dean and Bacon,[18)] who carried out the computation for a particular sample of isotopically dis-

ordered diatomic chain of 50 atoms. They pointed out that the modes corresponding to the higher eigenfrequencies are localized while those corresponding to the lower eigenfrequencies are not localized, and this feature had been missed in Rosenstock and McGill's calculation, because the length of their chain was too short. Later the computer experiments for normal modes are extended to larger systems by Payton and Visscher[19] (see Fig. 1). We shall calculate the rate of the exponential growth of the displacement for isotopically disordered chain in the low frequency limit. By invoking the IF-assumption we can infer to what extent the normal modes are localized as a function of frequency, mass ratio and concentration of one of the isotopes. The comparison of this theory with the results of the computer experiments seems to support the IF-assumption.

As to the transport phenomena of disordered systems Payton et al.[20] made computer experiments on the energy transport of the isotopically disordered harmonic chain in contact at its ends with heat reservoirs at temperature T_1 and T_N. On the other hand, for the regular harmonic chain Rieder et al.[21] and Nakazawa[22] independently made a theoretical calculation for the heat flux by obtaining the covariance matrix for the stationary state. They found that the heat flux is proportional to the temperature difference (T_1-T_N) rather than to the temperature gradient $(T_1-T_N)/N$. We shall obtain the

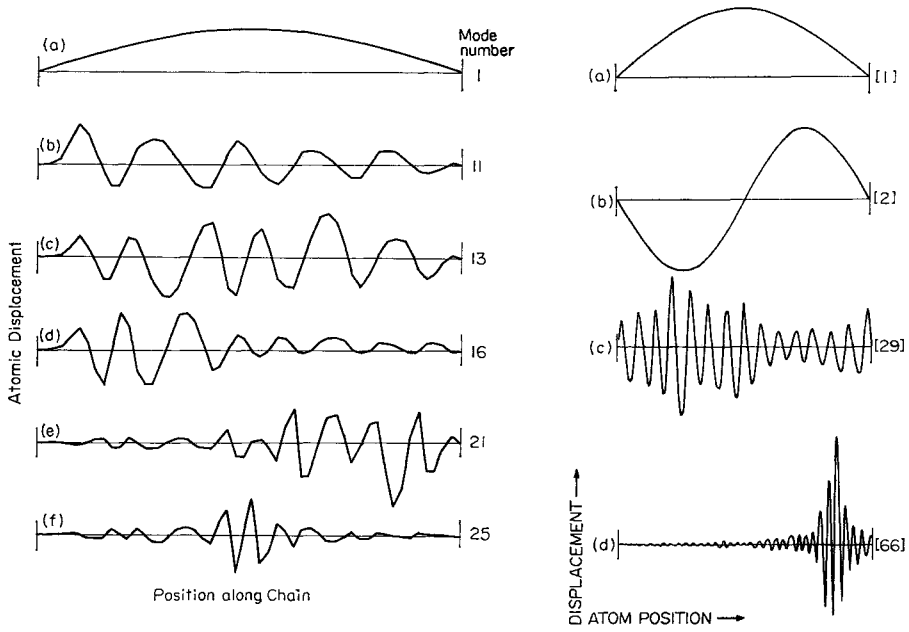

Fig. 1. Normal modes of an isotopically disordered harmonic chain, half-heavy atoms and half-light with a mass ratio of three. The mode numbering is from the lowest to the highest frequency. (i) $N=50$,[18] (ii) $N=200$.[19]

expression for the covariance matrix in terms of normal modes of the disordered harmonic chain in the limit of weak coupling with the heat reservoirs. Basing on the calculated rate of the exponential growth of normal modes and the IF-assumption, we shall show that the feature of the result of the computer experiment for the heat flux of the isotopically disordered harmonic chain can theoretically be reproduced.

Rubin[23] made a detailed study on the transmission properties of an isotopically disordered harmonic chain, including the theoretical calculation of the upper and lower bounds of the attenuation constants. Hori[24] pointed out that the attenuation constant is equal to the rate of the exponential growth of displacements. Recently, Rubin[25] calculated the low frequency limit of the attenuation constant, which exactly coincides with the rate of the exponential growth which we[1] obtained previously. While Rubin's theoretical estimate of the lower bound of the attenuation constant does not prove that the attenuation constant is positive throughout the whole frequency range, the use of Furstenberg's theorem neatly ensures this property.

As Ziman[26] remarked, the one-dimensional model has so different nature from the higher dimensional models that the former may not represent the feature of the wave functions of the three-dimensional systems in which many people are interested. However, even for the one-dimensional system we have not yet reached the satisfactory understanding of the nature of the eigenfunctions free from assumptions. In connection with this we do not know whether the spectrum is truly discrete or continuous; it is the problem which may be relevant to the localization of eigenfunctions.

Therefore, it will be worthwhile to try to deepen the knowledge of the one-dimensional system not only because there is the system like linear polymers where the one-dimensional character is dominant, but also for the understanding of the fundamental difference, if any, of the one-dimensional system from the higher dimensional ones. Thus, the purpose of this paper is to present our study hitherto made in order to give a theoretical unification of the various separate investigations and to extend the range of their applicability.

§2. Summary and plan of the paper

Consider an isotopically disordered harmonic chain with infinite length as a simple model of random systems. The displacement u_n of the n-th atom in the vibration with frequency ω satisfies the following set of equations

$$-m_n\omega^2 u_n = K(u_{n+1}+u_{n-1}-2u_n), \qquad (2\cdot1)$$

where K is the force constant and m_n is the mass of the atom at the n-th site.

We are primarily interested in the normal modes of the sufficiently long

finite chain, not the infinite chain as given in (2·1). However, since it is difficult to discuss the limiting behavior of the finite chain, we first study the infinite chain and then from the knowledge of the latter infer the feature of the former. In order to avoid the confusion caused by the complicated mathematics as well as for the sake of impatient reader, we summarize the main result of our study in this section leaving their proof and discussion to later sections.

First, we discuss the asymptotic behavior of the solution of (2·1) when the set of values u_0 and u_1 is given, where $|u_0|^2+|u_1|^2\neq 0$. Since the situation is the same for u_n with negative n we only consider u_n with positive n. The solution can be written in terms of the product of the transfer matrix $\boldsymbol{T}_n$ as

$$\begin{pmatrix} u_{N+1} \\ u_N \end{pmatrix} = \boldsymbol{T}_N \boldsymbol{T}_{N-1} \cdots \boldsymbol{T}_1 \begin{pmatrix} u_1 \\ u_0 \end{pmatrix}, \tag{2·2}$$

where

$$\boldsymbol{T}_n = \begin{pmatrix} 2-m_n\omega^2/K & -1 \\ 1 & 0 \end{pmatrix}. \tag{2·3}$$

For the regular chain where $m_n=m$, it is apparent that:
when $0<\omega^2\leqslant 4K/m$,

$$\overline{\lim_{N\to\infty}} \frac{1}{N} \ln |u_N|^2 = 0, \tag{2·4}$$

and when $\omega^2>4K/m$,

$$\begin{aligned} &\lim_{N\to\infty} \frac{1}{N} \ln |u_N|^2 = 2\lambda \quad \text{for } \frac{u_1}{u_0} \neq -e^{-\lambda}, \\ &\lim_{N\to\infty} \frac{1}{N} \ln |u_N|^2 = -2\lambda \quad \text{for } \frac{u_1}{u_0} = -e^{-\lambda}, \end{aligned} \tag{2·5}$$

where $\lambda=\cosh^{-1}(m\omega^2/2K-1)>0$.

On the other hand, for the random chain where masses $m_1, m_2 \cdots, m_n, \cdots$ are the sequence of independent real random variables with a common distribution function, we are concerned with the limiting property of the product of matrices or the limit theorem of the noncommuting random products.

In general, we let μ be a measure on $\mathrm{SL}(m, R)$, which is the group of m-dimensional unimodular matrices transforming the real vector space R^m into itself. Let G denote the smallest closed subgroup of $\mathrm{SL}(m, R)$ containing the support of μ. Let $X_1, X_2, \cdots, X_n, \cdots$ denote the sequence of the independent G-valued random variables with the common distribution μ. Then, Furstenberg's theorem runs as follows:

(Furstenberg's theorem)[16] Let G be a noncompact subgroup of $\mathrm{SL}(m, R)$ such that no subgroup of G of finite index is reducible. Then $\|X_n \cdots X_1 u\|$

grows exponentially as $n\to\infty$ with propability 1 for all u except for the zero vector. Here $\|\cdots\|$ denotes the norm of the vector.

In view of Furstenberg's theorem, identifying $\boldsymbol{T}_n$ as X_n our problem reduces to the study as to whether the closed subgroup G of $\mathrm{SL}(2,R)$ generated by the transfer matrices of the form given in (2·3) is noncompact and whether no subgroup of G given here with finite index is reducible. We call here the above two conditions as F-conditions.

Theorem 1 *If G contains at least two transfer matrices corresponding to different non-zero masses, then G satisfies F-conditions.*

Therefore, for the random chain where masses $m_1, m_2, \cdots, m_n, \cdots$ are the sequence of independent non-zero real valued random variables with a common distribution μ, there exists γ such that

$$\lim_{N\to\infty}\frac{1}{N}\ln\{|u_N|^2+|u_{N-1}|^2\}=2\gamma>0 \tag{2·6}$$

with probability 1.

The value of γ, which can be determined by solving the integral equation, cannot be given in a closed form in general. We shall prove

Theorem 2 *In the limit of $\omega\to 0$,*

$$\gamma=\langle(m-\langle m\rangle)^2\rangle\omega^2/8K\langle m\rangle, \tag{2·7}$$

where $\langle\cdots\rangle$ denotes the ensemble average and the suffix of the mass m is suppressed.

The proof of Theorems 1 and 2 will be given in §3. So far it is the first stage of our study. Next, we study the bounded solution of (2·1) such that $|u_n|<\infty$ for all n, which constitutes the second stage.

For the regular chain where $m_n=m$, we know that (2·1) either has no bounded solution (for $\omega^2>4K/m$), or has bounded solution which has no limit for u_N as $N\to\pm\infty$ (for $\omega^2\leqslant 4K/m$). No non-trivial localized bounded solution in the sense

$$\lim_{N\to\pm\infty}u_N=0 \tag{2·8}$$

exists for the regular system. The existence of such a solution in disordered system was inferred by Borland;[15] we shall closely look into it.

We prove in §4 the following theorem.

Theorem 3 *Let $u_n=\phi^{\pm}(n)$ be the particular solution of (2·1) such that $\phi^{\pm}(0)=0$, $\phi^{\pm}(\pm 1)=-1$. A necessary and sufficient condition for there to exist a non-trivial solution of (2·1) such that (2·8) holds is the following:*

Either $\lim_{N\to\pm\infty}\phi^{\pm}(N)=0$ *or*

(I) *There exists an infinite sequence of integers* $\{n(\nu)\}$ $(n(\nu)<n(\nu+1), \nu=0, \pm1, \pm2, \cdots)$ *for which*

$$c_{\pm} \equiv \lim_{\nu\to\pm\infty} \sum_{n=\pm1}^{n(\nu)\mp1} \frac{1}{\phi^{\pm}(n)\phi^{\pm}(n\pm1)} \tag{2·9}$$

exist and

$$\lim_{N\to\pm\infty} \lim_{\nu\to\pm\infty} \phi^{\pm}(N) \sum_{n=N}^{n(\nu)\mp1} \frac{1}{\phi^{\pm}(n)\phi^{\pm}(n\pm1)} = 0 \tag{2·10}$$

and

(II) c_+ *and* c_- *satisfy*

$$-m_0\omega^2 = K(c_+ + c_- - 2). \tag{2·11}$$

When the conditions (I) *and* (II) *are satisfied, then the only bounded solution of* (2·1) *is the localized solution satisfying* (2·8).

It is easy to show that for the regular system $\lim_{N\to\pm\infty} \phi^{\pm}(N)$ does not exist and the two conditions (I) and (II) are mutually exclusive, as it should be.

Now for the random chain we can prove on the basis of (2·6) and Theorem 3 that:

Theorem 4 *For the random chain, where* $m_{\pm1}, m_{\pm2}, \cdots, m_{\pm n}, \cdots$ *are the sequence of independent non-zero real random variables with a common distribution* μ, (2·9) *and* (2·10) *hold with probability* 1.

Let us call a set of sample chains where all the masses are specified except m_0 'a sample chain with variable m_0', since we may look upon such a set as if it is one sample which has a value of m_0 as a state variable. Then, any sample chain with variable m_0, except those with measure 0, can have a localized solution by setting the value of m_0 such that (2·11) holds. This fact indicates that if m_0 can have any value including negative values, then we can almost always construct for any given frequency and for any sequence of masses $m_{\pm1}, m_{\pm2}, \cdots, m_{\pm n}, \cdots$ a completely specified sample chain for which (2·1) has a localized solution.

It may happen, of course, that G may not contain $\boldsymbol{T}_0$ with m_0 that satisfies (2·11) for any possible set of values of c_+ and c_-. Such a frequency is the one forbidden as a normal frequency. For instance, if there is the minimum mass $\underline{m}$ such that $0<\underline{m}\leqq m_n$ $(-\infty<n<\infty)$ then the frequency ω with $\omega^2>4K/\underline{m}$ corresponds to such a forbidden frequency. Thus one may still suspect the existence of the localized solution in the physical system, since here m_0 should be positive.

However, we can state:

Theorem 5 *The probability that for a sample chain with variable* m_0 *which is positive to have a localized solution tends to* 1/2 *as* $\omega\to0$.

Theorem 6 *The localized solution has the asymptotic form for* $|n|\gg 1$ *such that*

$$|u_n|<U\exp[-(\gamma-\varepsilon)|n|], \tag{2·12}$$

where U *is a finite positive number independent of* n, $\gamma>0$ *and* $\varepsilon\to 0$ *as* $|n|\to\infty$. γ *is given by* (2·7) *in the limit of* $\omega\to 0$.

The third stage of our study should be the relation between the localized solution of the infinite system for given ω and the nature of normal modes of a given sample chain which is a large but finite system. We have not yet succeeded to formulate the *a priori* theory for the above relation, so we shall only study the consequences of the IF-assumption. Invoking the IF-assumption to Theorem 6, let us assume that essentially all the normal modes with $\gamma\gg 1/N$ of a finite chain of N atoms localize somewhere, say around the n_0-th site with the asymptotic form

$$|u_n|<U\exp[-\gamma|n-n_0|] \tag{2·13}$$

for $|n-n_0|\gg 1$, where U is a finite positive number and γ is given by (2·7). In §5 we compare (2·13) and (2·7) with the result of the computer calculation of normal modes, which supports the qualitative validity of (2·13).

In §6 we shall analyze the result of Payton, Rich and Visscher's computer experiment[20] on the thermal conductivity in a disordered harmonic chain. The equation of motion of the model of the experiment can be represented by

$$\begin{aligned} m_1\ddot{u}_1&=K(u_2-2u_1)-\lambda m_1\dot{u}_1+f_1(t),\\ m_n\ddot{u}_n&=K(u_{n+1}+u_{n-1}-2u_n),\quad (2<n<N-1)\\ m_N\ddot{u}_N&=K(u_{N-1}-2u_N)-\lambda m_N\dot{u}_N+f_N(t). \end{aligned} \tag{2·14}$$

The contact with the heat reservoirs of temperature T_1 and T_N, $(T_1-T_N=\Delta T>0)$, is represented by friction terms with constant λ together with the Gaussian random force $f_j(t)$, $(j=1, N)$, the ensemble average of which satisfying

$$\begin{aligned} &\overline{f_j(t)}=0,\\ &\overline{f_j(t)f_{j'}(t')}=2kT_j\lambda m_j\delta_{jj'}\delta(t-t'). \end{aligned} \tag{2·15}$$

By obtaining the stationary solution of the equation determining the evolution of the covariance matrix of displacements and momenta of atoms for such a system, we shall show that:

Theorem 7 *In the limit of* $\lambda\to 0$, *in the stationary state of the system given by* (2·14) *we have the equation*

$$\overline{u_n^2}=\frac{k}{m_n}\sum_\nu\left(\frac{T_1x_{\nu,1}^2+T_Nx_{\nu,N}^2}{x_{\nu,1}^2+x_{\nu,N}^2}\right)x_{\nu,n}^2, \tag{2·16}$$

where $u_{\nu,n}=x_{\nu,n}/\sqrt{m_n}$ *is the displacement of the n-th atom in the* ν*-th normal mode and*

$$\sum_n x_{\nu,n}^2=1. \tag{2·17}$$

The energy current is equal to the energy transmitted per unit time from the heat reservoir to the first atom, which is given, in virtue of (2·14) and (2·15), by

$$Q=\lambda(kT_1-m_1\overline{\dot{u}_1^2}). \tag{2·18}$$

For a regular chain we obtain from (2·16) and (2·17) in the limit of $\lambda\to 0$

$$Q=(\lambda k/2)\Delta T \tag{2·19}$$

in consistence with the result obtained by other authors.[21),22)]

For a disordered chain using (2·16) and (2·13) we obtain

$$Q=\bar{\kappa}\Delta T/N,\ \bar{\kappa}=k\lambda c\sqrt{N}\langle m\rangle/\sqrt{\langle(m-\langle m\rangle)^2\rangle}, \tag{2·20}$$

where $c=0(1)$ is a constant.

Payton et al. defined the thermal conductivity κ as the energy current divided by the gradient of the local temperature $\delta T/N$ rather than $\Delta T/N$, the relation between which is given from (2·18) by

$$\delta T=\Delta T-c_1 Q, \tag{2·21}$$

where c_1 is a constant. Hence, κ is given by

$$\kappa=\bar{\kappa}/(1-c_1\bar{\kappa}/N). \tag{2·22}$$

By suitably choosing two constants c and c_1 the concentration dependence of κ of the computer experiment can be well reproduced by the theory as shown in Fig. 2. In particular, when the concentration of mass m is p and that of mass 1 is $1-p$, the value of p for which κ is minimum is given by

$$p_{\min}=\frac{1}{1+m}, \tag{2·23}$$

which exactly coincides with the computer experiment independently of the values of c and c_1.

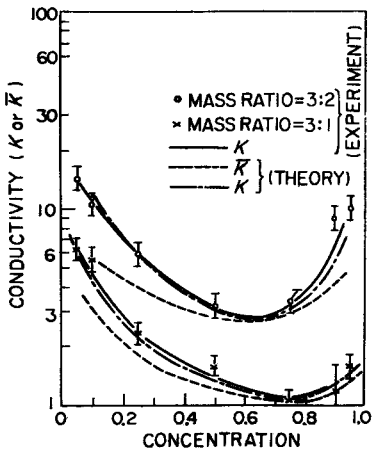

Fig. 2. Thermal conductivity coefficient κ or $\bar{\kappa}$ versus light atom concentration for the isotopically disordered harmonic chain. The experimental values are due to the computer experiment by Payton et al. (reference 19)).

One important result of our theory, which is not yet confirmed by the computer experiment, is the N-dependence of the thermal conductivity κ. According to (2·20) and (2·22) κ is proportional to $\sqrt{N}$ for large N, so that Fourier's law for thermal conduction does not hold. In most solids, except for quantum solids, at very low temperatures the amplitude of oscillation of atoms is very small. Therefore, the thermal conductivity is mainly determined by the scattering of phonons by impurities or boundaries and the effect of anharmonicity is not important, but it is usually presumed that Fourier's law does hold here, too.

If this presumption should be correct, we should look into the discrepancy between this presumption and our result for one-dimensional disorderd harmonic chain. At least there are three possibilities:

(1) IF-assumption is not correct for the derivation of the N-dependence of κ.

(2) In one-dimensional disorderded harmonic solids Fourier's law does not hold, but in the higher dimensional solids the situation is different.

(3) Even if anharmonicity is not important for determining the value of thermal conductivity, it is its presence that ensures the validity of Fourier's law.

The question as to which is the true cause of the discrepancy and how Fourier's law can be derived is an interesting future problem.

Allen and Ford[27] obtained a formally exact expression for the Kubo thermal conductivity for an infinite, one-dimensional chain of atoms which are connected by nearest-neighbor, harmonic springs of equal strength, and which are of equal mass m except within a finite section of the chain which contains disordered isotopic impurities of mass M. The thermal conductivity they obtained is in our notation

$$\kappa=\frac{k^2T}{2\pi\hbar}\int_0^{\Theta/T}\frac{Na}{|\Gamma_N(x)|^2}\frac{x^2e^x}{(e^x-1)^2}dx, \tag{2·24}$$

where N is the number of atoms in the above finite section, Θ is the Debye temperature, a is the nearest-neighbor atomic distance,

$$\lim_{N\to\infty}\frac{1}{N}\ln|\Gamma_N(x)|=\gamma, \tag{2·25}$$

$x=\hbar\omega/kT$, and γ is given by (2·6) or (2·7).

They concluded from the fact $\gamma>0$ that the thermal conductivity κ for finite N given in (2·24) is finite. As to the N-dependence, using the expression (2·7) valid for small value of x, the contribution from which is dominant for the integral in (2·24) when $N\gg1$, we obtain for $N\gg1$

$$\kappa=\frac{ka}{2\sqrt{\pi}}\sqrt{\frac{K\langle m\rangle}{\langle(m-\langle m\rangle)^2\rangle}}\sqrt{N}. \tag{2·26}$$*)

Apart from the validity of the Kubo formula itself, we think that (2·26) is the correct expression for the thermal conductivity based on the Kubo formula. This expression is valid for any concentration of random impurities so long as $N\gg 1$. It is of significance that (2·26) is derived without the IF-assumption; this fact may rule out the first of the above-mentioned three possibilities.

However, we must be careful that the Kubo thermal conductivity (2·26) is different from (2·20) and (2·22). In particular, when the concentration of mass m is p and that of mass 1 is $1-p$, the value of p for which κ is minimum is here given instead of (2·23) by

$$p_{\min}=\frac{1}{1+\sqrt{m}}, \tag{2·30}$$

in disagreement with the result of the computer experiment.

Although from our result we cannot say anything about the validity of the Kubo formula for thermal conductivity in the system where Fourier's law holds, our result indicates that care must be taken to calculate the energy flow in the system where Fourier's law does not hold, since in the absence of Fourier's law the energy flow is not necessarily determined by the temperature gradient alone.

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*) Allen and Ford obtained the following expression for γ in the low concentration of impurities:

$$\gamma=\frac{1}{2}\frac{R}{N}\ln\left[1+\frac{(1-M/m)^2x^2}{(\theta/T)^2-x^2}\right], \tag{2·27}$$

which coincides with (2·7) in the low concentration limit. Here R is the number of impurities. The correct use of (2·27) in (2·25) and (2·24) leads to the thermal conductivity which is proportional to $\sqrt{N}$ for $N\to\infty$ for fixed value of R/N, too. They also proposed the alternative expression for γ which they supposed to be valid for large R:

$$\gamma=\frac{b}{2}\frac{R}{N}(1-M/m)^2(T/\theta)x, \tag{2·28}$$

where b is a constant. They obtained using (2·28) in (2·24) and (2·25) the finite thermal conductivity in the limit of $N\to\infty$. However, the linear dependence of γ on x, which is vital for obtaining the finite κ, is not considered to be valid in view of our result (2·7).

Woll[28] also calculated using propagater formalism the Kubo formula for the thermal conductivity for a disordered harmonic chain in a slightly different model. In his model the impurities are randomly distributed throughout the entire chain. His result for the conductivity is, in the limit of $R/N\ll 1$,

$$\kappa=\frac{k\sqrt{K/m}}{4\pi^2(1-M/m)^2}\left(\frac{N}{R}\right)Na, \tag{2·29}$$

which is proportional to N for fixed value of the impurity concentration R/N. Because of subtlety of treatments inherent in the propagater formalism it is difficult to assess the validity of (2·29). However, if (2·29) is valid, then the energy flow should be determined by the temperature difference of both ends of the chain independently of the length of the chain as occurred in a regular chain, and the energy flow diverges in the limit of $R/N\to 0$. This property, however, seems to be at variance with the result of computer experiments.[20]

§3. Proof of Theorems 1 and 2

Theorem 1 First we show that F-conditions are satisfied if G contains two noncommuting matrices $\boldsymbol{T}_1$ and $\boldsymbol{T}_2$ whose traces are greater than 2 in the absolute value. Then one of the eigenvalues of $\boldsymbol{T}_i$ $(i=1, 2)$ is greater than 1 in the absolute value. Therefore the matrix elements of $\boldsymbol{T}_i^n$ become arbitrarily large if we choose a sufficiently large integer n. As G contains such $\boldsymbol{T}_i^n$, it cannot be compact. Next, let G_0 be a subgroup of G of finite index. Then for some integers n_i, $\boldsymbol{T}_i^{n_i} \in G_0$ $(i=1, 2)$; otherwise, there exist infinitely many cosets $T_i^n G_0$ $(n=1, 2, 3, \cdots)$ of G in contradiction with the finiteness of the index of G_0. $\boldsymbol{T}_i^{n_i}$ have the same non-degenerate eigenstates as $\boldsymbol{T}_i$, and $\boldsymbol{T}_1$ and $\boldsymbol{T}_2$ are noncommuting, so that $\boldsymbol{T}_1^{n_1}$ and $\boldsymbol{T}_2^{n_2}$ are also non-commuting. Therefore, G_0 is irreducible.

To prove Theorem 1, we show that we can construct the above mentioned two matrices from two arbitrary transfer matrices $\boldsymbol{T}$, $\boldsymbol{T}'$ corresponding to different non-zero masses. If the absolute values of the traces of $\boldsymbol{T}$ and $\boldsymbol{T}'$ are both greater than 2, there is no problem. So we assume that $|\mathrm{Tr}\,\boldsymbol{T}|<2$. It is easily shown that in the representation which diagonalizes $\boldsymbol{T}$, $\boldsymbol{T}'$ is a matrix of the following type

$$\begin{pmatrix} a & b \\ b^* & a^* \end{pmatrix}, \tag{3·1}$$

where a and b are complex numbers and * denotes the complex conjugate. We mention that the product of two matrices of this type is also of this type. A unimodular matrix of this type must satisfy a condition $|a|^2-|b|^2=1$, and is generally expressed using three real parameters. When the absolute value of its trace is smaller than 2, it is expressed as

$$\begin{aligned} a &= \cos\theta + i \sin\theta \cosh 2\chi, \\ b &= e^{i\delta} \sin\theta \sinh 2\chi, \end{aligned}$$

where $0 \leqq \theta < 2\pi$, $0 \leqq \chi < \infty$, $0 \leqq \delta < 2\pi$. A transformation which diagonalizes this matrix is given by

$$\begin{aligned} \boldsymbol{S} &= \begin{pmatrix} \cosh\chi & ie^{i\delta}\sinh\chi \\ -ie^{-i\delta}\sinh\chi & \cosh\chi \end{pmatrix}, \\ \boldsymbol{S}^{-1} &= \begin{pmatrix} \cosh\chi & -ie^{i\delta}\sinh\chi \\ ie^{-i\delta}\sinh\chi & \cosh\chi \end{pmatrix}. \end{aligned} \tag{3·2}$$

Note that $\boldsymbol{S}$ and $\boldsymbol{S}^{-1}$ are also of the type of (3·1). When the absolute value of the trace of a unimodular matrix is greater than 2, it is expressed as

$$\begin{aligned} a &= \pm\cosh\Theta + i \sinh\Theta \sinh 2\chi, \\ b &= e^{i\delta} \sinh\Theta \cosh 2\chi, \end{aligned} \tag{3·3}$$

where $-\infty<\theta<\infty$, $0\leqq\chi<\infty$, $0\leqq\delta<2\pi$.

Now the construction runs as follows. In the first stage of construction we show how to obtain a composite transfer matrix $\widetilde{T}$ whose trace is greater than 2 in the absolute value and which is noncommuting with T'. Let $T_1(n)\equiv T^n T'$. If we assume that T and T' are expressed by the parameters $(\theta, 0, 0)$ and $(\theta', \chi', \delta')$ respectively, then

$$\begin{aligned}\mathrm{Tr}\, T_1(n) &= 2(\cos\theta'\cos n\theta-\sin\theta'\cosh 2\chi'\sin n\theta)\\ &= 2|a'|\cos(n\theta+\varphi'),\end{aligned}$$

where

$$\begin{aligned}a' &\equiv \cos\theta'+i\sin\theta'\cosh 2\chi'\\ &\equiv |a'|e^{i\varphi'}.\end{aligned}$$

Here we must treat the two cases separately according as θ/π is rational or irrational.

Case 1) The case when θ/π is irrational

In this case we can make $|n\theta+\varphi'|$ arbitrarily small with mode 2π by choosing n suitably. Since $|a'|>1$, we can choose a n_1 and make $\mathrm{Tr}\, T_1(n_1)>2$. $\widetilde{T}\equiv T_1(n_1)$ and T' are noncommuting. This $\widetilde{T}$ is a desired matrix, and the first stage ends here.

Case 2) The case when θ/π is rational

Let $\theta=(q/p)\pi$, where p and q are prime to each other. In this case $n\theta$ takes only $2p$ discrete values $0, \pi/p, 2\pi/p, \cdots, (2p-1)\pi/p$ with mode 2π. This time T^n can become the unit matrix. So we make a condition that T^n should not become the unit matrix and choose the integer n so as to make $|n\theta+\varphi'|$ as small as possible with mode 2π. Let n_1 be such a number and $T_1\equiv T_1(n_1)$. Then, as $|n_1\theta+\varphi'|<\pi/p$, following inequality holds for $p\geqq 2$.

$$\mathrm{Tr}\, T_1>2|a'|\cos\frac{\pi}{p}. \tag{3·4}$$

It is easily seen that T_1 and T' are noncommuting. If $\mathrm{Tr}\, T_1>2$, then the first stage ends here. But if $\mathrm{Tr}\, T_1<2$, we repeat the similar construction using T_1 instead of T. That is, let $T_2(n)\equiv T_1^n T'$ and choose the integer n so as to make $\mathrm{Tr}\, T_2(n)$ as large as possible. Let $(\theta_1, \chi_1, \delta_1)$ be the parameters to express T_1 and let S_1 and S_1^{-1} be the corresponding transformation matrix given in (3·2). Now we change the representation and diagonalize T_1. In this representation

$$T_1=\begin{pmatrix} e^{i\theta_1} & 0\\ 0 & e^{-i\theta_1}\end{pmatrix},$$

$$T_1'\equiv S_1^{-1}T'S_1\equiv\begin{pmatrix} a_1' & b_1'\\ b_1'^* & a_1'^*\end{pmatrix},$$

and

$$\mathrm{Tr}\, \boldsymbol{T}_2(n) = 2|a_1'| \cos(n\theta_1 + \varphi_1').$$

If θ_1/π is irrational, we can choose a n_2 and make $\mathrm{Tr}\, \boldsymbol{T}_2(n_2) > 2$ and the first stage ends here as before. But, if θ_1/π is rational ($\theta_1 = (q_1/p_1)\pi$, where p_1 and q_1 are prime to each other), we can say only that

$$\mathrm{Tr}\, \boldsymbol{T}_2 > 2|a_1'| \cos\frac{\pi}{p_1}. \tag{3·5}$$

From (3·4), we have the following inequalities.

$$\cos\frac{q_1}{p_1}\pi > |a'| \cos\frac{\pi}{p} > \cos\frac{\pi}{p}, \tag{3·6}$$

i.e. $$p_1 > p.$$

If $\mathrm{Tr}\, \boldsymbol{T}_2 > 2$, then the first stage ends here. But if $\mathrm{Tr}\, \boldsymbol{T}_2 < 2$, we must repeat the similar construction.

In the worst case, we may construct an infinite sequence of matrices $\boldsymbol{T}_1, \boldsymbol{T}_2, \cdots, \boldsymbol{T}_n, \cdots$ whose traces are all smaller than 2 in the absolute value and θ_i/π are all rational ($\theta_i = (q_i/p_i)\pi$, p_i and q_i are prime to each other). But we can show that such case does not hold and we can make the first stage end after a finite times of repetition of the construction. If we assume the existence of such an infinite sequence, then in the same way as we obtained (3·5) and (3·6), we have

$$p < p_1 < p_2 < \cdots < p_n < \cdots, \tag{3·7}$$

and

$$\mathrm{Tr}\, \boldsymbol{T}_{i+1} > 2|a_i'| \cos\frac{\pi}{p_i}, \quad (i = 1, 2, \cdots) \tag{3·8}$$

where a_i' is the $(1, 1)$ element of $\boldsymbol{T}'$ in the representation which diagonalizes $\boldsymbol{T}_i$. We will show in the following that there exists a number $A_c (> 1)$ such that if $|a_i'| < A_c$, there appears $|a_j'| > A_c$ within a finite times of repetition of the construction. Now let N be an integer such that $\cos(\pi/p_N) > A_c^{-1}$. Such N exists because of (3·7). If $|a_N'| > A_c$, we have $\mathrm{Tr}\, T_{N+1} > 2$ by (3·8) contrary to the first assumption. Even if $|a_N'| < A_c$, within a finite times of repetition of the construction there appears $|a_{N+l}'| > A_c$ and from (3·7) and (3·8) we have

$$\mathrm{Tr}\, \boldsymbol{T}_{N+l+1} > 2|a_{N+l}'| \cos\frac{\pi}{p_{N+l}} > 2A_c \cos\frac{\pi}{p_N} > 2,$$

contrary to the first assumption.

We must now examine the sequence $\{|a_i'|\}$ and show the above mentioned

property. Let $(\theta_i, 0, 0)$, $(\theta_{i+1}, \chi_{i+1}, \delta_{i+1})$ and $(\theta'_i, \chi'_i, \delta'_i)$ be respectively the parameters to express $\boldsymbol{T}_i$, $\boldsymbol{T}_{i+1}$ and $\boldsymbol{T}'$ in the representation which diagonalizes $\boldsymbol{T}_i$. There is a relation $\boldsymbol{T}_{i+1}=\boldsymbol{T}_i^m\boldsymbol{T}'$ for some integer m. Expressing the (1, 2) elements of both hand sides by parameters, we have

$$e^{i\delta'_{i+1}}\sin\theta_{i+1}\sinh 2\chi_{i+1}=e^{i(m\theta_i+\delta'_i)}\sin\theta'_i\sinh 2\chi'_i,$$

i.e.
$$|\sin\theta_{i+1}|\sinh 2\chi_{i+1}=|\sin\theta'_i|\sinh 2\chi'_i. \tag{3·9}$$

Let $\boldsymbol{S}_{i+1}$ be the transformation matrix which diagonalizes $\boldsymbol{T}_{i+1}$. Then

$$a'_{i+1}=[\boldsymbol{S}_{i+1}^{-1}\boldsymbol{T}'\boldsymbol{S}_{i+1}]_{11}$$

and expressing the both sides by parameters, we have

$$\cos\theta'_{i+1}+i\sin\theta'_{i+1}\cosh 2\chi'_{i+1}=\cos\theta'_i+i\sin\theta'_i \times\{\cosh 2\chi_{i+1}\cosh 2\chi'_i-\sinh 2\chi_{i+1}\sinh 2\chi'_i\cos(\delta_{i+1}-\delta'_i)\}.$$

As $\cosh 2\chi_{i+1}\cosh 2\chi'_i-\sinh 2\chi_{i+1}\sinh 2\chi'_i\cos(\delta_{i+1}-\delta'_i)\geqslant\cosh 2(\chi_{i+1}-\chi'_i)>0$, we obtain $\theta'_{i+1}=\theta'_i=\cdots=\theta'$ and

$$\cosh 2\chi'_{i+1}=\cosh 2\chi_{i+1}\cosh 2\chi'_i-\sinh 2\chi_{i+1}\sinh 2\chi'_i\cos(\delta_{i+1}-\delta'_i) \geqslant\cosh 2(\chi_{i+1}-\chi'_i). \tag{3·10}$$

Now as $\theta'_i=\theta'$, (3·9) becomes

$$\sinh 2\chi_{i+1}=\left|\frac{\sin\theta'}{\sin\theta_{i+1}}\right|\sinh 2\chi'_i.$$

Because $\pi/p_{i+1}\leqslant\theta_{i+1}<\pi/p_i$, there exists an integer M, such that for $i\geqslant M$

$$|\sin\theta'/\sin\theta_{i+1}|>4$$

and the relation between χ_{i+1} and χ'_i is plotted in Fig. 3. Let $x=\chi_c>0$, and $y=3\chi_c$ be a solution of the simultaneous equations

$$\begin{cases}\sinh 2y=4\sinh 2\chi\\ y=3x.\end{cases}$$

Then, for $\chi'_i<\chi_c$, $\chi_{i+1}>3\chi'_i$ as can be seen from Fig. 3. Substituting this inequality into (3·10), we have

$$\cosh 2\chi'_{i+1}>\cosh 4\chi'_i.$$

Therefore for $\chi'_i<\chi_c$ we have

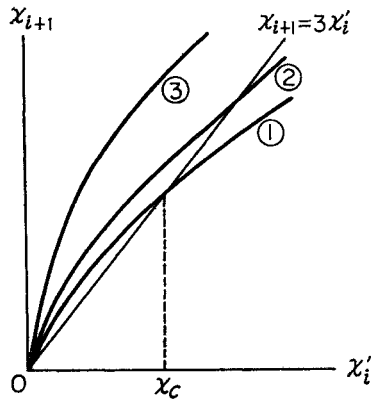

Fig. 3. Schematic relation between χ_{i+1} and χ'_i (arbitrary scale).

$\sinh 2\chi_{i+1}=m\sinh 2\chi'_i$

1···$m=4$ 2···$m=m_2>4$

3···$m=m_3>m_2$

$$\chi'_{i+1}>2\chi'_i . \tag{3·11}$$

As $|a'_i|$ is expressed by parameters as

$$|a'_i|=\sqrt{\cos^2\theta'+\sin^2\theta'\cosh^2\chi'_i}\,, \tag{3·12}$$

the above mentioned property of $\{|a'_i|\}$ follows from (3·11) if we put

$$A_c\equiv\sqrt{\cos^2\theta'+\sin^2\theta'\cosh^2\chi_c}\,.$$

In the first stage of the construction, a matrix $\widetilde{T}$ was constructed by finite times of multiplication of matrices T and T' whose traces are both smaller than 2 in the absolute value. Of course, $\widetilde{T}$ is contained in G and $\widetilde{T}$ and T' are noncommuting and $\mathrm{Tr}\,\widetilde{T}>2$. Now we construct a matrix $\widetilde{T}'$ in the similar way as we constructed $\widetilde{T}$. This time, we use T' and $\widetilde{T}$ respectively instead of T and T'. As $\mathrm{Tr}\,\widetilde{T}>2$, we must use (3·3) to express $\widetilde{T}$ by parameters. The argument is essentially the same as before except for some modifications. For example, (3·7), (3·8) hold also this time, but $|\tilde{a}_i|$ is given not by (3·12) but by

$$|\tilde{a}_i|=\sqrt{\cosh^2\widetilde{\Theta}+\sinh^2\widetilde{\Theta}\cosh^2\chi_i}\geqslant\cosh\widetilde{\Theta}>1.$$

Therefore, it is easier this time to show that the second stage ends within a finite times of repetition of the construction. If the given matrices are such that $|\mathrm{Tr}\,T|<2$, $|\mathrm{Tr}\,T'|>2$, then we need only the second stage of construction mentioned above. Thus the proof of Theorem 1 is now complete.

Theorem 2 In this theorem, the rate γ of the exponential growth of vectors in Theorem 1 is calculated in the limiting case of $\omega\to 0$. First, we quote a theorem due to Furstenberg[16] and show the procedure one should follow to obtain γ in the general case. Let μ be a measure on $\mathrm{SL}(m,R)$, and let G denote the smallest subgroup of $\mathrm{SL}(m,R)$ containing the support of μ. μ need not be absolutely continuous. $\{X_n\}$ denotes the G-valued variables with distribution μ. We are interested in the action of G on R^m. The real $(m-1)$ dimensional projective space P^{m-1} is obtained from $R^m-\{0\}$ by identifying two vectors if each is a scalar multiple of the other. G acts on P^{m-1} as well as on R^m. Let ν be a distribution on P^{m-1}, and let $g\nu$ denote the distribution which gx has if x has distribution ν. We define the convolution $\mu*\nu$ of μ and ν as a weak integral by

$$\mu*\nu=\int g\nu\, d\mu(g).$$

If $\mu*\nu=\nu$, we call ν a stationary measure for μ on P^{m-1}. Consider a function on $G\times(R^m-\{0\})$ defined by

$$\sigma(g,u)=\|gu\|/\|u\|,$$

where $\|\cdots\|$ denotes the norm of vector. $\sigma(g, u)$ depends only on g and $\bar{u}\in P^{m-1}$. We set $\rho_1=\log\sigma$. Then, we have the following theorem (Theorem 8·5 in the Furstenberg's paper).

(Theorem) If G is irreducible and $\int\|g\|d\mu(g)<\infty$, the expression

$$\iint\rho_1(g,\xi)d\mu(g)d\nu(\xi)$$

for a stationary measure ν for μ is independent of the stationary measure ν. Denoting the common value by $\alpha_\mu(\rho_1)$, we have, with probability 1,

$$n^{-1}\log\|X_n\cdots X_1u\|\to\alpha_\mu(\rho_1)$$

for all nonzero vectors $u\in R^m$.

Now we turn to the calculation of γ for a particular case. In this case, G is a group of 2×2 transfer matrices given in (2·3). If we define state vectors by the transpose of (u_{n+1}, u_n), they are transfered as in (2·2). If we define the state ratios by $z_n\equiv u_n/u_{n-1}$, they satisfy the following equation, as is seen from (2·1).

$$z_{n+1}=2-\frac{m_n}{K}\omega^2-\frac{1}{z_n}, \tag{3·13}$$

where, the masses m_n are the random variables with a common probability density $p(m_n)$. P^{m-1} in the above therorem is identical with the space of state ratio. In order to calculate γ we must find a stationary distribution of state ratio z. But, it is more convenient to make a variable transformation from z to ϕ as

$$z\equiv\frac{\cos(\phi+\lambda)}{\cos\phi}=\cos\lambda-\sin\lambda\tan\phi, \tag{3·14}$$

where $2\cos\lambda\equiv2-(M/K)\omega^2$, $M\equiv\langle m\rangle$, and ϕ is defined in the interval $-\pi/2<\phi<\pi/2$. In terms of this new variable ϕ, (3·13) becomes

$$\tan\phi_{n+1}=\tan(\phi_n+\lambda)+\frac{m_n-M}{K}\omega^2\operatorname{cosec}\lambda.$$

From this equation ϕ_{n+1} is determined as a function of ϕ_n. We write this relation as $\phi_{n+1}=\Phi(\phi_n; m_n)$ and its inverse relation as $\phi_n=\bar{\Phi}(\phi_{n+1}; m_n)$. Then the stationary distribution $F(\phi)$ of ϕ which we seek, satisfies the following equation.

$$F(\phi)=\int F(\Psi(\phi; m))\frac{d\Psi(\phi; m)}{d\phi}p(m)dm. \tag{3·15}$$

As we are interested in the limit $\omega\to0$, we expand $\Psi(\phi; m)$ as a power series of ω and obtain

$$\Psi(\phi;\, m)=\phi-\sqrt{\frac{M}{K}}\,\omega\left(1+\frac{\Delta m}{M}\cos^2\phi\right)-\frac{(\Delta m)^2}{MK}\omega^2\sin\phi\cos^3\phi+\cdots, \quad (3\cdot16)$$

where $\Delta m\equiv m-M$ and $\cdots$ denotes the higher order terms of ω than the retained terms. Though strictly speaking, (3·16) only holds with mode π, we neglect this remark for a while and try to find a solution of (3·15). Further, we assume that $F(\phi)$ can be expanded as a power series of ω as

$$F(\phi)=F_0(\phi)+\omega F_1(\phi)+\omega^2F_2(\phi)+\cdots. \quad (3\cdot17)$$

If we substitute (3·16) and (3·17) into (3·15) and make a Taylor expansion of $F_i(\Psi(\phi;\, m))$ about ϕ, $(i=0, 1, 2, \cdots)$, we obtain the following equations for $F_0(\phi)$ and $F_1(\phi)$ by comparing the first three order terms of the both hand sides of (3·15).

$$\frac{dF_0}{d\phi}=0,$$

$$\frac{dF_1}{d\phi}=-F_0(\phi)\frac{\langle(\Delta m)^2\rangle}{2M\sqrt{MK}}(\cos 4\phi+\cos 2\phi). \quad (3\cdot18)$$

We notice that the solutions of these equations have the period π. Normalizing the solution in the interval $-\pi/2<\phi<\pi/2$ we can think it as a stationary solution of (3·15) where ϕ is confined in the interval $-\pi/2<\phi<\pi/2$. Now, the rate γ is given in terms of $F(\phi)$ as

$$\gamma=\int_{-\pi/2}^{\pi/2}F(\phi)\log\left|\frac{\cos(\phi+\lambda)}{\cos\phi}\right|d\phi,$$

and is calculated to the order of ω^2 as follows. First, by rearranging the terms we obtain

$$\gamma=\int_{-\pi/2}^{\pi/2}\{F(\phi-\lambda)-F(\phi)\}\log|\cos\phi|\,d\phi.$$

As λ is of the first order of ω, we next make a Taylor expansion of $F(\phi-\lambda)$ about ϕ and obtain

$$\gamma=-\sqrt{\frac{M}{K}}\,\omega\int_{-\pi/2}^{\pi/2}\frac{dF(\phi)}{d\phi}\log|\cos\phi|\,d\phi+\cdots.$$

Substituting (3·17) and (3·18) into the above equation, we have the final result

$$\gamma=\frac{\langle(\Delta m)^2\rangle}{2MK\pi}\omega^2\int_{-\pi/2}^{\pi/2}(\cos 4\phi+\cos 2\phi)\log|\cos\phi|\,d\phi+\cdots$$

$$=\frac{\langle(\Delta m)^2\rangle}{8MK}\omega^2+\cdots.$$

§4. Proof of Theorems 3, 4, 5 and 6

Theorem 3 Let $\psi^{\pm}(n)$ be the particular solution of (2·1) such that $\psi^{\pm}(0)=1$, $\psi^{\pm}(\pm 1)=0$. Then it is easily seen from (2·1) that $\phi^{+}(n)$ and $\psi^{+}(n)$ satisfy the following relation.

$$\begin{aligned}&\phi^{+}(n)\psi^{+}(n+1)-\phi^{+}(n+1)\psi^{+}(n)=\phi^{+}(n-1)\psi^{+}(n)-\phi^{+}(n)\psi^{+}(n-1)\\&\quad=\cdots=\phi^{+}(0)\psi^{+}(1)-\phi^{+}(1)\psi^{+}(0)=1.\end{aligned}\tag{4·1}$$

Any solution of (2·1) is generally expressed in terms of two independent solutions $\phi^{+}(n)$ and $\psi^{+}(n)$ as

$$u_n=u_0\psi^{+}(n)-u_1\phi^{+}(n).\quad(n=0,1,2,\cdots)\tag{4·2}$$

First we assume that u_n is a non-trivial solution such that

$$\lim_{n\to\pm\infty}u_n=0,\tag{4·3}$$

and examine the property which $\phi^{+}(n)$ should have in this case. We consider two cases separately according as $\lim_{n\to\infty}\phi^{+}(n)$ exists or not.

Case 1) *The case when* $\lim_{n\to\infty}\phi^{+}(n)$ *exists*

Let $\lim_{n\to\infty}\phi^{+}(n)=\varPhi$. If $u_0\neq 0$, we have from (4·2)

$$\psi^{+}(n)=\frac{1}{u_0}\{u_n+u_1\phi^{+}(n)\}$$

and $\lim_{n\to\infty}\psi^{+}(n)=u_1\varPhi/u_0$ also exists. Then, taking the limit of $n\to\infty$ of (4·1), we have a contradictory relation $0=\varPhi\cdot u_1\varPhi/u_0-\varPhi\cdot u_1\varPhi/u_0=1$. Therefore, $u_0=0$ and as $u_n=-u_1\phi^{+}(n)$, we have

$$\lim_{n\to\infty}\phi^{+}(n)=0.\tag{4·4}$$

Case 2) *The case when* $\lim_{n\to\infty}\phi^{+}(n)$ *does not exist*

In this case there exist a positive number ε and an infinite sequence of integers $\{n(\nu);\ \nu=1,2,3,\cdots\}$ such that $|\phi^{+}(n(\nu))|>\varepsilon$; otherwise, $\lim_{n\to\infty}\phi^{+}(n)=0$ would exist contrary to the assumption. And this time $u_0\neq 0$; otherwise $u_n=-u_1\phi^{+}(n)$ and $\lim_{n\to\infty}u_n$ would not exist contrary to (4·3). From (4·2) we now have the following relation for the sequence $\{n(\nu)\}$.

$$\left|\frac{\psi^{+}(n(\nu))}{\phi^{+}(n(\nu))}-\frac{u_1}{u_0}\right|=\left|\frac{u_{n(\nu)}}{u_0\phi^{+}(n(\nu))}\right|<\left|\frac{u_{n(\nu)}}{u_0\varepsilon}\right|.$$

As $\lim_{\nu\to\infty}u_{n(\nu)}=0$ by (4·3), $\lim_{\nu\to\infty}\psi^{+}(n(\nu))/\phi^{+}(n(\nu))=u_1/u_0$ exists. Dividing the both sides of (4·1) by $\phi^{+}(n)\phi^{+}(n+1)$, we have

$$\frac{\psi^+(n+1)}{\phi^+(n+1)}-\frac{\psi^+(n)}{\phi^+(n)}=\frac{1}{\phi^+(n)\phi^+(n+1)}.$$

Taking sum over n from 1 to $l-1$, we have

$$\frac{\psi^+(l)}{\phi^+(l)}=\sum_{n=1}^{l-1}\frac{1}{\phi^+(n)\phi^+(n+1)},$$

where, if $\phi^+(n)=0$ for some integer n, we must do the following replacement.

$$\frac{1}{\phi^+(n-1)\phi^+(n)}+\frac{1}{\phi^+(n)\phi^+(n+1)}\to\frac{2-m_n\omega^2/K}{\phi^+(n-1)\phi^+(n+1)}. \tag{4·5}$$

This replacement, which is also an identity for n such that $\phi^+(n)\neq 0$, is justified by taking into account (2·1). Though we do not mention explicitly, such replacement should be done also in the similar situation which will appear in the following. In this way

$$\lim_{\nu\to\infty}\sum_{n=1}^{n(\nu)-1}\frac{1}{\phi^+(n)\phi^+(n+1)}=\frac{u_1}{u_0} \tag{4·6}$$

exists and

$$\begin{aligned}u_n&=u_0\phi^+(n)\left\{\frac{\psi^+(n)}{\phi^+(n)}-\frac{u_1}{u_0}\right\}\\&=u_0\phi^+(n)\left\{\sum_{l=1}^{n-1}\frac{1}{\phi^+(l)\phi^+(l+1)}-\lim_{\nu\to\infty}\sum_{l=1}^{n(\nu)-1}\frac{1}{\phi^+(l)\phi^+(l+1)}\right\}\\&=-u_0\phi^+(n)\lim_{\nu\to\infty}\sum_{l=n}^{n(\nu)-1}\frac{1}{\phi^+(l)\phi^+(l+1)},\end{aligned} \tag{4·7}$$

where, if $\phi^+(n)=0$, this relation should be replaced by the following as is seen from (4·1).

$$u_n=-u_0\cdot\frac{1}{\phi^+(n+1)}. \tag{4·8}$$

In terms of $\phi^+(n)$, (4·3) is expressed as

$$\lim_{n\to\infty}\lim_{\nu\to\infty}\phi^+(n)\sum_{l=n}^{n(\nu)-1}\frac{1}{\phi^+(l)\phi^+(l+1)}=0. \tag{4·9}$$

So far we considered the right half part ($n\geqslant 0$) of the chain. For the left half part ($n\leqslant 0$) of the chain, we can do essentially the same argument as above. For example, we can express the general solution as

$$u_n=u_0\psi^-(n)-u_{-1}\phi^-(n).\quad(n=0,-1,-2,\cdots)$$

We should consider two cases according as $\lim_{n\to-\infty}\phi^-(n)$ exists or not. Here we mention only that for the existence of $\lim_{n\to-\infty}\phi^-(n)$ the same case holds as for

the existence of $\lim_{n\to\infty}\phi^+(n)$.

Finally to obtain a complete solution of (2·1), we must adjust the three displacements u_1, u_0, u_{-1} as to satisfy the following equation.

$$-m_0\omega^2 u_0=K(u_1+u_{-1}-2u_0).$$

Dividing the both sides by u_0, we can express this condition in terms of $\phi^\pm(n)$ if we use (4·6).

Thus we have obtained a necessary condition in terms of $\phi^\pm(n)$ for the existence of a non-trivial solution of (2·1) such that $\lim_{n\to\pm\infty}u_n=0$:

Either $\lim_{n\to\pm\infty}\phi^\pm(n)=0$ or

(I) There exists an infinite sequence of integers $\{n(\nu)\}$ $(n(\nu)<n(\nu+1)$, $\nu=0, \pm1, \pm2, \cdots)$ for which

$$c_\pm\equiv\lim_{\nu\to\pm\infty}\sum_{l=\pm1}^{n(\nu)\mp1}\frac{1}{\phi^\pm(l)\phi^\pm(l\pm1)} \tag{2·9}$$

exists and

$$\lim_{n\to\pm\infty}\lim_{\nu\to\pm\infty}\phi^\pm(n)\sum_{l=n}^{n(\nu)\mp1}\frac{1}{\phi^\pm(l)\phi^\pm(l\pm1)}=0 \tag{2·10}$$

and

(II) c_+ and c_- satisfy

$$-m_0\omega^2=K(c_++c_--2). \tag{2·11}$$

It is easily seen that the above condition is also sufficient for the existence of a non-trivial solution u_n of (2·1) such that $\lim_{n\to\pm\infty}u_n=0$.

Theorem 4 In this theorem we show that the two conditions (2·9) and (2·10) are satisfied with probability 1 for the random chain, where $m_{\pm1}$, $m_{\pm2}, \cdots$ are the sequence of independent non-zero real random variables with a common distribution μ. Here we consider only the conditions for the right half part $(n>0)$ of the chain. We prove the theorem by examining a majorant series for the series in (2·9) and a majorant sequence for the sequence in (2·10).

As $\phi^+(n)$ is a particular solution of (2·1) with a given set of values of $u_0=0$ and $u_1=-1$, the relation in (2·6) applies to $\phi^+(n)$. Thus for any sufficiently small positive number $\varepsilon>0$ there exists an integer N such that for $n>N$

$$\exp[2(\gamma-\varepsilon)l]<\phi^+(l)^2+\phi^+(l-1)^2<\exp[2(\gamma+\varepsilon)l]. \tag{4·10}$$

From (4·10) we cannot have any lower bounds for $|\phi^+(l)|$ $(l\geqslant N)$ and they may become very small including the case of becoming zero. As they appear in (2·9) and (2·10) as products of their inverse, small $|\phi^+(l)|$ may

contribute significantly to the series in (2·9) and (2·10). So we consider two cases separately according as $\phi^+(l)$ satisfies an inequality

$$\phi^+(l^2)>\tfrac{1}{2}\exp[2(\gamma-\varepsilon)l] \tag{4·11}$$

or not.

Case 1) The case when $\phi^+(l)$ does not satisfy (4·11)

In this case we have the following lower bounds for $\phi^+(l\pm1)$ by (4·10).

$$\begin{aligned}&\phi^+(l-1)^2>\tfrac{1}{2}\exp[2(\gamma-\varepsilon)l],\\&\phi^+(l+1)^2>\tfrac{1}{2}\exp[2(\gamma-\varepsilon)(l+1)].\end{aligned} \tag{4·12}$$

Therefore this case never holds for the consecutive sites, and we can have an upper bound for the combined two consecutive terms containing $\phi^+(l)$ by virtue of (4·12) and the identity (4·5).

$$\begin{aligned}\left|\frac{1}{\phi^+(l-1)\phi^+(l)}+\frac{1}{\phi^+(l)\phi^+(l+1)}\right|&=\left|\frac{2-m_l\omega^2/K}{\phi^+(l-1)\phi^+(l+1)}\right|\\&<2\widetilde{M}\exp[-(\gamma-\varepsilon)(2l+1)]\\&<\widetilde{M}\{\exp[-(\gamma-\varepsilon)(2l-1)]+\exp[-(\gamma-\varepsilon)(2l+1)]\},\end{aligned} \tag{4·13}$$

where $\widetilde{M}\equiv\underset{l}{\mathrm{Max}}|2-m_l\omega^2/K|$.

Case 2) The case when $\phi^+(l)$ satisfies (4·11)

If $\phi^+(l+1)(\phi^+(l-1))$ does not satisfy (4·11), then the contribution of $1/\phi^+(l)\phi^+(l+1)(1/\phi^+(l-1)\phi^+(l))$ is already estimated in (4·13). So we need only to estimate the contribution from the remaining terms for which both $\phi^+(l)$ and $\phi^+(l\pm1)$ satisfy (4·11). Then it is easily seen that

$$\left|\frac{1}{\phi^+(l)\phi^+(l\pm1)}\right|<2\exp[-(\gamma-\varepsilon)(2l\pm1)]. \tag{4·14}$$

Thus we have the following majorant series by (4·13) and (4·14).

$$\begin{aligned}\sum_{l=N}^{n(\nu)-1}\frac{1}{\phi^+(l)\phi^+(l+1)}&\leqslant M\sum_{l=N}^{n(\nu)-1}\exp[-(\gamma-\varepsilon)(2l+1)]\\&\leqslant\frac{M\exp[-(\gamma-\varepsilon)(2N+1)]}{1-\exp[-(\gamma-\varepsilon)]},\end{aligned}$$

where $M\equiv\mathrm{Max}(2,\widetilde{M})$, and for $n\geqslant N$

$$\begin{aligned}\left|\phi^+(n)\sum_{l=n}^{n(\nu)-1}\frac{1}{\phi^+(l)\phi^+(l+1)}\right|&\leqslant M\phi^+(n)\frac{\exp[-2(\gamma-\varepsilon)n]}{1-\exp[-2(\gamma-\varepsilon)]}\\&\leqslant M\frac{\exp[-(\gamma-3\varepsilon)n]}{1-\exp[-2(\gamma-\varepsilon)]},\end{aligned} \tag{4·15}$$

where we used an inequality of $|\phi^+(n)|<\exp[(\gamma+\varepsilon)n]$ obtained from (4·10).

From these inequalities it is easily seen that (2·9) and (2·10) hold with probability 1 for this case.

Theorem 5 In this theorem we examine the possibility to satisfy the condition (2·11)

$$m_0\omega^2/K=2-(c_++c_-)$$

in the limiting case of $\omega\to 0$. To satisfy this condition by choosing a positive mass m_0, it is necessary and sufficient for $c_\pm$ to satisfy the following inequality.

$$c_++c_-<2. \tag{4·16}$$

Now $c_\pm$ are random variables which are defined in terms of $\phi^\pm(n)$. Their values are determined by the sequence of masses $m_{\pm 1}, m_{\pm 2}, \cdots$ and as is shown in (4·6) they are also expressed as $c_\pm=u_{\pm 1}/u_0$, where u_n is a non-trivial solution of (2·1) such that $\lim_{n\to\pm\infty} u_n=0$. We now wish to find the probability distribution of $c_\pm$. We will show that this probability distribution is the same as the stationary distribution of z_n considered in the proof of Theorem 2. It is convenient to use the notation which we used in the proof of Theorem 2. Then $c_\pm=z_{\pm 1}$, and using (3·13) we have

$$z_1=\cfrac{1}{a_1-\cfrac{1}{a_2-\ddots-\cfrac{1}{a_n-\cfrac{1}{z_{n+1}}}}},$$

where $a_n=2-m_n\omega^2/K$. By Theorem 4, the existence of the limit of $n\to\infty$ of this continued fraction is guaranteed, and its value is determined by the sequence $m_1, m_2, m_3, \cdots$. In the same way z_2 is also expressed as a continued fraction which is determined by the sequence $m_2, m_3, m_4, \cdots$. z_1 and z_2 are related by

$$z_1=\frac{1}{2-m_1\omega^2/K-z_2}. \tag{4·17}$$

As m_n are independent random variables, it is easily seen that the distribution $F(z_1)$ of $c_+=z_1$ is stationary with respect to the transformation (4·17) where m_1 is a random variable with distribution μ. Such a stationary distribution is exactly what we have obtained in the proof of Theorem 2, and is given by (3·14), (3·17) and (3·18).

$$c_+=\cos\lambda-\sin\lambda\tan\phi_+,$$

$$F(\phi_+)=\frac{1}{\pi}+\cdots,$$

where $2\cos\lambda=2-\langle m\rangle\omega^2/K$ and $\cdots$ denotes the higher order terms of ω. It is easily seen that c_+ and c_- are mutually independent and have the common distribution. The condition (4·16) is expressed in terms of $\phi_\pm$ in the limit of $\omega\to 0$ as

$$\tan\phi_+ + \tan\phi_- > 0, \quad \text{i.e.} \quad \sin(\phi_+ + \phi_-) > 0. \tag{4·18}$$

The region in (ϕ_+, ϕ_-) plane satisfying (4·18) is shown in Fig. 4 as the dashed region, and the limit of $\omega\to 0$ the point (ϕ_+, ϕ_-) is uniformly distributed in the square $-\pi/2<\phi_+<\pi/2$, $-\pi/2<\phi_-<\pi/2$. Therefore, the probability to find sample chains with such $c_\pm$ as to satisfy (4·16) tends to 1/2 as $\omega\to 0$.

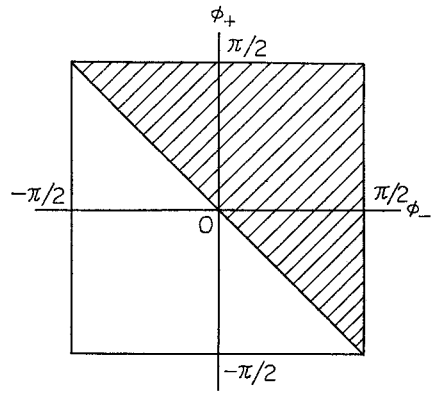

Fig. 4. The region in (ϕ_+, ϕ_-) plane satisfying (4·18).

Theorem 6 In this theorem we examine the asymptotic form of u_n. By (4·7) and (4·8), u_n is expressed in terms of $\phi^+(n)$ as

$$u_n = -u_0\phi^+(n)\lim_{\nu\to\infty}\sum_{l=n}^{n(\nu)-1}\frac{1}{\phi^+(l)\phi^+(l+1)} \quad \text{if } \phi^+(n)\neq 0$$

$$= -u_0\cdot\frac{1}{\phi^+(n+1)} \quad \text{if } \phi^+(n)=0.$$

Then by (4·13) and (4·15) we have for any sufficiently small positive number ε and an appropriate integer N,

$$|u_n| \leqslant U\exp[-(\gamma-\varepsilon)n]$$

for $n\geqslant N$, where U is a finite positive number independent of n. We can make ε arbitrarily small, though we must then take large N accordingly.

§5. Comparison of (2·13) and (2·7) with numerically calculated normal modes

According to (2·13), the normal mode is spacially well localized if and only if $\gamma N/2\gg 1$, or by virtue of (2·7) if and only if

$$\omega \gg 4\sqrt{\frac{K\langle m\rangle}{N\langle(m-\langle m\rangle)^2\rangle}} \equiv \omega_d\,, \tag{5·1}$$

where N is the number of atoms in the chain.

Let us call the right side of (5·1) demarcation frequency between localization and non-localization of normal modes. The demarcation frequency tends to zero as N tends to infinity, so that almost all the normal modes in any frequency range should be localized if the number of atoms is sufficiently large.

In the low frequency range where (2·7) is valid, the normal frequency is approximately given by

$$\omega_n = \sqrt{\frac{K}{\langle m \rangle}} \frac{n}{N} \pi, \tag{5·2}$$

where n is the mode number labelled in the increasing order of normal frequency. Then, the demarcation mode number n_d corresponding to the demarcation frequency is given by

$$n_d = \frac{4}{\pi} \sqrt{N \langle m \rangle / \sqrt{\langle (m - \langle m \rangle)^2 \rangle}}. \tag{5·3}$$

Thus if IF-assumption is valid, (5·3) gives the order of magnitude of the number of normal modes which are not well localized. We use the term 'the order of magnitude', because the notion of 'well-localized' cannot be sharply defined. However, we can clearly assert that among N normal modes all the normal modes except for low frequency modes, the number of which is of the order of $\sqrt{N}$, are well localized.

Equation (5·3) is valid for any isotopically disordered harmonic chain where the probability of the occupation of isotopes at different sites is uniform and uncorrelated. We can get the dependence of the number of non-well-localized modes on the concentration and mass ratio r through (5·3).

In Table I we give some numerical examples of the demarcation mode number of the isotopically disordered diatomic chain where the concentration of the two isotopes is the same.

Table I. Demarcation mode number, n_d, that is, the number of non-well-localized modes in the isotopically disordered diatomic chain.

mass ratio r \ N	16	50	200
2	15	27	54
3	10	18	36
5	8	14	27

The numerical calculation of normal modes were carried out for $r=3$ by Dean and Bacon[18] ($N=50$), and by Payton and Visscher[19] ($N=200$), and for $r=2$ by Rosenstock and McGill[17] ($N=16$). Some of their results are illustrated in Fig. 1, which can be favorably compared with Table I. Incidentally, it is interesting to imagine that Rosenstock and McGill, who suggested that the nature of normal modes of a disordered chain would be similar to that of a regular chain, would have concluded differently if

their calculation were made for $r \geq 3$ even though the chain length was as short as $N=16$.

We may go into the details of comparison by introducing the notion of the probable number of localized sites s_ν for the ν-th mode, which is defined by

$$s_\nu = \left[\sum_{n=1}^{N} \left(x_{\nu,n}^2 - \frac{1}{N} \right)^2 \right]^{-1}, \tag{5·4}$$

where $x_{\nu,n} = \sqrt{m_n}\, u_{\nu,n}$, $u_{\nu,n}$ being the displacement of the n-th atom in the ν-th normal mode normalized as

$$\sum_{n=1}^{N} x_{\nu,n}^2 = 1.$$

If the normal mode essentially localizes over s lattice sites, then for $N \gg s \gg 1$, $x_{\nu,n}^2 = O(1/s)$ for the s lattice sites and the contribution to the sum in the right side of (5·4) from these s sites is $O(1/s)$. On the other hand the contribution from all the other sites is $O(1/N)$, so that the right side of (5·4) is $O(s)$, which justifies the nomenclature.

The notion of the probable number of localized sites has the merit that it can be used for any dimensional system. However, because of the lack of the detailed data of the numerical calculations available to the authors, we conclude this section without utilizing this notion, only saying that (2·13) and (2·7) is in good qualitative agreement with numerical calculations.

§6. Thermal conductivity in the disordered harmonic chain

——Proof of Theorem 7——

In general the Hamiltonian of our chain can be written in the form

$$H = \tfrac{1}{2} \sum_{i=N+1}^{2N} x_i^2 + \tfrac{1}{2} \sum_{i,j=1}^{N} \Phi_{ij} x_i x_j , \tag{6·1}$$

where

$$x_i = \begin{cases} \sqrt{m_i}\, u_i & (i = 1, 2, \cdots, N) \\ \sqrt{m_i}\, \dot{u}_{i-N}, & (i = N+1, \cdots, 2N) \end{cases}$$

$$\Phi_{ij} = \frac{K}{\sqrt{m_i m_j}} (2\delta_{i,j} - \delta_{i,j+1} - \delta_{i,j-1}), \quad (i \neq 1,\ j \neq N)$$

$$\Phi_{1j} = \frac{K}{\sqrt{m_1 m_j}} (2\delta_{1,j} - \delta_{1,j-1}) = \Phi_{j1} ,$$

$$\Phi_{Nj} = \frac{K}{\sqrt{m_N m_j}} (2\delta_{N,j} - \delta_{N,j+1}) = \Phi_{jN} .$$

When the chain has contacts with heat reservoirs as represented by

(2·14) and (2·15), the time development of the covariance matrix $\boldsymbol{b}=\{b_{ij}\}$, $(b_{ij}=\overline{x_i x_j})$ is given by[21]

$$\frac{d}{dt}\boldsymbol{b}(t)=\boldsymbol{d}-\boldsymbol{a}\boldsymbol{b}(t)-\boldsymbol{b}(t)\tilde{\boldsymbol{a}}, \tag{6·2}$$

where $\tilde{\boldsymbol{a}}$ is the transpose of $\boldsymbol{a}$;

$$\boldsymbol{a}=\begin{pmatrix}\boldsymbol{0} & -\boldsymbol{1}\\ \boldsymbol{\Phi} & \boldsymbol{\mathcal{R}}\end{pmatrix}, \quad \boldsymbol{d}=\begin{pmatrix}\boldsymbol{0} & \boldsymbol{0}\\ \boldsymbol{0} & \boldsymbol{\varepsilon}\end{pmatrix}. \tag{6·3}$$

Here $\boldsymbol{\Phi}$, $\boldsymbol{\mathcal{R}}$, $\boldsymbol{\varepsilon}$ are the $N\times N$ matrices whose (ij)-element is Φ_{ij},

$$\mathcal{R}_{ij}=\lambda(\delta_{i,1}+\delta_{i,N})\delta_{i,j}\,, \tag{6·4}$$

and $\varepsilon_{ij}=2kT_i\mathcal{R}_{ij}$, respectively.

In order to introduce dimensionless quantities we put

$$\begin{aligned}&\boldsymbol{\Phi}=\bar{\omega}^2\boldsymbol{G}, \quad \bar{\omega}^2=K/\langle m\rangle, \quad \boldsymbol{G}=\widetilde{\boldsymbol{G}},\\ &\boldsymbol{\mathcal{R}}=\lambda\boldsymbol{R},\\ &\boldsymbol{\varepsilon}=2kT\lambda(\boldsymbol{R}+\eta\boldsymbol{E}),\end{aligned} \tag{6·5}$$

where

$$T=(T_1+T_N)/2, \quad \eta=(T_1-T_N)/(2T), \tag{6·6}$$

and

$$E_{ij}=\delta_{i,j}(\delta_{i,1}-\delta_{i,N}).$$

Writing the $2N\times 2N$ covariance matrix $\boldsymbol{b}$ in the partitioned form

$$\boldsymbol{b}=\begin{pmatrix}\boldsymbol{x} & \boldsymbol{z}\\ \tilde{\boldsymbol{z}} & \boldsymbol{y}\end{pmatrix}, \tag{6·7}$$

and introducing $\boldsymbol{X}$, $\boldsymbol{Y}$ and $\boldsymbol{Z}$ by

$$\begin{aligned}&\boldsymbol{x}=(kT/\bar{\omega}^2)[\boldsymbol{G}^{-1}+\eta\boldsymbol{X}],\\ &\boldsymbol{y}=kT[\boldsymbol{1}+\eta\boldsymbol{Y}],\\ &\boldsymbol{z}=\lambda^{-1}kT\eta\boldsymbol{Z},\end{aligned} \tag{6·8}$$

one obtains from (6·2) the following equations in the stationary state.

$$\boldsymbol{X}=\widetilde{\boldsymbol{X}}, \quad \boldsymbol{Y}=\widetilde{\boldsymbol{Y}}, \quad \boldsymbol{Z}=-\widetilde{\boldsymbol{Z}}, \tag{6·9}$$

$$\boldsymbol{Y}=\boldsymbol{X}\boldsymbol{G}+\boldsymbol{Z}\boldsymbol{R}, \tag{6·10}$$

$$\tilde{\lambda}[2\boldsymbol{E}-\boldsymbol{Y}\boldsymbol{R}-\boldsymbol{R}\boldsymbol{Y}]=\boldsymbol{G}\boldsymbol{Z}-\boldsymbol{Z}\boldsymbol{G}. \tag{6·11}$$

The quantity $\tilde{\lambda}$ in (6·11) is $\tilde{\lambda}=\lambda^2/\bar{\omega}^2$. Now, our problem is to solve (6·9) $\sim$(6·11) for $\boldsymbol{Y}$ in the limit of $\tilde{\lambda}\to 0$.

Writing as

$$\boldsymbol{Z}=\boldsymbol{Z}^{(0)}+\tilde{\lambda}\boldsymbol{Z}^{(1)}, \tag{6·12}$$

and substituting it into (6·11), we find that the zeroth order term in $\tilde{\lambda}$ satisfies

$$\boldsymbol{G}\boldsymbol{Z}^{(0)}-\boldsymbol{Z}^{(0)}\boldsymbol{G}=0. \tag{6·13}$$

Let us take the representation in which $\boldsymbol{G}$ is diagonal:

$$\begin{aligned}&\boldsymbol{G}=\{G_{\mu\nu}\},\\ &G_{\mu\nu}=G_\mu\delta_{\mu,\nu}.\end{aligned} \tag{6·14}$$

Hereafter we use Greek letter for the suffix in this new representation and Latin letter for the former representation. Since $\boldsymbol{\Phi}$ is the dynamical matrix for the harmonic chain, μ, ν is the label of normal modes and

$$G_\mu=\omega_\mu^2\langle m\rangle/K,$$

where ω_μ is the normal frequency of the μ-th mode.

Using (6·14) in (6·13) we have

$$Z^{(0)}_{\mu\nu}=0 \qquad \text{for } \mu\neq\nu,$$

since there is no degeneracy in the normal frequency in our chain.*) By virtue of (6·9), the diagonal element of $\boldsymbol{Z}^{(0)}$ also vanishes, so that

$$\boldsymbol{Z}^{(0)}=\boldsymbol{0}.$$

Then, from (6·10), (6·9) and (6·5) we have up to the zeroth order

$$\boldsymbol{Y}=\boldsymbol{X}\boldsymbol{G}=\boldsymbol{G}\boldsymbol{X},$$

so that

$$X_{\mu\nu}=X_\mu\delta_{\mu,\nu}, \tag{6·15}$$

$$Y_{\mu\nu}=X_\mu G_\mu\delta_{\mu,\nu}. \tag{6·16}$$

Substituting (6·16) into (6·11) we have

$$2E_{\mu\nu}-(X_\mu G_\mu+X_\nu G_\nu)R_{\mu\nu}=(G_\mu-G_\nu)Z^{(1)}_{\mu\nu}, \tag{6·17}$$

from which we obtain

*) In our chain each atom is coupled only with its nearest neighbors, so that, the state ratio z_N is a function of ω and z_1, by (3·13). The boundary condition specifies the value of z_1 and z_N and thereby the normal frequency ω for given chain. This means, in turn, that z_1 is a (one-valued) function of ω. Since the atomic displacement u_n is uniquely determined by (2·2) by z_1 up to the multiplicative constant as a function ω, we have only one linearly independent solution for any ω.

$$X_\mu G_\mu = E_{\mu\mu}/R_{\mu\mu}\,, \tag{6·18}$$

$$Z^{(1)}_{\mu\nu} = (1-\delta_{\mu,\nu})\,[2E_{\mu\nu} - (E_{\mu\mu}/R_{\mu\mu} - E_{\nu\nu}/R_{\nu\nu})R_{\mu\nu}]\,/(G_\mu - G_\nu). \tag{6·19}$$

Noting that the matrix element of the transformation matrix which makes $\boldsymbol{G}$ diagonal is nothing but the normal coordinate $X_{\mu,n}$, we obtain from (6·16)

$$Y_{nm} = \sum_{\mu,\nu} x_{\mu,n} Y_{\mu\nu} x_{\nu,m} = \sum_{\mu} x_{\mu,n} x_{\mu,m} X_\mu G_\mu\,.$$

Here, $x_{\mu,n}$ satisfies:

$$\sum_{\mu} x_{\mu,n} x_{\mu,m} = \delta_{n,m} \quad \text{and} \quad \sum_{n} x_{\mu,n} x_{\nu,n} = \delta_{\mu,\nu}\,. \tag{6·20}$$

From (6·6) and (6·4) we get

$$E_{\mu\mu} = x^2_{\mu,1} - x^2_{\mu,N}\,, \quad R_{\mu\mu} = x^2_{\mu,1} + x^2_{\mu,N}\,,$$

so that by virtue of (6·18) we obtain

$$Y_{nm} = \sum_{\mu} \frac{x^2_{\mu,1} - x^2_{\mu,N}}{x^2_{\mu,1} + x^2_{\mu,N}} x_{\mu,n} x_{\mu,m}\,. \tag{6·21}$$

Therefore,

$$\begin{aligned}
\overline{\dot{u}_n^2} &= \frac{1}{m_n}\overline{x^2_{n+N}} \\
&= \frac{1}{m_n} y_{nn} \\
&= \frac{kT}{m_n}\left(1 + \frac{T_1 - T_N}{2T} Y_{nn}\right) \\
&= \frac{k}{m_n} \sum_{\mu} \frac{T_1 x^2_{\mu,1} + T_N x^2_{\mu,N}}{x^2_{\mu,1} + x^2_{\mu,N}} x^2_{n,\mu}\,.
\end{aligned} \tag{2·16}$$

Thus, Theorem 7 is proved.

In virtue of (2·16), (2·18) and (6·20) the energy current can be written as

$$Q = \lambda k \Delta T \sum_{\mu} \frac{x^2_{\mu,1} x^2_{\mu,N}}{x^2_{\mu,1} + x^2_{\mu,N}}\,. \tag{6·22}$$

Incidentally, it is to be noted that in the weak coupling limit of $\tilde{\lambda} \to 0$, by virtue of (6·18) and (6·19), other elements of the covariance matrix (6·7) can also be written down in terms of the normal coordinates and normal frequency.

Now, we estimate the value of Q using (6·22) and (2·13). We have shown in §5 that among N normal modes the low frequency modes the number of which is of the order of n_d are not well localized, whereas other modes are exponentially localized. We may thus assume that

$$x_{\mu,1}^2 \simeq x_{\mu,N}^2 \simeq \frac{1}{N} \quad \text{for } \mu < \bar{c}n_d\,,$$
$$x_{\mu,1}x_{\mu,N} \simeq o\left(\frac{1}{N}\right) \quad \text{for } \mu > \bar{c}n_d\,, \tag{6·23}$$

where $\bar{c}$ is the numerical factor of the order of magnitude of 1.

Therefore, we obtain

$$Q \simeq \lambda k \Delta T \left\{ \frac{\bar{c}n_d}{2N} + o\left(\frac{1}{N}\right) \right\}. \tag{6·24}$$

Substituting (5·3) into (6·24) we get for $N \gg 1$

$$Q \simeq \lambda k \Delta T \frac{2}{\pi} \bar{c} \frac{\langle m \rangle}{\sqrt{\langle (m - \langle m \rangle)^2 \rangle}} \frac{1}{\sqrt{N}}.$$

Finally, putting $c = (2/\pi)\bar{c}$, we obtain (2·20). Here, we note that only the low frequency modes the number of which is of the order of $\sqrt{N}$ contribute to the energy current.

As mentioned in §2, the theoretical expression (2·22) of the thermal conductivity agrees well with the result of the computer experiments as shown in Fig. 2. This also seems to support *a posteriori* the IF-assumption.

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References

1) H. Matsuda, T. Miyata and K. Ishii, *Proceedings of the International Conference on Statistical Mechanics, Kyoto 1968* [Suppl. to J. Phys. Soc. Japan **26** (1969), 40].
2) P. Dean, Proc. Roy. Soc. **254** (1960), 507.
3) J. Hori, *Spectral Properties of Disordered Chains and Lattices* (Pergamon Press, Oxford, 1968).
4) B. I. Halperin, Adv. in Chem. Phys. **13** (1967), 123.
5) E. H. Lieb and D. C. Mattis, *Mathematical Physics in One-Dimension* (Academic Press, New York, 1966), Chaps. 2 and 3.
6) H. Matsuda and K. Okada, Prog. Theor. Phys. **34** (1965), 539.
7) H. Matsuda and T. Miyata, Prog. Theor. Phys. Suppl. Extra Number (1968), 450.
8) J. Hori, Prog. Theor. Phys. Suppl. No. 46 (1970).
9) H. Matsuda, Prog. Theor. Phys. Suppl. No. 36 (1966), 97.
10) H. Matsuda and N. Ogita, Prog. Theor. Phys. **38** (1967), 81.
11) K. Okada and H. Matsuda, Prog. Theor. Phys. **39** (1968), 1153.
12) P. W. Anderson, Phys. Rev. **109** (1958), 1492.
13) N. F. Mott and W. D. Twose, Adv. in Phys. **10** (1961), 107.

14) R. Makinson and A. Roberts, Proc. Phys. Soc. **79** (1962), 222.
15) R. E. Borland, Proc. Roy. Soc. A**274** (1963), 529.
16) H. Furstenberg, Trans. Amer. Math. Soc. **108** (1963), 3.
17) H. B. Rosenstock and R. E. McGill, J. Math. Phys. **3** (1962), 200.
18) P. Dean and M. D. Bacon, Proc. Phys. Soc. **81** (1963), 642.
19) D. N. Payton, III and W. M. Visscher, Phys. Rev. **156** (1967), 1032.
20) D. N. Payton, III, M. Rich and W. M. Visscher, Phys. Rev. **160** (1967), 706.
21) Z. Rieder, J. L. Lebowitz and E. Lieb, J. Math. Phys. **8** (1967), 1073.
22) H. Nakazawa, Prog. Theor. Phys. **39** (1968), 236.
23) R. J. Rubin, J. Math. Phys. **9** (1968), 2252.
24) J. Hori, Prog. Theor. Phys. Suppl. No. 46 (1970).
25) R. J. Rubin, J. Math. Phys. **11** (1970), 1857.
26) J. M. Ziman, J. Phys. (London) **C2** (1968), 1532.
27) K. R. Allen and J. Ford, Phys. Rev. **176** (1968), 1046
28) E. J. Woll, Jr., Phys. Rev. **137** (1965), A95.