Journal of Statistical Physics, Vol. 3, No. 2, 1971

Approach to Equilibrium of Coupled Harmonic Oscillator Systems. II

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Received August 6, 1970

The approach to equilibrium of a finite segment of an infinite chain of harmonically coupled masses is studied in several variations. The chain is taken as completely free, or it is bound at $x_0 = 0$; ordinary coordinates and momenta or Schrödinger variables are used to treat the dynamics; and the inital distribution of heat-bath variables is chosen to be canonical or noncanonical. Equipartition of energy is found in all cases. Brownian drifts are obtained for the free chain with ordinary variables, but when this is excluded, the equilibrium entropy is found to be canonical and extensive when the initial heat bath is canonical, but less than canonical and slightly nonextensive when the initial heat bath is noncanonical. The modifications of the entropy do not contribute to the heat capacity of the system.

KEY WORDS: Entropy; information theory; approach to equilibrium; coupled oscillators; Liouville function; nonequilibrium statistical mechanics, noncanonical equilibrium; harmonic chain.

1. INTRODUCTION

In the first paper of this series[1] (hereinafter denoted by *I*), we have treated the temporal evolution of a finite segment (the system) of an infinite linear chain of coupled harmonic oscillators. The parts of chain that are not in the system are regarded as a heat bath. The exact dynamical solution of the equations of motion yields the temporal behavior of each coordinate and momentum in the chain in terms of the initial values of all the coordinates and momenta.

Statistical mechanics was introduced by recognizing that our knowledge of these initial values, especially those of the heat bath, is inexact, and should properly be specified probabilistically. In *I*, we chose the initial probability density of the heat

Supported in part by the United States Atomic Energy Commission.

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bath to be a product of individual Gaussian probability densities of the coordinates and momenta, rather than the more usual canonical expression. We demonstrated that, even with this noncanonical initial description of the heat bath, energy is equipartitioned, temperature is defined naturally in terms of appropriate variances, and many of the usual properties of equilibrium were attained.

In our treatment of the simple chain, however, the Brownian drift of the system led to an ever-increasing entropy, as is physically plausible, rather than to true equilibrium. (For the more complicated harmonically bound chain, also treated in *I*, a true equilibrium was reached, but the Gaussian initial probability densities were very nearly canonical for this system, and the treatment given was not exact.) In addition, nearest-neighbor momentum correlations were found to persist as $t \to \infty$, so that the quasiequilibrium state was not one of canonical equilibrium.

We have discussed the underlying logical basis for our approach in *I*, and in somewhat more general terms in another paper.[2] In the present paper, we give exact equilibrium (where possible) results of calculations for the simple chain in eight variations, represented by (1) Gaussian or canonical initial distributions, (2) ordinary or Schrödinger[3] variables, and (3) the free chain, or one with x_0 fixed at its origin. The Schrödinger variables are essentially momenta and spring stretchings, rather than momenta and coordinates; they therefore reveal nothing about the Brownian motion of the entire system, even when it is present. The chain with x_0 fixed is prevented from drifting. We can, with these choices, separate out the effects of initial distribution from the consequences of Brownian drift.

We show that equilibrium need not be canonical, that entropy is not necessarily extensive for some systems or choices of variables, and that our initial knowledge of the heat bath may lead to an equilibrium entropy of the system that is less than the canonical one.

In Section 2, we review the dynamics briefly; in Section 3, we present the statistical procedures; and in subsequent sections, the results are presented and discussed.

2. DYNAMICS

We consider an infinite linear chain of equal masses m, connected by springs of constant k, for which the Hamiltonian is

$$H = \sum_{n=-\infty}^{\infty} [(p_n^2/2m) + (k/2)(x_{n+1} - x_n)^2] \tag{1}$$

The solutions of the equations of motion are well known to be

$$x_n(t) = \sum_{r=-\infty}^{\infty} [x_{n+r}(0) f_r(t) + p_{n+r}(0)\, g_r(t)/2m\omega] \tag{2a}$$

and

$$p_n(t) = m\dot{x}_n(t) \tag{2b}$$

where $\omega^2 = k/m$, and with $\tau = 2\omega t$, we can write

$$f_r(t) = J_{2r}(\tau) \tag{3}$$

and

$$g_r(t) = \int_0^\tau J_{2r}(y)\, dy \tag{4}$$

All solutions for the semiinfinite chain, where $x_0(t) = 0$ for all t, can be derived from Eqs. (2), merely by requiring that $x_n(0) = -x_{-n}(0)$ and $p_n(0) = -p_{-n}(0)$.

The dynamics may be elegantly treated by use of the Schrödinger variables[3]:

$$\xi_{2n} = m^{1/2}\dot{x}_n = p_n/m^{1/2} \tag{5a}$$

and

$$\xi_{2n+1} = k^{1/2}(x_n - x_{n+1}) = \omega m^{1/2}(x_n - x_{n+1}) \tag{5b}$$

The equations of motion then become simply

$$2\dot{\xi}_n = \xi_{n-1} - \xi_{n+1} \tag{6}$$

with the solution

$$\xi_n(t) = \sum_{r=-\infty}^{\infty} \xi_{r+n}(0)\, J_r(\tau) \tag{7}$$

The inverse of the Schrödinger transformation is trivial for the momenta; for the coordinates, it is given by

$$x_n = x_0 - k^{-1/2} \sum_{r=0}^{n-1} \xi_{2r+1}\,, \qquad n > 0 \tag{8a}$$

and

$$x_n = x_0 + k^{-1/2} \sum_{r=0}^{|n|-1} \xi_{-(2r-1)}\,, \qquad n < 0 \tag{8b}$$

The coordinate x_0 is thus explicit in all the Schrödinger coordinate inverses; in order to convert spring elongations into coordinate displacements, one must have a reference point.

3. ENTROPY AND THE COVARIANCE MATRIX

The entropy function to be used here, as in *I*, is given by

$$S_N = -k_B \int_\Gamma \rho_N(t) \ln(h^N \rho_N)\, d\Gamma \tag{9}$$

where $\rho_N(t)$ is the reduced Liouville function for the system of N masses and their connecting springs, k_B is Boltzmann's constant, h is a constant with the units of action, and Γ is the $2N$-dimensional phase volume of the system. The reduced Liouville function is nothing more than the time-dependent probability density that describes our state of knowledge of the system variables as a consequence of the dynamical evolution expressed in the equations of motion and the initial statistical description of the system and heat bath. As already explained,[1,2] $\rho_N(t)$ can best be calculated by means of the characteristic function, or Fourier transform, of the complete Liouville function of the chain. The calculation, which need not be repeated here, yields the expression

$$\rho_N(X, t) = (2\pi)^{-N} (\det W)^{-1/2} \exp[-\tilde{X} W^{-1} X/2] \tag{10}$$

where X is a $2N$-component vector, the transpose of which is

$$\tilde{X}(t) = (x_1 x_2 \cdots x_N p_1 p_2 \cdots p_N) \tag{11}$$

and W is the so-called covariance matrix, given as

$$W = \begin{pmatrix} W & G \\ \tilde{G} & Q \end{pmatrix} \tag{12}$$

where $M = (M_{ij})$, $G = (G_{ij})$, $Q = (Q_{ij})$, and these matrix elements are given by the time-dependent statistical averages

$$M_{ij} = \langle x_i(t)\, x_j(t) \rangle \tag{13}$$

$$Q_{ij} = \langle p_i(t)\, p_j(t) \rangle \tag{14}$$

and

$$G_{ij} = \langle x_i(t)\, p_j(t) \rangle \tag{15}$$

When $\rho_N(t)$, as given by Eq. (10), is used in Eq. (9), the entropy function becomes

$$S_N(t) = Nk_B + k_B \ln[\hbar^{-N} (\det W)^{1/2}] \tag{16}$$

where $\hbar = h/2\pi$. Thus, it is seen that only the covariance matrix W is needed for the purpose of finding the entropy, and the matrix elements of W can be calculated directly from the initial probability density by use of Eqs. (2). We have, for example,

$$M_{ij} = \int x_i(t)\, x_j(t)\, \rho(0) \prod_{n=-\infty}^{\infty} dx_n(0)\, dp_n(0) \tag{17}$$

where $x_i(t)$ is expressed in terms of the initial values of the coordinates and momenta, as given in Eq. (2a). The specification of $\rho(0)$ permits the integrations to be carried out directly.

In the case of Schrödinger variables, we have, in analogy to Eq. (10),

$$\rho_N(\Xi, t) = (2\pi)^{-N} (\det W_\xi)^{1/2} \exp(-\tilde{\Xi} W_\xi^{-1} \Xi/2) \tag{18}$$

where $\Xi(t)$ is the $2N$-component vector of the ξ_n, the transpose of which is

$$\tilde{\Xi}(t) = (\xi_1 \xi_3 \cdots \xi_{2N-1} \xi_2 \xi_4 \cdots \xi_{2N}) \tag{19}$$

and W_ξ is defined in analogy to W of Eq. (12), with $M_{ij} = \langle \xi_{2i-1}(t)\, \xi_{2j-1}(t) \rangle$, $Q_{ij} = \langle \xi_{2i} \xi_{2j} \rangle$, and $G_{ij} = \langle \xi_{2i-1} \xi_{2j} \rangle$. The entropy is identical in form to Eq. (16), and need not be rewritten.

4. PRESENTATION OF RESULTS

Two distinct dynamical problems have been treated—the free chain and the chain with $x_0 = 0$ for all t. Each of these has been treated in terms of ordinary coordinates and momenta and in terms of Schrödinger variables. Finally, each variation of the dynamics has been treated with both canonical and Gaussian initial distributions of the variables. Details of the calculations are, in most cases, not particularly interesting; they are available, as long as the supply lasts, upon request.[4]

In the present paper, we have made the minor simplification that the initial system variables are zero-centered, rather than centered around nonzero initial expectation values. Very little extra effort, other than notational inconvenience, is required to include the nonzero initial expectation values. Since we have already treated such systems,[1,2] however, and since these nonthermal terms do not contribute to the entropy or to any of the final equilibrium properties of the system, we have not carried them along.

Notational economy is effected by the use of a variety of four-index symbols $(a, b; c, d)$, etc., that are defined in the appendix. Results of the calculations with canonical initial distributions for the four dynamical treatments are presented in Section 5; those with Gaussian initial distribution are found in Section 6.

5. CANONICAL INITIAL CONDITIONS

The initial probability density for the system and heat bath is given in terms of ordinary variables, taken at $t = 0$, as

$$\begin{aligned}\rho(0) = &\prod_{n=1}^{N-1} \frac{\exp[-(x_{n+1} - x_n)^2/2\alpha^2]}{\alpha(2\pi)^{1/2}} \prod_{n=1}^{N} \frac{\exp[-p_n^2/2\delta^2]}{\delta(2\pi)^{1/2}} \\ &\times \prod_{n=N}^{\infty} \frac{\exp[-(x_{n+1} - x_n)^2/2\epsilon^2]}{\epsilon(2\pi)^{1/2}} \prod_{n=N+1}^{\infty} \frac{\exp[-p_n^2/2\zeta^2]}{\zeta(2\pi)^{1/2}} \\ &\times \prod_{n=-1}^{-\infty} \frac{\exp[-(x_{n+1} - x_n)^2/2\epsilon^2]}{\epsilon(2\pi)^{1/2}} \prod_{n=0}^{-\infty} \frac{\exp[-p_n^2/2\zeta^2]}{\zeta(2\pi)^{1/2}} \\ &\times \frac{\exp[-x_0^2/2\phi^2]}{\phi(2\pi)^{1/2}}\end{aligned} \tag{20}$$

where the final factor represents our initial knowledge of one coordinate. The average initial energy terms are seen to be, for the system,

$$\langle p_n^2\rangle_0/2m = \delta^2/2m \tag{21a}$$

and

$$(k/2)\langle(x_{n+1} - x_n)^2\rangle_0 = k\alpha^2/2 = m\omega^2\alpha^2/2 \tag{21b}$$

and for the heat bath,

$$\langle p_n^2\rangle_0/2m = \zeta^2/2m = k_B T_h/2 \tag{22a}$$

and

$$(k/2)\langle(x_{n+1} - x_n)^2\rangle_0 = m\omega^2\epsilon^2/2 = k_BT_p/2 \tag{22b}$$

where kinetic and potential temperatures have been here defined.

In the sense that T_k and T_p are not necessarily equal, the initial probability density of the heat bath is a slight generalization of the canonical one, carried along whenever it is convenient to do so.

The initial probability density in terms of Schrödinger variables, obtainable directly from Eq. (20) by use of Eqs. (5a) and (5b), will not be written out here.

Results of the calculations for elements of the covariance matrix W and the entropy S are summarized in the following subsections.

5.1. Canonical, Schrödinger Variables, Free Chain

For $t = 0$, the following results are direct consequences of Eq. (20):

$$\begin{aligned}
&\langle\xi_i\xi_j\rangle_0 = \langle\xi_i^2\rangle_0\,\delta_{ij}, \qquad \langle x_0\xi_i\rangle_0 = 0 \\
&\langle\xi_{2n}^2\rangle_0 = \delta^2/m, \quad 1 \leqslant n \leqslant N; \qquad \langle\xi_{2n}^2\rangle_0 = \zeta^2/m, \quad n \neq \{1, N\} \\
&\langle\xi_{2n+1}^2\rangle_0 = m\omega^2\alpha^2, \quad 0 \leqslant n \leqslant N-1; \qquad \langle\xi_{2n+1}^2\rangle = m\omega^2\epsilon^2, \quad n \neq \{0, N-1\} \\
&\langle x_0^2\rangle_0 = \phi^2.
\end{aligned} \tag{23}$$

For any t, the results are

$$\begin{aligned}
&\langle\xi_{2j+1}(t)\,\xi_{2i+1}(t)\rangle \\
&\quad = [(\delta^2 - \zeta^2)/m](1, N; 2r-2j-1, 2r-2i-1) \\
&\qquad + m\omega^2(\alpha^2 - \epsilon^2)(0, N; 2r-2j, 2r-2i) \\
&\qquad + (\zeta^2/2m)[\delta_{ji} - J_{2(j-i)}(2\tau)] + (m\omega^2\epsilon^2/2)[\delta_{ji} + J_{2(j-i)}(2\tau)]
\end{aligned} \tag{24}$$

$$\begin{aligned}
&\langle\xi_{2i}(t)\,\xi_{2j}(t)\rangle \\
&\quad = (\zeta^2/m)(-\infty, \infty; 2r-2i, 2r-2j) + [(\delta^2 - \zeta^2)/m](1, N; 2r-2i, 2r-2j) \\
&\qquad + m\omega^2\epsilon^2(-\infty, \infty; 2r+1-2i, 2r+1-2j) + m\omega^2(\alpha^2 - \epsilon^2) \\
&\qquad \times (0, N-1; 2r+1-2i, 2r+1-2j)
\end{aligned} \tag{25}$$

$$\begin{aligned}
&\langle\xi_{2j+1}(t)\,\xi_{2i}(t)\rangle \\
&\quad = [(m\omega^2\epsilon^2/2) - (\zeta^2/2m)]\,J_{2i-2j-1}(2\tau) + [(\zeta^2 - \delta^2)/m] \\
&\qquad \times (1, N; 2r-2i, 2r-1-2j) \\
&\qquad + m\omega^2(\epsilon^2 - \alpha^2)(0, N-1; 2r+1-2i, 2r-2j)
\end{aligned} \tag{26}$$

$$\begin{aligned}\langle x_0(t)\,\xi_{2i}(t)\rangle &= (2\omega\sqrt{m})^{-1}\{(\zeta^2/m)(-\infty,\infty;2r-2i,2r]+[(\delta^2-\zeta^2)/m]\\&\quad\times(1,N;2r-2i,2r]+m\omega^2\epsilon^2(-\infty,\infty;2r+1-2i,2r+1]\\&\quad+m\omega^2(\alpha^2-\epsilon^2)(0,N-1;2r+1-2i,2r+1]\}\end{aligned}\tag{27}$$

and

$$\begin{aligned}\langle x_0(t)\,\xi_{2j+1}(t)\rangle &= -(2\omega\sqrt{m})^{-1}\{(\zeta^2/m)(-\infty,\infty;2r-2j-1,2r]\\&\quad+[(\delta^2-\zeta^2)/m](1,N;2r-2j-1,2r]\\&\quad+m\omega^2\epsilon^2(-\infty,\infty;2r-2j,2r+1]+m\omega^2(\alpha^2-\epsilon^2)\\&\quad\times(0,N-1,2r-2j,2r+1]\}\end{aligned}\tag{28}$$

where $\tau = 2\omega t$, and the four-index symbols $(\cdot)$ and $(\cdot]$, which are sums of Bessel functions or their integrals, are defined in the appendix.

As $t \to \infty$, these expressions decay to

$$\begin{aligned}\langle\xi_{2j+1}\xi_{2i+1}\rangle_\infty &= \langle\xi_{2j}\xi_{2i}\rangle_\infty = [(\zeta^2/2m)+(m\omega^2\epsilon^2/2)]\delta_{ji}\\\langle\xi_{2j+1}\xi_{2i}\rangle_\infty &= 0\end{aligned}\tag{29}$$

and

$$\langle x_0\xi_{2j+1}\rangle_\infty = \langle x_0\xi_{2j}\rangle_\infty = (4\omega\sqrt{m})^{-1}\,[(\zeta^2/m)+(m\omega^2\epsilon^2)]\tag{30}$$

The initial and ultimate values of (det W) and S are found to be

$$\det W_\xi(0) = (\omega\alpha\delta)^{2N}\tag{31}$$

$$\det W_\xi(\infty) = (k_B T)^{2N}\tag{32}$$

where $T = (T_p + T_k)/2$, from Eqs. (22) and (29),

$$S_\xi(0) = Nk_B + Nk_B\ln(\alpha\delta/\hbar)\tag{33}$$

and

$$S_\xi(\infty) = Nk_B + Nk_B\ln(k_B T/\hbar\omega)\tag{34}$$

It is of interest to note that even though the initial kinetic and potential temperatures in the heat bath may be unequal, the final temperatures, as seen in Eq. (29), *are* equal, as a result of equipartitioning of energy. The initial and final covariance matrices are diagonal, as shown by Eqs. (23) and (29). The entropies of Eqs. (33) and (34) are of the same form when T in Eq. (34) is recognized to be the geometric mean of the final kinetic and potential temperatures, and we write $\omega\alpha\delta = k_B(T_{p0}T_{k0})^{1/2}$, in terms of the initial kinetic and potential temperatures of the system, which are defined by replacing δ and ζ by α and ϵ, respectively, in Eqs. (22). It is noted that [det $W(0)$] and $S(0)$ are unchanged for the next three variations of the problem.

5.2. Canonical, Ordinary Variables, Free Chain

The results for this section follow directly from Eqs. (5), (8), and the results of Section 5.1 First, we write

$$\langle x_0^2(t)\rangle = \phi^2 + [(\delta^2 - \xi^2)/(2m\omega)^2][1, N; 2r, 2r] + [(\alpha^2 - \epsilon^2)/4][0, N-1; 2r+1, 2r+1] + [\zeta^2\tau/(2\omega m)^2]\Big[\int_0^{2\tau} J_0(x)\,dx - J_1(2\tau)\Big] + [\epsilon^2\tau/4]\Big[2\int_0^{\tau} J_0(x)\,dx - \int_0^{2\tau} J_0(x)\,dx + J_1(2\tau) - 2J_1(\tau)\Big] \tag{35}$$

Then, from Eqs. (8) with $1 \leqslant r, s \leqslant N$, we obtain

$$\langle x_r(t)\,x_s(t)\rangle = \langle x_0^2(t)\rangle - (\omega\sqrt{m})^{-1}\sum_{j=0}^{r-1}\langle x_0(t)\,\xi_{2j+1}(t)\rangle - (\omega\sqrt{m})^{-1}\sum_{j=0}^{s-1}\langle x_0(t)\,\xi_{2j+1}(t)\rangle + (\omega^2 m)^{-1}\sum_{i=0}^{r-1}\sum_{j=0}^{s-1}\langle \xi_{2i+1}(t)\,\xi_{2j+1}(t)\rangle \tag{36}$$

where the required averages have been given in Eqs. (24), (28), and (35). Similarly, we have

$$\langle p_i(t)\,p_j(t)\rangle = m\langle \xi_{2i}(t)\,\xi_{2j}(t)\rangle \tag{37}$$

and

$$\langle x_i(t)\,p_j(t)\rangle = m^{1/2}\langle x_0(t)\,\xi_{2j}(t)\rangle - \omega^{-1}\sum_{r=0}^{i-1}\langle \xi_{2r+1}(t)\,\xi_{2j}(t)\rangle \tag{38}$$

At $t = 0$, from Eq. (20), we start with

$$\langle p_i(0)\,p_j(0)\rangle = m\langle \xi_{2i}^2(0)\rangle\,\delta_{ij} = \delta^2\delta_{ij}, \qquad 1 \leqslant i \leqslant N \tag{39a}$$

$$= \zeta^2\delta_{ij}, \qquad i \notin \{1, N\} \tag{39b}$$

$$\langle x_n(0)\,x_{n+r}(0)\rangle = \phi^2 + n\alpha^2, \qquad r \geqslant 0, \quad 1 \leqslant n \leqslant N \tag{40}$$

$$\langle x_i(0)\,p_j(0)\rangle = 0, \tag{41}$$

and

$$\langle (x_{n+1} - x_n)^2\rangle_0\,(m\omega^2/2) = m\omega^2\alpha^2/2 = k_B T_{k0}/2 \tag{42}$$

As $t \to \infty$, the corresponding results are

$$\langle p_i p_j\rangle_\infty/2m = (\delta_{ij}/2)[(\zeta^2/2m) + (m\omega^2\epsilon^2/2)] = (k_B T/2)\,\delta_{ij} \tag{43}$$

$$\langle x_n x_{n+r}\rangle_\infty = \langle x_0^2\rangle_\infty - (r/2m\omega^2)[(\zeta^2/2m) + (m\omega^2\epsilon^2/2)] \tag{44}$$

$$\langle x_n p_r\rangle_\infty = k_B T/4\omega \tag{45}$$

and

$$\langle x_0^2(t)\rangle \to \phi^2 + N[(\delta^2 - \zeta^2)/(2\omega m)^2 + (\alpha^2 - \epsilon^2)/4] + (\tau/4)[(\zeta/\omega m)^2 + \epsilon^2 - (\zeta/\omega m)^2 J_1(2\tau) + \epsilon^2 J_1(2\tau) - 2\epsilon^2 J_1(\tau)] \quad (46)$$

where $\tau = 2\omega t$.

The free chain drifts with time, as expected, since there is no constraint to anchor it. For $\tau \gg N$, the dominant term in Eq. (46) is

$$\langle x_0^2(t)\rangle \approx \tau k_B T/2m\omega^2 = tk_B T/m\omega \quad (47)$$

A diffusivity may be obtained from the relation $\langle x_0^2\rangle = 2Dt$, yielding

$$D_c = k_B T/2m\omega \quad (48)$$

in agreement with Hemmer's result.[5]

The covariance matrix elements for $t \to \infty$ are given by Eqs. (43)–(45), but because of the diffusion of the entire chain, both det W and S are expected to increase without limit. Nevertheless, we can write det W_N in terms of $\langle x_0^2\rangle$ for $\omega t \gg N$ as

$$\det W_N(t) \to (k_B T/\omega)^{2N} [(m\omega^2\langle x_0^2\rangle/k_B T) - O(N)] \quad (49)$$

where, in order for this approximation to be valid, terms of the order of N are negligible compared to the $\langle x_0^2\rangle$ term. By use of Eqs. (18) and (47), we write the entropy as

$$S_N(t) \to Nk_B + Nk_B \ln(k_B T/\hbar\omega) + (k_B/2)\ln(\omega t) \quad (50)$$

It is thus seen that, except for the Brownian drift term, the entropy of Eq. (50) agrees with that of Eq. (34) for the same system in terms of Schrödinger variables. The time-dependent term in (50) is not proportional to N, and therefore is not extensive; it serves as a reminder that thermodynamic entropy is not intrinsically and fundamentally extensive for all choices of systems.

5.3. Canonical, Schrödinger Variables, x_0 Fixed

The elements of the covariance matrix, when x_0 is fixed at the origin, are obtained from evident symmetry operations on the results of Section 5.1. At $t = 0$, the conditions are the same as those given by Eqs. (23), except that $\phi = 0$. For any t, we obtain

$$\begin{aligned}\langle \xi_{2j+1}(t)\, \xi_{2i+1}(t)\rangle &= [(\zeta^2/2m) + (m\omega^2\epsilon^2/2)]\,\delta_{ij} + [(m\omega^2\epsilon^2/2) - (\zeta^2/2m)] \\ &\quad \times [J_{2j-2i}(2\tau) + J_{2j+2i+2}(2\tau)] \\ &\quad + [(\delta^2 - \zeta^2)/m] \sum_{r=1}^{N} (J_{2i+1-2r} - J_{2i+1+2r})(J_{2j+1-2r} - J_{2j+1+2r}) \\ &\quad + m\omega^2(\alpha^2 - \epsilon^2) \sum_{r=0}^{N-1} (J_{2j-2r} + J_{2j+2r+2})(J_{2i-2r} + J_{2i+2r+2}) \end{aligned} \quad (51)$$

$$\begin{aligned}\langle \xi_{2j}(t)\, \xi_{2i}(t)\rangle &= [(\zeta^2/2m) + (m\omega^2\epsilon^2/2)]\,\delta_{ij} + [(m\omega^2\epsilon^2/2) - (\zeta^2/2m)] \\ &\quad \times [J_{2j+2i}(2\tau) - J_{2j-2i}(2\tau)] \end{aligned} \quad (52)$$

and

$$\begin{aligned}\langle \xi_{2j}(t)\, \xi_{2i+1}(t) \rangle &= [(m\omega^2\epsilon^2/2) - (\zeta^2/2m)][J_{2j+2i+1} - J_{2i-2j+1}] \\ &+ [(\delta^2 - \zeta^2)/m] \sum_{r=1}^{N} (J_{2j-2r} - J_{2j+2r})(J_{2i+1-2r} - J_{2i+1+2r}) \\ &+ m\omega^2(\alpha^2 - \epsilon^2) \sum_{r=0}^{N-1} (J_{2j-2r-1} + J_{2j+2r+1})(J_{2i-2r} + J_{2i+2r+2}) \end{aligned} \tag{53}$$

where the arguments of the Bessel functions are all $2\tau = 4\omega t$.

As $t \to \infty$, these matrix elements become

$$\langle \xi_{2j+1}\xi_{2i+1} \rangle_\infty = \delta_{ji} k_B T \tag{54a}$$

$$\langle \xi_{2j}\xi_{2i} \rangle_\infty = \delta_{ji} k_B T \tag{54b}$$

and

$$\langle \xi_{2j}\xi_{2i+1} \rangle_\infty = 0 \tag{54c}$$

where $k_B T = (\zeta^2/2m) + (m\omega^2\epsilon^2/2)$, as before. These ultimate matrix elements are the same as those of Section 5.1, showing that the covariance matrix and the entropy at equilibrium are not affected by the process of fixing x_0, provided that variables are so chosen that the Brownian motion is concealed.

5.4. Canonical, Ordinary Variables, x_0 Fixed

The elements of the covariance matrix follow from Eqs. (5) and (8) and the results of Section 5.3. Only the results as $t \to \infty$ will be given here. These, giving a simpler covariance matrix than when x_0 is free, are found to be

$$\langle x_n x_{n+r} \rangle_\infty = n k_B T/m\omega^2, \qquad r \geqslant 0 \tag{55a}$$

$$\langle p_i p_j \rangle_\infty = \delta_{ij} m k_B T \tag{55b}$$

and

$$\langle x_i p_j \rangle_\infty = 0 \tag{55c}$$

Although some x–x correlations exist, as seen in Eq. (55a), these arise merely from the displacement of the nth particle resulting in origin shifts of all particles further away from x_0 than the nth, and they contribute nothing to the entropy. The equilibrium entropy is found to be

$$S_N(\infty) = Nk_B + Nk_B \ln(k_B T/\hbar\omega) \tag{56}$$

in agreement with all the others except that of Section 5.2, where Brownian motion modifies the result.

6. NONCANONICAL INITIAL CONDITIONS

The initial probability density for the system and heat bath considered in this section is identical to that of Eq. (20) in the momentum terms, except that the coordinate terms are replaced by Gaussian factors in the coordinates themselves, rather than in the spring stretchings, as follows, with the prime on the product denoting omission of variables numbered 1 — N:

$$\rho(0) = \prod_{n=1}^{N} \frac{\exp[-x_n^2/2\alpha^2]}{\alpha(2\pi)^{1/2}} \prod_{n=1}^{N} \frac{\exp[-p_n^2/2\delta^2]}{\delta(2\pi)^{1/2}} \times \prod{}' \frac{\exp[-x_n^2/2\epsilon^2]}{\epsilon(2\pi)^{1/2}} \prod{}' \frac{\exp[-p_n^2/2\zeta^2]}{\zeta(2\pi)^{1/2}} \tag{57}$$

where the coordinates and momenta are those at $t = 0$. Expectation values of the system coordinates and momenta are here chosen as zero at $t = 0$, although they can be chosen more generally without undue complication. Except for this somewhat restricted choice of initial expectation values, which does not affect the final result, Eq. (57) is the same probability density that we have treated in previous papers.[1,2] The average initial variances are seen by inspection to be, for the system,

$$\langle p_n^2 \rangle_0 = \delta^2 \tag{58a}$$

$$\langle x_n^2 \rangle_0 = \alpha^2 \tag{58b}$$

and for the heat bath,

$$\langle p_n^2 \rangle_0 = \zeta^2 \tag{59a}$$

and

$$\langle x_n^2 \rangle_0 = \epsilon^2 \tag{59b}$$

The initial kinetic temperature of the heat bath is just that given by Eq. (22a), but for the potential temperature, we have

$$(k/2)\langle (x_{n+1} - x_n)^2 \rangle_0 = m\omega^2\epsilon^2 = k_B T_p/2 \tag{60}$$

further emphasizing that ϵ has different meanings in Eqs. (20) and (57). No problem of comparison will arise, however, if results are expressed in terms of temperatures rather than variances.

We note here that, in addition to Eq. (60), nearest-neighbor spring stretchings are not independent; we have

$$\langle (x_{n+1} - x_n)(x_n - x_{n-1}) \rangle_0 = - \langle x_n^2 \rangle_0 , \tag{61}$$

an evident result, since the displacement x_n stretches one of its connected springs and compresses the other. This claimed knowledge, that the initial stretchings of adjacent springs are not independent, is the basis for the result that the equilibrium entropy of the system is smaller than its canonical value, since the equilibrium reduced Liouville function reflects, in its departure from the canonical one, a persistent interdependence of adjacent elements of the chain.

Results of the calculations for elements of the covariance matrix W and the entropy S are summarized in the following sections.

6.1. Noncanonical, Ordinary Variables, Free Chain

The results of this section have already appeared,[1,2] but they will be included for completeness. For any t, we find

$$\langle x_i(t)\, x_j(t)\rangle = (\epsilon^2/2)[\delta_{ij} + J_{2i-2j}(2\tau)] + (\zeta/2\omega m)^2 \Big\{\tau \Big[\int_0^{2\tau} J_0(y)\,dy - J_1(2\tau) - \sum_{n-1}^{|i-j|} \int_0^{2\tau} J_{2n-1}(y)\,dy\Big\} + (\alpha^2 - \epsilon^2)(1, N; 2r - 2i, 2r - 2j) + [(\delta^2 - \zeta^2)/(2\omega m)^2][1, N; 2r - 2i, 2r - 2j\Big] \tag{62}$$

$$\langle p_i(t)\, p_j(t)\rangle = (\zeta^2/2)[\delta_{ij} + J_{2i-2j}(2\tau)] + [(\epsilon\omega m)^2/2][J_{2i-2j+2}(2\tau) + J_{2i-2j-2}(2\tau) - 2J_{2i-2j}(2\tau) + 2\delta_{ij} - \delta_{i,j-1} - \delta_{i,j+1}] + (\alpha^2 - \epsilon^2)(2\omega m)^2 (1, N; \overline{2r - 2i}, \overline{2r - 2j}) + (\delta^2 - \zeta^2)(1, N; 2r - 2i, 2r - 2j) \tag{63}$$

and

$$\langle x_i(t)\, p_j(t)\rangle = (\alpha^2 - \epsilon^2)(2\omega m)(1, N; 2r - 2i, \overline{2r - 2j}) + (\delta^2 - \zeta^2)(2\omega m)^{-1}[1, N; 2r - 2i, 2r - 2j) + [\epsilon^2(2\omega m)/4][dJ_{2i-2j}(2\tau)/d\tau] + \zeta^2(4\omega m)^{-1}\int_0^{2\tau} J_{2i-2j}(y)\,dy \tag{64}$$

As $\tau \gg N$, these become

$$\langle x_n(t)\, x_{n+r}(t)\rangle \to \langle x_1^2(t)\rangle - r(\zeta/2\omega m)^2, \qquad r \geqslant 0 \tag{65}$$

$$\langle p_n(t)\, p_{n+r}(t)\rangle \to (\zeta^2/2)\,\delta_{0r} + [(m\omega\epsilon)^2/2](2\delta_{0r} - \delta_{ir} - \delta_{-1r}) \tag{66}$$

$$\langle x_i(t)\, p_j(t)\rangle \to \zeta^2/4\omega m \tag{67}$$

and

$$\langle x_1^2(t)\rangle \to (\zeta/2\omega m)^2\,\tau[1 - J_1(2\tau)] + (\epsilon^2/2) + (\delta^2 - \zeta^2)\,N/(2\omega m)^2 \tag{68}$$

where the last two terms in Eq. (68) are negligible compared to the τ terms, as is the $J_1(2\tau)$ term for large τ. The diffusivity is here seen to be

$$D_n = \zeta^2/4\omega m^2 = k_B T_k/4m\omega \tag{69}$$

as reported in I.[1] Thus, the noncanonical diffusivity depends only on the kinetic temperature, in contrast to the canonical result of Eq. (48).

The entropy diverges because of the Brownian drift, as in the canonical case of Eq. (50), and it is fairly complicated even in the nondivergent terms. Since these terms will be exhibited in the next three variations of the problem, the entropy for this formulation will not be presented. The initial entropy, however, is found to be

$$S_N(0) = Nk_B + Nk_B \ln(\alpha\delta/\hbar) = Nk_B \ln[k_B(T_{k0}T_{p0}/2)^{1/2}/\hbar\omega] + Nk_B \tag{70}$$

6.2. Noncanonical, Schrödinger Variables, Free Chain

The elements of the covariance matrix as $t \to \infty$ are found to be

$$\langle \xi_{2i+1}\xi_{2j}\rangle_\infty = 0 \tag{71a}$$

$$\langle \xi_{2r}\xi_{r+2n}\rangle_\infty = (\zeta^2/2m)\,\delta_{0n} + (m\omega^2\epsilon^2/2)(2\delta_{0n} - \delta_{1n} - \delta_{-1n}) \tag{71b}$$

$$= \langle \xi_{2r+1}\xi_{2r+2n+1}\rangle_\infty \tag{71c}$$

The persistence of nearest-neighbor correlations should be noted. If Eqs. (71) are chosen as the covariance matrix elements at $t = 0$, the covariance matrix $W_N(t)$ is found to be independent of time, showing that these results do indeed prescribe an equilibrium state, though not a canonical one.

The use of Eq. (60) for T_p, the definition of Eq. (22a) for T_k, and the definition $T = (T_p + T_k)/2$ enable us to write

$$\det W_\xi(\infty) = k_B^{2N} \begin{vmatrix} D_N & 0 \\ 0 & D_N \end{vmatrix} \tag{72}$$

where the $N \times N$ matrix D_N is given by

$$D_N = \begin{pmatrix} T & -T_p/4 & 0 & 0 & \cdots & 0 \\ -T_p/4 & T & -T_p/4 & 0 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & -T_p/4 & T \end{pmatrix} \tag{73}$$

If we now write $\det D_N = T^N P_N(\gamma)$, where $\gamma = T_p/2T$ and P_N is a polynomial in γ, we find that

$$P_N(\gamma) = 2^{-N} \sum_{j,k=0}^{N} (-)^j \binom{k}{j}\binom{N+1}{2k+1} \gamma^{2j} \tag{74}$$

For large N, we find that

$$2P_{N+1}/P_N \to 1 + (1 - \gamma^2)^{1/2} \tag{75}$$

For $\gamma = 1/2$ (when $T_p = T_k = T$), the result of Eq. (75) is

$$P_{N+1}(1/2)/P_N(1/2) \approx 0.933 \tag{76}$$

and numerical analysis of the polynomial set yields the very good approximation

$$P_N(1/2) \approx [(15/16)/(0.933)^2](0.933)^N \approx 1.078(0.933)^N, \qquad N \geqslant 2 \tag{77}$$

Since $(\det W_\xi)^{1/2} = (k_B T)^N P_N(\gamma)$, we obtain from Eq. (18) and approximation (77) for $\gamma = 1/2$,

$$S_\xi(\infty) \approx Nk_B + Nk_B \ln(0.933 k_B T/\hbar\omega) + k_B \ln(1.078), \qquad N \geqslant 2 \tag{78}$$

The expression (78) for the equilibrium entropy contains a small nonextensive term, which is negligible for large N, and a numerical factor (0.933) multiplying T that shows clearly the less-than-canonical value of the equilibrium entropy. In general, for any γ, the factor 0.933 in Eq. (78) is replaced by $[1 + (1 - \gamma^2)^{1/2}]/2$, and the nonextensive term is still unimportant for large N. Since the definitions of T, T_p, and γ require that $\gamma \leqslant 1$, the extensive part of the entropy will always be less than (or equal to, when $\gamma = 0$, which is unphysical) the canonical entropy for the same system. At $t = 0$, the entropy of this system is that given by Eq. (70) plus the nonextensive term $k_B \ln(N + 1)$.

6.3. Noncanonical, Ordinary Variables, x_0 Fixed

The elements of the covariance matrix are given in this case for any time t as

$$\begin{aligned}\langle x_i(t)\, x_j(t)\rangle = {} & (\alpha^2 - \epsilon^2)\{(1, N; 2r - 2i, 2r - 2j) - (1, N; 2r - 2i, 2r + 2j) \\ & - (1, N; 2r + 2i, 2r - 2j) + (1, N; 2r + 2i, 2r + 2j)\} \\ & + (\epsilon^2/2)\{\text{same, except} \quad (-\infty, \infty;\ldots)\} \\ & + (\delta^2 - \zeta^2)(2\omega m)^{-2}\{\text{same, except} \quad [1, N;\ldots]\} \\ & + (\zeta^2/2)(2\omega m)^{-2}\{\text{same, except} \quad [-\infty, \infty;\ldots]\}\end{aligned} \tag{79a}$$

$$\begin{aligned}\langle p_i(t)\, p_j(t)\rangle = {} & (2m\omega)^2(\alpha^2 - \epsilon^2)\{(1, N; \overline{2r - 2i}, \overline{2r - 2j}) - (1, N; \overline{2r - 2i}, \overline{2r + 2j}) \\ & - (1, N; \overline{2r + 2i}, \overline{2r - 2j}) + (1, N; \overline{2r + 2i}, \overline{2r + 2j})\} \\ & + (\epsilon^2/2)(2m\omega)^2\{\text{same, but with} \quad (-\infty, \infty; \overline{\cdots}, \overline{\cdots})\} \\ & + (\delta^2 - \zeta^2)\{(1, N; 2r - 2i, 2r - 2j) + \text{etc.}\} \\ & + (\zeta^2/2)\{\text{same, but with} \quad (-\infty, \infty; \cdots, \cdots)\}\end{aligned} \tag{79b}$$

and

$$\begin{aligned}\langle x_i(t)\, p_j(t)\rangle = {} & (\alpha^2 - \epsilon^2)(2\omega m)\{(1, N; 2r - 2i, \overline{2r - 2j}) - (1, N, 2r - 2i, \overline{2r + 2j}) \\ & - (1, N; 2r + 2i, \overline{2r - 2j}) + (1, N; 2r + 2i, 2r + 2j)\} \\ & + (\epsilon^2/2)(2\omega m)\{\text{same, but with} \quad (-\infty, \infty; \cdots, \cdots,)\} \\ & + (\delta^2 - \zeta^2)(2\omega m)^{-1}\{[1, N; 2r - 2i, 2r - 2j) + \text{etc.}\} \\ & + (\zeta^2/2)(2\omega m)^{-1}\{\text{same, but with} \quad [-\infty, \infty; \cdots, \cdots)\}\end{aligned} \tag{79c}$$

As $t \to \infty$, these become

$$\langle x_n x_{n+r} \rangle_\infty = (\epsilon^2/2)\, \delta_{0r} + [2n\zeta^2/(2\omega m)^2], \qquad r \geqslant 0 \tag{80a}$$

$$\langle p_n p_{n+r} \rangle_\infty = (\zeta^2/2)\, \delta_{0r} + [(m\omega\epsilon)^2/2](2\delta_{0r} - \delta_{ir} - \delta_{-1r}) \tag{80b}$$

and

$$\langle x_n p_r \rangle_\infty = 0 \tag{80c}$$

The determinant of the equilibrium covariance matrix can be written

$$\det W_N(\infty) = (k_B \zeta^2/2\omega^2 m)^N \begin{vmatrix} E_N & 0 \\ 0 & D_N \end{vmatrix} \tag{81}$$

where D_N is given by Eq. (73), and E_N is the matrix

$$E_N = \begin{pmatrix} \sigma+1 & 1 & 1 & \cdots & 1 \\ 1 & \sigma+2 & 2 & \cdots & 2 \\ 1 & 2 & \sigma+3 & \cdots & 3 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 1 & 2 & 3 & \cdots & \sigma+N \end{pmatrix} \tag{82}$$

where $\sigma = (m\omega\epsilon/\zeta)^2 = (T_p/2T_k)$. Then, $\det W_N(\infty)$ becomes

$$\det W_N(\infty) = (k_B \zeta^2/2\omega^2 m)(\det D_N)(\det E_N) \tag{83}$$

where $\det D_N$ has already been evaluated in the previous section, and $\det E_N$ is found to be

$$\det E_N = \sum_{n=0}^{N} \left(\frac{4\sigma+1}{4}\right)^n \left[\binom{N}{2n}\left(\frac{2\sigma+1}{2}\right)^{N-2n} + \frac{1}{2}\binom{N}{2n+1}\left(\frac{2\sigma+1}{2}\right)^{N-2n-1}\right] \tag{84}$$

For the condition that $T = T_p = T_k$, so that $\sigma = \gamma = 1/2$, we obtain the very good approximations

$$\det D_N \approx (0.933T)^N (1.078), \qquad N \geqslant 2 \tag{85}$$

as before, and

$$\det E_N \approx (1.866)^N (0.790), \qquad N \geqslant 2 \tag{86}$$

where $0.790 = 2.75/(1 + \sqrt{3}/2)^2$, and $2.75 = \det E_2(1/2)$. A combination of these results yields

$$S_N(\infty) \approx Nk_B + Nk_B \ln(0.933 k_B T/\hbar\omega) + k_B \ln(0.924), \qquad N \geqslant 2 \tag{87}$$

which agrees with Eq. (78) except for the small, nonextensive term.

6.4. Noncanonical, Schrödinger Variables, x_0 Fixed

The results for this section are identical with those of Section 6.2, just as the Schrödinger-variable description of equilibrium was found to be identical in the two comparable canonical examples.

7. DISCUSSION

In all the variations of the problem, the initial state of the heat bath permits the definition of kinetic and potential temperatures by use of $k_BT/2$ = mean kinetic/potential energy of a mass/spring, and in all cases the final kinetic and potential temperatures of the system were found to be equal to the *arithmetic* mean of the initial heat-bath temperatures. Thus, equipartition of energy is easily demonstrated.

The behavior of the entropy function provides several useful insights. The initial entropy in each case depends upon the product of system-variable variances, as seen in Eqs. (33) and (70). This product, in turn, can be written as the *geometric* mean of initial kinetic and potential temperatures, as was done at the end of Section 5.1. This result suggests that we examine the final form of the entropy for a similar dependence, and indeed it exists. The equality of final potential and kinetic temperatures, because of equipartition, obscures the fact that $T = (T_kT_p)^{1/2}$ in the entropy formulas. Examination of the covariance matrix W, however, shows, as in Eqs. (54), for example, that the equilibrium value of det W becomes the product of two determinants, one involving only the coordinates and the other only the momenta. These do not always become diagonal, but one can clearly be seen to yield a coordinate-related quantity that can be called the final potential temperature, and the other a momentum-related quantity called the kinetic temperature. Thus, in all cases, the final temperature turns out to be the geometric mean, from (det $W)^{1/2}$, of the (equal) kinetic and potential temperatures.

These two temperatures are measures of the variances in the coordinates and momenta, just as the initial temperatures were given in terms of initial variances. When quantum systems are considered, the uncertainty principle bounds from below the product of coordinate and momentum variances. Thus, for example, the logarithmic term in Eq. (70) is prevented from being negative by the uncertainty principle.

Although the entropy calculations herein are entirely classical and expressions such as Eq. (34) are not correct for the quantum mechanical entropy, the point here is that the entropy variable is $k_BT/\hbar\omega$, which is equivalent to $[\langle(\delta x)^2\rangle\langle(\delta p)^2\rangle]^{1/2}/\hbar$, a quantity that cannot become zero, and in fact should always be greater than unity. The entropy function, then, is well-behaved for our best possible measurements of initial conditions, and it increases as the mechanical-variable variances become larger, i.e., as our knowledge of these variables becomes less precise.

When the heat bath is chosen to be canonical, the final entropies are found to be extensive, except in Section 5.2, where a single reference coordinate was needed to locate the position of the entire system, independent of N. This nonextensive term is time-dependent, increasing without limit as the system drifts, but the remaining contributions to the entropy are the usual thermal ones. Eliminating the Brownian drift by setting $x_0 = 0$ for all t, or concealing it by the choice of Schrödinger variables, gives rise to the correct classical canonical equilibrium entropy of the system. On the other hand, the choice of independent Gaussian distributions for the heat-bath variables results in small nonextensive contributions to the entropy even when the Brownian drift is excluded. In the thermodynamic limit ($N \to \infty$), these terms disappear, but they do serve as a reminder that the entropy is not fundamentally and necessarily an extensive quantity.

In all cases, if the system comes to equilibrium with a heat bath at temperature T_1, and then is allowed to come to equilibrium with another *similarly* defined heat bath and temperature T_2, the entropy change is found to be

$$S_N(T_2) - S_N(T_1) = Nk_B \ln(T_2/T_1) \tag{88}$$

so that the definition of the heat bath does not intrude upon the measured entropy change of a system.

Finally, the physical picture of the noncanonical equilibrium is entirely reasonable. As best seen in terms of the Schrödinger variables of Section 6.2, nearest-neighbor (anti) correlations persist at equilibrium. These represent the shortening of one spring and lengthening of the other as the mass between them moves, and the oppositely directed motions of masses on opposite ends of the same spring. Perhaps the real surprise is the realization that these motions are absent in the canonical system.

It is interesting to observe that these correlations reduce the entropy of the system only if we know about them; they limit the freedom of the phase trajectory, in its coverage of the $2N$-dimensional phase space, without contributing to observable quantities such as heat capacity. The result implies, for ordinary thermodynamics and statistical mechanics, that hidden correlations among the microscopic variables may exist without in any way making their presence known via the usual thermodynamic observations, in support of a comment made by Blatt.[6]

APPENDIX

The four-index symbols used in Sections 5 and 6 are defined as

$$[a, b; c, d] = \sum_{r=a}^{b} \int_0^{\tau} J_c(y)\, dy \int_0^{\tau} J_d(z)\, dz \tag{A.1}$$

$$(a, b; c, d] = \sum_{r=a}^{b} J_c(\tau) \int_0^{\tau} J_d(y)\, dy \tag{A.2}$$

$$[a, b; c, d) = \sum_{r=a}^{b} \int_0^{\tau} J_c(y)\, dy\, J_d(\tau) \tag{A.3}$$

$$(a, b; c, d) = \sum_{r=a}^{b} J_c(\tau)\, J_d(\tau) \tag{A.4}$$

$$(a, b; \bar{c}, d) = \sum_{r=a}^{b} J_c'(\tau)\, J_d(\tau) \tag{A.5}$$

$$(a, b; c, \bar{d}) = \sum_{r=a}^{b} J_c(\tau)\, J_d'(\tau) \tag{A.6}$$

and

$$(a, b; \bar{c}, \bar{d}) = \sum_{r=a}^{b} J_c'(\tau)\, J_d'(\tau) \tag{A.7}$$

where $J'(\tau) = dJ(\tau)/d\tau$, and the summations are always over the index r, which must appear in c and d.

Some specific infinite sums that have been used are

$$\begin{aligned}(-\infty, \infty; 2r+1, 2r+1+m) &= \sum_{r=-\infty}^{\infty} J_{2r+1}(\tau)\, J_{2r+1+m}(\tau) \\ &= \tfrac{1}{2}[J_m(0) - J_m(2\tau)]\end{aligned} \tag{A.8}$$

$$(-\infty, \infty; 2r, 2r+m) = \tfrac{1}{2}[J_m(0) + J_m(2\tau)] \tag{A.9}$$

$$\begin{aligned}(-\infty, \infty; 2r-2n, 2r-2m) &= (-\infty, \infty; 2r, 2r+2n-2m) \\ &= (-\infty, \infty; 2r, 2r+2m-2n)\end{aligned} \tag{A.10}$$

$$(-\infty, \infty; 2r-2m, 2r] = (1/2)\int_0^{2\tau} J_{2m}(y)\, dy \tag{A.11}$$

$$(-\infty, \infty; 2r+1-2m, 2r+1] = (1/2)\int_0^{2\tau} J_{2m}(y)\, dy + \int_0^{\tau} J_{2m}(y)\, dy \tag{A.12}$$

$$(-\infty, \infty; 2r-2j-1, 2r] = -(1/2)\int_0^{2\tau} J_{2j+1}(y)\, dy \tag{A.13}$$

$$(-\infty, \infty; 2r-2j, 2r+1] = (1/2)\int_0^{2\tau} J_{2j+1}(y)\, dy - \int_0^{\tau} J_{2j+1}(y)\, dy \tag{A.14}$$

$$[-\infty, \infty; 2r, 2r] = \tau\left[\int_0^{2\tau} J_0(y)\, dy - J_1(2\tau)\right] \tag{A.15}$$

$$[-\infty, -\infty; 2r-2n, 2r-2m] = [-\infty, \infty; 2r, 2r] - \sum_{j=1}^{|n-m|}\int_0^{2\tau} J_{2j-1}(y)\, dy \tag{A.16}$$

$$\begin{aligned}(-\infty, \infty; \overline{2r-2n}, \overline{2r-2m}) &= (1/8)[J_{2n-2m+2}(2\tau) + J_{2m-2m-2}(2\tau) - J_{2n-2m}(2\tau) \\ &\quad + 2\delta_{nm} - \delta_{n,m-1} - \delta_{n,m+1}]\end{aligned} \tag{A.17}$$

and

$$(-\infty, \infty; 2r-2n, \overline{2r-2m}) = (1/4)\, dJ_{2n-2m}(2\tau)/d\tau \tag{A.18}$$

Other, similar results can be obtained from obvious symmetry properties or from direct evaluation of the infinite sums, using standard identities. These results and their derivations are available in limited supply.[4]

REFERENCES

1. M. A. Huerta and H. S. Robertson, *J. Stat. Phys.* **1**:393 (1969).
2. H. S. Robertson and M. A. Huerta, *Am. J. Phys.* **38**:619 (1970).
3. E. Schrödinger, *Ann. Phys.* **44**:916 (1914).
4. M. A. Huerta, "Approach to Equilibrium of Infinite Chains of Coupled Harmonic Oscillators," Thesis, Miami (1969); MIAPH-TP-69.24.
5. P. C. Hemmer, "Dynamic and Stochastic Types of Motion in the Linear Chain," Thesis, Trondheim, Norway (1959).
6. J. M. Blatt, *Progr. Theoret. Phys.* **22**:745 (1959).