Heat conduction and sound transmission in isotopically disordered harmonic crystals*

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We investigate some kinetic properties of an isotopically disordered harmonic crystal. We prove rigorously that for almost all disordered chains the transmission coefficient of a plane wave with frequency ω, $t_N(\omega)$, decays exponentially in N, the length of the disordered chain, with the decay constant proportional to ω^2 for small ω. The response of this system to an incident wave is related to the nature of the heat flux $J(N)$ in a disordered chain of length N placed between heat reservoirs whose temperatures differ by $\Delta T > 0$. We clarify the relationship between the works of various authors in the heat conduction problem and establish that for all models $J(N) \to 0$ as $N \to \infty$ in a disordered system. The exact asymptotic dependence of $J(N)$ on N eludes us, however. We also investigate the heat flow in a simple stochastic model for which Fourier's law is shown to hold. Similar results are proven for two-dimensional systems disordered in one direction.

1. INTRODUCTION

There does not exist at the present time any dynamical system for which kinetic laws can be proven to hold. A kinetic law relates fluxes to gradients, e. g., Fourier's law of heat conduction. Indeed the two "standard models" of equilibrium statistical mechanics, that of the noninteracting gas for an ideal fluid and the perfect harmonic crystal for the ideal solid do not obey any macroscopic kinetic laws. The next dynamical model, in order of complexity, is the isotopically disordered harmonic system where the masses of the individual particles are independent identically distributed random variables. This paper studies the transport properties of such a system, particularly those of the disordered harmonic chain: We give new rigorous proofs of some already known (or conjectured) results and derive a few new ones.

We consider a disordered chain in which left and right end particles are coupled by some mechanism to heat baths at different temperatures; call them T_L and T_R, $T_L - T_R = \Delta T$. Using some description of the coupling to the heat baths,[1] we can compute the steady state energy flow across the chain. If $J(N)$ is the flow across a particular chain of length N and $\langle J(N) \rangle$ the average of $J(N)$ over the different choices of the N masses we identify $N^{-1} \Delta T$ as the "temperature gradient" across the chain and define the average conductivity of chains with length N by $K(N) = \langle J(N) \rangle / (\Delta T / N)$. Fourier's law will hold if $K(N) \to K$ as $N \to \infty$ with K a finite, strictly positive, constant. Fourier's law certainly fails for periodic systems. In these $J(N)$ tends to a nonzero constant as N increases, i. e., $K(N)$ grows linearly with N. This was proven for the homogeneous chain in[1] and for the general periodic chain in.[2] The behavior of $J(N)$ does not depend on the dimensionality of the system: Hellemann[3] investigated two-dimensional homogeneous cylindrical systems with general couplings and found the same behavior for $J(N)$ (see also Nakazawa[4]). For truly disordered chains the situation is entirely different. Here Casher and Lebowitz[2] proved that $J(N) \to 0$ as $N \to \infty$ for almost every random chain (almost all is defined here with respect to the probability measure on the chains constructed from the individual distribution of each mass). Ideally we would like to decide if $\lim_{N \to \infty} K(N)$ is finite, zero, or infinite. Regretably we still cannot do this in a definite way. Some heuristic

arguments suggest[5] that for the linear chain $K(N)$ decreases as $N^{-1/2}$. This, if true, implies that the random chain is an even poorer heat conductor than a real system and would presumably be a peculiarity related to the chain being one-dimensional. We would then have to look at two- and three-dimensional random harmonic systems to obtain models in which Fourier's law holds.

Intuitively, we picture the heat baths exciting the ends of the chain and setting up vibrations which travel along the chain. These vibrations are linear combinations of the chain's normal modes. The energy flow therefore depends on the fraction of normal modes which have significant amplitudes at both ends of the chain. We could say that a normal mode which has significant amplitude at both ends is an efficient heat carrier. In periodic systems (i. e., m_i is periodic in i) nearly every mode is efficient and so that heat flow $J(N)$ through a periodic chain of length N approaches a nonzero limit with increasing chain length. In a disordered system on the other hand nearly every mode is "localized" and so relatively few are efficient heat conductors. This leads to $J(N) \to 0$ as $N \to \infty$ for these systems.

The difference between the normal modes in periodic and disordered systems is reflected in the spectrum of the corresponding infinite chains and the character of plane wave solutions to the lattice equations of motion [a plane wave solution is one of the type $\mathbf{u}(t) = \mathbf{u}(0)e^{i\omega t}$]. In a periodic chain the frequency spectrum consists of allowed bands separated by gaps. The bands are actually the spectrum of an infinite-dimensional self-adjoint matrix operator. The spectrum of this operator is absolutely continuous. At allowed frequencies the plane wave solutions are bounded periodic functions on the chain. For frequencies in the band gaps the plane wave solutions grow or decrease exponentially. In a disordered chain the corresponding spectrum is more complicated. For almost all chains the corresponding infinite matrix operator does not have any absolutely continuous spectrum.[2] Indeed for every frequency $\omega > 0$ the plane wave solutions of the equations of motion of the semiinfinite chain (1-2) grow exponentially for almost all chains. Borland[6] was the first to appreciate this exponential growth (he used it to explain the frequent occurence of localized modes in random systems). A rigorous proof of the existence of exponentially

growing solutions for infinite chains was, however, only obtained when Matsuda and Ishii[5] proved that the powerful results of Furstenberg[7] apply to this system.

The harmonic chain

We will now specify more precisely the dynamical system with which we are primarily concerned here. The harmonic chain is a one-dimensional system of particles coupled together by harmonic springs. The force between two adjacent particles is proportional to the change in the length of the connecting spring: When both particles are in their equilibrium position this force is zero. At the nth site there is a particle with mass m_n whose displacement from its equilibrium position at time t is $u_n(t)$. The center of mass movement of a finite chain of length N can be removed by constraining the first and last particles by additional harmonic forces. The Hamiltonian for the system with the spring constant set equal to one, is then

$$H = \sum_{n=1}^{N} \tfrac{1}{2} m_n \dot{u}_n^2 + \sum_{n=1}^{N-1} \tfrac{1}{2}(u_n - u_{n+1})^2 + \tfrac{1}{2} u_1^2 + \tfrac{1}{2} u_N^2. \qquad (1.1)$$

This is often described as a chain with fixed boundary conditions because it is also obtained by considering a chain beginning with a particle labelled 0 and ending with one labelled $N+1$ and demanding that $u_0 = u_{N+1} \equiv 0$. The equation of motion for the chain is

$$M_N \ddot{u}(t) + \Phi_N u(t) = 0. \qquad (1.2)$$

$u(t)$ is the column vector $[u_1(t), \ldots, u_N(t)]$, M_N is the diagonal matrix with entries $m_1 \cdots m_N$. Φ_N is the $N \times N$ tridiagonal matrix with entries $(\Phi_N)_{ii} = 2$, $(\Phi_N)_{ij} = -1$ for $|i-j| = 1$ and $(\Phi_N)_{ij} = 0$ otherwise.

This harmonic chain has N normal modes, i.e., solutions of the form $u(t) = u(0) e^{i\omega t}$. Any solution of (1.2) with specified initial conditions is a linear combination of these solutions. For a normal mode (1.2) becomes

$$M_N \omega^2 u(0) = \Phi_N u(0)$$

or

$$\omega^2 (M_N^{1/2} u(0)) = M_N^{-1/2} \Phi_N (M_N^{-1/2} M_N^{1/2} u(0)) \qquad (1.3)$$

The normal mode frequencies are thus (determined by) the eigenvalues of the symmetric matrix $H_N = M_N^{-1/2} \Phi_N M_N^{-1/2}$.

These ideas extend to a semiinfinite (or infinite) harmonic chain. Again m_n and u_n are the mass of the nth particle and its displacement from its equilibrium position; n runs from 1 (or $-\infty$) to ∞. We will assume that all m_i are bounded above and below. The equations of motion for the semiinfinite chain are

$$m_n \ddot{u}_n + 2u_n - u_{n-1} - u_{n+1} = 0 \quad (n > 1), \qquad (1.4)$$

$$m_1 \ddot{u}_1 + 2u_1 - u_2 = 0.$$

The energy

$$E(t) = \sum_{n=1}^{\infty} \tfrac{1}{2} m_n \dot{u}_n^2 + \sum_{n=1}^{\infty} \tfrac{1}{2}(u_n - u_{n+1})^2 + \tfrac{1}{2} u_1^2$$

is a conserved quantity and so the set of solutions to (1.4) with finite initial energy span a Hilbert space h whose norm is just the energy functional. For these

solutions (1.4) can be written

$$M \ddot{u}(t) + \Phi u(t) = 0. \qquad (1.5)$$

Φ is the bounded self-adjoint tridiagonal matrix operator on h with entries $\Phi_{ii} = 2$, $\Phi_{ij} = -1$ if $|i-j| = 1$ and $\Phi_{ij} = 0$ otherwise. M is the infinite diagonal matrix with entries m_i. It is a bounded operator on h. The "allowed" frequencies ω^2 are points in the spectrum of the symmetric operator $H = M^{-1/2} \Phi M^{-1/2}$ with $\|H\| \leq 4/\bar{m}$, $\bar{m} = \min_i \{m_i\}$.

Models of stationary heat flow

In this paper we are interested primarily in the behavior of the thermal conductivity of a random harmonic crystal. Since we are interested in a stationary flow we need to have our system coupled at its ends (left and right) to some kind of inexhaustible heat reservoirs which are maintained at temperatures T_L and T_R so that energy will flow steadily across the system from left to right due to the temperature difference $T_L - T_R = \Delta T > 0$.

In this note we use two models for the heat bath and its coupling to the chain. These were developed by Lebowitz et al.[1,2] and by Rubin and Greer.[8] In Lebowitz's model the heat bath is a Maxwellian gas of very light molecules. These gas molecules collide with the end particles of the chain. At each collision the momentum of the end particle is altered in a discontinuous way. Using the Maxwell—Boltzmann distribution for the velocities of the gas particles prior to a collision we can compute the probability per unit of time that the momentum of an end (chain) particle will jump from p to p'. This will depend on the gas temperature and the frequency of these collisions. The frequency is incorporated into a constant λ measuring the coupling between the particle and the heat bath. Finally we get a modified Liouville equation for the Gibbs ensemble density $\mu(u_1 \ldots u_N, p_1 \ldots p_N, t)$ of the system,[1,2] $(p_i = m_i \dot{u}_i)$,

$$\frac{\partial \mu}{\partial t} = \sum_{i,j=1}^{2N} \left[\frac{\partial}{\partial x_i} (a_{ij} x_j \mu) + \tfrac{1}{2} d_{ij} \left(\frac{\partial^2 \mu}{\partial x_i \partial x_j} \right) \right]. \qquad (1.6)$$

$x = (x_1, \ldots x_{2N}) = (u_1 \ldots u_N, p_1 \ldots p_N)$ and a_{ij} and d_{ij} are entries in the $2N \times 2N$ matrix

$$a = \begin{pmatrix} 0 & -M_N^{-1} \\ \Phi_N & L \end{pmatrix}, \qquad d = \begin{pmatrix} 0 & 0 \\ 0 & 2M_N L T \end{pmatrix}.$$

L and T are diagonal $N \times N$ matrices with entries

$$L_{ii} = \lambda(\delta_{i1} + \delta_{iN}).$$

$$T_{ii} = T_L \delta_{i1} + T_R \delta_{iN}.$$

λ represents the coupling of the baths to the system ($\lambda \geq 0$). When $\lambda = 0$ the system is isolated and follows the equations of motion given in (1.2). The solution of Liouville's equation (1.6) with $\lambda = 0$ has the form

$$\mu[x_1 \cdots x_{2N}; t] = \mu[x_1(-t) \cdots x_{2N}(-t); 0]$$

where $x_i(t)$ is the solution of (1.2) with initial values $x_1 \cdots x_{2N}$. In this case μ will not approach any stationary state. For $\lambda > 0$, however, any initial distribution ap-

proaches a unique stationary distribution which is a generalized Gaussian. The expected value of the heat flow across the system in the stationary state, for a specified set of masses $\{m_i\}$, is[2]

$$J(N) = \pi^{-1}(T_L - T_R)\lambda^2 m_1 m_N \int_{-\infty}^{\infty} \omega^2 \, |Z(\omega)_{1N}^{-1}|^2 \, d\omega$$

$$= \pi^{-1}(T_L - T_R)\lambda^2 m_1 m_N \int_{-\infty}^{\infty} \omega^2 j_N(\omega) \, d\omega. \qquad (1.7)$$

Here $Z(\omega)$ is the $N \times N$ matrix $\Phi_N - \omega^2 M_N - i\omega M_N L$ and

$$j_N(\omega)$$
$$= \{2m_1 m_N \lambda^2 \omega^2 + K_{1,N}^2 + \lambda^2 \omega^2 (m_N^2 K_{1,N-1}^2 + m_1^2 K_{2,N}^2)$$
$$+ \lambda^4 \omega^4 m_1^2 m_N^2 K_{2,N-1}^2\}^{-1}. \qquad (1.8)$$

$K_{ij}(\omega^2)$ is the determinant of the submatrix of $\Phi - \omega^2 M$ beginning with the ith row and column and ending at the jth row and column.

Rubin and Greer's model[8] is rather different. In it the chain of N particles (which constitutes the system) is connected at either end to semiinfinite chains of identical particles. Initially the left-and right-hand chains are in thermal equilibrium at temperatures T_L and T_R, respectively. We can follow the time developement of the infinite system from a specified initial state and at any later time we can compute such quantities as the local temperature or energy flow. More interestingly we can find their average values over the ensemble of initial states and then calculate the steady state value approached as $t \to \infty$, of these averaged quantities. In the next section we give a simpler rederivation of Rubin's result relating the stationary heat flow $\hat{J}(N)$ in his model to the integral of the square of the transmission coefficient $t_N^2(\omega)$. This uses a method introduced by Ford, Kac, and Mazur.[9] Our approach is quite similar to that of Casher and Lebowitz.[2]

In Sec. 3 we use Furstenberg's theorem to prove rigorously an earlier result of Rubin, based on an explicit but not entirely rigorous computation that, in a chain with random masses, $N^{-1} \lim |t_N(\omega)| \to -\gamma(\omega)$ as $N \to \infty$, with $\gamma(\omega) > 0$ for $\omega \neq 0$. It follows from this that $\hat{J}(N)$ like $J(N) \to 0$ as $N \to \infty$ for almost all random chains. We also show that $\gamma(\omega)$ is a continuous function of ω for small ω and $\gamma(\omega)/\omega^2 \to$ const for $\omega \to 0$. The latter result was proven earlier by Matsuda and Ishii[5] using a perturbation expansion.

In Sec. 4 we use the Casher–Lebowitz expression for the heat flux, $J(N)$ to derive an explicit expression for the nonvanishing heat flow in an infinite periodic diatomic chain and in a uniform chain containing a single impurity. We then, in Sec. 5, derive rigorously an expression for the weak coupling limit of the heat flux $J(N, \lambda)$ where λ is the coupling to the heat reservoirs, i.e., we compute $\lim_{\lambda \to 0} \lambda^{-1} J(N, \lambda)$ and find it in agreement with the perturbation result of Matsuda and Ishii.[5] We note however that the interchange of the limits $\lambda \to 0$ and $N \to \infty$ should not be expected to be valid when the heat flow vanishes as $N \to \infty$. This is shown explicitly in Sec. 6 where we construct a nondynamical model which obeys Fourier's law of heat conduction.

Section 7 discusses the generalization of the Rubin formalism to a two-dimensional harmonic square lattice in which the masses in each column are the same and the heat flow is along the x-axis. We find, as ex-

pected,[2] that when the system is periodic the heat flux per unit cross-sectional area does not vanish when the length of the system becomes infinite. When the masses in the different columns are random, then the analog of the Casher–Lebowitz argument for chains, based on the Furstenberg theorem, shows that the flux vanishes. The difference between the two flows is, as in the case of chains, a reflection of the difference between the spectral measure of periodic and random harmonic systems and, in Sec. 8, we give an explicit proof that the spectrum of a simple harmonic chain is absolutely continuous.[2]

Finally in Sec. 9 we discuss briefly the relation between the heat flow in Rubin's and Lebowitz's model. We also discuss there what strengthening of the Furstenberg theorem is needed for obtaining the asymptotic N-dependence of $J(N)$ or $\hat{J}(N)$. Appendices A–C contain some technical details.

2. THE HEAT FLOW IN RUBIN'S MODEL

The first step is to look at a finite analog of the infinite chain. Particles of unit mass are placed at sites $-S$ to 0, from sites 1 to N particles of random mass and from sites $N+1$ to $N+S+2$ particles of unit mass are placed. The random masses are assumed for simplicity to be all greater than one and are identically distributed, independent random variables. At $t=0$ we know the position and momenta of every particle in the chain. The left-hand segment of unit masses is just a chain driven by an external force u_1. Explicitly

$$\ddot{\eta}(t) + \Omega^2 \eta(t) = g(t), \qquad (2.1)$$

where

$$\eta(t) = (u_0, u_{-1}, \ldots, u_{-S}), \quad \Omega^2 = \Phi_{S+1},$$

$$g(t) = (u_1(t), 0, \ldots, 0).$$

Ω^2 has the spectral representation

$$\Omega^2 = \sum_{a=1}^{S+1} \omega_a^2 \, |\xi_a\rangle \langle \xi_a| \qquad (2.2)$$

where

$$\omega_a^2 = 4 \sin^2\left(\frac{a\pi}{S+2}\right) \quad \text{and} \quad \xi_a(j) = \left(\frac{2}{S+2}\right)^{1/2} \sin\left(\frac{ja\pi}{S+2}\right),$$

$$1 \leq j \leq S+1.$$

If

$$\eta(0) = \sum_{a=1}^{S+1} b_a \, \xi_a,$$
$$\dot{\eta}(0) = \sum_{a=1}^{S+1} v_a \, \xi_a, \qquad (2.3)$$

then as is known

$$u_0(t) = g_1(t) + \int_0^t A_S(t-s) u_1(s) \, ds, \qquad (2.4)$$

where

$$g_1(t) = \sum_a [(\cos \omega_a t) b_a + \omega_a^{-1}(\sin \omega_a t) v_a] \xi_a(1),$$

$$A_a(t) = \sum_a \omega_a^{-1}(\sin \omega_a t) \xi_a^2(1). \qquad (2.5)$$

The initial energy of the particles $-S, \ldots, 0$ is $\frac{1}{2}\sum_a (v_a^2 + \omega_a^2 b_a^2)$. The b_a and v_a have a Boltzmann (Gaussian) distribution at temperature T_L and so we can compute the statistical properties of g. When $S \to \infty$

$$u_0(t) = g_1(t) + \int_0^t A(t-s) u_1(s) \, ds, \qquad (2.6)$$

$$A(t) = (2/\pi) \int_0^\pi \omega^{-1}(k) \, (\sin^2 k) \, \sin[t\,\omega(k)] \, dk, \qquad (2.7)$$

$$\omega(k) = 2 \sin(k/2),$$

$$\langle g_1(t) \rangle = 0,$$

$$\langle g_1(t) g_1(t+s) \rangle = (T_L/\pi) \int_0^\pi \omega^{-2}(k) \, (\sin^2 k) \cos[\omega(k)s] dk, \qquad (2.8)$$

where we have set Boltzmann's constant equal to one. Similarly,

$$u_{N+1}(t) = g_N(t) + \int_0^\infty A(t-s) u_N(s) \, ds. \qquad (2.9)$$

g_N has identical properties to g_1 when T_R replaces T_L.

Here $g_1(t)$ and $g_N(t)$ are to be interpreted as "independent Gaussian random variables" with mean zero and covariances given by (2.8) for g_1 and a corresponding expression with T_R replacing T_L for g_N. We set $\mathbf{g} = (g_1, 0, \ldots, g_N)$.

Using (2.6) and (2.9) we have a closed set of equations for the particles 1 to N:

$$m_1 \ddot{u}_1 + 2u_1 - u_2 = u_0 = g_1 + A * u_1,$$

$$m_2 \ddot{u}_2 + 2u_2 - u_3 - u_1 = 0$$

$$\cdot$$
$$\cdot$$
$$\cdot$$

$$m_{N-1} \ddot{u}_{N-1} + 2u_{N-1} - u_{N-2} - u_N = 0,$$

$$m_N \ddot{u}_N + 2u_N - u_{N-1} = u_{N+1} = g_N + A * u_N. \qquad (2.10)$$

The same set of equations was obtained by Magalinskii.[10]

In the Fourier representation (2.10) takes the form

$$[\Phi_N - M_N \omega^2 - A(\omega) U_N] \, \mathbf{u}(\omega) = \mathbf{g}(\omega) \qquad (2.11)$$

where U_N is the N by N diagonal matrix with entries $(U_N)_{ii} = (\delta_{i1} + \delta_{iN})$. In Appendix A we show that the $N \times N$ matrix $Y_N(\omega) = \Phi_N - M_N \omega^2 - A(\omega) U_N$ is nonsingular for all real values of ω except $\omega^2 = 0$ and 4. These singularities are integrable. We specify that $\mathbf{u}(t)$ and $\mathbf{g}(t)$ vanish when $t < 0$. It is important that we include this carefully in the calculation. $\mathbf{u}(t)$ is the sum of a particular solution of the inhomogeneous equation (2.10) and a general solution of the homogeneous equation which matches the initial values of $\mathbf{u}$ and $\dot{\mathbf{u}}$. In Appendix B we show that the general solution decays at least as fast as $t^{-1/2}$. This represents the diffusion of energy into the chain and so initial data on the N particles does not contribute to the steady state heat flow. A solution of the inhomogeneous equation is

$$\mathbf{u}(t) = (2\pi)^{-1} \int_{-\infty}^\infty \exp(i\omega t) \, Y_N(\omega)^{-1} \, \mathbf{g}(\omega) \, d\omega. \qquad (2.12)$$

The value of $A(\omega)$ and the statistical properties of $\mathbf{g}(\omega)$ are easily computed as continuations of the associated Laplace transforms. We obtain

$$A(\omega) = \tfrac{1}{2}[2 - \omega^2 - i\omega(4 - \omega^2)^{1/2}]$$

$$\langle \mathbf{g}(\omega) \rangle = 0,$$

$$\langle g_i(\omega) g_j(\sigma) \rangle = (T_L \delta_{i1} + T_R \delta_{iN}) \, \delta_{ij} \, [\bar{g}(\omega) + \bar{g}(\sigma)] \, \hat{\theta}(\sigma + \omega),$$

$$\bar{g}(\omega) = \tfrac{1}{2}[(4 - \omega^2)^{1/2} - i\omega],$$

$$\hat{\theta}(\omega) = \lim_{\epsilon \to 0_+} (\epsilon + i\omega)^{-1}. \qquad (2.13)$$

We choose the branch of $z^{1/2}$ which is cut from 0 to ∞ along the positive real axis. For later use we note that when ω is real

$$A(\omega) - A(-\omega) = -i\omega (4 - \omega^2)_+^{1/2}, \quad |\omega| < 2,$$

$$A(\omega) - A(-\omega) = 0, \qquad |\omega| \geq 2,$$

$$\bar{g}(\omega) + \bar{g}(-\omega) = (4 - \omega^2)_+^{1/2}, \quad |\omega| < 2,$$

$$\bar{g}(\omega) + \bar{g}(-\omega) = 0, \qquad |\omega| \geq 2,$$

$$(2.14)$$

where $(x)_+^{1/2}$ is the positive square root of $x \geq 0$.

We can now compute the average heat flow past particle 1 at time t:

$$\hat{J}(N, t) = \langle \dot{u}_1(u_1 - u_0) \rangle$$
$$= \langle \dot{u}_1(u_1 - g_1 - A * u_1) \rangle \qquad (2.15)$$

Substituting from (2.12) and using (2.13) and (2.14) gives the following expression for the stationary heat flux in Rubin's model,

$$\hat{J}(N) \equiv \lim_{t \to \infty} \hat{J}(N, t) = \pi \, (T_L - T_R) \int_0^2 \omega^2 \, (4 - \omega^2) \, |\Delta_N(\omega)|^{-2} \, d\omega, \qquad (2.16)$$

$$\Delta_N(\omega) = \det[Y_N(\omega)].$$

In deriving this we use the result

$$\lim_{t \to \infty} \lim_{\epsilon \to 0_+} \int_{-\infty}^\infty \exp[i(\omega + \sigma)t] \, [\epsilon + i(\omega + \sigma)]^{-1} \, f(\sigma) \, d\sigma = \pi f(-\omega) \qquad (2.17)$$

when f is a continuous, integrable function.

It is interesting to note that only the frequencies in the allowed band of the infinite chain which, because we considered only heavy impurities, contains all the characteristic frequencies of the finite chain, contribute to $\hat{J}(N)$. Any solution $\mathbf{u}(t)$ which vanishes when $t < 0$ must contain contributions from almost all real frequencies [because $\mathbf{u}(\omega)$ is a nonzero analytic function in the lower half plane and so its boundary values $\mathbf{u}(\omega)$ can only vanish on a set of measure zero]. As time increases however the contribution from frequencies outside the allowed band falls to zero.

We can relate $\hat{J}(N)$ to the transmission coefficients of the segment $1, \ldots, N$ for plane waves with frequencies from 0 to 2. To calculate the transmission coefficient of an incoming plane wave with frequency ω we only need to find a solution of the equations of motion which to the right of the segment $1, \ldots, N$ is a combination of an incoming and a reflected wave and to the left is a pure outgoing wave, i.e.,

$$u_j(t) = D \, \exp[-i(\omega t + kj)] + R \exp[-i(\omega t - kj)], \quad j \geq N,$$

$$u_j(t) = \exp[-i(\omega t + kj)], \qquad j \leq 0, \qquad (2.18)$$

$$\omega = \omega(k) = 2 \sin(k/2).$$

Clearly $|D|^{-1}$ is the transmission coefficient $t_N(\omega)$ and the argument of D^{-1} is the phase shift of the plane wave. Also R/D is the reflection coefficient with $|R/D|^2 = 1 - t_N^2$. Using the transfer matrix approach, we find

$$\begin{bmatrix} u_{N+1} \\ u_N \end{bmatrix} = \begin{bmatrix} \exp[-ik(N+1)] & \exp[+ik(N+1)] \\ \exp(-ikN) & \exp(+ikN) \end{bmatrix} \begin{bmatrix} D \\ R \end{bmatrix}$$

$$= T_N T_1 \ldots T_0 \begin{pmatrix} u_0 \\ u_1 \end{pmatrix}, \qquad (2.19)$$

$$\begin{bmatrix} u_0 \\ u_{-1} \end{bmatrix} = \begin{bmatrix} 1 \\ \exp(+ik) \end{bmatrix}$$

where T_j is the "transfer matrix,"

$$T_j = \begin{bmatrix} 2 - m_j \omega^2 & -1 \\ 1 & 0 \end{bmatrix}. \qquad (2.20)$$

We find that

$$|D(k)|^{-1} = |2\sin k| \; |K_{1,N} - \exp(-ik)(K_{2,N} + K_{1,N-1})$$
$$+ \exp(-2ik)K_{2,N-1}|^{-1}$$
$$= t_N(\omega), \qquad (2.21)$$

where $K_{i,j}(\omega^2)$ is defined in (1.8).

The expression for $t_N(\omega)$ is related simply to $\Delta_N(\omega)$ in (2.16),

$$\Delta_N(\omega) = K_{1,N} - \exp(-ik)(K_{2,N} + K_{1,N-1}) + \exp(-2ik)K_{2,N-1}. \qquad (2.22)$$

The final result is then

$$\hat{J}(N) = (4\pi)^{-1}(T_L - T_R)\int_0^2 d\omega \, t_N^2(\omega). \qquad (2.23)$$

This agrees with the result of Rubin and Greer. [8]

For periodic chains $t_N(\omega)$ approaches, as $N \to \infty$, a finite value different from zero for ω in the spectrum of this chain. This spectrum consists of bands in the interval $\omega \in [0, 2]$. For ω not in the spectrum $t_N(\omega)$ vanishes as $\exp[-N\delta(\omega)]$, where $\delta(\omega) = (\omega - \omega_0)^2$ and ω_0 is band edge nearest ω. Indeed, for $m_i = 1$, for all i, $t_N(\omega) = 1$. Thus $\hat{J}(N)$ will approach a finite positive value as $N \to \infty$ in periodic chains. The situation is quite different in random chains where, as will be shown in the next section, $t_N(\omega)$ goes to zero, exponentially in N for almost all chains.

3. GROWTH OF SOLUTIONS TO THE LATTICE EQUATIONS

We consider a semiinfinite chain with masses m_i, $i \geq 1$. A plane wave solution with frequency ω satisfies the equation [cf (1.3)–(1.5)]

$$(2 - m_N \omega^2)u_N = u_{N+1} + u_{N-1}. \qquad (3.1)$$

This is more conveniently written in the transfer matrix notation

$$\begin{bmatrix} u_{N+1} \\ u_N \end{bmatrix} = \begin{bmatrix} 2 - m_N \omega^2 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} u_N \\ u_{N-1} \end{bmatrix}$$
$$= T_N(\omega) \begin{bmatrix} u_N \\ u_{N-1} \end{bmatrix}. \qquad (3.2)$$

T_N is in the matrix group $SL(2, R)$. In disordered chains the sequence $\{u_N(\omega)\}$ grows exponentially with N for almost every sequence of masses and almost all initial values of u_0 and u_1. This was first proven by Matsuda and Ishii[5] using a theorem of Furstenberg.[7] Here a brief summary of the theorem and its application is given.

We see from (3.2) that the asymptotic behavior of $u_N(\omega)$ is determined by the behavior of products of the transfer matrices T_j associated with the chain.

Furstenberg's theorem deals with products of matrices in the groups $SL(m, R)$ when the matrices themselves are random variables.

Theorem (Furstenberg,[7] Theorem 8.5): Suppose that G is a subgroup of $SL(m, R)$ such that

(i) G is not compact;

(ii) no subgroup of G with finite index in G is reducible;

(iii) there is a probability measure μ on G.

Then for almost all sequences $\{g_N : N \geq 1\}$ chosen from G we have

$$\lim_{N \to \infty} \frac{1}{N} \log \|g_N \cdots g_1 u\| = \gamma > 0 \qquad (3.3)$$

for any nonzero vector u in R^N.

Remark: A real analytic group G is reducible if it has a faithful finite-dimensional continuous representation and if every finite-dimensional continuous representation of G is semisimple, i.e., if G has a representation as linear transformations on a finite-dimensional vector space V the only subspaces of V which are invariant under the action of G are $\{0\}$ and V itself. In our case G is a subgroup of $SL(2, R)$ and so there is always a faithful representation as matrices acting on R^2. The remaining condition must be checked explicitly. γ can be explicitly calculated in terms of certain measures on the projective space P^{m-1}. These measures are determined by μ and the induced action of G on P^{m-1}. In the statement of this theorem almost all is meant in the sense of the standard measure on the product of a countable number of copies of G which can be obtained from the basic measure μ on G.

Matsuda and Ishii have proven the following result. Their argument has been greatly simplified by Yoshioka.[11]

Theorem (Matsuda and Ishii, Theorem 1): If there are at least two different masses present, the subgroup of $SL(2, R)$ generated by the transfer matrices $\left(\begin{smallmatrix} 2-m_1\omega^2 & -1 \\ 1 & 0 \end{smallmatrix}\right)$ obeys conditions (i) and (ii) (for $\omega^2 > 0$).

The mass m is a random variable with probability distribution $dp(\cdot)$ and the measure μ on the subgroup is determined by $dp(\cdot)$. The corresponding γ is written as $\gamma(\omega)$ and by (3.3) $\gamma(\omega) > 0$ for $\omega \neq 0$. $\gamma(\omega)$ can be calculated from the following equations, when ω^2 is small, i.e., η defined in (3.4b) is real,[5]

$$\gamma(\omega) = \int_{-\pi/2}^{\pi/2} \log \left| \frac{\cos(\theta + \eta)}{\cos\theta} \right| dG(\theta), \qquad (3.4a)$$

where

$$2\cos\eta = 2 - \langle m \rangle \omega^2,$$
$$\langle m \rangle = \int_0^\infty m \, dp(m). \qquad (3.4b)$$

$dG(\cdot)$ is a probability measure on $(-\frac{1}{2}\pi, \frac{1}{2}\pi)$ which satisfies

$$G(A) = \int_0^\infty G[\Psi(A,m)]\,dp(m) \qquad (3.5)$$

for every measurable set A in $(-\frac{1}{2}\pi, \frac{1}{2}\pi)$. Here $\Psi(A,m) = \{\Psi(\theta,m) : \theta \in A\}$ and

$$\tan[\Psi(\theta,m) + \eta] = \tan\theta - 2\left[\frac{m - \langle m\rangle}{\langle m\rangle}\right]\tan\frac{\eta}{2}. \qquad (3.6)$$

The integral in (3.4) is absolutely convergent and can be shown to be independent of the particular measure dG used, provided that $dG(\cdot)$ obeys (3.5). These are Eqs. (3.14) and (3.15) in Ref. 5.

We now give a nonperturbative proof of Theorem 2 in Ref. 5. This deals with the low frequency behavior of $\gamma(\omega)$.

Theorem: For small values of ω, $\gamma(\omega)$ is continuous in ω and

$$\lim_{\omega \to 0_+} \frac{\gamma(\omega)}{\omega^2} = \frac{1}{8}\frac{\langle m^2\rangle - \langle m\rangle^2}{\langle m\rangle}.$$

Proof: We always choose ω so small that η is real. Then the stationary measures $dG(\theta,\eta)$ (explicitly showing the dependence on η) can be chosen to depend continuously on η (see Lemmas 1.2, 2.2, and 2.3 in Ref. 7). Then because the integral defining $\gamma(\omega)$ converges absolutely we can write $\gamma(\omega)$ as the sum of terms similar to

$$A(\omega) = \int_0^{1/2\pi - \epsilon} \log|\cos\theta|\,dG(\theta,\eta) + a(\epsilon,\eta),$$
$$a(\epsilon,\eta) = \lim_{\delta \to 0_+}\int_{1/2\pi - \epsilon}^{1/2\pi - \delta}\log|\cos\theta|\,dG(\theta,\eta) \qquad (3.7)$$

and absolute convergence also means that $\lim_{\epsilon\to 0_+} a(\epsilon,\eta) = 0$. So by choosing η and η' (corresponding to ω and ω') sufficiently close together and also choosing ϵ small enough, we can make $A(\omega) - A(\omega')$ arbitrarily small. Consequently, $\gamma(\omega)$ is a continuous function of ω.

$$2\gamma(\omega) = \int_{-\pi/2}^{\pi/2}\log\left(\frac{\cos^2(\theta + \eta)}{\cos^2\theta}\right)dG(\theta,\eta)$$
$$= \int_{-\pi/2}^{\pi/2}\log\cos^2[\Psi(\theta,m) + \eta]\,dG[\Psi(\theta,m),\eta]$$
$$= \int_{-\pi/2}^{\pi/2}\log\cos^2\theta\,dG(\theta,\eta). \qquad (3.8)$$

$\Psi(\theta,m)$ can be calculated from (3.6) to second order in η. Using this gives

$$\log\cos^2[\Psi(\theta,m) + \eta] = \log\cos^2\theta - a\sin 2\theta + a^2 f(\theta) + O(a^3),$$
$$f(\theta) = -\sin\theta\cos^3\theta. \qquad (3.9)$$
$$a = 2\left(\frac{m - \langle m\rangle}{\langle m\rangle}\right)\tan(\tfrac{1}{2}\eta).$$

Since $\gamma(\omega)$ is independent of m, (3.8) is not changed if we integrate it over $dp(m)$. We obtain

$$2\gamma(\omega) = \int_0^\infty dp(m)\int_{-\pi/2}^{\pi/2} - a\sin^2\Phi(\theta,m)\,dG(\theta,\eta)$$
$$+ \int_0^\infty dp(m)\int_{-\pi/2}^{\pi/2} a^2 f[\Phi(\theta,m)]\,dG(\theta,\eta)$$
$$+ O(\eta^3). \qquad (3.10)$$

$\Phi(\theta,m)$ is the inverse of Ψ and expanding in powers of a gives

$$\sin 2\Phi(\theta,m) = \sin 2(\theta + \eta) + 2a\cos^2(\theta + \eta)\cos 2(\theta + \eta)$$

$$+ O(a^2). \qquad (3.11)$$

Then to second order in a

$$2\gamma(\omega) = \int dp(m)\cdot a \int \{\sin 2\theta + 2\cos 2\theta\,[\eta + a\cos^2\theta]\}$$
$$dG(\theta,\eta)$$
$$- \int dp(m)\,a^2\int\cos^2\theta\cos 2\theta\,dG(\theta,\eta). \qquad (3.12)$$

Finally, we find

$$\lim_{\omega \to 0_+}[\gamma(\omega)/\omega^2] = \frac{1}{2}\cdot\langle m\rangle\int dp(m)\left(\frac{m - \langle m\rangle}{\langle m\rangle}\right)^2$$
$$\times\int_{-\pi/2}^{\pi/2}\cos 2\theta\cos^2\theta\,dG(\theta,0). \qquad (3.13)$$

We can choose $dG(\theta,0)$ to be $\pi^{-1}\,d\theta$ and so finally get the result of the theorem.

We can use this result to connect Sec. 2 with earlier work by Rubin[12] on the transmission of plane waves through random chains. We can rewrite (2.21) as

$$2|\sin k|\,t_N^{-1}(\omega) = \left|(1, -e^{-ik})\cdot T_1\cdots T_N\begin{bmatrix}1\\e^{ik}\end{bmatrix}\right|. \qquad (3.14)$$

Furstenberg[7] has not only shown that the norm of $T_1\cdots T_N u$ grows exponentially with N but also that the vector converges to a fixed direction (depending on u). Consequently, we can use (3.13) to calculate

$$\lim_{N\to\infty}[-(1/N)\log t_N^2(\omega)] = 2\gamma(\omega). \qquad (3.15)$$

This relationship was previously proven by Minami and Hori[13] using a different method. If each mass can take the values m and $m(1+Q)$ with probabilities q and p, we see from (2.13) that

$$\lim_{\omega\to 0_+}\frac{2\gamma(\omega)}{\omega^2} = \left(\frac{m}{4}\right)\frac{pq\,Q^2}{1+pQ}. \qquad (3.15')$$

Rubin's normalization of frequency is equivalent to taking $m = 4$. The mean spacing between the heavy particles is $\sum_{r=0}^\infty (r+1)q^r p = p^{-1}$. In Rubin's notation this is C^{-1} and so for small ω, $2\gamma(\omega)$ behaves as $C(1 - C)Q^2(1 + QC)^{-1}\omega^2$. This agrees with Rubin's result (Eq. 4.4, Ref. 12). (Note, however, that Rubin's N differ from ours by a factor of C.) Because $t_N^2(\omega)$ decays exponentially with N for almost all random chains, we can use the argument of Ref. 2 to conclude that $\langle\hat{J}(N)\rangle \to 0$ as $N \to \infty$.

Sulem and Frisch[14] have recently examined the transmission of light through a one-dimensional system in which the refractive index takes different constant values on successive intervals. These values are independent, identically distributed random variables. They used an argument based on the random ergodic theorem to show that almost all such systems are totally reflecting. The method of Ref. 12 shows that Furstenberg's theorem applies to their model.[15]

4. CALCULATION OF HEAT FLOW IN SPECIAL CASES

The heat flow through an arbitrary chain of masses given by (1.7) can only rarely be explicitly calculated. In Ref. 2, Casher and Lebowitz checked that it agrees with Ref. 1 for the infinite isotropic chain. Two more examples are given here; the infinite diatomic chain and the infinite isotropic chain in which a single impurity is imbedded. The spectrum of both systems contains an

absolutely continuous part and so the limiting value of the heat flux, J, is nonzero (Ref. 2 and Sec. 8).

A. The infinite diatomic chain

This is an infinite periodic chain in which m is m_1 when j is odd and m_2 when j is even. From Ref. 2 the heat flow through an infinite periodic chain whose unit cell contains the masses $m_1 \cdots m_c$ is just

$$J = \pi^{-1} m_1 m_c \lambda \Delta T \int d\omega \, |\omega \sin q| \, |c(\omega)|,$$
$$c(\omega)^{-1} = (1 + \lambda^2 \omega^2 m_1 m_c)(m_c K_{1,c-1} + m_1 K_{2,c}). \tag{4.1}$$

Only frequencies in the allowed bands will contribute to J. These are just the values of ω^2 for which

$$|K_{1,c}(\omega) - K_{2,c-1}(\omega)| \leqslant 2. \tag{4.2}$$

For a wave vector q they are the solutions of

$$K_{1,c}(\omega) - K_{2,c-1}(\omega) = 2 \cos q$$

as q ranges from 0 to π. For the diatomic chain these are

$$\omega^2 = (m_1^{-1} + m_2^{-1})(1 \pm \phi(q)).$$
$$\phi(q)^2 = 1 - \mu(1 - \cos q), \tag{4.3}$$
$$\mu = 2 m_1 m_2 (m_1 + m_2)^{-2}.$$

The acoustical branch of the spectrum is given by the negative sign and the optical branch by the positive sign. Then (4.1) reduces to

$$J = 2(1 + M\lambda^2)^{-1} \pi^{-1} \lambda \Delta T \int_0^\pi dq \sin^2 q \, |\phi(q)|^{-2}$$
$$\times [(1 + M\lambda^2)^2 - (M\lambda^2 \phi(q)^2)]^{-1},$$
$$M = m_1 + m_2. \tag{4.4}$$

A partial fraction expansion of the integrand gives

$$\frac{1}{x^2} + \left(\frac{2\mu - 1}{(1+x)^2}\right)(\phi^2)^{-1}$$
$$- \left(\frac{(2\mu x^2 + 2x + 1)(2x + 1)}{x^2(1+x)^2}\right)[(1+x)^2 - x^2\phi^2]^{-1}.$$

Using $\phi^2 = \cos^2(\tfrac{1}{2}q) + (1 - 2\mu)\sin^2(\tfrac{1}{2}q)$, each term becomes a simple trigonometric integral and we get

$$J = \frac{8\lambda^{-3}\Delta T}{M^2(1+x)(1-\delta^2)} \{(1+x)^2 - x^2\delta - (1+2x)^{1/2}[1$$
$$+ 2x + x^2(1 - \delta^2)]\} \tag{4.5}$$

where $x = M\lambda^2$ and we have set $|m_2 - m_1| = M\delta$. This agrees with (3.13) in Ref. 1c when $m_1 = m_2 = m$. Near $\delta = 0$, J is a decreasing function of δ so that starting from a monatomic chain and keeping M fixed J will initially decrease as $|m_1 - m_2|$ is increased.

B. A single impurity in an infinite isotropic chain

When a finite number of impurities are added to an infinite isotropic chain the spectrum of the new chain still contains an absolutely continuous piece. At most a finite number of isolated eigenvalues will be added to the original spectrum. These eigenvalues correspond when the impurities are light to highly localized normal modes. Using the techniques of Ref. 2 it is clear that they will not contribute to the heat flux through the in-

finite chain. In principle we can use (1.7) to calculate the limiting value, J, for any set of impurities. There seems to be a simple expression for J only for a single impurity and even this cannot be evaluated in terms of elementary functions. It was found more convenient to use techniques similar to those of Sec. 2 on the Langevin equation approach used by Ishii.[16] [The results will be exactly equivalent to those obtained from (1.7).] The final result, for a single impurity of mass m in the middle of a chain of unit masses, is (for details see Appendix D)

$$J = (2\pi)^{-1} \lambda \Delta T \int_0^\pi d\theta \sin^2\theta \, (1+u^2)[(1+u^2)^2 + u^2 v^2]^{-1},$$
$$\tag{4.6}$$
$$u^2 = \lambda^2 \omega^2, \quad v = (m-1)\omega^2, \quad \omega^2 = 2(1 - \cos\theta).$$

When $m = 1$, this agrees with (3.13) in Ref. 1c.

5. HEAT FLOW IN A WEAKLY COUPLED CHAIN

We give here an exact derivation of the asymptotic behavior of the heat flow in Lebowitz's model when the coupling constant λ of the chain to the heat baths is small. This is of interest because in the limit $\lambda \to 0$ the dependence of the heat flux $J(N, \lambda)$ [where we have indicated the explicit dependence of $J(N)$ on λ] on the amplitude of the normal modes at the ends of the chain becomes transparent. For small λ the integrand in (1.7) is large when $K_{1,N}(\omega^2) = 0$, i.e., at the normal mode frequencies of the chain. We will only treat those chains whose normal modes are distinct. This is not an important restriction (see Ref. 17 for a discussion of this point). Our theorem is also Theorem 7 in Ref. 5.

Theorem: Consider a chain of masses $\{m_i : i = 1, \cdots, N\}$ which has distinct normal mode frequencies $\{\omega_i^2 : i = 1 \cdots N\}$ and corresponding normal modes $\{u_i : i = 1 \cdots N\}$. u_i is normalized by $\sum_{j=1}^N m_j u_i(j)^2 = 1$. Then

$$\lim_{\lambda \to 0} \lambda^{-1} J(N, \lambda) = \pi^{-1} m_1 m_N \Delta T \sum_{i=1}^N \frac{m_1 u_i(1)^2 m_N u_i(N)^2}{m_1 u_i(1)^2 + m_N u_i(N)^2}. \tag{5.1}$$

Proof: If ω_i^2 is a simple zero of $K_{1,N}(\omega^2)$, then when ω^2 is near ω_i^2

$$K_{1,N}(\omega^2) = (\omega^2 - \omega_i^2)K'_{1,N}(\omega_i^2) + O(\omega^2 - \omega_i^2)^2 \tag{5.2}$$

where the prime indicates derivative. Hence the contribution of ω_i^2 to (1.7) is

$$J^{(i)}(N, \lambda) = m_1 m_N \Delta T \, |K'_{1,N}(\omega_i^2)| \, \tau(\omega_i^2)^{-1/2}, \tag{5.3}$$

where

$$\tau(\omega^2) = 2 m_1 m_N + m_1^2 K_{2,N}^2(\omega^2) + m_N^2 K_{1,N-1}^2(\omega^2).$$

Using the identity

$$K_{1,N}(\omega^2)K_{2,N-1}(\omega^2) - K_{1,N-1}(\omega^2)K_{2,N}(\omega^2) = -1, \tag{5.4}$$

(5.3) reduces to

$$J^{(i)}(N, \lambda) = m_1 m_N \Delta T \, |K'_{1,N}(\omega_i^2)|^{-1} \, |K_{1,N-1}(\omega_i)|$$
$$[m_N K_{1,N-1}^2 + m_1]^{-1}. \tag{5.5}$$

The normal mode associated with ω_i^2 is just u_i and

$$u_i(j) = K_{1,j-1}(\omega_i^2)N(\omega_i)^{-1},$$
$$N(\omega_i)^2 = \sum_{j=1}^N m_j K_{1,j-1}^2(\omega_i). \tag{5.6}$$

Considering the equations

$$(2 - m_{j+1}\omega^2)K_{1j} = K_{1j+1} + K_{1j-1},$$

$$- m_{j+1}K_{1j} + (2 - m_{j+1}\omega^2)K'_{1j} = K'_{1j+1} + K'_{1j-1} \qquad (5.7)$$

and multiplying the first by K'_{1j} and the second by K_{1j} and substracting, we get

$$m_{j+1}K_{1j}^2 = (K_{1j-1}K'_{1j} - K'_{1j-1}K_{1j}) - (K_{1j}K'_{1j+1} - K'_{1j}K_{1j+1})$$
$$= \phi_j - \phi_{j+1}. \qquad (5.8)$$

Thus

$$\sum_{j=0}^{N-1} m_{j+1}K_{1j}^2 = \phi_0 - \phi_{N+1},$$

$$\phi_0 = K_{1,-1} - K'_{10} - K'_{11}K_{10} = 0,$$

and if $\omega^2 = \omega_i^2$, where $K_{1,N}(\omega_i^2) = 0$, then

$$\sum_{j=0}^{N-1} m_{n+1}K_{1j}^2(\omega_i^2) = N(\omega_i^2) = K'_{1N}(\omega_i^2)K_{1N+1}(\omega_i^2). \qquad (5.9)$$

So (5.5) reduces to the term in (5.1) associated with ω_i^2 and the proof is complete.

Matsuda and Ishii have argued in Ref. 5 that this supports the conjecture that $\langle J(N, \lambda)\rangle$ decreases as $N^{-3/2}$. We want to point out, however, that even if one could establish that, for random chains, the right side of (5.1) behaves as $N^{-3/2}$ when $N \to \infty$ this would not necessarily tell us anything about the behavior of $J(N, \lambda)$ as $N \to \infty$ for any fixed $\lambda > 0$. What (5.1) gives is the large N behavior of $\lim_{\lambda\to 0} \lambda^{-1} J(N, \lambda)$ and this need not be the same as the large N behavior of $\lambda^{-1}J(N, \lambda)$ for $\lambda > 0$. They will agree for periodic chains where $\lambda^{-1} J(N, \lambda)$ approaches a finite nonzero limit as $N \to \infty$ for any $\lambda > 0$. We surmise that for a system obeying Fourier's law the asymptotic form of the heat flux may be of the form

$$J(N, \lambda) \sim \lambda(\Delta T)/(1 + \gamma\lambda N)^{-1}, \qquad (5.10)$$

where γ is related to the resistance to heat flow in the interior of the system, e.g., the degree of anharmonicity in a anharmonic crystal, or the "degree of disorder" $\langle(m - \langle m\rangle)^2\rangle$ in a random crystal if indeed such a system obeys Fourier's law. If this surmise is right then the two asymptotic behaviors will not be the same. This surmise is based (or strengthened) by the behavior of the heat flow in a simple stochastic model system discussed in the next section.

6. RANDOM REFLECTION MODEL

This is a simple system which transports energy and has a Fourier law behavior. It is a variation of one originally considered by Lebowitz and Frisch.[18] It is a dilute gas of noninteracting particles which move linearly along a cylinder. At either end of the cylinder is a heat bath and barriers are placed at random positions along the cylinder. When a gas particle meets a barrier it will either pass through without changing its velocity or it will be reflected with its velocity exactly reversed. The probability of reflection is r and of transmission $1 - r$. At each end it can be directly reflected with probability $1 - \lambda$ or with probability λ it is reflected back with a random velocity. This random velocity is independent of the incident velocity and has a Maxwellian distribution characterized by the temperature of the heat baths. These are T_0 on the left and T_1 on the right

$(T_0 > T_1)$. Thus λ plays the role of coupling to the heat baths as before, $0 \leqslant \lambda \leqslant 1$. Since the total number of particles is constant, the total number flowing to the right at any point will, in a steady state exactly balance the total number flowing to the left. The first group will presumably be more energetic and so energy will be carried along the cylinder.

We look at the steady state situation. There are N barriers and between barriers i and $i + 1$, the number of particles in a unit volume with velocities between v and $v + dv$ is $f_i(v)\, dv$.

Let

$$f_i^+(v) = f_i(v), \qquad v > 0,$$
$$f_i^-(v) = f_i(-v), \qquad v > 0, \qquad (6.1)$$

be the densities for those particles flowing to the right and those flowing to the left. $f_0^\pm$ and $f_N^\pm$ are the corresponding densities for the particles between the heat baths and the first and last barriers. At each barrier the net flux of particles with velocities near v must be zero. So

$$f_i^+(v) = r f_i^-(v) + (1 - r)f_{i-1}^+(v), \qquad N \geqslant i > 0.$$
$$f_i^-(v) = r f_i^+(v) + (1 - r)f_{i+1}^-(v), \qquad N > i \geqslant 0. \qquad (6.2)$$

At the left the flux of particles incident on the heat bath with velocities near v is $v f_0^-(v)\, dv$. This is redistributed by direct and diffuse reflection so

$$v f_0^+(v) = (1 - \lambda) v f_0^-(v) + \lambda v g_0(v)\int_0^\infty u f_0^-(u)\, du. \qquad (6.3)$$

$g_0(v)$ is proportional to the Maxwellian distribution of particles in the heat bath at temperature T_0. It is normalized so as to conserve the total flux striking the edge of the cylinder. So $g_0(v) = \beta_0 m \exp(-\beta_0 m v^2)$, $\beta_0 = (kT_0)^{-1}$. g_1 is defined similarly. So

$$f_0^+(v) = (1 - \lambda)f_0^-(v) + \lambda g_0(v)\int_0^\infty u f_0^-(u)\, du \qquad (6.4)$$

and

$$f_N^-(v) = (1 - \lambda)f_N^+(v) + (\lambda)g_1(v)\int_0^\infty (u)\, du. \qquad (6.5)$$

The solution of these equations, for $0 \leqslant i \leqslant N$, is

$$f_i^+ = \nu[g_0 + C_i(g_1 - g_0)],$$
$$f_i^- = \nu[g_1 + C_{N-i}(g_0 - g_1)], \qquad (6.6)$$

where $C_j = \alpha + j\beta$ with,

$$\alpha = (1 - \lambda)(1 - r)/[(2 + \lambda)(1 - r) + r\lambda N],$$
$$\beta = \lambda r/[(2 - \lambda)(1 - r) + r\lambda N] \qquad (6.7)$$

and ν is the total flux of particles flowing in either direction, i.e., $\int_0^\infty v f_i^+(v)\, dv = \int_0^\infty v f_i^-(v)\, dv = \nu$ for $N \geqslant i \geqslant 0$. The next flux of energy from left to right is

$$\int_0^\infty \tfrac{1}{2}m v^3[f_i^+(v) - f_i^-(v)]\, dv = \frac{\nu\lambda(1 - r)}{(2 - \lambda)(1 - r) + \lambda r N}$$
$$\times k(T_0 - T_1) = \bar{J}(N, \lambda). \qquad (6.8)$$

The heat flux $J(N, \lambda)$ has the form conjectured in (5.10). It depends only on the number of barriers present and does not depend at all on their spacing (because there is no attenuation between adjacent barriers). In particular, it does not depend on the length of the cylinder. However, if we suppose that in a cylinder of

length L the number of barriers present is randomly distributed with a Poisson distribution whose mean is ρL the average heat flow will be

$$\langle J(L, \lambda) \rangle = \sum_{n=0}^{\infty} \frac{(\rho L)^n}{n!} \exp(-\rho L) \bar{J}(n, \lambda). \tag{6.9}$$

In the limit

$$\lim_{L \to \infty} \left[\frac{L \langle J(L, \lambda) \rangle}{T_0 - T_1} \right] = \nu k (1 - r)/r\rho, \tag{6.10}$$

is independent of λ, Eq. (6.10) depends on the asymptotic expansion

$$\sum_{n=0}^{\infty} \frac{t^n}{n!} \frac{e^{-t}}{n+b} = \frac{1}{t} + 0 \left(\frac{1}{t^2} \right) \tag{6.11}$$

as $t \to \infty$, for fixed positive b.

Exactly the same result holds if the barriers are placed with a constant density ρ along the cylinder. So we can say that the thermal conductivity of this model is

$$K = \nu k (1 - r) \cdot (r\rho)^{-1}. \tag{6.12}$$

Decreasing the barrier spacing means that ρ increases and then K will tend to zero.

7. A SIMPLE TWO-DIMENSIONAL MODEL

This is a cylindrical system in which the masses in each column are identical although from column to column the mass may vary randomly. The cylindrical analog of Lebowitz's model has been examined by Nakazawa.[4] We will combine the method of Sec. 2 with his method to examine the cylindrical analog of Rubin's model. Each column of the cylinder contains p masses and the displacement of the particle in the ith column and the ath row is x_{ia}. Its mass is m_i. When $-S \le i \le 0$ and $N + 1 \le i \le N + S + 2$, $m_i = 1$; when $1 \le i \le N$ the m_i are independent, identically distributed random variables. The particle at site (i, a) is coupled by harmonic forces of unit strength to those at $(i-1, a)$ and $(i+1, a)$ and by forces of strength μ to those at $(i, a-1)$ and $(i, a+1)$. The equation of motion of this system, with $x_{i,p+1} = x_{i,1}$, is

$$m_i \ddot{x}_{i,a} + (2x_{i,a} - x_{i-1,a} - x_{i+1,a}) + \mu(2x_{i,a} - x_{i,a-1} - x_{i,a+1})$$
$$= 0. \tag{7.1}$$

We exploit cylindrical symmetry by forming the sums

$$x_i(\theta_l) = p^{-1/2} \sum_{a=1}^{p} x_{i,a} \exp(i \theta_l a) \tag{7.2}$$

where $1 \le l \le p$, $\theta_l = 2\pi l/p$. Then (7.1) becomes

$$M\ddot{x}(\theta_l) + \Omega^2(\theta_l) x(\theta_l) = 0, \tag{7.3}$$

where M is the diagonal matrix with entries m_i, $\Omega^2(\theta)$ the tridiagonal matrix with diagonal entries $2 + 4\mu \sin^2 \frac{1}{2}\theta$ and off diagonal entries -1 and $x(\theta_l)$ is the column vector whose ith entry is $x_i(\theta_l)$, $-S \le i \le N + S + 2$. These are identical to the equations of motion (1.2) of a linear chain with different coupling strengths between adjacent particles.

We have the inversion formula

$$x_{i,a} = p^{-1/2} \sum_{l=1}^{p} x_i(\theta_l) \eta^{-la}. \tag{7.4}$$

In terms of these coordinates the energy in the left-hand piece of the cylinder is

$$\frac{1}{2} \sum_{l=1}^{p} \{ \dot{x}'(\theta_l) \cdot \dot{x}'(\theta_l) + x'(\theta_l) \cdot \Omega^2(\theta_l) x'(\theta_l) \}. \tag{7.5}$$

Here $x'(\theta_l) = \{ x_i(\theta_l) : -S \le i \le 0 \}$.

We can repeat the analysis of Sec. 2 to obtain a closed set of equations of motion for the columns 1 through N. If the left- and right-hand pieces are initially in thermal equilibrium at temperatures T_L and T_R we find, after letting $S \to \infty$ and then $p \to \infty$, that the analog of (2.6) and (2.7) are

$$x_0(\theta, t) = g_1(\theta, t) + \int_0^T A(t - s) x_1(\theta, s) ds,$$

$$A(t) = \frac{2}{\pi} \int_0^\pi \omega(k)^{-1} \sin[t\omega(k)] \sin^2 k \, dk,$$

$$\langle g_1(t) \rangle = 0,$$

$$\langle g_1(t) g_1(t+s) \rangle = \pi^{-1} k \, T_L \int_0^\pi \omega(k)^2 \sin^2 k \cos[s\omega(k)] dk,$$

$$\omega(k)^2 = 4(\sin^2 \frac{1}{2} k + \mu \sin^2 \frac{1}{2}\theta) \tag{7.6}$$

(in the limit $p \to \infty$, θ_l becomes a continuous parameter θ ranging from 0 to 2π). In deriving these we note that the $S \times S$ matrix $\Omega^2(\theta)$ has eigenvalues $4(\sin^2 \frac{1}{2}\phi_j + \mu \sin^2 \frac{1}{2}\theta]$ with $\phi_j = j\pi/S + 1$ $(1 \le j \le S)$ and eigenvectors $\xi_j = [2/(S+1)]^{1/2} (\sin\phi_j, \cdots, \sin S\phi_j)$.

The average energy flowing past the particle at site $(1, a)$ (from left to right) is

$$\hat{J}(N, t) = \langle \dot{x}_{1,a} (x_{1,a} - x_{0,a}) \rangle = p^{-1} \sum_{l=1}^{p} \langle \dot{x}_1(\theta_l) - x_0(\theta_l) \} \rangle. \tag{7.7}$$

When $p \to \infty$, $\hat{J}(N, t)$ becomes

$$\hat{J}(N, t) = (2\pi)^{-1} \int_0^{2\pi} \dot{x}_1(\theta) [x_1(\theta) - x_0(\theta)] d\theta. \tag{7.8}$$

This is just a superposition of currents from harmonic chains with coupling matrices $\Omega^2(\theta)$ so that repeating the analysis of Sec. 2 we obtain, when $t \to \infty$ (setting Boltzmann's constant equal to unity),

$$\hat{J}(N) = (4\pi)^{-1} \Delta T \int_0^\pi d\theta \int_0^\infty d\omega \mid \det Y(\omega, \theta) \mid^{-2}$$
$$\times i\omega[\hat{A}(\omega) - \hat{A}(-\omega)] [\hat{g}(\omega) + \hat{g}(-\omega)]. \tag{7.9}$$

$\hat{A}$ and $\hat{g}$ are the Fourier transforms of A and g and are obtained by analytic continuation of their Laplace transforms. $Y(\omega, \theta)$ is the $N \times N$ matrix $\Omega^2(\theta) - \omega^2 M - \hat{A}(\omega) L$. We find that when $4\mu \sin^2 \frac{1}{2}\theta \le \omega^2 \le 4 + 4\mu \sin^2 \frac{1}{2}\theta$, then

$$\hat{A}(\omega) - \hat{A}(-\omega) = -i(\omega^2 - 4\mu \sin^2 \frac{1}{2}\theta)^{1/2} (4 + 4\mu \sin^2 \frac{1}{2}\theta - \omega^2)^{1/2}, \tag{7.10}$$

$$\hat{g}(\omega) + \hat{g}(-\omega) = \omega^{-1}(\omega^2 - 4\mu \sin^2 \frac{1}{2}\theta)^{1/2} (4 + 4\mu \sin^2 \frac{1}{2}\theta - \omega^2)^{1/2}$$

and that they are zero otherwise. Thus, calling R the range of the ω integration, we obtain

$$\hat{J}(N) = \Delta T \int_0^\pi d\theta \int_R d\omega \mid \det Y(\omega, \theta) \mid^2 (\omega^2 - 4\mu \sin^2 \frac{1}{2}\theta)$$
$$\times (4 + 4\mu \sin^2 \frac{1}{2}\theta - \omega^2). \tag{7.11}$$

We simplify this by introducing the parametrization $\omega^2 = 4 \sin^2 \frac{1}{2}k_1 + 4\mu \sin^2 \frac{1}{2}k_2$ which is valid for all ω^2 in the range of integration of (7.11); then

$$\hat{J}(N) = \Delta T \int_0^\pi \int_0^\pi dk_1\, dk_2 \cos \tfrac{1}{2}k_1 \left(\frac{\sin^2 \tfrac{1}{2}k_1}{\sin^2 \tfrac{1}{2}k_1 + \mu \sin^2 \tfrac{1}{2}k_2} \right)^{1/2}$$

$$|f(k_1, k_2)|^2,$$

$$f(k_1, k_2) = 2\, \sin k_1 \cdot (\det Z_N(k_1, k_2))^{-1},$$

$$Z_N = \Omega^2(k_2) - M\omega^2 - \exp(ik_1)\, L. \qquad (7.12)$$

L is the diagonal matrix with entries $L_{ii} = (\delta_{i1} + \delta_{iN})$ and in this representation of ω^2, $\hat{A}(\omega) = \exp(ik_1)$.

We can relate $\hat{J}(N)$ to the transmission properties of the columns 1 to N. The incident and transmitted plane waves are

$$x_{j,a} = \exp[-i(\omega t + k_1 j + k_2 a)] \qquad , j \leq 1,$$

$$x_{j,a} = D \exp[-i(\omega t + k_1 j + k_2 a)] \qquad (7.13)$$

$$+ R \exp[-i(\omega t - k_1 j + k_2 a)] \qquad , j \geq N.$$

Using the equations of motion (7.3) for a plane wave with frequency ω, we find

$$\begin{bmatrix} x_{j+1}(\theta) \\ x_j(\theta) \end{bmatrix} = \begin{bmatrix} 2 + 4\mu \sin^2 \tfrac{1}{2}\theta - m_j \omega^2 & -1 \\ 1 & 0 \end{bmatrix}$$
$$\begin{bmatrix} x_j(\theta) \\ x_{j-1}(\theta) \end{bmatrix}. \qquad (7.14)$$

Applying (7.13) yields

$$\begin{bmatrix} \exp(-ik_1(N+1)) & \exp[ik_1(N+1)] \\ \exp(-ik_1 N) & \exp(ik_1 N) \end{bmatrix} \begin{bmatrix} D \\ R \end{bmatrix}$$

$$= T_N \cdots T_1(k_1, k_2) \begin{bmatrix} \exp(-ik_1) \\ 1 \end{bmatrix}, \qquad (7.15)$$

where

$$T_j(k_1, k_2) = \begin{bmatrix} 2 + 4\mu \sin^2 \tfrac{1}{2}k_2 - m_j \omega^2 & -1 \\ 1 & 0 \end{bmatrix}.$$

This yields for the transmission coefficient, t_N, in analogy with (2.21),

$$|D_N(k_1, k_2)|^{-1} = |f(k_1, k_2)| = |t_N(k_1, k_2)|. \qquad (7.16)$$

Substituting in (7.12) gives

$$\hat{J}(N) = k\Delta T \int_0^\pi \int_0^\pi dk_1\, dk_2 \cos\tfrac{1}{2}k_1$$

$$\times \left[\frac{\sin^2\tfrac{1}{2}k_1}{\sin^2\tfrac{1}{2}k_1 + \mu\sin^2\tfrac{1}{2}k_2} \right]^{1/2} |t_N(k_1, k_2)|^2. \qquad (7.17)$$

We can compare this with Nakazawa's result[4] for the heat flow in the cylindrical analog of Lebowitz's model

$$J(N) = \pi^{-2} k\, m_1\, m_N \lambda^2 \Delta T \int_0^\pi d\theta \int_{-\infty}^\infty \omega^2 |\det Y(\omega, \theta)|^{-2}\, d\omega,$$

$$Y(\omega, \theta) = \Omega^2(\theta) - \omega^2 M - i\omega\lambda ML. \qquad (7.18)$$

When the mass sequence m_i is periodic, the results of the next section extend to show that the semiinfinite matrix $K(\theta) = M^{-1/2} \Omega^2(\theta) M^{-1/2}$ has only an absolutely

continuous spectrum and so from Ref. 2 we see that both $J(N)$ and $\hat{J}(N)$ have strictly positive limits as $N \to \infty$. An examination of Theorem 1 in Ref. 5 shows that Furstenberg's theorem holds for any subgroup of $SL(2, R)$ which is generated by two noncommuting matrices $\begin{bmatrix} a_i & -1 \\ 1 & 0 \end{bmatrix}$ $(i = 1, 2)$. (See also Ref. 11.) Consequently, for a disordered cylindrical system $J(N)$ and $\hat{J}(N)$ will tend to zero as $N \to \infty$ for almost every choice of masses in the columns. We can use Sec. 3 to find the asymptotic behavior of $t_N(k_1, k_2)$ for large N. Equation (7.15) gives

$$|t_N(k_1, k_2)|^{-1} = |2 \sin k_1|^{-1} \left| [1, -\exp(ik_1)]\, T_N \cdots T_1 \right.$$

$$\left. \times \begin{pmatrix} 1 \\ e^{ik_1} \end{pmatrix} \right|.$$

An extension of Theorem 8.1 in Ref. 7 shows that the angle between the rows and the angle between the columns of $T_N \cdots T_1$ converges to zero as N increases. So for any k_1, the angle between the vector $T_N \cdots T_1$ $\binom{1}{e^{ik_1}}$ and the vector $\binom{1}{1}$ tends to zero. If $k_1 \neq 0$, this shows that $|t_N(k_1, k_2)|^{-1}$ grows exponentially with N. The analog of (3.15) is now as follows: when $k_1 \neq 0$, $\lim_{N \to \infty} - (1/N) \log |t_N(k_1, k_2)| = \gamma(k_1, k_2)$. When $k_1 = 0$, t_N is identically zero. The analog of $\gamma(\omega)$ (3.4a) is now $\gamma(\mathbf{k})$.

Theorem: For small $|\mathbf{k}|$, $\gamma(\mathbf{k})$ is continuous in $\mathbf{k}$ and

$$\lim_{|\mathbf{k}| \to 0} \frac{\gamma(\mathbf{k})}{g(\mathbf{k})} = \frac{1}{8} \frac{\langle m^2 \rangle - \langle m \rangle^2}{\langle m \rangle}, \qquad (7.19)$$

where

$$g(\mathbf{k}) = (k_1^2 + \mu k_2^2)^2\ k_1^2 + \mu \left(1 - \frac{1}{\langle m \rangle}\ k_2^2 \right)^{-1}$$

(we assume $m_i \geq 1$, all i).

Proof: Adapting the calculation of Sec. 3 to the family of transfer matrices $T_j(k_1, k_2)$ yields

$$\gamma(\mathbf{k}) = \int_{-\pi/2}^{\pi/2} \log \left| \frac{\cos(\theta + \eta)}{\cos \theta} \right| dG(\theta, \eta) \qquad (7.20)$$

where

$$G(A) = \int_0^\infty G[\Psi(A, m)]\, dp(m),$$

$$\tan \phi = \tan[\Psi(\phi, m) + \eta] + [(m - \langle m \rangle)/\sin\eta]\, \omega^2,$$

$$2\cos\eta = 2 + 4\mu \sin^2\tfrac{1}{2}k_2 - 4\langle m \rangle (\sin^2\tfrac{1}{2}k_1 + \mu \sin^2\tfrac{1}{2}k_2). \qquad (7.21)$$

If $a = [(m - \langle m \rangle)/\sin\eta]\, \omega^2$ then (3.12) gives

$$\gamma(\mathbf{k}) = \int_0^\infty dp(m) \cdot a^2 \int_{-\pi/2}^{\pi/2} \cos 2\theta \cos^2\theta\, dG(\theta, \eta) + O(\eta^3). \qquad (7.22)$$

This gives the result.

8. SPECTRUM OF PERIODIC CHAINS

We consider a infinite periodic chain whose basic cell contains the masses $m_1 \cdots m_A$. It is easy to see that the allowed bands for the chain are specified by the algebraic condition

$$|\mathrm{Tr}\, T(\omega)| \leq 2, \qquad (8.1)$$

where $T(\omega) = T_A \cdots T_1(\omega)$ is the transfer matrix for one cell of the chain. These bands form the spectrum of the self-adjoint infinite matrix operator $H = M^{-1/2} \Phi M^{-1/2}$ introduced in Sec. 1. H acts on the Hilbert space l^2 and has a cyclic vector, viz. $\psi = (1, 0, 0 \cdots)$. So H has a simple spectrum whose spectral type (Ref. 19, Chap. VII) is precisely the type of the measure μ_Ψ on $[0, \infty)$ determined by

$$(\Psi, H^k \Psi) = \int_0^\infty x^k \, d\mu_\Psi \quad (k \geq 0). \tag{8.2}$$

Theorem: The spectrum of a semiinfinite periodic lattice is absolutely continuous.

Proof: We will evaluate the left side of (8.2) for finite periodic systems and then let the length tend to infinity. We will see that there is a unique measure satisfying (4.2) and that it is absolutely continuous. We also normalize the lightest mass to 1 so that all $m_i \geq 1$. The spectrum of H will therefore be in $[0, 4]$.

Let P_N be the projection on l^2 which projects any vector onto its first NA entries. Then $H_N = P_N H P_N$ is the operator introduced in Sec. 1 corresponding to a periodic lattice with N cells. For each $k \geq 1$, the operators H_N^k converge strongly to H^k. Suppose that a chain containing N cells has normal modes with frequencies ω_a^2, $a = 1 \cdots NA$. The corresponding displacements are

$$u(a, jA + p) = d_p(\omega_a) \sin[(jA + p)K_a],$$
$$K_a = \pi a(NA + 1)^{-1}, \quad 1 \leq p \leq A, \quad 0 \leq j \leq N - 1. \tag{8.3}$$

$d_p(a)$ are certain constants depending on a. Using the transfer matrix method (8.2) can be a solution to the lattice equations only if

$$\text{Tr } T(\omega_a^2) = 2 \cos A K_a. \tag{8.4}$$

The normalization condition for (4.3) is

$$1 = |u(a)|^2 = \frac{1}{2} \sum_{p=1}^A |d_p(a)|^2 [N - \cos 2K_a(p - 1)]. \tag{8.5}$$

So

$$(\Psi, H_N^k \Psi) = 2N^{-1} \sum_{a=1}^{NA} F(\omega_a^2) \omega_a^{2k} + O(N^{-2})$$

with

$$F(\omega^2) = \sum_{p=1}^A d_p(\omega)^2. \tag{8.6}$$

Each $d_p(\omega)$ is a cofactor in a certain determinant and so $F(\omega^2)$ is a bounded continuous function. The spacing of the wave vectors K_a in a long finite chain is very nearly $\pi(NA)^{-1}$. Rewriting this in terms of the frequencies ω_a^2 and letting $N \to \infty$ gives

$$\cdot (\Psi, H^k \Psi) = 2A \pi^{-1} \int \left| \frac{dK}{d\omega^2} \right| \omega^{2k} F(\omega^2) \, d(\omega^2) \tag{8.7}$$

provided that $dK/d\omega^2$ makes sense. The integral is over the values of ω^2 for which $|\text{tr } T(\omega)| \leq 2$, i.e., the allowed frequency bands. Using (4.4) in the limit $N \to \infty$ gives

$$2 \cos AK = \text{Tr } T(\omega^2) = g(\omega^2), \tag{8.8}$$

So

$$\left| \frac{dK}{d\omega^2} \right| = (2A)^{-1} g'(\omega^2) (4 - g^2)^{-1/2}$$
$$= (2A)^{-1} h(\omega^2). \tag{8.9}$$

Any singularities occuring in this ratio are integrable and so

$$(\Psi, H^k \Psi) = \pi^{-1} \int h(\omega^2) F(\omega^2) \omega^{2k} \, d\omega^2 = \int x^k p(x) \, dx. \tag{8.10}$$

$p(x)$ is an integrable function over the spectrum of the chain. Since H is bounded we also have

$$(\Psi, f(H)\Psi) = \int f(x) p(x) \, dx \tag{8.11}$$

for any polynomial f and consequently for all measurable functions f. Spectral theory now tells us that $p(x) \, dx$ is unique and consequently the spectrum of H is absolutely continuous.

9. DISCUSSION

The expression for the heat flux $J(N)$ in (1.7) and for $\hat{J}(N)$ in (2.16) [or (2.23)] differ essentially in that (1.7) contains an integral over all ω while the integration in (2.16) is restricted to the spectrum of the homogeneous chain with unit masses. (The difference in integrands is presumably due to the nature of the coupling between the system and heat baths in the two models.) It seems intuitively clear that the reason why frequencies outside the spectrum do not contribute to $\hat{J}(N)$ is that all such modes would be damped out in the homogeneous stretches of the side chains when $S \to \infty$. Indeed the integral in (1.7) will reduce to an integral only over the spectrum of the chain when we take a chain of length $N + 2S$ in which $m_j = 1$ if $1 \leq j \leq S$ and $N + S + 1 \leq j \leq 2S + N$. Using expansions similar to those in Appendix C, it is easy to see that $\lim_{S \to \infty} J(N + 2S)$ becomes an integral over $[0, 4]$ involving only the determinants $K_{1,r}$, etc. There does not, however, seem to be a compact expression for this flux.

In any case, as we have seen, both $J(N)$ and $\hat{J}(N)$ approach nonvanishing limits when $N \to \infty$ in periodic systems and go to zero in random systems. The latter result follows from the behavior of the integrands $j_N(\omega)$ and $t_N^2(\omega)$ which, by Furstenberg's theorem, vanish for almost all chains as $\exp[-N\gamma(\omega)]$ as $N \to \infty$ for fixed ω, with $\gamma(\omega) > 0$ for $\omega \neq 0$. The difficulty with using Furstenberg's theorem for the evaluation of the asymptotic form of $J(N)$ or $\hat{J}(N)$ (the latter ought to be easier since the integration is over a finite range) is that the approach to the limit in Furstenberg's theorem, i.e., in (3.15), is not known to be uniform in ω for $\omega \neq 0$. We need some such kind of uniformity to decide for certain whether Fourier's law is obeyed by random harmonic systems.

ACKNOWLEDGMENTS

APPENDIX A

We show that the matrix $Y(\omega) = \Phi - M\omega^2 - A(\omega)U$ in Sec. 1 is nonsingular for real ω except at $\omega^2 = 0$ and 4. If $\omega^2 \leq 4$, we write $\omega = 2 \sin(\theta/2)$ and if $D(\omega) = \det Y(\omega)$

vanishes we have

$$\cos\theta(K_{1,r}+K_{2,r-1})=K_{2,r}+K_{1,r-1},$$
$$\sin\theta(K_{1,r}-K_{2,r-1})=0. \tag{A1}$$

If θ is different from 0 and π, then $K_{2,r-1}=K_{1,r}$ and (3.4) implies $K_{2,r}K_{1,r-1}=1+K_{1,r}^2$ so that $|\cos\theta|\geq 1$. Equality is only possible if $\theta=0$ or π, i.e., $\omega^2=0$ or 4. When $\omega^2=0$, $A(\omega)=1$ and $D=0$. When $\omega^2=4$, D need not vanish and will only have a simple zero. If $\omega^2>4$, we consider a square matrix C with $2N+r$ rows and columns:

$$C=\Phi-M\omega^2 \tag{A2}$$

with Φ the usual tridiagonal matrix and M and diagonal matrix with entries $M_{ii}=1$ if $1\leq i\leq N$ and $N+r+1\leq i\leq 2N+r$ and $M_{ii}=m_j$ if $i=N+j$, $j=1\cdots r$. Then

$$\det C=d(N-2)^2K_{1,r}-d(N)\,d(N-2)(K_{1,r-1}+K_{2,r})$$
$$+d(N)^2K_{2,r-1}, \tag{A3}$$

$$d(N)=(-1)^N\frac{\sinh(N+1)\theta}{\sinh\theta}\quad\text{when }\omega^2=4\cos h^2\theta.$$

Also, using Rayleigh's theorem,[20] we can find lower bounds on the eigenvalues of the matrix $M^{-1/2}\Phi M^{-1/2}$ and so prove that when N is large

$$|\det C|\geq(\omega^2)^r\,d(2N)m_1\cdots m_r. \tag{A4}$$

So $\lim_{N\to\infty}\exp(-2N\theta)\,|C|=|D(\omega)|>0$. The only zeros in $D(\omega)$ then are cancelled by the zeros in the numerator of (1.24).

APPENDIX B

We show that for an infinite harmonic chain with $m_j=1$ except possibly when $N\geq j\geq 1$ that if $u_j=0=\dot u_j$ at $t=0$ except when $N\geq j\geq 1$ then $|u_j(t)|$ falls off as $t^{-1/2}$ when $N\geq j\geq 1$. We check the case when $\dot u(0)=0$ but $u(0)\neq 0$. Then

$$u(t)=(2\pi)^{-1}\int_C \exp(i\omega t)\,(\Phi-M\omega^2-a(\omega)L)^{-1}u(0)\,d\omega. \tag{B1}$$

C is a contour obtained as the limit of semicircles in the upper half plane with radius R and centre $-i\epsilon$ (ϵ very small and positive). The integrand may have some poles in the upper half plane and has a cut along the real axis from -2 to $+2$. The poles contribute exponentially decreasing terms and the cut a term of type

$$\int_{C_1}\omega^2(4-\omega^2)\,[P(\omega)+iQ(\omega)\,(4-\omega^2)^{1/2}]^{-1}\exp(i\omega t)\,d\omega. \tag{B2}$$

P and Q are polynomials in ω and the integrand has only the singularity due to the branch in the square root. C_1 is a contour enclosing the interval $(-2,2)$. We can easily check that if f and f' are integrable $\int_{-2}^2 f(\omega)\exp(i\omega t)\,d\omega$ falls off at least as t^{-1} and that $\int_{-2}^2 f(\omega)\,(4-\omega^2)^{1/2}\exp(i\omega t)\,d\omega$ falls off at least as $t^{-1/2}$. This proves the claim.

APPENDIX C

We give here the detailed computation for the heat flow along an infinite isotropic chain containing a single impurity. Using the Langevin equation approach of Ishii[5,16] and the method of Sec. 2 we find that the heat flow across a segment of r masses, $m_1\cdots m_r$, embeded in isotropic chains of length N is just

$$J=\lambda^2\,k\,T\,m_1\,m_r\int_{-2}^2\omega^2|b(\omega)|^4\,|\det Z(\omega)|^{-2}\,d\omega. \tag{C1}$$

$Z(\omega)=\Phi-M\omega^2-a(\omega)L$ is the standard $r\times r$ matrix. $a(\omega)$ and $b(\omega)$ are given by

$$(d_{N+1}-i\omega\lambda\,d_N)\,a(\omega)=d_N-i\omega\lambda\,d_{N-1},$$
$$(d_{N+1}-i\omega\lambda\,d_N)\,b(\omega)=1, \tag{C2}$$

where $d_p(\omega)=\sin(p+1)\theta/\sin\theta$ if $\omega^2=2(1-\cos\theta)$.

We can use the methods of Ref. 2 to show that as $N\to\infty$ this reduces to an integral over the spectrum of the infinite homogeneous chain (if any $m_j<1$ then there are some localized modes with frequencies greater than 2 but an explicit examination shows that these do not contribute to J as $N\to\infty$). This integral is only tractable when $r=1$. In that case putting $\phi=(2N+1)\theta$ and letting $N\to\infty$, we get

$$J=(2\pi)^{-1}m\,\lambda^2\,k\,T\int_0^{2\pi}d\omega\,\omega^2(\theta)\sin^2\theta$$
$$\times\int_0^{2\pi}d\phi\,|F(\theta,\phi)|^{-2}, \tag{C3}$$

$$F(\theta,\phi)=a\cos 2\phi+b\sin 2\phi+e-if,$$
$$a=\cos 2\theta+u^2-v\sin 2\theta,$$
$$b=\sin 2\theta+v(\cos 2\theta+u^2), \tag{C4}$$
$$e-if=-v(1+u^2)-2iu\sin\theta.$$

Standard manipulations will reduce (C3) to (4.6).

[1](a) P.G. Bergmann and J.L. Lebowitz, Phys. Rev. 99, 578 (1965). (b) J.L. Lebowitz, Phys. Rev. 114, 1192 (1959). (c) Z. Rieder, J.L. Lebowitz, and E. Lieb, J. Math. Phys. 8, 1073 (1967).
[2]A. Casher and J.L. Lebowitz, J. Math Phys. 12, 1701 (1971).
[3]R.H.G. Gellemann, "Heat Transport in Harmonic and Anharmonic Lattices," thesis, Yeshiva University, 1971.
[4]H. Nakazawa, Suppl. Progr. Theor. Phys. 45, 231 (1970).
[5]H. Matsuda and K. Ishii, Suppl. Prog. Theor. Phys. 45, 56 (1970).
[6]R.E. Borland, Proc. Roy. Soc. A274, 529 (1963).
[7]H. Furstenberg, Trans. Am. Math. Soc. 108, 377 (1963).
[8]R.J. Rubin and W.L. Greer, J. Math. Phys. 12, 1686 (1971).
[9]G.W. Ford, M. Kac, and P. Mazur, J. Math. Phys. 6, 504 (1965).
[10]V.B. Magalinskii, Zh. Eksp. Teor. Fiz. 36, 1942 (1959) [Sov. Phys. JETP 9, 1381 (1959)].
[11]Y. Yoshioka, "On the Singularity of the Spectral Measures of a Semi-Infinite Random System" (to be published).
[12]R.J. Rubin, J. Math. Phys. 9, 2252 (1968); J. Math. Phys. 11, 1857 (1970).
[13]S. Minami and J. Hori; Suppl. Prog. Theor. Phys. 45, 87 (1970).
[14]P.L. Sulem and H. Frisch, J. Plasma Phys. 8, 217 (1972).
[15]U. Frisch, C. Froeschle, J.P. Scheidecker, and P.L. Sulem, Phys. Rev. A 8, 1416 (1973).
[16]K. Ishii, "Localization of eigenstates and transport phenomena in one-dimensional disordered systems," preprint, Research Institute for Fundamental Physics, Kyoto University, 1972.
[17]W.M. Visscher, Prog. Theor. Phys. 46, 729 (1971).
[18]J.L. Lebowitz and H.L. Frisch, Phys. Rev. 107, 917 (1957).
[19]M. Reed and B. Simon, Methods of Modern Mathematical Physics (Academic, New York, 1972), Vol. I.
[20]A. Maradudin, E. Montroll, and G. Weiss, Theory of Lattice Dynamics in the Harmonic Approximation (Academic, New York, 1963).