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$$\langle|D_N(i\omega)|^2\rangle_c = \frac{1}{2} + \left(\frac{1}{2} + \frac{1}{8}\frac{Q^2C^2}{1+QC}\right)\left(1 - 2\frac{Q^2(1-C)}{1+QC}\omega^2\right)^{-N}$$
$$- \frac{1}{8}\frac{Q^2C^2}{1+QC}\left[1 + 2(1-C)\left(\frac{8}{C^2} + \frac{Q^2}{1+QC}\right)\omega^2\right]^{-N}$$
$$\times \cos\left[4NC^{-1}\omega(1+QC)^{\frac{1}{2}}\right]$$

and

$$\lim_{N\to\infty} N^{-1}\ln\left[\langle|D_N(i\omega)|^2\rangle_c\right] = -\ln\left(1 - 2\frac{Q^2(1-C)}{1+QC}\omega^2\right)$$
$$\cong 2\frac{Q^2(1-C)}{1+QC}\omega^2, \quad \omega \ll 1,$$

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Heat Flow in Regular and Disordered Harmonic Chains*

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We investigate the steady state heat flux J in a large harmonic crystal containing different masses whose ends are in contact with heat baths at different temperatures. Calling ΔT the temperature difference and $\mathfrak{L}$ the distance between the ends, we are interested in the behavior of $J/\Delta T$ as $\mathfrak{L} \to \infty$. For a perfectly periodic harmonic crystal, $J/\Delta T$ approaches a fixed positive value as $\mathfrak{L} \to \infty$ corresponding to an infinite heat conductivity. We show that this will be true also for a general one-dimensional harmonic chain (arbitrary distribution of different masses) if the spectral measure of the infinite chain contains an absolutely continuous part. We also show that for an infinite chain containing two different masses, the cumulative frequency distribution is continuous and that the spectrum is not exhausted by a denumerable number of points, i.e., the spectrum cannot consist entirely of point eigenvalues with a denumerable number of limit points. Using a theorem of Matsuda and Ishii, we show that for a random chain, corresponding to the mass at each site being an independent random variable, the heat flux approaches zero as $\mathfrak{L} \to \infty$, with probability one. This implies that the spectrum of a disordered chain has, with probability one, no absolutely continuous part.

1. INTRODUCTION

Equilibrium statistical mechanics as developed by Gibbs gives a prescription for calculating the free energy of an arbitrary physical system from its microscopic Hamiltonian. It is natural to ask whether this prescription really yields, for systems containing very many particles, free energy densities with the properties required of them by macroscopic thermodynamic theory? While this question can be readily answered in the affirmative for idealized systems such as "ideal" gases and "ideal" harmonic crystals, it is only more recently that this and more was proven rigorously for systems with realistic interactions between their microscopic constituents.[1] This puts equilibrium statistical mechanics in a sound mathematical position, notwithstanding the fact that actual computations on complex real systems can still only be done in approximate ways. At least we know that the quantities we are trying to compute really exist.

The situation in nonequilibrium statistical mechanics is much less satisfactory. Results comparable to those obtained for equilibrium statistical mechanics are not yet in sight. In particular, there is no proof at present that it is possible, even in principle, to compute transport coefficients, e.g., heat conductivity, viscosity, etc., from the microscopic Hamiltonian of a system. (We are speaking here of a "proof" not of faith followed, or preceded, by approximate computations.

Such computations are very important, perhaps the most important thing to do, but they do not constitute a proof and might just be wrong.) These coefficients play the same role in macroscopic transport theory as the pressure, specific heat, etc., do in macroscopic equilibrium theory. All we can do rigorously at present is to study the nonequilibrium behavior of model systems with well-defined Hamiltonians. Even here we are, however, in a worse situation than in the equilibrium case. It was discovered quite early that the nonequilibrium properties (unlike the equilibrium properties) of the ideal gas and the ideal harmonic, crystal differ qualitatively from those of real systems. In particular, it is impossible to define transport coefficients for these systems. We are therefore forced, in studying transport processes, to use more complex models than the ideal systems mentioned earlier. One such model system, which *may* have well-defined transport coefficients, is the random harmonic crystal which we shall study in this paper.[2]

To be more specific, we wish to find the "steady state" energy flux in a system in contact with heat reservoirs at different temperatures T_α. Following the general principles of statistical mechanics,[3] we identify the observable properties of such a system with averages over a "suitable" phase space ensemble. To obtain such a Gibbs ensemble, we use a formalism developed in earlier papers[4,5] and look for the stationary solution of a generalized Liouville equation having the form

$$\frac{\partial \mu(x,t)}{\partial t} + (\mu, H) = \sum_\alpha \int [\mathcal{K}_\alpha(x,x')\mu(x',t) - \mathcal{K}_\alpha(x',x)\mu(x,t)]\,dx'. \tag{1.1}$$

Here x is a point in the phase space of the system, $H(x)$ is the Hamiltonian of the system, (μ, H) is the Poisson bracket describing the motion of the isolated system, and $\mathcal{K}_\alpha(x,x')\,dx\,dt$ is the conditional probability that when the system is at the point x' in its phase space it will, due to its interaction with the αth reservoir, make a transition to the volume element dx, about x, in the time interval dt. It is assumed here that the reservoirs are "stationary" so that the $\mathcal{K}_\alpha$ are independent of the time. Multiplying (1.1) by H and integrating over x, we obtain

$$\frac{\partial \langle H\rangle}{\partial t} = \sum_\alpha \int \mathcal{K}_\alpha(x,x') \times [H(x) - H(x')]\mu(x',t)\,dx\,dx' = \sum_\alpha J_\alpha, \tag{1.2}$$

where J_α is the energy flux from the αth reservoir. (We refer the reader to Refs. 4 and 5 for a detailed discussion.)

The stationary ensemble density is obtained from (1.1) by setting the time derivative there equal to zero. When all the reservoirs have the same temperature, this will be an equilibrium canonical ensemble while for reservoirs at different temperatures this ensemble will represent a system in a steady nonequilibrium state through which heat is flowing. In the steady state we have, of course, $\sum J_\alpha = 0$. Thus, if the geometry is set up in such a way that the system is in contact with only two reservoirs, one "on the left" at a temperature T_L and "one on the right" at a temperature T_R with $T_L > T_R$, and if the system has a uniform "cross section" S and "length" $\mathfrak{L}$, then we expect that in the stationary state the heat flux $J = J_L = -J_R$ should, for macroscopic size systems, be related via Fourier's law to the average temperature gradient $(T_L - T_R)/\mathfrak{L}$. More precisely, J should have the property that the quantity $\kappa(\mathfrak{L}) \equiv (J/S)/[(T_L - T_R)/\mathfrak{L}]$ should approach a well-defined limit κ when $\mathfrak{L} \to \infty$. If this κ exists, we would identify it with the heat conductivity of the system at temperature T when $T_L \to T_R \to T$.

This formalism was applied in I to a harmonic crystal with some particular forms of interaction with the heat reservoirs. The stationary nonequilibrium ensemble density for such a harmonic system was found to be a generalized Gaussian. The covariance matrix of this Gaussian was obtained there explicitly for a one-dimensional chain of equal masses with nearest neighbor interactions whose end atoms are in contact with heat reservoirs at temperature T_L and T_R. Identifying the number of particles in the chain with its length $\mathfrak{L}$, it was found there that, in the stationary nonequilibrium state, $\kappa(\mathfrak{L}) \sim \mathfrak{L}$, i.e., the heat flux achieves a constant value, for fixed $T_L - T_R$, independent of the length of the chain $\mathfrak{L}$. A similar result obtains for any perfectly periodic harmonic crystal corresponding to an "infinite" heat conductivity if one can speak of a heat conductivity in this case.[6] We therefore thought it of interest to investigate the case of a random harmonic crystal, i.e., what happens, in the same situation, to a crystal whose atoms are not all of the same mass, with the different masses distributed at "random." There seems to be no *a priori* way of deciding on what should happen in this case. On the one hand, it seems reasonable, and in apparent agreement with some machine computations,[7] that such a system would have, even in only one dimension, a well-defined heat conductivity; the reasoning is that the normal modes are scattered by the impurities inhibiting the flow of energy. On the

other hand, one can argue for a behavior similar to that found in the regular chain since the system is still harmonic. A computation by Matsuda and Ishii[8] suggests a compromise giving a $\kappa(\mathfrak{L}) \sim \sqrt{\mathfrak{L}}$, i.e., $J \sim \mathfrak{L}^{-\frac{1}{2}}$ for fixed $T_L - T_R$ (cf. also Ref. 9).

In this paper we describe our work on this problem. Unfortunately, we do not have a definite result for the asymptotic behavior of $\kappa(\mathfrak{L})$ but can show rigorously only that the heat flux J will not vanish as $\mathfrak{L} \to \infty$ if the spectral measure of the infinite chain has an absolutely continuous part. We also show, using a theorem of Matsuda and Ishii,[8] that, for a random chain, $J \to 0$ as $\mathfrak{L} \to \infty$ with probability one with $\langle J \rangle \geq O(\mathfrak{L}^{-\frac{3}{2}})$. This may suggest that the eigenfrequencies of a disordered chain are all isolated, but this is not so, as we show that the spectrum of an infinite chain in which the masses can have only two different values contains a nondenumerable infinity of points and is thus, in particular, not exhausted by a set of discrete eigenvalues having a denumerable number of accumulation points. This result is based on a proof that the cumulative frequency distribution of such a chain is continuous. These results suggest that the spectrum of a disordered chain may be of the singular continuous type, i.e., its continuous spectrum may have its support in a kind of Cantor set. They also raise the possibility that in more realistic systems, too, the existence of transport coefficients may require the absence of an absolutely continuous spectrum, while the irreversible decay of local disturbances requires the absence of localized bound states (corresponding to a point spectrum). Our results are based on a new general formalism for expressing J which brings out its relation to the normal mode spectrum. This also yields some new results for periodic chains showing explicitly how their infinite heat conductivity arises from their having an absolutely continuous spectrum.

2. FORMAL EXPRESSION FOR HEAT FLUX IN GENERAL HARMONIC SYSTEM

We consider a harmonic crystal made up of particles of masses $m_j, j = 1, \cdots, A$. (In I we assumed that all particles have the same mass.) Some of these particles are coupled to external heat reservoirs which are labeled by the same index as the particles. The particles of the jth reservoir, which interact via impulsive collisions with the jth crystal atom, have (prior to each collision) a Maxwellian velocity distribution with temperature T_j. Assuming that the masses of the jth reservoir particles are very small compared to m_j, the integral operators on the right side of (1.1) become Fokker–Planck type differential operators[4,5] and the generalized Liouville equation for $\mu(x, t)$ assumes the form, cf. Eq. (I.2.2),

$$\frac{\partial \mu(x,t)}{\partial t} = \sum_{i,j=1}^{2N} \left\{ \frac{\partial}{\partial x_i} (a_{ij} x_j \mu) + \tfrac{1}{2} d_{ij} \frac{\partial^2 \mu}{\partial x_i \partial x_j} \right\}. \quad (2.1)$$

Here x_i, $i = 1, \cdots, N$, $N \equiv sA$ (s the dimensionality of the space) are the Cartesian coordinates of the particles relative to their equilibrium positions. x_1, x_2, x_s are the coordinates of particle one, etc., while x_j, $j = i + N$, is the momentum conjugate to x_i, a and d are $2N \times 2N$ matrices made up of $N \times N$ matrices

$$\mathsf{a} = \begin{pmatrix} 0 & -\mathsf{M}^{-1} \\ \mathbf{\Phi} & \mathsf{L} \end{pmatrix}, \quad \mathsf{d} = \begin{pmatrix} 0 & 0 \\ 0 & 2\mathsf{MLT} \end{pmatrix}. \quad (2.2)$$

Here $\mathbf{\Phi}$ is the positive-definite symmetric force matrix of the system, M is the diagonal mass matrix of the system (with $M_{11} = M_1, \cdots, M_{ss} = M_s$, etc.), T is the diagonal temperature matrix of the reservoirs (with $T_{11} = T_1, \cdots, T_{ss} = T_s$, etc., and we have set Boltzmann's constant equal to 1), and L is a diagonal matrix with positive or zero elements which describes the reservoir system coupling; $L_{11} = \lambda_1, \cdots, L_{ss} = \lambda_s$, etc., with the λ_i the Fokker–Planck friction constant between the ith crystal atom and the ith reservoir, λ_i being zero if the ith particle is not coupled to any reservoir (cf. I, Sec. 2).

The fundamental solution of Eq. (1.1) can be shown[5] to be a generalized Gaussian. The time evolution of the moments of the distribution function μ may be obtained directly from (1.1) and are seen to satisfy the equations

$$\frac{d\langle x \rangle}{dt} = -\mathsf{a}\langle x \rangle, \quad \langle x_i \rangle \equiv \int x_i \mu(x,t)\, dx, \quad (2.3)$$

$$\frac{d\langle xx \rangle}{dt} = \mathsf{d} - \mathsf{a}\langle xx \rangle - \langle xx \rangle \mathsf{a},$$

$$\langle x_i x_j \rangle = \int x_i x_j \mu(x,t)\, dx. \quad (2.4)$$

The solutions of (2.3) and (2.4) are

$$\langle x(t) \rangle = \exp[-\mathsf{a}t]\langle x(0) \rangle, \quad (2.5)$$

$$\langle x(t)x(t) \rangle = \exp[-\mathsf{a}t]\langle x(0)x(0) \rangle \exp[-\tilde{\mathsf{a}}t] + \int_0^t ds \exp[-\mathsf{a}s]\mathsf{d} \exp[-\tilde{\mathsf{a}}s] \quad (2.6)$$

where $\tilde{\mathsf{a}}$ denotes the transpose of a.

The requirement that $\mathbf{\Phi}$ be positive definite ensures that none of the eigenvalues of $\mathbf{\Phi}$ vanishes. The further requirement that if Q is an eigenvector of $\mathbf{\Phi}$, then $\mathsf{LMQ} \neq 0$ (i.e., there are no normal modes of the isolated system for which *all* the particles which are in contact with the external reservoirs are always

at their equilibrium positions[10]) insures that all eigenvalues of a have positive real parts. This can be readily seen by noting that if $\boldsymbol{\xi} = (\mathbf{Q}; \mathbf{P})$ is an eigenvector of a with eigenvalue α, i.e., $\xi_i = Q_i$ for $i \leq N$, $\xi_{i+N} = P_i$, then we have

$$\tilde{\mathbf{Q}}\boldsymbol{\Phi}\mathbf{Q} - \alpha\tilde{\mathbf{Q}}\mathsf{LM}\mathbf{Q} + \alpha^2\tilde{\mathbf{Q}}\mathsf{M}\mathbf{Q} = 0. \quad (2.7)$$

Since LM is a positive (diagonal) matrix, we see that if α is real, it has to be positive while, if $\operatorname{Im}\alpha \neq 0$, we find by taking the imaginary part of (2.7) that

$$\operatorname{Re}\alpha = \tfrac{1}{2}(\tilde{\mathbf{Q}}\mathsf{LM}\mathbf{Q})/(\tilde{\mathbf{Q}}\mathsf{M}\mathbf{Q}) > 0. \quad (2.8)$$

Returning now to (2.5) and (2.6), we see that $\langle x(t)\rangle$ vanishes as $t \to \infty$ and

$$\lim_{t\to\infty}\langle x(t)x(t)\rangle = \int_0^\infty ds \exp[-\mathsf{a}s]\mathsf{d}\exp[-\tilde{\mathsf{a}}s]. \quad (2.9)$$

Hence the suitable stationary Gibbsian ensemble describing our harmonic system is a Gaussian with the covariance matrix (2.9) which thus contains all the information about the macroscopic properties of the stationary state. In order to obtain this covariance matrix in a more convenient form, we define the two $N \times N$ matrices

$$[\mathsf{F}(t)]_{ij} = [\exp(-\mathsf{a}t)]_{i,N+j},$$
$$[\mathsf{G}(t)]_{ij} = [\exp(-\mathsf{a}t)]_{N+i,N+j},$$
$$i,j = 1,\cdots,N. \quad (2.10)$$

Using the explicit form of a in (2.2), we find that $\mathsf{F}(t)$ and $\mathsf{G}(t)$ satisfy the equations

$$\mathsf{M}\dot{\mathsf{F}}(t) = \mathsf{G}(t); \quad \mathsf{M}\ddot{\mathsf{F}}(t) + \mathsf{ML}\dot{\mathsf{F}}(t) + \boldsymbol{\Phi}\mathsf{F} = 0, \quad (2.11)$$

with the initial conditions $\mathsf{F}(0) = 0$, $\mathsf{G}(0) = 1$ (the unit matrix).

It is now readily seen that

$$(2\pi)^{-1}\int_{-\infty}^{\infty} d\omega e^{-i\omega t}\mathsf{Z}^{-1}(\omega) = \begin{cases}\mathsf{F}(t) & \text{for } t \geq 0\\ 0 & \text{for } t < 0\end{cases}, \quad (2.12)$$

where $\mathsf{Z}(\omega)$ is an $N \times N$ matrix

$$\mathsf{Z}(\omega) = \boldsymbol{\Phi} - i\omega\mathsf{ML} - \omega^2\mathsf{M}. \quad (2.13)$$

Use has been made here of (2.7) and (2.8), which show that all the zeros of $\mathsf{Z}(\omega)$ are in the lower half of the complex ω plane occurring at values of $\omega = -i\alpha$, α an eigenvalue of a. We may now express the stationary correlations (2.9) in terms of the impedance matrix $\mathsf{Z}(\omega)$. Decomposing $\langle x(\infty)x(\infty)\rangle$ into four $N \times N$ matrices, we find

$$\langle q(\infty)q(\infty)\rangle = \pi^{-1}\int_{-\infty}^{\infty} d\omega\mathsf{Z}^{-1}(\omega)\mathsf{LMT}\mathsf{Z}^{-1}(-\omega), \quad (2.14a)$$

$$\langle q(\infty)p(\infty)\rangle\mathsf{M}^{-1} = \pi^{-1}\int_{-\infty}^{\infty} d\omega\mathsf{Z}^{-1}(\omega)[i\omega\mathsf{LMT}]\mathsf{Z}^{-1}, \quad (2.14b)$$

$$\mathsf{M}^{-1}\langle p(\infty)p(\infty)\rangle\mathsf{M}^{-1} = \pi^{-1}\int_{-\infty}^{\infty} d\omega\mathsf{Z}^{-1}(\omega)[\omega^2\mathsf{LMT}]\mathsf{Z}^{-1}(-\omega). \quad (2.14c)$$

Equations (2.14) may be evaluated explicitly for the case when all the reservoirs have the same temperature $T_i = T$. We expect that in this case the stationary ensemble will be the canonical equilibrium ensemble with temperature T. This can be readily confirmed for (2.14c), for example. Noting that the matrix $-\omega\mathsf{LM}$ is just the imaginary part of $\mathsf{Z}(\omega)$, we find

$$\mathsf{M}^{-1}\langle p(\infty)p(\infty)\rangle\mathsf{M}^{-1} = T(2\pi i)^{-1}\int_{-\infty}^{\infty} d\omega[\mathsf{Z}^{-1}(\omega) - \mathsf{Z}^{-1}(-\omega)]\omega = 2T\operatorname{Re}\left\{(2\pi i)^{-1}\int_{-\infty}^{\infty} d\omega[\omega\mathsf{Z}^{-1}(\omega)]\right\}. \quad (2.15)$$

Closing the contour of integration in (2.15) along an infinite semicircle in the upper half-plane yields the expected result

$$\langle p(\infty)p(\infty)\rangle = \mathsf{M}T, \quad \text{when } T_l = T \text{ for all } l. \quad (2.16)$$

Incidentally we have found the sum rule

$$\pi^{-1}\int_{-\infty}^{\infty} d\omega\mathsf{Z}^{-1}(\omega)[\omega^2\mathsf{ML}]\mathsf{Z}^{-1}(-\omega) = \mathsf{M}^{-1}. \quad (2.17)$$

When the temperatures are not all the same, heat flows into the system from the different reservoirs. Applying (1.2) to our system, we find at all times

$$\langle\dot{H}(t)\rangle = \sum_j \lambda_j[T_j - m_j^{-1}\langle p_j^2(t)\rangle] = \sum_j J_j(t). \quad (2.18)$$

For the heat flux in the steady state, we have, using (2.14) and (2.17),

$$J_l = \sum_j (T_l - T_j)\lambda_l m_l m_j\lambda_j(\pi^{-1})\int_{-\infty}^{\infty} d\omega\omega^2\,|[\mathsf{Z}^{-1}(\omega)]_{lj}|^2. \quad (2.19)$$

Note that due to the symmetry of $\mathsf{Z}(\omega)$ the sum over all J_l vanishes as it should in a steady state.

Henceforth we shall specialize to the case of two heat reservoirs of temperatures T_L and T_R, coupled with equal strength λ to the first and last particles of a one-dimensional chain which consists of A particles, i.e., $T_1 = T_L$, $T_A = T_R$, $\lambda_1 = \lambda_A = \lambda$, $\lambda_j = 0$ for $j \neq 1, A$. Designating $\det[\boldsymbol{\Phi} - \omega^2\mathsf{M}]$ by K, we note that the cofactor C_{1A} of Z_{1A} is equal to that of $(\boldsymbol{\Phi} - \omega^2\mathsf{M})_{1A}$ and that $\det\mathsf{Z}$ may be expressed as a

quadratic function of λ. We are thus led to

$$J = (T_L - T_R)\lambda^2 m_1 m_A \int_{-\infty}^{\infty} \frac{d\omega}{\pi} \frac{\omega^2 |C_{1A}(\omega)|^2}{(K_{1,A} - \lambda^2\omega^2 m_1 m_A K_{2,A-1})^2 + \lambda^2\omega^2(m_A K_{1,A-1} + m_1 K_{2,A})^2}, \quad (2.20)$$

where $K_{l,m}(\omega^2)$ is det $(\Phi - \omega^2 M)$ for a chain which starts from the lth particle and ends with the mth one.

Restricting the system further by assuming nearest neighbor forces of unit strength with particles 1 and A tied by springs to fixed positions

$$\Phi_{ij} = 2\delta_{ij} - \delta_{i+1,j} - \delta_{i,j+1}, \quad i, j = 1, \cdots, A, \quad (2.21)$$

leads to $|C_{1A}|^2 = 1$. Moreover, both $K_{1,A}$ and $K_{2,A}$ now satisfy the same recursion relation, namely

$$K_{j,A} = (2 - m_A\omega^2)K_{j,A-1} - K_{j,A-2}, \quad j = 1, 2, \cdots. \quad (2.22)$$

Using Eq. (2.22) for A and $A - 1$ leads to

$$K_{1,A}K_{2,A-1} - K_{1,A-1}K_{2,A} = \text{const independent of } A. \quad (2.23)$$

Evaluating (2.23) for $A = 2$ yields

$$K_{1,A}K_{2,A-1} - K_{1,A-1}K_{2,A} = -1. \quad (2.24)$$

This enables us to eliminate the cross terms in the denominator of Eq. (2.20) with the result

$$\begin{aligned} J_A &= (T_L - T_R)m_1 m_A \frac{\lambda^2}{\pi} \int_{-\infty}^{\infty} d\omega\omega^2/[2m_1 m_A\lambda^2\omega^2 \\ &\quad + (K_{1,A}^2 + \lambda^2\omega^2 m_A^2 K_{1,A-1}^2) \\ &\quad + \lambda^2\omega^2 m_1^2(K_{2,A}^2 + \lambda^2\omega^2 m_A^2 K_{2,A-1}^2)] \\ &\equiv (T_L - T_R)\int_0^{\infty} d\omega j_A(\omega). \end{aligned} \quad (2.25)$$

Equation (2.25) is an expression for the steady state heat flux in a harmonic chain containing A particles with masses $m_1, m_2, \cdots, m_A$. We shall be interested from now on in the behavior of the right side of (2.25) as $A \to \infty$.

3. PERIODIC CHAINS

We shall now specialize the analysis of the last section to the case of a periodic chain with a unit cell containing C particles of masses $m_1, \cdots, m_C$, $m_{C+1} = m_1$, etc. The chain contains N such cells, $A = NC$. It will be shown that for this system the heat flux in (2.25) does not vanish when $N \to \infty$ (i.e., the "heat conductivity" grows proportionally to the length of the chain as discussed in Sec. 1).

To proceed we note that the recursion relation (2.22) may be written as a 2×2 matrix equation[8]

$$\begin{aligned} Q_A &\equiv \begin{pmatrix} K_{1,A} & -K_{2,A} \\ K_{1,A-1} & -K_{2,A-1} \end{pmatrix} \\ &= \begin{pmatrix} 2 - m_A\omega^2 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} K_{1,A-1} & -K_{2,A-1} \\ K_{1,A-2} & -K_{2,A-2} \end{pmatrix} \\ &= Q_1 Q_{A-1}, \end{aligned} \quad (3.1)$$

where $K_{1,1} = 2 - m_1\omega^2$, $K_{1,0} = K_{2,1} = 1$, $K_{2,0} = 0$. This leads immediately for $A = NC$ to

$$Q_A = (Q_C)^N. \quad (3.2)$$

The behavior of the integrand in (2.25) depends on the eigenvalues of Q_C. Since Q_C is unimodular and real its eigenvalues have the form $\exp(\pm iq)$ with q real or pure imaginary. In fact q is real whenever ω is such that

$$-2 \leq \text{tr } Q_C \equiv K_{1,C} - K_{2,C-1} = 2\cos q \leq 2. \quad (3.3)$$

This corresponds to wave vectors q with which waves will propagate through the lattice with one of the frequencies in the band $\omega_j(q)$, $j = 1, \cdots, C$. The $\omega_j^2(q)$ are the C roots of the polynomial equation $\text{tr } Q_C(\omega^2) = 2\cos q$, $\text{tr } Q_C$ being a polynomial of order C in ω^2 and the $\omega_j^2(q)$ are positive for q real. To see that there is always some range of ω for which q is real we note that, for $\omega = 0$, Q_C has the form

$$Q_C(0) = \begin{pmatrix} C + 1 & -C \\ C & -C + 1 \end{pmatrix} \quad (3.4)$$

so that $\text{tr } Q_C(0) = 2$. The first-order correction to the trace is negative:

$$\text{tr } Q_C = 2 - \omega^2 C \sum_{\nu=1}^{C} m_\nu + O(\omega^2). \quad (3.5)$$

There will thus always be some $\omega_0 > 0$ such that $|\text{tr } Q_C| \leq 2$ for $0 \leq \omega \leq \omega_0$.

Returning now to (3.2), we may verify that

$$\begin{aligned} Q_A = [Q_C]^N &= [\cos Nq]\,\mathbb{1} \\ &\quad + [(\sin Nq)/\sin q][Q_C - (\cos q)\,\mathbb{1}], \end{aligned} \quad (3.6)$$

where $\mathbb{1}$ is the 2×2 unit matrix. We now note that the denominator of the integrand in (2.25) can be written as $|z_A|^2$, where z_A is the matrix element

$$z_A = (1, -i\lambda m_A\omega)Q_A \begin{pmatrix} 1 \\ i\lambda m_2\omega \end{pmatrix}. \quad (3.7)$$

Using (3.5), we find

$$z_A = (1 + \lambda^2\omega^2 m_1 m_C)\cos Nq + (\sin Nq/\sin q) \times [z_C - (1 + \lambda^2\omega^2 m_1 m_C)\cos q], \quad (3.8)$$

where

$$z_C = [K_{1,C} - \lambda^2 m_1 m_C \omega^2 K_{2,C-1}] - i\lambda\omega[m_1 K_{2,C} + m_C K_{1,C-1}]. \quad (3.9)$$

By writing $J(N, C)$ for J_A, Eq. (2.25) now assumes the form

$$J(N, C) = [(T_L - T_R)m_1 m_C \lambda^2 \pi^{-1}] \times \int_{-\infty}^{\infty} d\omega\omega^2 |(1 + \lambda^2\omega^2 m_1 m_C)\cos Nq + (\sin Nq/\sin q) \times [z_C - (1 + \lambda^2\omega^2 m_1 m_C)\cos q]|^{-2}. \quad (3.10)$$

The dependence of the heat flux on N, the number of cells of the chain, is entirely explicit in (3.10), z_C depending on ω (or q) but is independent of N. We note that as $N \to \infty$ only values of ω (more properly intervals of ω) for which q is real $|K_{1,C} - K_{2,C-1}| \leq 2$ will make a finite contribution to $J(N, C)$, since for imaginary q the integrand will decrease exponentially with N. Hence, to obtain $J(N, C)$ as $N \to \infty$, we may change variables from ω to q and restrict the range over q to the interval $[0, 2\pi]$. For large N the terms in the integrand of (3.10) which do not involve Nq may be regarded as constant while Nq changes by 2π. Calling the integrand in (3.10) $F(q, Nq)$, we may write

$$\int_0^{2\pi} dqF(q, Nq) = \sum_{j=0}^{N-1} \int_{2\pi j/N}^{2\pi(j+1)/N} dqF(q, Nq) = \frac{1}{2\pi}\sum_{j=0}^{N-1} \frac{2\pi}{N}\int_{2\pi j}^{2\pi(j+1)} dxF\left(\frac{x}{N}, x\right) \xrightarrow[N\to\infty]{} \frac{1}{2\pi}\int_0^{2\pi} dq \int_0^{2\pi} F(q, \theta)\, d\theta. \quad (3.11)$$

Carrying out the indicated integration over Nq in (3.10) and going back to the variable ω, we obtain, using also (3.9),

$$\lim_{N\to\infty} J(N, C) = (T_L - T_R)m_1 m_C \lambda\pi^{-1} \int d\omega\, |\omega \sin q| \times |(1 + \lambda^2\omega^2 m_1 m_C)[m_C K_{1,C-1} + m_1 K_{2,C}]|^{-1}, \quad (3.12)$$

the integration being over the region $|K_{1,C} - K_{2,C-1}| \leq 2$ [i.e., over the frequency bands of ω^2: $\min \omega_j^2(k) \leq \omega^2 \leq \max \omega_j^2(k), j = 1, \cdots, C$, which are the solutions of (3.3), $0 \leq k \leq 2\pi$; cf. discussion after Eq. (3.3)]. It is seen from (3.12) that $J \sim \lambda$ for $\lambda \to 0$ and $J \sim \lambda^{-1}$ when $\lambda \to \infty$. This was noted in I, where J was computed for the case of a chain with equal masses, which corresponds to a special case of (3.12) where $C = 1$. In that case, setting $m_1 = m$, we have, $2\cos q = 2 - m\omega^2$, $K_{1,0} = K_{2,1} = 1$, and the integration is over the interval $0 \leq \omega^2 \leq 4/m$. Changing the integration variable to q, we obtain, for the heat flow in an infinite chain with all masses $m_j = m$,

$$J = (T_L - T_R)\lambda(2\pi)^{-1} \times \int_0^{2\pi} dq \sin^2 q[1 + 2m\lambda^2(1 - \cos q)]^{-1} = \tfrac{1}{2}(m^2\lambda^3)^{-1}[T_L - T_R] \times [1 + 2m\lambda^2 - (1 + 4m\lambda^2)^{-\frac{1}{2}}], \quad (3.13)$$

the same result as was obtained in (I.4.6).

4. ASYMPTOTIC HEAT FLUX AND THE SPECTRUM

In this section we shall return to the general formula (2.25) and investigate the connection between the behavior of J_A as $A \to \infty$ and the nature of the spectrum of the semi-infinite chain. [For the periodic chain we have seen in (3.12) that $J_\infty > 0$ is given by an integral over the spectrum of the chain.]

To this end, consider the semi-infinite diagonal matrix M, whose entries are the masses $\{m_\nu\}$, $\nu = 1, 2, \cdots$. The proper frequencies squared of the associated harmonic chain are the eigenvalues of the semi-infinite Hermitian matrix

$$H = \mathsf{M}^{-\frac{1}{2}}\mathbf{\Phi}\mathsf{M}^{-\frac{1}{2}}, \quad (4.1)$$

where $\mathbf{\Phi}$ is the force matrix given in (2.21) with $A = \infty$. Regarded as an operator acting on the Hilbert space of sequences with the L_2 norm, H is bounded, nonnegative, and self-adjoint. In the usual Dirac notation,

$$\langle\nu|\, H\, |\Psi\rangle = -(m_{\nu-1}m_\nu)^{-\frac{1}{2}}\psi_{\nu-1} + 2m_\nu^{-1}\psi_\nu - (m_\nu m_{\nu+1})^{-\frac{1}{2}}\psi_{\nu+1}, \quad \psi_0 \equiv 0. \quad (4.2)$$

$$0 \leq \langle\Psi|\, H\, |\Psi\rangle \leq 4\, \|\Psi\|^2/m', \quad m' = \min\{m_\nu\} = 1, \quad (4.3)$$

and we are assuming that the $\{m_\nu\}$ have a lower bound which we set equal to unity. We see from Eq. (4.3) that the spectral support of H is contained in the interval $[0, 4]$. The spectrum is characterized by the family of spectral projections $E(\lambda)$ satisfying[11]

$$H = \int_0^4 dE(\lambda)\lambda, \quad (4.4)$$

$$E(0) = 0, \quad E(4) = 1. \quad (4.5)$$

Let H operate on the sequence Ψ:

$$\psi_\nu = \sqrt{m_\nu} \cdot K_{\nu-1}(\omega^2), \quad \psi_0 = 0, \tag{4.6}$$

where $K_\nu(\omega^2)$ is the determinant $K_{1,\nu}$ defined in Sec. 2 which satisfies the recurrence relation (2.22), $K_0 = 1$. It is seen from (4.2) that

$$H\Psi = \omega^2\Psi. \tag{4.7}$$

It follows from this that the matrix elements of $E(\lambda)$ can be written in the form[11]

$$\langle \nu | E(\lambda) | \nu' \rangle = (m_\nu m_{\nu'})^{\frac{1}{2}} \int_0^\lambda d\rho(x) K_{\nu-1}(x) K_{\nu'-1}(x), \qquad K_0 = 1, \tag{4.8}$$

where $\rho(x)$ is the spectral measure of H with respect to the vector $|1\rangle$. Since for cyclic vectors the different spectral measures of H are "equivalent," we shall refer to ρ simply as the spectral measure of H. The spectrum of H is the support of the measure $\rho(x)$. It follows from (4.5) and (4.8) that

$$\rho(x) = 0 \text{ for } x < 0, \quad \rho(x) = m_1^{-1} \text{ for } x > 4, \tag{4.9}$$

$$\int_0^4 d\rho(x) K_\nu^2(x) = m_{\nu+1}^{-1} \leq 1. \tag{4.10}$$

[For a chain with all $m_\nu = m$, $\rho'(x) = \pi^{-1}(x/m)^{\frac{1}{2}}(1 - x/4)^{\frac{1}{2}}$ for $0 \leq x \leq 4$].

It is seen from (4.10) that if $\rho(x)$ has an absolutely continuous part with support in a set X of Lebesgue measure $\delta > 0$, then $\exists\, B, B < \infty$, such that $d\rho(x)/dx > B^{-1}$ for $x \in X$ and thus

$$\int_X dx K_\nu^2(x) < B. \tag{4.11}$$

Furthermore, the determinants $K_{2,\nu}(\omega^2)$ which also occur in Eq. (2.25) play the same role with respect to an identical chain except for the first mass which is set equal to ∞. The operator H associated with this chain differs from H in (4.1) by a 2×2 matrix. Hence the absolutely continuous parts of their spectra coincide.[11] We now find, on assuming that the masses m_ν have also an upper bound, that the integral of the reciprocal of the integrand in (2.25) over a set $X' \subset X$

$$\int_{X'} d\omega j_A^{-1}(\omega) \leq B' < \infty, \tag{4.12}$$

where X' is the set $X - [0, \delta/2]$ and B' is a constant independent of A. It therefore follows by the Schwartz inequality that J_A is bounded below, i.e., $\exists \epsilon > 0$ such that

$$J_A \geq \epsilon(T_L - T_R) \quad \text{for all} \quad A \tag{4.13}$$

for fixed $\lambda \neq 0$. Hence we conclude that if the spectrum of the infinite chain with bounded masses $\{m_\nu\}$ has an absolutely continuous part, then the heat conductivity of a segment containing $\mathfrak{L}$ particles has a lower bound $\kappa(\mathfrak{L}) \geq \epsilon(\mathfrak{L})$ and thus *a priori* goes to infinity as $\mathfrak{L} \to \infty$.

We shall now use a theorem of Matsuda and Ishii,[8] which they derived on the basis of a theorem by Furstenberg, to show that for almost all random chains the heat flux $J_A \to 0$ as $A \to \infty$. By a random chain we mean a chain whose masses $m_1, m_2, \cdots$ are a sequence of independent positive random variables with a common distribution $p(m)$ which gives a nonvanishing probability for at least two different masses. A weak form of the Matsuda–Ishii theorem states that for such a chain

$$K_N^2(\eta) \to \infty \quad \text{as} \quad N \to \infty \quad \text{for all} \quad \eta \neq 0, \tag{4.14}$$

with probability one.

It follows from our previous discussion that when $m_\nu \geq 1$ for all possible chains, only the interval $0 \leq \omega \leq 2$ can make a finite contribution to the integral in (2.25). We therefore have

$$J_A = (T_L - T_R) \int_0^2 d\omega j_A(\omega). \tag{4.15}$$

Taking the average of J_A over the probability distribution of the masses m_ν, we have

$$\langle J_A \rangle = (T_L - T_R) \int_0^2 d\omega \langle j_A(\omega) \rangle. \tag{4.16}$$

It follows from (4.14) that

$$\langle j_A(\omega) \rangle \to 0 \quad \text{for} \quad 0 < \omega \leq 2. \tag{4.17}$$

We also have from (2.25) that

$$j_A(\omega) \leq (2\pi)^{-1} \quad \text{for all} \quad \omega; \tag{4.18}$$

hence, by the Lebesgue theorem,[12]

$$\lim_{A \to \infty} \langle J_A \rangle = 0. \tag{4.19}$$

Since $J_A \geq 0$, it follows from (4.19) that for any $\delta > 0$

$$\text{Prob}\,(J_A \geq \delta, \text{ for all } A) = 0. \tag{4.20}$$

Combining (4.20) with our previous result (4.13), we find that the probability that the spectrum of an infinite random chain has an absolutely continuous part is zero.

It will be shown in the next section that the spectrum of a chain containing two different masses cannot consist entirely of a denumerable number of points. Since it will also with probability one not contain an absolutely continuous part, it will "generally" either contain a singular continuous part or have a point

spectrum with a nondenumerable number of limit points.

5. FREQUENCY DISTRIBUTION FUNCTION AND SPECTRUM OF A BINARY CHAIN

We shall be concerned in this section with the simplest type of chain containing unequal masses, i.e., the mass of the νth atom m_ν can take on only two values,

$$m_\nu = 1 \text{ or } M, \quad M > 1, \quad \nu = 1, 2, \cdots, \infty. \tag{5.1}$$

The "average" properties of this system when the $\{m_\nu\}$ are assumed to be a set of independent random variables have, as mentioned earlier, been extensively investigated.[2] We recall this here only to emphasize that the main discussion in this section is *not* concerned with any probability distributions or averages but pertains to a specific chain with specified $\{m_\nu\}$ for *all* positive integer ν.

As was done in the last section, we let H denote the semi-infinite matrix $\mathsf{M}^{-\frac{1}{2}}\mathbf{\Phi}\mathsf{M}^{-\frac{1}{2}}$. We also let H_A denote the $A \times A$ matrix consisting of the first A rows and columns of H. The eigenvalues of H_A, which are the squares of the normal frequencies of the chain containing A atoms with masses m_ν, $\nu = 1, \cdots, A$, are the zeros of the equation $K_A(\eta) = 0$ and will be designated by η_A^i, $i = 1, \cdots, A$. As is well known, $0 < \eta_A^i < 4$ and all the η_A^i are distinct for M finite. Let $AG_A(\eta)$ be the number of eigenvalues of H_A which are smaller than η. $G_A(\eta)$ is a monotonic step function,

$$G_A(\eta) = A^{-1} \sum_{\eta_A^i < \eta} 1, \quad G_A(0) = 0, \quad G_A(4) = 1, \tag{5.2}$$

i.e., $G_A(\eta)$ is the integrated normalized density of states. Since a set of uniformly bounded monotonic positive functions is compact, it is always possible to choose a subsequence of $G_A(\eta)$ which will converge to a function $G(\eta)$ as $A \to \infty$.

$G(\eta)$ need not be unique as may be seen by considering a chain for which $m_\nu = 1$, $\nu \leq N$, $m_\nu = M$, $N < \nu \leq N^2$, $m_\nu = 1$, $N^2 < \nu \leq N^4$, etc., with $N > 1$. Lederman's theorem [cf. Ref. 2(a)] asserts that the change in the number of eigenvalues of H_A in a given interval $[\eta_1, \eta_2]$ when a given number, say T, of the masses m_ν are changed is bounded by T. It is thus readily seen that we may choose sequences $G_A(\eta)$ which will converge to either $G^{(1)}(\eta)$ or $G^{(m)}(\eta)$, where $G^{(m)}(\eta)$ is the frequency distribution of the infinite chain, all of whose masses are equal to m.

We shall now show that

$$G(\eta) \text{ is continuous,} \tag{5.3}$$

the spectrum of the infinite chain, i.e., of H, contains a nondenumerable infinity of points. (5.4)

Following Rubin,[7] let $A_1, A_2, \cdots$ designate the positions of the heavy mass particles, $m_{A_\nu} = M$, and let $a_\nu = A_\nu - A_{\nu-1}$ with $A_0 \equiv 0$. Define the variable k and the quantity Δ by

$$\omega = 2 \sin (k/2), \quad \Delta(k) = (M - 1) \tan (k/2), \tag{5.5}$$

and note that $0 \leq \omega \leq 2$ corresponds to $0 \leq k \leq \pi$. It may now be verified that the determinants K_N satisfying the recurrence relation (2.22) can be expressed, for $A_\nu \leq N < A_{\nu+1}$, as

$$K_N = |R_\nu| \, (\sin k)^{-1} \sin [\tfrac{1}{2}\theta(N)], \tag{5.6}$$

where (suppressing the dependence on ω or k whenever possible)

$$R_0 = 1, \quad R_\nu = r_\nu R_{\nu-1},$$
$$r_\nu = 1 - i\Delta + i\Delta e^{i\theta_\nu}, \quad \nu \geq 1, \tag{5.7}$$
$$\theta(N) = \theta_{\nu+1} - 2k(A_{\nu+1} - N - 1),$$
$$A_\nu \leq N < A_{\nu+1}. \tag{5.8}$$

The $\theta_\nu(k)$ are continuous functions of k with $\theta(0) = 0$ and satisfy the recurrence relations

$$\exp [i(\theta_{\nu+1} - \theta_\nu)] = \exp [2ika_{\nu+1}](\bar{r}_\nu/r_\nu)$$
$$\text{for} \quad \nu \geq 1, \quad \theta_1 = 2kA_1, \tag{5.9}$$

with $\bar{r}_\nu$ denoting the complex conjugate of r_ν. It can be verified that these $\theta_\nu(k)$ and the $\theta(N, k)$ are monotonic functions of k for real k whose derivative with respect to k is given by

$$\frac{d\theta_{\nu+1}}{dk} - 2(A_{\nu+1} - N - 1)$$
$$= \frac{d}{dk}\theta(N)$$
$$= 2\Big((N + 1 - A_\nu) + |R_\nu|^{-2}$$
$$\times \sum_{i=1}^{\nu} (a_i |R_{i-1}^2| + 2\Delta' \sin^2 k \, |K_{A_i-1}^2|)\Big),$$
$$A_\nu \leq N < A_{\nu+1}, \tag{5.10}$$

where

$$\Delta'(k) = (M - 1)/[2 \cos^2 (k/2)]. \tag{5.11}$$

Using the recurrence relation (5.7) yields the bounds

$$0 < C^{-\nu} \leq |R_\nu| \leq [(1 + \Delta^2)^{\frac{1}{2}} + \Delta]^\nu \equiv C^\nu \tag{5.12}$$

so that the zeros of K_N, i.e., the eigenvalues of H_N, occur at those values of k for which $\theta(N, k) = 2\pi j$, with j a positive integer. Since there are altogether N such zeros in the interval $0 < k < \pi$, we must have

$\theta(N, \pi) = 2\pi(N+1)$ [we have here $(N+1)$ rather than N to take care of the zeros of $\sin k$ in the denominator of (5.6)]. In general $G_N(\eta) = j/N$ in the interval $2j\pi < k \leq 2(j+1)\pi$, $j = 0, \cdots, N$ (with the relation $\eta = 4\sin^2 k/2$).

To prove (5.3), we write $K_N(\eta)$ in (5.6) as a product over its zeros

$$K_N = M^{\nu} \prod_{i=1}^{N} (\eta_N^i - \eta), \quad 0 < \eta_N^i < 4, \qquad A_\nu \leq N < A_{\nu+1}. \quad (5.13)$$

A discontinuity at the point $\eta_0 \neq 0$ or 4 ($\eta_0 = 0$ or 4 is excluded by Rayleigh's theorem) in the integrated density of states $G(\eta)$ means that η_0 is an accumulation point for a finite fraction of the zeros η_N^i, i.e., if $f(N, \epsilon)$ is the fraction of zeros of K_N in the interval $I = [\eta_0 - \frac{1}{2}\epsilon, \eta_0 + \frac{1}{2}\epsilon]$, then $N \to \infty$, followed by $\epsilon \to 0, f(N, \epsilon) \to p > 0$. We thus have

$$|K_N|^{1/N} \leq M[4^{(1-f)}\epsilon^f] \quad \text{for} \quad \eta \text{ in } I, \quad (5.14)$$

where $f = f(N, \epsilon)$. On the other hand, $|\sin[\frac{1}{2}\theta(N)]|$ must, according to (5.10), take on the value 1 at Nf points η_N^i inside I. At those points

$$|K_N|^{1/N} = (|R_\nu|/|\sin k|)^{1/N} \geq C^{-\nu/N} \geq C^{-1} \quad (5.15)$$

by (5.12). It is clear that (5.14) and (5.15) cannot be satisfied simultaneously for arbitrary ϵ and $M < \infty$ if $f(N, \epsilon) \to p > 0$ independent of ϵ. We thus conclude that

$$G_N(\eta + \epsilon/2) - G_N(\eta - \epsilon/2) = f(N, \epsilon) \to 0$$

as

$$N \to \infty \quad \text{and} \quad \epsilon \to 0, \quad (5.16)$$

for all η, and thus that $G(\eta)$ is continuous. This will be true for each limiting frequency distribution $G(\eta)$ if there is more than one for the infinite chain in question.

A similar analysis can also be applied to the average cumulative frequency distribution of a random chain[2]

$$\langle G(\eta) \rangle = \lim_{N \to \infty} \langle G_N(\eta) \rangle. \quad (5.17)$$

Taking the logarithms of Eqs. (5.14) and (5.15), we again find that

$$\lim_{\epsilon \to 0} \lim_{N \to \infty} \langle f(N, \epsilon) \rangle = 0 \quad (5.18)$$

and hence $\langle G(\eta) \rangle$ is continuous. The average frequency distribution $\langle G(\eta) \rangle$ determines all the equilibrium thermodynamic properties of the random chain[2] and has been shown elsewhere to be unique.[13,14]

It follows that since $G(\eta)$ increases continuously from 0 to 1 as η goes from 0 to 4 that the points of increase of $G(\eta)$ in the interval $[0, 4]$ are nondenumerable. Indeed it follows from Rayleigh's theorem that the number of normal frequencies in the interval $[(1-\delta)2\pi^{-1}M^{-\frac{1}{2}}\omega, \omega] = [\omega', \omega]$ for a chain containing A atoms of masses 1 and M has a lower bound which may be put in the form

$$G_A(\eta) - G_A(\eta') \geq \delta/\pi \quad \text{for} \quad \eta = \omega^2 < 4, \quad 0 \leq \delta \leq 1. \quad (5.19)$$

Eq. (5.4) now follows if we can show that every point of increase of $G(\eta)$ for $0 < \eta \leq \eta_0$, $\eta_0 > 0$, is in the spectrum of H.

To prove this, assume that the point $\bar{\eta}$ is not in the spectrum of H. Then $\exists\ \epsilon > 0$ such that, for any sequence of normalized vectors[11] $\phi^{(n)}$,

$$\|(H - \eta)\phi^{(n)}\| \geq \epsilon, \quad \|\phi^{(n)}\| = 1 \quad (5.20)$$

whenever $\eta \in I = [\bar{\eta} - \epsilon/2, \bar{\eta} + \epsilon/2]$. The norm here is the L_2 norm in the space of sequences. Let $\phi^{(n)}$ be the sequence obtained by cutting off the sequence Ψ in (4.6) after n terms and normalizing it

$$\phi_j^{(n)} = \begin{cases} m_j^{\frac{1}{2}} K_{j-1}(\eta)/C_n, \\ \qquad 1 \leq j \leq n, \quad C_n = \left(\sum_{l=0}^{n-1} K_l^2 m_{l+1} \right)^{\frac{1}{2}}, \\ 0, \qquad j > n. \end{cases} \quad (5.21)$$

Substitution of the explicit matrix elements of H given in (4.2) into (5.20) yields

$$\|(H - \eta)\phi^{(n)}\| = (m_n^{-1}K_n^2 + m_{n+1}^{-1}K_{n-1}^2) \Big/ \sum_{l=0}^{n-1} K_l^2 m_{l+1} \geq \epsilon, \quad (5.22)$$

or, since $m_\nu \geq 1$, we have for $A_\nu \leq N < A_{\nu+1}$

$$\sum_{l=1}^{N} K_l^2 \leq (1 + \epsilon^{-1})[K_N^2 + K_{N-1}^2] \leq 2C^2(\sin k)^{-2}(1 + \epsilon^{-1})\,|R_\nu|^2, \quad (5.23)$$

where the last inequality follows from (5.6) and (5.12).

On the other hand, it follows from Eqs. (5.6)–(5.9) that

$$|R_\nu|^2 = \{\sin^2 k/\sin^2 \tfrac{1}{2}[\theta(N) - \theta(N-1)]\} \times |K_N - \exp\{\tfrac{1}{2}i[\theta(N) - \theta(N-1)]\}\rho_N K_{N-1}|^2, \quad (5.24)$$

where $A_\nu \leq N < A_{\nu+1}$ and

$$\rho_N = \begin{cases} 1, & \text{if } A_\nu < N, \\ |r_\nu|, & \text{if } A_\nu = N. \end{cases} \quad (5.25)$$

Moreover, we find from (5.6)–(5.9) that, for any mass M, $\exists\ k_0(M) > 0$ such that, for $k \leq k_0(M)$, $\{\sin^2 k/\sin^2 \frac{1}{2}[\theta(N) - \theta(N-1)]\} < M$. Hence, we have, using (5.11), that

$$\frac{d\theta(N)}{dk} \leq 2(N + 1 - A_\nu) + \sigma \sum_{l=0}^{N} \frac{K_l^2}{|R_\nu|^2}, \qquad k < k_0, \quad A_\nu \leq N < A_{\nu+1}, \quad (5.26)$$

where $\sigma < \infty$ is independent of N. Combining (5.26) with (5.23), we obtain an upper bound on the number of η_N^i in the interval I whenever $\bar{\eta} \leq \eta_0 < 4 \sin^2 (k_0/2)$. This upper bound shows that $\bar{\eta}$ cannot be a point of increase of $G(\eta)$ if, in the sequence of chains of length N for which $G_N(\eta) \to G(\eta)$, we can find a subsequence in which the distance from the end of the chain to the nearest atom with mass M, $(N - A_\nu)$ is of $o(N)$. For such chains then (5.4) is true. It seems clear that we can always choose our first sequence H_N so that this is true unless all the masses m_ν for $\nu > A_l$, $l < \infty$ are equal to unity, in which case $G(\eta)$ will equal $G^{(1)}(\eta)$, corresponding to a chain all of whose masses are unity, and the spectrum of H will have the same[11] absolutely continuous part as the chain whose $m_\nu = 1$ for all ν, i.e., its support will be the interval $[0, 4]$.

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APPENDIX: LOWER BOUND ON THE AVERAGE HEAT FLUX

Although we have no way of directly averaging the expression (2.25), a crude lower bound on J_A may be obtained when the m's are independent random variables by averaging the denominator of the integrand in (2.25).

To this end, we note that $K_{1,A}^2$ is the (11) entry of the (4×4) matrix obtained by taking the direct product of the (2×2) matrix Q_A with itself. It is readily established that

$$\mathsf{Q}_A \times \mathsf{Q}_A = \begin{bmatrix} f_A^2 & -f_A & -f_A & 1 \\ f_A & 0 & -1 & 0 \\ f_A & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} \cdots \begin{bmatrix} f_1^2 & -f_1 & -f_1 & 1 \\ f_1 & 0 & -1 & 0 \\ f_1 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \tag{A1}$$

where $f_\nu \equiv 2 - m_\nu \omega^2$. Averaging $\mathsf{Q}_A \times \mathsf{Q}_A$ thus reduces to taking the average of a 4×4 matrix and raising it to the Ath power:

$$\langle (\mathsf{Q}_A \times \mathsf{Q}_A) \rangle = \begin{bmatrix} f^2 + g^2 & -f & -f & 1 \\ f & 0 & -1 & 0 \\ f & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}^A \equiv (\mathsf{F})^A, \tag{A2}$$

where $f = 2 - \langle m \rangle \omega^2$, $g^2 = \langle (m - \langle m \rangle)^2 \rangle \omega^4$. A direct check of the characteristic equation associated with the matrix F shows that its eigenvalues are of the form

$$\lambda_1 = \lambda, \quad \lambda_2 = \lambda^{-\frac{1}{2}} e^{i\alpha}, \quad \lambda_3 = \lambda^{-\frac{1}{2}} e^{-i\alpha}, \quad \lambda_4 = 1, \tag{A3}$$

where $\lambda > 1$. Evidently the dominant term in $\langle K_{1,A}^2 \rangle$ is the one associated with λ_1. An explicit calculation involving the solution of the third-order characteristic equation as $\omega^2 \to 0$ leads to the result

$$\langle K_{1,A}^2 \rangle \simeq e^{cA\sigma\omega^2}, \tag{A4}$$

where $\sigma \equiv \langle (m - \langle m \rangle)^2 \rangle$ and c is a numerical coefficient. Using the estimate (A4) in (2.25) gives[9]

$$\frac{\langle J_A \rangle}{(T_L - T_R)} \geq O[(A\sigma)^{-\frac{3}{2}}]. \tag{A5}$$

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always sufficient, that there be no part of the crystal which is "isolated" from all the atoms which are in contact with the reservoirs.

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Mathematics of the Measurement Problem in Quantum Mechanics

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The mathematical structure of the simplest nontrivial hidden variable theory is derived. The core of the resulting theory is an essentially unique nonlinear differential equation which gives a causal description of the continuous collapse of the wavefunction during a measurement. It is shown that the simplest collapse equation is the same as the equation given ad hoc by Bohm and Bub.

INTRODUCTION

The many papers written since von Neumann's initial paper on the subject of the possible existence of hidden variable theories of quantum mechanics have been thoroughly reviewed and criticized by several authors.[1] In this paper I do not intend to either attack or defend ideas expressed by previous authors on the subject of hidden variables. Instead I will derive the explicit mathematical structure of what I believe is the simplest nontrivial hidden variable theory. The core of the resulting theory is an essentially unique nonlinear differential equation which gives a causal description of the continuous collapse of the wavefunction during a measurement. The simplest collapse equation turns out to be the same as the equation given ad hoc by Bohm and Bub.[2]

DERIVATION OF THE FORM OF THE SIMPLEST HIDDEN VARIABLE THEORY

In my previous papers on this subject[3,4] I have tried to explore the mathematical consequences of the Bohm–Bub theory with the intent of helping to bring it to an experimental test. Due to the complexity of the equations I was not entirely successful. I feel that no real experimental tests of the theory have been conducted or proposed for the following three reasons.[5] First the nonlinearity of the collapse equation makes the theory very difficult to analyze. Secondly the theory is not fully interpreted by Bohm and Bub. The main collapse parameter γ is left practically arbitrary, as are the hidden variables themselves. Since the theory was introduced primarily as a counterexample to various theorems claiming that such a theory could not exist, this lack of completeness is understandable.[6] The third, and perhaps most significant, reason for the lack of experimental tests is the ad hoc and artificial way in which the theory was originally introduced. I will show that a combination of very general and reasonable requirements concerning quantum mechanics, physical measurement, and mathematical simplicity leads inescapably to an equation of the Bohm–Bub type and to a corresponding set of hidden variables. I had previously hoped that a simpler hidden variable theory might exist, but it seems that this hope was false.

If quantum mechanics is interpreted as a statistical theory of quantum ensembles and not as a physical theory concerning individual quanta, then there is no need to introduce the idea of the collapse of the wavefunction during measurement. However, individual quanta do exist experimentally; thus many physicists would like to believe, lacking any other theory, that quantum mechanics applies to the individual. The problem one then faces is that of explaining how the probabilities are changed to certainties by the process of measurement. The so-called projection postulate, first introduced by von Neumann, is the standard explanation of this process; yet, due to its almost metaphysical character, its validity cannot be taken seriously by most physicists.

In classical physics, probabilities enter due to our lack of knowledge of a large number of classical parameters, and not as intrinsic properties of the real world. Furthermore, the probabilities are generally