

Properties of a Harmonic Crystal in a Stationary Nonequilibrium State*

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The stationary nonequilibrium Gibbsian ensemble representing a harmonic crystal in contact with several idealized heat reservoirs at different temperatures is shown to have a Gaussian Γ space distribution for the case where the stochastic interaction between the system and heat reservoirs may be represented by Fokker-Planck-type operators. The covariance matrix of this Gaussian is found explicitly for a linear chain with nearest-neighbor forces in contact at its ends with heat reservoirs at temperatures T_1 and T_N , N being the number of oscillators. We also find explicitly the covariance matrix, but not the distribution, for the case where the interaction between the system and the reservoirs is represented by very "hard" collisions. This matrix differs from that for the previous case only by a trivial factor. The heat flux in the stationary state is found, as expected, to be proportional to the temperature difference ($T_1 - T_N$) rather than to the temperature gradient $(T_1 - T_N)/N$. The kinetic temperature of the j th oscillator $T(j)$ behaves, however, in an unexpected fashion. $T(j)$ is essentially constant in the interior of the chain decreasing exponentially in the direction of the hotter reservoir rising only at the end oscillator in contact with that reservoir (with corresponding behavior at the other end of the chain). No explanation is offered for this paradoxical result.

1. INTRODUCTION

IN a series of papers¹⁻³ Lebowitz and Bergmann developed a general formalism for describing the time evolution of a Gibbs ensemble representing a system in contact with one or more idealized heat reservoirs (temperature baths). They imagine the reservoirs made up of an infinite number of identical noninteracting components each of which interacts with the system at most once. This interaction is impulsive and it is assumed that prior to this interaction the components of each reservoir have an equilibrium distribution with some specified temperature T_α , where $\alpha = 1, \dots, n$, specifies the different reservoirs. Under these conditions the Γ space ensemble density of the system $\mu(x, t)$ satisfies the generalized Liouville equation

$$\frac{\partial \mu(x, t)}{\partial t} + (\mu, H) = \sum_{\alpha=1}^n \int [K_\alpha(x, x')\mu(x', t) - K_\alpha(x', x)\mu(x, t)] dx'. \quad (1.1)$$

Here $x = (\mathbf{q}_1, \dots, \mathbf{q}_N, \mathbf{p}_1, \dots, \mathbf{p}_N)$ is a point in the phase space of the system, $H(x)$ is the Hamiltonian of the system, (μ, H) is the Poisson bracket between μ and H , and the right side of (1.1) represents the effect of collisions with reservoir components on the

evolution of μ . $K(x, x') dx dt$ is the conditional probability that when the system is at the point x' in its Γ space it will suffer a collision in the time interval dt as a result of which it will jump to the region $(x, x + dx)$.

Under very general conditions $\mu(x, t)$ approaches, as $t \rightarrow \infty$, a stationary distribution $\mu_s(x)$. This stationary distribution will correspond to the system being in equilibrium if the temperature of all the reservoirs is the same; otherwise $\mu_s(x)$ will represent a stationary nonequilibrium state in which there are heat currents flowing through the system. (More general nonequilibrium situations may also be represented in this manner.^{1,4}) It is to be expected for a physical system of macroscopic size, whose interaction with the heat reservoirs is confined to specified "surface regions," that its bulk properties in the stationary state will depend only on the temperature of the reservoirs and not on the details of the interaction (this, of course, is expected to be true when the reservoirs all have the same temperature); e.g., the properties of a "long" metal bar should not depend on whether its ends are in contact with water or with wine "heat reservoirs" at temperature T_1 and T_2 .

(We are assuming here "good" heat contact between reservoirs and system so that regions of the system in direct contact with a given reservoir are essentially at the "temperature" of that reservoir.) This belief justifies the idealization of the reservoirs already made in deriving (1.1) and the further drastic simplification made below, and thus, we expect, for realistic systems,

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¹ P. G. Bergmann and J. L. Lebowitz, *Phys. Rev.* **99**, 578 (1955); J. L. Lebowitz and P. G. Bergmann, *Ann. Phys. (N.Y.)* **1**, 1 (1957).

² J. L. Lebowitz, *Phys. Rev.* **114**, 1192 (1959).

³ J. L. Lebowitz, *Rend. Scuola Intern. Fis. XIV Corso Bologna, Italy* (1961).

⁴ J. L. Lebowitz and A. Shimony, *Phys. Rev.* **128**, 1945 (1962); E. P. Gross and J. L. Lebowitz, *ibid.* **104**, 1528 (1956).

that the stationary state found from our model will correctly represent, in the Gibbs ensemble sense, such a physical system in a steady nonequilibrium state.

To obtain an explicit simple form for the right side of (1.1) we imagine the system to contain at its surface n pistons of mass M_α . The α th reservoir will consist of point particles of mass m_α at uniform densities ρ_α always having a Maxwellian velocity distribution at temperature T_α prior to a collision with the α th piston. During such an elastic collision there will be an exchange of momentum in some specified direction. Under these conditions the kernel $K_\alpha(x, x')$ may be specified explicitly [cf. Eq. (2.3), Ref. 2]. Still further simplification is achieved when $m_\alpha \ll M_\alpha$ so that the piston velocity is changed very little during a collision. The effect of the collisions with the reservoirs on the time evolution of $\mu(x, t)$ may then be represented by a Fokker-Planck-type term,^{2,5} and (1.1) assumes the form

$$\frac{\partial \mu(x, t)}{\partial t} + (\mu, H) = \sum_{\alpha=1}^n \lambda_\alpha \frac{\partial}{\partial P_\alpha} \left[P_\alpha \mu + k T_\alpha M_\alpha \frac{\partial}{\partial P_\alpha} \mu \right]. \quad (1.2)$$

Here (Q_α, P_α) are the coordinates and momentum of the α th piston (the pistons being part of the system) and λ_α is the "friction constant" of the α th piston given by [Eq. (3.3), Ref. 2]

$$\lambda_\alpha = \rho_\alpha A_\alpha (8 m_\alpha k T_\alpha / \pi M_\alpha^2)^{\frac{1}{2}}, \quad (1.3)$$

where A_α is the collision cross section (or area) of the α th piston. It is easy to show² that $\mu(x, t)$ satisfying (1.2) will in general approach, as $t \rightarrow \infty$, a stationary value $\mu_s(x)$.

Up to now we have not specified the nature of our system which determines $H(x)$. We now consider the case where our system is a harmonic crystal and the pistons are just some of the particles of the system. (Their location need not be specified at the moment.) It is then shown in Sec. 2 that the stationary solution of (1.2), which $\mu(x, t)$ will approach as $t \rightarrow \infty$, is a Gaussian in the coordinates and momenta of the system (corresponding to the canonical distribution when the temperatures of all the reservoirs are equal; $T_\alpha = T$). The explicit form of the stationary distribution, i.e., the covariance matrix of the Gaussian, is found in Sec. 3 for the special case of a one-dimensional crystal of N particles with nearest-neighbor interactions in which the first particle is in contact with a reservoir at temperature T_1 and the

last with a reservoir at temperature T_N and $\lambda_1 = \lambda_N$. The general form of the distribution for this system, including its time dependence, has also been discussed independently by Bils.⁶ Since we are interested in this system solely as a model, we do not worry about the drastic simplifications made in the right side of (1.1) to arrive at (1.2) or the further one, $\lambda_1 = \lambda_N$, required to obtain an explicit stationary nonequilibrium ensemble in Γ space. What is unfortunate, however, is that the harmonic crystal is *not* a realistic physical system. As is well known,⁷ the harmonic crystal has an "infinite" heat conductivity; i.e., the heat flux is not proportional to the temperature gradient when one considers the relaxation of this system from some initial nonequilibrium state. This is reflected in the true stationary state considered here by the fact that the heat flux is proportional (when $N \gg 1$, or strictly speaking in the limit $N \rightarrow \infty$), to the temperature difference between the ends of the system, $(T_1 - T_N)$, rather than to the temperature gradient $(T_1 - T_N)/N$, which would be the case if there was any anharmonic coupling. This is also reflected in the form of $T(j)$, the kinetic temperature of the j th harmonic oscillator which is uniform throughout the linear chain, being equal to $\frac{1}{2}(T_1 + T_N)$, except near the edges where it varies exponentially in a backward way; i.e., with $T_1 > T_N$, $T(j)$ will decrease from its mean value as $j \rightarrow 1$ jumping to a higher value, close to T_1 , for $j = 1$. Also the heat flux, $J(\lambda)$, will vary with λ , the strength of the coupling to the reservoirs, in an unphysical way, reaching a maximum at $\lambda = \frac{1}{2}\sqrt{3}\omega$, (where $m\omega^2$ is the force constant between the oscillators), and vanishing as ω^2/λ for $\lambda \rightarrow \infty$. This may perhaps be understood as a mismatching between the frequencies of the reservoirs and the oscillators. We have no explanation for the abnormal behavior of $T(j)$.

An alternate idealization of the stochastic interaction between the reservoirs and the system is to imagine that after *each* collision with a component of the α th reservoir the momentum P_α will have a Maxwellian distribution at the temperature T_α ,

$$h_\alpha(P) = (M_\alpha k T_\alpha / 2\pi)^{\frac{1}{2}} \exp[-P^2 / 2M_\alpha k T_\alpha]. \quad (1.4)$$

This is an opposite extreme of the small momentum transfer considered before and corresponds to the pistons and reservoir components having the same mass.^{1,2} We simplify this further by assuming that

⁶ O. Bils, "On the Non-Stationary Equilibrium of a Finite Chain of Coupled Oscillators" (to be published).

⁷ G. Klein and I. Prigogine, *Physica* **19**, 1053 (1953); P. C. Hemmer, *Kgl. Norske Videnskab. Selskab. Fork.* **33**, 101 (1960); E. I. Takizawa and K. Kobayasi, *Chinese J. Phys.* **1**, 59 (1963); E. Teramoto, *Progr. Theoret. Phys.* (Kyoto) **28**, 1059 (1962); R. Rubin, *Phys. Rev.* **131**, 964 (1963).

⁵ J. L. Lebowitz and P. Resibois, *Phys. Rev.* **139**, A1101 (1965).

the probability of a collision with a reservoir component in a time interval dt is given by $\lambda'_\alpha dt$, independent of the state of the system. These assumptions lead to a modified Krook type of collision kernel⁴ and Eq. (1.2) assumes the form

$$\frac{\partial \mu(x, t)}{\partial t} + (\mu, H) = \sum_\alpha \lambda'_\alpha \left\{ h_\alpha(P_\alpha) \int \mu(x, t) dP_\alpha - \mu(x, t) \right\}. \quad (1.5)$$

While the stationary solution of (1.5) for a harmonic crystal is no longer a Gaussian the stationary covariance matrix of the linear chain and hence the kinetic temperature and heat flux, is of the same form as before. The only change is that the system acts as if the temperature difference $(T_1 - T_N)$ was reduced by the factor $[1 + (\omega^2/\lambda^2)\varphi_1]$, where φ_1 depends on ω and λ . These assertions about the covariance matrix are proved in Sec. 3.

2. STATIONARY STATE OF A HARMONIC CRYSTAL

The Hamiltonian of a harmonic crystal containing N particles, each being s dimensional, may be written in the general form⁶

$$H = \frac{1}{2} \sum_{i=1}^{2N} x_i^2 + \frac{1}{2} \sum_{i,j=1}^N \Phi_{ij} x_i x_j; \quad N = sN'. \quad (2.1)$$

Here the $x_i, i = 1, \dots, N$, are the Cartesian coordinates of the particles, (relative to their equilibrium positions), while $x_j, j = i + N$, is the momentum conjugate to x_i (we have set the mass of the particles equal to unity). The generalized Liouville equation (1.2) now has the form

$$\frac{\partial \mu(x, t)}{\partial t} = \sum_{i=1}^{2N} \frac{\partial}{\partial x_i} (\xi_i \mu) + \frac{1}{2} \sum_{i,j=1}^{2N} \frac{\partial^2}{\partial x_i \partial x_j} (d_{ij} \mu), \quad (2.2)$$

where

$$\xi_i = \sum_{j=1}^{2N} a_{ij} x_j \quad (2.3)$$

and a_{ij} and d_{ij} are elements of $2N$ by $2N$ matrices \mathbf{a} and \mathbf{d} which we write in the partitioned form

$$\mathbf{a} = \begin{pmatrix} \mathbf{0} & -\mathbf{I} \\ \Phi & \mathcal{R} \end{pmatrix}, \quad \mathbf{d} = \begin{pmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \epsilon \end{pmatrix}. \quad (2.4)$$

Here $\mathbf{0}$ and \mathbf{I} are the null and unit N by N matrices, Φ_{ij} is defined in (2.1), $\mathcal{R}_{ij} = \lambda_\alpha \delta_{\alpha i} \delta_{ij} [\lambda_\alpha$ given in (1.3) with $M_\alpha = 1]$ and $\epsilon_{ij} = 2kT_i \mathcal{R}_{ij}$. The general time-

dependent solution of (2.2) may be found⁶ by diagonalizing the right side of (2.2) as was done by Wang and Uhlenbeck⁹ for fluctuations in electrical circuits. (Wang and Uhlenbeck consider only the case corresponding to all the T_α being the same.) It is clear, however, from an inspection of (2.2) that its stationary solution μ_s [corresponding to setting $\partial \mu / \partial t = 0$ in (2.2)], which is all that is of interest to us in this problem, has the general form

$$\mu_s(x) = (2\pi)^{-N} \text{Det} [\mathbf{b}^{-\frac{1}{2}}] \exp \left[-\frac{1}{2} \sum_{i,j=1}^{2N} b_{ij}^{-1} x_i x_j \right]. \quad (2.5)$$

The matrix \mathbf{b} is the positive definite covariance matrix, and is related to expectation values in the stationary state by

$$b_{ij} = \langle x_i x_j \rangle = \int \mu_s(x) x_i x_j dx \quad (2.6)$$

and we have

$$A_i = \langle x_i \rangle = \int \mu_s(x) x_i dx = 0. \quad (2.7)$$

Substituting (2.5) into (2.2) and equating terms yields the basic, necessary, and sufficient equation

$$\mathbf{a} \cdot \mathbf{b} + \mathbf{b} \cdot \mathbf{a}^\dagger = \mathbf{d}, \quad (2.8)$$

where \mathbf{a}^\dagger is the transpose of \mathbf{a} . Once \mathbf{b} is known all the properties of the stationary state, e.g., heat flux, local kinetic temperature, etc., are readily available. [It is clear that when all the $T_\alpha = T$ then $\epsilon = 2kT\mathcal{R}$ and $\mu_s(x) \sim e^{-\beta H(\omega)}$, $\beta = (kT)^{-1}$; i.e, the stationary state is the equilibrium state at temperature T .]

The uniqueness of the stationary solution $\mu_s(x)$ for the case where the coupling with the reservoirs does not vanish and the phase space of the crystal is not divided into different isolated parts (i.e., the representative phase point of the system can move between any two regions via a combination of its natural motion and collision with the reservoirs) follows from the general results of Ref. 1, explicitly verifiable here, that an arbitrary initial distribution will approach a unique $\mu_s(x)$ as $t \rightarrow \infty$. For the harmonic crystal in which there are no "torn bonds" isolating some parts this condition of ergodicity is clearly satisfied. The uniqueness of μ_s for the linear chain is shown explicitly in the next section.

Equations (2.7) and (2.8) are consequences of the general equations satisfied by the time-dependent expectation values $A_i(t)$ and $b_{ij}(t)$ defined with $\mu_s(x) \rightarrow \mu(x, t)$ in (2.6)–(2.7). We then have from (1.2)

$$(d/dt)\mathbf{A}(t) = -\mathbf{a} \cdot \mathbf{A}(t) \quad (2.9)$$

⁶ Cf., for example, A. A. Maradudin, E. W. Montroll, and G. H. Weiss, *Theory of Lattice Dynamics in the Harmonic Approximation* (Academic Press Inc., New York, 1963); E. W. Montroll, Third Berkeley Symp. Math. Stat. and Prob. 3, 209 (1957).

⁹ M. C. Wang and G. E. Uhlenbeck, Rev. Mod. Phys. 17, 323 (1945).

and

$$(d/dt)\mathbf{b}(t) = \mathbf{d} - \mathbf{a} \cdot \mathbf{b}(t) - \mathbf{b}(t) \cdot \mathbf{a}^\dagger. \quad (2.10)$$

For the case where $\mu(x, t)$ satisfies Eq. (1.5) the expectation values of the coordinates and momenta $\mathbf{A}'(t)$ again satisfy (2.9) (with λ_α replaced by λ'_α) while the covariance matrix $\mathbf{b}'(t)$ now satisfies the equation

$$(d/dt)\mathbf{b}'(t) = \frac{1}{2}\mathbf{d} - \mathbf{a} \cdot \mathbf{b}'(t) - \mathbf{b}'(t) \cdot \mathbf{a}^\dagger + \mathbf{r} \cdot \mathbf{b}'(t) \cdot \mathbf{r} \quad (2.11)$$

with

$$\mathbf{r} = \begin{pmatrix} 0 & 0 \\ 0 & \mathcal{R}^\dagger \end{pmatrix}. \quad (2.12)$$

In the stationary state \mathbf{A}' and \mathbf{A} again vanish while \mathbf{b}' or \mathbf{b} satisfy (2.11) or (2.10) with the left sides set equal to zero.

3. EXPLICIT SOLUTION FOR A LINEAR CHAIN

We consider now a one-dimensional harmonic crystal (chain of pistons) with nearest-neighbor interactions, whose ends are rigidly fixed.⁸ The interaction with the reservoirs takes place at the first and last piston, $\alpha = 1, N$ and we set

$$\begin{aligned} \lambda_1 = \lambda_N = \lambda, \quad T_1 = T(1 + \eta), \\ T_N = T(1 - \eta); \quad |\eta| \leq 1. \end{aligned} \quad (3.1)$$

The N by N matrices Φ , \mathcal{R} , and ϵ now have the form

$$\Phi = \omega^2 \mathbf{G}; \quad G_{ij} = 2\delta_{ij} - \delta_{i+1,j} - \delta_{i,j+1} \quad (\text{for } j = 1 \text{ through } N - 1), \quad (3.2)$$

$$G_{Nj} = G_{jN} = \begin{cases} 0, & j < N - 1, \\ -1, & j = N - 1, \\ 2, & j = N, \end{cases}$$

$$\mathcal{R} = \lambda \mathbf{R}; \quad \mathbf{R}_{ij} = \delta_{ij}(\delta_{i1} + \delta_{iN}), \quad (3.3)$$

$$\epsilon = 2kT\lambda(\mathbf{R} + \eta \mathbf{E}); \quad E_{ij} = \delta_{ij}(\delta_{i1} - \delta_{iN}). \quad (3.4)$$

We now write the $2N$ by $2N$ covariance matrix \mathbf{b} in the partitioned form

$$\mathbf{b} = \begin{pmatrix} \mathbf{x} & \mathbf{z} \\ \mathbf{z}^\dagger & \mathbf{y} \end{pmatrix}. \quad (3.5)$$

The N by N matrices \mathbf{x} , \mathbf{y} , and \mathbf{z} give, respectively, the correlations in the stationary state, among the coordinates, momenta and between the coordinates and momenta

$$x_{ij} = \langle q_i q_j \rangle, \quad y_{ij} = \langle p_i p_j \rangle, \quad z_{ij} = \langle q_i p_j \rangle. \quad (3.6)$$

To obtain the deviation of these correlations from their equilibrium values at uniform temperature T ,

corresponding to $\eta = 0$, we write

$$\mathbf{x} = (kT/\omega^2)[\mathbf{G}^{-1} + \eta \mathbf{X}], \quad (3.7)$$

$$\mathbf{y} = kT[\mathbf{I} + \eta \mathbf{Y}], \quad (3.8)$$

$$\mathbf{z} = \lambda^{-1} kT \eta \mathbf{Z}. \quad (3.9)$$

Using now (2.8) we find the following equations for \mathbf{X} , \mathbf{Y} , \mathbf{Z} :

$$\mathbf{Z} = -\mathbf{Z}^\dagger, \quad (3.10)$$

$$\mathbf{Y} = \mathbf{X}\mathbf{G} + \mathbf{Z}\mathbf{R}, \quad (3.11)$$

$$2\mathbf{E} - \mathbf{Y}\mathbf{R} - \mathbf{R}\mathbf{Y} = \nu[\mathbf{G}\mathbf{Z} - \mathbf{Z}\mathbf{G}]. \quad (3.12)$$

In addition, \mathbf{X} and \mathbf{Y} are required to be symmetric

$$\mathbf{X} = \mathbf{X}^\dagger, \quad \mathbf{Y} = \mathbf{Y}^\dagger, \quad (3.13)$$

while \mathbf{b} is required to be positive definite. The quantity ν in (3.12) is $\nu = \omega^2/\lambda^2$, and is the only dimensionless parameter to remain in the problem.

To obtain an explicit solution of (3.10)–(3.13) we first note that the left side of (3.12), $2\mathbf{E} - \mathbf{Y}\mathbf{R} - \mathbf{R}\mathbf{Y}$, is a bordered matrix (it has nonvanishing elements only in the first and last rows and columns). Hence $\mathbf{G}\mathbf{Z} - \mathbf{Z}\mathbf{G}$ must also be bordered. Using the explicit form of \mathbf{G} , (3.2), together with the antisymmetry requirement (3.10), it is easy to show that \mathbf{Z} is necessarily a skew-symmetric Toeplitz matrix when $\mathbf{G}\mathbf{Z} - \mathbf{Z}\mathbf{G}$ is a bordered matrix, and \mathbf{Z} may therefore be written in the form

$$\mathbf{Z} = \begin{pmatrix} 0 & \varphi_1 & \varphi_2 & & \varphi_{N-2} & \varphi_{N-1} \\ -\varphi_1 & & & & & \varphi_{N-2} \\ -\varphi_2 & & & & & \varphi_2 \\ & & & & & \varphi_1 \\ & & & & & 0 \\ -\varphi_{N-1} & & & & -\varphi_2 & -\varphi_1 & 0 \end{pmatrix}. \quad (3.14)$$

The quantities $\varphi_1, \dots, \varphi_N$ are simply related to the entries in the bordered matrix in the left side of (3.12) and turn out to be

$$\nu \varphi_j = \delta_{j1} - Y_{1j} = \delta_{j1} + Y_{N,N-j+1}, \quad (3.15)$$

where $\varphi_N \equiv 0$ by definition. Equation (3.15) implies certain obvious restrictions on \mathbf{Y} in order that (3.12) has a solution.

Next, Eq. (3.11), together with the fact that \mathbf{Y} is symmetric implies that

$$\mathbf{X}\mathbf{G} - \mathbf{G}\mathbf{X} = -(\mathbf{R}\mathbf{Z} + \mathbf{Z}\mathbf{R}). \quad (3.16)$$

Once again, the right side of (3.16) is a bordered matrix, which is known in terms of the φ 's. Unlike \mathbf{Z} ,

however, \mathbf{X} is required to be symmetric and we find that one solution is a Hankel matrix:

$$\mathbf{X} = \begin{pmatrix} \varphi_1 & \varphi_2 & \varphi_3 & \cdots & \cdots & \varphi_{N-2} & \varphi_{N-1} & 0 \\ & & & & & & & \varphi_{N-1} \\ & & & & & & & \vdots \\ & & & & & & & \vdots \\ & & & & & & -\varphi_2 & \\ & & & & & & -\varphi_1 & \end{pmatrix} \quad (3.17)$$

The solution to (3.16) is, however, not unique. We could add to (3.17) any symmetric matrix that commutes with \mathbf{G} . Because all the eigenvalues of \mathbf{G} are nondegenerate, such a matrix must be of the form $\tilde{\mathbf{X}} = P(\mathbf{G})$, where P is any polynomial. Nevertheless, $\tilde{\mathbf{X}}$ is required to vanish as a consequence of our last condition, (3.11).

Substitution of (3.14) and (3.17) into the right side of (3.11) gives an expression for \mathbf{Y} in terms of the φ 's. This, when combined with (3.15) yields an equation for the φ 's, namely,

$$\sum_{j=1}^{N-1} K_{ij} \varphi_j = \delta_{i1} \quad (3.18)$$

where \mathbf{K} is the $(N - 1)$ -square matrix

$$\mathbf{K} = \begin{pmatrix} \nu + 2 & -1 & & & & \\ -1 & \nu + 2 & -1 & & & \\ & -1 & \nu + 2 & -1 & & \\ & & -1 & \nu + 2 & -1 & \\ & & & -1 & \nu + 2 & -1 \\ & & & & -1 & \nu + 2 \end{pmatrix} \quad (3.19)$$

The matrix \mathbf{Y} is then the Hankel matrix

$$\mathbf{Y} = \mathbf{E} - \nu \mathbf{X} \quad (3.20)$$

It is to be noted that both \mathbf{X} and \mathbf{Y} are antisymmetric about the ‘‘cross’’ diagonal [i.e., the $(1, N) - (N, 1)$ diagonal], a state of affairs that reflects the fact that changing the sign of η corresponds to interchanging the reservoirs at the ends of the chain. Were we to add a matrix $\tilde{\mathbf{X}} = P(\mathbf{G})$ to \mathbf{X} , as discussed above, then \mathbf{X} would acquire a symmetric component about the ‘‘cross’’ diagonal. By (3.11) \mathbf{Y} , too, would acquire such a component. But (3.15) precludes this possibility.

We conclude then, that the solution to (3.10)–(3.13) is given uniquely by (3.14), (3.17), and (3.20), assuming, of course that (3.18) has a unique solution. That this is so follows from the fact that \mathbf{K} is positive definite for all $\nu \geq 0$.

To find φ we use Cramer’s rule. Consider the general M -square version of K and let D_M denote its determinant. Then

$$\varphi_j = (D_{N-1})^{-1} \times (\text{cofactor of } K_{1j} \text{ in } D_{N-1}). \quad (3.21)$$

But, it is easily seen that the cofactor of K_{1j} is simply D_{N-1-j} . The computation of D_M is simple. We observe that if we consider D_M to be a function of the parameter $x = 1 + \frac{1}{2}\nu$, then $D_M(x) = 2xD_{M-1}(x) - D_{M-2}(x)$, while $D_0(x) = 1$ and $D_1(x) = 2x$. This is just the recursion relation for $U_M(x)$, the Chebyshev polynomial of the second kind. Using the fact that $U_M(\cosh \theta) = \sinh(M + 1)\theta / \sinh \theta$, and defining α by

$$\cosh \alpha = 1 + \frac{1}{2}\nu \quad (3.22)$$

we obtain

$$\varphi_j = \sinh(N - j)\alpha / \sinh N\alpha. \quad (3.23)$$

For large N and fixed j we have the asymptotic formula:

$$\varphi_j = e^{-j\alpha} = (\varphi_1)^j, \quad (3.24)$$

and

$$\varphi_1 = e^{-\alpha} = 1 + \frac{1}{2}\nu - \frac{1}{2}(4\nu + \nu^2)^{\frac{1}{2}}. \quad (3.25)$$

For $\nu \rightarrow 0$ or ∞ we have

$$\varphi_1(\nu) \rightarrow \begin{cases} 1 - \nu^{\frac{1}{2}}, & \text{as } \nu \rightarrow 0, \\ \nu^{-1}, & \text{as } \nu \rightarrow \infty. \end{cases} \quad (3.26)$$

Finally, we note that \mathbf{b} is necessarily positive definite, a property that can be proved directly from (2.8) using the fact that Φ is positive definite.

For the case of hard collisions, $\mu(x, t)$ satisfying (1.5) and $\mathbf{b}'(t)$ satisfying (2.11), the corresponding matrices \mathbf{X}' , \mathbf{Y}' , and \mathbf{Z}' will also satisfy Eq. (3.10) and (3.11) while (3.12) is now replaced by

$$\mathbf{E} - \mathbf{Y}'\mathbf{R} - \mathbf{R}\mathbf{Y}' + \mathbf{R}\mathbf{Y}'\mathbf{R} = \nu[\mathbf{G}\mathbf{Z}' - \mathbf{Z}'\mathbf{G}] \quad (3.27)$$

with ν now given by λ'^2/ω^2 . These equations may be brought into the same form as (3.10)–(3.12) by the replacements

$$\begin{aligned} \mathbf{X}' &= (1 + \nu\varphi_1)^{-1}\mathbf{X}, & \mathbf{Y}' &= (1 + \nu\varphi_1)^{-1}\mathbf{Y}, \\ \mathbf{Z}' &= (1 + \nu\varphi_1)^{-1}\mathbf{Z}, \end{aligned} \quad (3.28)$$

which corresponds simply to the replacement of the temperature difference η by η^* , where

$$\eta^* = \frac{\eta}{(1 + \nu\varphi_1)} \rightarrow \begin{cases} \eta & \text{as } \nu \rightarrow 0, \\ \frac{1}{2}\eta & \text{as } \nu \rightarrow \infty. \end{cases} \quad (3.29)$$

4. PROPERTIES OF THE STATIONARY STATE

Kinetic Temperature

The kinetic temperature of the j th particle is given by

$$kT(j, \nu; N) = \langle p_j^2 \rangle = kT[1 + \eta Y_{jj}] = \langle x_i \partial H / \partial x_i \rangle \quad (4.1)$$

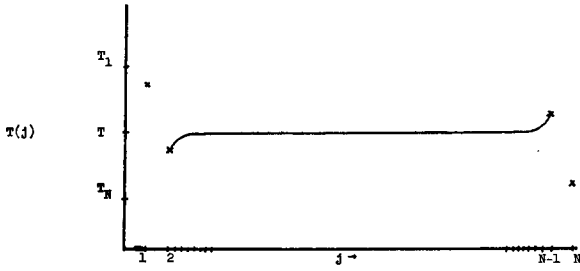


FIG. 1. Typical behavior of $T(j)$.

the last equality holding for all $i = 1, \dots, 2N$ indicating some kind of equipartition for the stationary nonequilibrium state. In the limit of $N \rightarrow \infty$ we have

$$T(j, \nu) = \begin{cases} T[1 - \eta\nu(\varphi_1)^{2j-1}], & 1 < j < \frac{1}{2}N, \\ T[1 + \eta\nu(\varphi_1)^{2j'-1}], & 1 < j' = N - j < \frac{1}{2}N, \end{cases} \quad (4.2)$$

and

$$\begin{aligned} T(1, \nu) &= T_1 - \nu\varphi_1 T\eta, \\ T(N, \nu) &= T_N + \nu\varphi_1 T\eta, \end{aligned} \quad (4.3)$$

with φ_1 given by (3.25) and $T_1 = T(1 + \eta)$, $T_N = T(1 - \eta)$. The temperature of the linear chain thus deviates from its average value $T = \frac{1}{2}(T_1 + T_N)$ only at its edges where it changes exponentially over a length $\ell(\nu)$;

$$\ell(\nu) \rightarrow \begin{cases} \frac{1}{2}\nu^{-\frac{1}{2}}, & \nu \rightarrow 0, \\ \frac{1}{2}(\ln \nu)^{-1}, & \nu \rightarrow \infty. \end{cases}$$

It is a totally unexpected result of this model that the kinetic temperature *drops* below the average value at the second particle and then *increases* exponentially as we move away from the hot reservoir (cf. Fig. 1).

For the case of hard collisions (4.2) is unchanged except for the replacement of η by η^* , while (4.3) now has the form

$$\begin{aligned} T'(1, \nu) &= T_1 - 2\nu\varphi_1 T\eta^*, \\ T'(N, \nu) &= T_N - 2\nu\varphi_1 T\eta^*. \end{aligned} \quad (4.5)$$

Heat Flux

It is easy to show that the energy flux across a plane separating the $(i - 1)$ th particle from the i th particle

is given by⁷

$$j_{i-1,i} = \omega^2 \langle q_{i-1} p_i \rangle = \omega^2 Z_{12} \equiv J, \quad i = 2, \dots, N - 1.$$

The equalities hold in the stationary state where the flux is constant throughout the system and coincides with the energy flux $j_1 = -j_N$, coming from the reservoir at the left and going into the reservoir at the right, which is given by² $\lambda k [T_1 - T(1, \nu)]$. We then have using (3.25)

$$\begin{aligned} J(\lambda, \omega) &= (\omega^2/\lambda)kT\varphi_1\eta \xrightarrow{N \rightarrow \infty} \frac{1}{2}(\omega^2/\lambda)kT[1 + (\nu/2) \\ &\quad - \frac{1}{2}\nu(1 + 4/\nu)^{\frac{1}{2}}](T_1 - T_N) \\ &= \frac{1}{2}(\omega^2/\lambda)k(T_1 - T_N) \quad \text{for } \lambda \gg \omega \\ &= \frac{1}{2}\lambda k(T_1 - T_N) \quad \text{for } \lambda \ll \omega. \end{aligned} \quad (4.6)$$

As expected the heat flux for the harmonic crystal is proportional to $(T_1 - T_N)$ rather than to the temperature gradient $(T_1 - T_N)/N$, i.e., the "heat" conductivity⁷ is proportional to the size of the system.

The behavior of $J(\lambda, \omega)$ for fixed ω is very peculiar. For small λ , $\lambda \ll \omega$, J is proportional to λ as it should be, and is independent of ω , the whole chain behaving as if it were just one tight piston. As λ increases J reaches a maximum at $\lambda = \frac{1}{2}\sqrt{3}\omega$, $J_{\max} = \frac{1}{6}k(T_1 - T_N)\omega$, and then decreases, vanishing as λ^{-1} when $\lambda \rightarrow \infty$; the system now behaves, in the stationary state, as if the oscillators at the two ends are at the temperatures of the corresponding reservoirs, while the remainder are in equilibrium at temperature T . This latter behavior is quite unexpected. For a physical system (anharmonic coupling) we would expect $J(\lambda)$ to reach a limiting value proportional to the heat conductivity of the system times the temperature gradient.

For the case of hard collisions

$$J'(\lambda, \omega) = (1 + \nu\varphi_1)^{-1}J(\lambda, \omega) \rightarrow \begin{cases} J(\lambda, \omega), & \nu \rightarrow 0, \\ \frac{1}{2}J(\lambda, \omega), & \nu \rightarrow \infty. \end{cases}$$

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