Local Dynamics in an Infinite Harmonic Chain

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Abstract: By the method of recurrence relations, the time evolution in a local variable in a harmonic chain is obtained. In particular, the autocorrelation function is obtained analytically. Using this result, a number of important dynamical quantities are obtained, including the memory function of the generalized Langevin equation. Also studied are the ergodicity and chaos in a local dynamical variable.

1. Introduction

A harmonic chain has been a useful model for a variety of dynamical phenomena, such as the lattice vibrations in solids, Brownian motion and diffusion. It has also been a useful model for testing theoretical concepts, such as the thermodynamic limit, irreversibility and ergodicity. One can study these properties in a harmonic chain. In this work, we shall touch on most of these issues analytically.

The dynamics in a chain of nearest-neighbor (nn) coupled monatomic oscillators (defined in Section 3) has been studied in the past almost exclusively by means of normal modes [1]. If there are N oscillators in a chain, the single-particle or individual coordinates of the oscillators q_i, $i = 1, 2, ..N$, are replaced by the total or collective coordinates Q_j, $j = 1, 2, ..N$. In the space of the collective coordinates, the "collective" oscillators are no longer coupled. As a result, their motions are simply periodic. Each collective oscillator would have a unique frequency associated with it (if degeneracy due to symmetry could be ignored).

On the one hand, this collective picture is very helpful in understanding the dynamics of a harmonic chain by avoiding what might be a complicated picture due to a set of motions of coupled single particles. If only the collective behavior is required, this approach is certainly sufficient.

On the other hand, if one wishes to know the dynamics of a single oscillator in a chain, the traditional approach becomes cumbersome. Why would one wish to know the dynamics of one oscillator in a chain? There may be a defect in a chain, for example. It may be a heavier or lighter mass than its neighbors'. Diffusivity is attributed to the motions of single oscillators. For these and other physical reasons that will become apparent, there is a need to study how a single oscillator embedded in a chain evolves in time. We shall term it local dynamics to be distinguished from total dynamics.

In the 1980s, a new method of calculating the time evolution in a Hermitian system was developed, known as the method of recurrence relations [2]. It solves the Heisenberg equation of motion for a dynamical variable of physical interest, which may be the momentum of a single particle, the number or current density. Although it was intended to deal with dynamical variables of quantum origin, *i.e.*, operators, it was found to be applicable to classical variables by replacing commutators with Poisson brackets. During the past three decades, this method has been widely applied to a variety of dynamical issues emanating from the electron gas, lattice spins, lattice vibrations and classical fluids. For reviews, see [3–7]. For a partial list of recent papers, see [8–21].

Formally, this method shows what types of solutions are admissible [22]. It provides a deeper insight into the memory function and the Langevin equation. It has also provided a basis from which to developed the ergometric theory of the ergodic hypothesis.

In Section 2, we will briefly introduce the method of recurrence relations, mostly by assertion, referring the proofs to the original sources and review articles. In Section 3, the dynamics of a local variable (a single particle) in an infinite harmonic chain will be solved by the method of recurrence relations. Some useful physical applications will follow to complete this work.

2. Method of Recurrence Relations

Let A be a dynamical variable, e.g., a spin operator, and $H(A)$ an N-body Hamiltonian. The number of particles N is not restricted initially. The Hamiltonian H must however be Hermitian, which means that there is to be no dissipation in the dynamics of A. The time evolution of A is to be given by the Heisenberg equation of motion:

$$\dot{A}(t) = i[H, A(t)] \tag{1}$$

with $\hbar = 1$ and $[H, A] = HA - AH$. If A is a classical variable, the rhs of Equation (1) is to be replaced by the Poisson brackets.

A formal solution for Equation (1) may be viewed in geometrical terms. Let $A(t)$ be a vector in an inner product space S of d dimensions. This space is spanned by d basis vectors f_k, $k = 0, 1, ..d - 1, d \geq 2$. These basis vectors are mutually orthogonal:

$$(f_k, f_{k'}) = 0 \ \ if \ \ k' \neq k \tag{2}$$

where (,) denotes an inner product, which defines the space S. Observe that they are time independent. In terms of these, $A(t)$ may be expressed as:

$$A(t) = \sum_k a_k(t) f_k \tag{3}$$

where a_k, $k = 0, 1, ..d - 1$, is a set of functions or basis functions conjugate to the basis vectors. They carry time dependence.

As t evolves, this vector $A(t)$ evolves in this space S. Its motion in S is governed by Equation (1), so that it is H specific. Since $||A(t)|| = ||A||$, that is $(A(t), A(t)) = (A, A)$, the "length" of $A(t)$ in S is an invariant of time. As t evolves, $A(t)$ may only rotate in S. This means that there is a Bessel equality, which limits what kind of rotation is allowed.

Since both the basis vectors and functions are only formally stated, Equation (3) is not yet useful. One does not know what is d, the dimensionality of S. To make it useful, we need to realize S, an abstract space by defining the inner product in a physically-useful way.

2.1. Kubo Scalar Product

We shall realize S by the Kubo scalar product (KSP) as follows: let X and Y be two vectors in S. The inner product of X and Y is defined as:

$$(X, Y) = 1/\beta \int_0^\beta d\lambda < X(\lambda) Y^* > - < X >< Y^* > \tag{4}$$

where $\beta = 1/k_B T$, T temperature, $< .. >$ means an ensemble average, $*$ means Hermitian conjugation and:

$$X(\lambda) = e^{\lambda H} X e^{-\lambda H} \tag{5}$$

Equation (4) is known as KSP in many body theory [23]. There is a deep physical reason for using KSP to realize S [24]. When realized by KSP, it shall be denoted $\bar{S}$.

2.2. Basis Vectors

We have proved that the basis vectors in $\tilde{S}$ satisfy the following recurrence relation, known as RR I:

$$f_{k+1} = \dot{f}_k + \Delta_k f_{k-1}, \ \ k = 0, 1, 2, .., d-1 \tag{6}$$

where $\dot{f}_k = i[H, f_k]$, $\Delta_k = ||f_k|| / ||f_{k-1}||$, with $f_{-1} = 0$ and $\Delta_0 = 1$.

If $k = 0$ in Equation (6), $f_1 = \dot{f}_0$. With $f_0 = A$ (by choice), f_1 is obtained and, therewith, Δ_1.

Given Δ_1, by setting $k = 1$ in Equation (6), one can calculate f_2, therewith Δ_2. If proceeding in this manner, $f_d = 0$ for some finite value of d giving a finite dimensional $\bar{S}$ or $f_d \neq 0$ as $d \to \infty$ giving an infinite dimensional $\bar{S}$. By RR I, we can determine d and, thus, generate all of the basis vectors needed to span $A(t)$ in $\bar{S}$ for a particular H. In addition, we can construct the hypersurface σ:

$$\sigma = (\Delta_1, \Delta_2, ..\Delta_{d-1}) \tag{7}$$

As we shall see, the dynamics is governed by σ. The Δ's known as the recurrants are successive ratios of the norms of f_k. They are static quantities, so that they are in principle calculable as a function of parameters, such as temperature, wave vectors, *etc.*, for a given H. They collectively define the shape of $\bar{S}$, constraining what kind of trajectory is possible for $A(t)$.

2.3. Basis Functions

If RR I is applied to Equation (1), it yields a recurrence relation for the basis functions: with $a_{-1} = 0$,

$$\Delta_{k+1} a_{k+1} = -\dot{a}_k + a_{k-1}, \ \ k = 0, 1, ..d-1 \tag{8}$$

where $\dot{a}_k = d/dt \ a_k$. Equation (8) is known as RR II. It is actually composed of two recurrence relations, one for $k = 0$ (because of $a_{-1} = 0$) and another for the rest $k = 1, 2, ..d-1$.

There is an important boundary condition on a_k. By Equation (3), $A(t = 0) = A = f_0$. Thus, $a_0(t = 0) = 1$ and $a_k(t = 0) = 0$, $k \neq 0$. These basis functions are autocorrelation functions. For example, $a_0 = (A(t), A)/(A, A), a_1 = (A(t), f_1)/(f_1, f_1) = (A(t), \dot{A})/(\dot{A}, \dot{A})$, *etc.* Hence, the static and dynamic information is to be contained in them.

2.4. Continued Fractions

If a_0 is known, the rest of the basis functions can be obtained one by one by RR II. To obtain it, let $L_z a_k(t) = \tilde{a}_k(z)$, $k = 0, 1, ..d-1$, where L_z is the Laplace transform operator. The RR II is transformed to:

$$1 = z\tilde{a}_0 + \Delta_1 \tilde{a}_1 \tag{9}$$

$$\tilde{a}_{k-1} = z\tilde{a}_k + \Delta_{k+1} \tilde{a}_{k+1}, \ \ k = 1, 2, ..d-1 \tag{10}$$

From Equation (9), $\tilde{a}_0$ is obtained in terms of $\tilde{b}_1 = \tilde{a}_1 / \tilde{a}_0$. By setting $k = 1$ in Equation (10), $\tilde{b}_1$ in terms of $\tilde{b}_2 = \tilde{a}_2 / \tilde{a}_1$. Proceeding term by term, we obtain the continued fraction form for $\tilde{a}_0$:

$$\tilde{a}_0(z) = 1/(z + \Delta_1/(z + ... + \Delta_{d-1}/z))..) \tag{11}$$

If the hypersurface is determined, the continued fraction may be summable. By taking L_z^{-1} on Equation (11), we can obtain $a_0(t)$:

$$a_0(t) = 1/2\pi i \int_c \tilde{a}_0(z) e^{zt} dz, \ \ Re \ z > 0 \tag{12}$$

where by c, we mean that the contour is to be on the right of all singularities contained in the rhs of Equation (11). If $a_0(t)$ is thus determined, the rest of the basis functions can be obtained one by one by

RR II. Hence, $A(t)$ (see Equation (3)) is completed solved if formally. This recurrence relation analysis can be implemented for a harmonic chain, described in Section 3.

3. Local Dynamics in a Harmonic Chain

Consider a classical harmonic chain of N equal masses in periodic boundary conditions (N even number, m mass and κ the coupling constant) defined by the Hamiltonian:

$$H = \sum_{-N/2}^{N/2-1} p_i^2/2m \; + \; 1/2\kappa \; (q_i - q_{i+1})^2 \tag{13}$$

where p_i and q_i are the momentum and the coordinate of mass m at site i, and sites $-N/2$ and $N/2-1$ are nns. Let $A = p_0$ the momentum of mass m at Site 0. The time evolution of p_0 follows from the method of recurrence relations: in units $m = \kappa = 1$,

$$p_0(t) = a_0(t) \; p_0 \; + \; a_1(t) \; ((q_{-1} \; + \; q_1)/2 \; - \; q_0) \; + \; a_2(t) \; (p_{-1} + p_1) + ... \tag{14}$$

Let HC denote a harmonic chain of N masses defined by Equation (13). It has been shown that for HC, $d = N + 1$ and that there are N recurrants in the hypersurface [25]. If the recurrants are expressed in our dimensionless units, the hypersurface has a symmetric structure in the form: $\sigma(N = 2) = (2, 2), \sigma(N = 4) = (2, 1, 1, 2), \sigma(N = 6) = (2, 1, 1, 1, 1, 2),$ *etc*. We can conclude that for N oscillators (N even number), Δ_1 and $\Delta_N = 2$ and $\Delta_k = 1, \; k = 2, 3, ..N - 1$, giving a general form:

$$\sigma(N) = (2, 1, 1,, ..1, 1, 2) \tag{15}$$

If these recurrants are substituted in Equation (11), they will realize Equation (11). If $N \rightarrow \infty (d \rightarrow \infty)$,

$$\sigma = (2, 1, 1, ...) \tag{16}$$

Taking this limit breaks the front-end symmetry. Equation (11) is summable:

$$\tilde{a}_0(z) = \frac{1}{\sqrt{4 + z^2}} \tag{17}$$

By taking the inverse transform, see Equation (12), we obtain:

$$a_0(t) = J_0(2t) \tag{18}$$

where J is the Bessel function. This is a known result [26,27]. By RR II, we obtain:

$$a_k(t) = J_k(2t), \; k = 1, 2, .. \tag{19}$$

Therewith, we have obtained the complete time evolution of p_0 in an infinite HC.

Observe that $a_0(t \rightarrow \infty) = 0$. The vanishing of the autocorrelation function at $t = \infty$ is an indication of irreversibility. It is possible in a Hermitian system only by the thermodynamic limit being taken. This property is an important consideration for the ergodicity of the dynamical variable $A = p_0$, to be considered later [28].

Langevin Dynamics

The equation of motion for A may also be expressed by the generalized Langevin equation [29]:

$$d/dt \; A(t) + \int_0^t M(t - t')A(t')dt' = F(t) \tag{20}$$

where M and F are the memory function and the random force, resp. They are important quantities in many dynamical issues, most often given phenomenologically or approximately [23]. For an infinite HC, we can provide exact expressions for them.

In obtaining a continued fraction for $\tilde{a}_0(z)$, we have introduced $\tilde{b}_k = \tilde{a}_k / \tilde{a}_{k-1}$, $k = 1, 2, ..d - 1$. By convolution, we can determine b_k. They are the basis functions for $\bar{S}_1$, a subspace of $\bar{S}$, spanned by f_k, $k = 1, 2, ..d - 1$. They satisfy RR II with the boundary condition that $b_1(t = 0) = 1$ and $b_k(t = 0) = 0$ if $k \neq 1$, with $b_0 = 0$. The hypersurface for this subspace is the same as Equation (7) with Δ_1 removed. One can also express $\tilde{b}_1(z)$ in a continued fraction:

$$\tilde{b}_1(z) = 1/(z + \Delta_2/(z + \Delta_3/(z + .. + \Delta_{d-1}/z))..) \tag{21}$$

The random force is a vector in $\bar{S}_1$; thus,

$$F(t) = \sum b_k(t) f_k \tag{22}$$

and:

$$M(t) = \Delta_1 b_1(t) \tag{23}$$

For the infinite HC, $\sigma_1 = (1, 1, 1, ..)$, summable to:

$$\tilde{b}_1(z) = 1/2 \ (\sqrt{z^2 + 4} - z) \tag{24}$$

By the inverse Laplace transform, we obtain:

$$b_1(t) = J_1(2t)/t \tag{25}$$

and the rest by RR II. Therewith, we have obtained exact expressions for the two Langevin quantities.

4. Dispersion Relation for Harmonic Chain

Equation (11) for $\tilde{a}_0$ shows that if d the dimensionality of $\bar{S}$ is finite, the continued fraction may be expressed as a ratio of two polynomials in z. For HC, let us denote the lhs of Equation (11) by $\check{\Psi}_N(z)$ and the rhs of Equation (11) the continued fraction by two polynomials as:

$$\check{\Psi}_N(z) = P_N(z)/Q_N(z) \tag{26}$$

Since every Q_N is found to contain $z(z^2 + 4)$ as a common factor, we express it as:

$$Q_N = z(z^2 + 4)q_N, \ N = 2, 4, 6, .. \tag{27}$$

Below, we list $P's$ and $q's$ for several values of N, sufficient to draw a general conclusion therefrom:

(a) $N = 2$, $\sigma = (2, 2)$
 $P_2 = z^2 + 2$,
 $q_2 = 1$
(b) $N = 4$, $\sigma = (2, 1, 1, 2)$
 $P_4 = z^4 + 4z^2 + 2$
 $q_4 = z^2 + 2$
(c) $N = 6$; $\sigma = (2, 1, 1, 1, 1, 2)$
 $P_6 = z^6 + 6z^4 + 9z^2 + 2$
 $q_6 = z^4 + 4z^2 + 3$
(d) $N = 8$; $\sigma = (2, 1, 1, 1, 1, 1, 1, 2)$
 $P_8 = z^8 + 8z^6 + 20z^4 + 16z^2 + 2$

$q_8 = z^6 + 6z^4 + 10z^2 + 4$

(e)　$N = 10$; $\sigma = (2, 1, 1, 1, 1, 1, 1, 1, 1, 2)$
$P_{10} = z^{10} + 10z^8 + 35z^6 + 50z^4 + 25z^4 + 2$
$q_{10} = z^8 + 8z^6 + 21z^4 + 20z^2 + 5$

(f)　$N = 12$; $\sigma = (2, 1, 1, 1, 1, 1, 1, 1, 1, 1, 1, 2)$
$P_{12} = z^{12} + 12z^{10} + 54z^8 + 112z^6 + 105z^4 + 36z^2 + 2$
$q_{12} = z^{10} + 10z^8 + 36z^6 + 56z^4 + 35z^2 + 6$

If $z = 2i\sin\alpha$, $\alpha \neq 0$, the above polynomials have simple expressions for all orders of N:

$$P_N = 2\cos N\alpha \tag{28}$$

$$q_N = \sin N\alpha / \sin 2\alpha, \ \sin 2\alpha \neq 0 \tag{29}$$

4.1. Zeros of q_N

The dispersion relation can be deduced from z_k the zeros of q_N:

$$q_N(z) = \Pi(z - z_k) \tag{30}$$

From Equation (29),

$$\sin N\alpha_k = 0 \tag{31}$$

with $\sin 2\alpha_k \neq 0$ and $\alpha_k \neq 0$. Hence,

$$\alpha_k = (\pi/N)k, \ k = \pm 1, \pm 2, .. \pm (N/2 - 1) \tag{32}$$

Hence, with k given above,

$$z_k = 2i\sin\alpha_k \tag{33}$$

One may also write:

$$\Pi(z - z_k)|_{z=2i\sin\alpha} = \sin N\alpha / \sin 2\alpha \tag{34}$$

Since $Q_N = z(z^2 + 4)q_N$ (see Equation (26)), the prefactor contributes to the zeros of Q_N. They may be included in Equation (32) if the range of k is made to includes zero and $N/2$.

4.2. $a_0(t)$ for Finite N

Given the zeros of Q_N, it is now straightforward to obtain $a_0(t)$ by Equation (12). For example, if $N = 6$,

$$a_0(t) = 1/6[1 + 2\cos t + 2\cos\sqrt{3}t + \cos 2t] \tag{35}$$

A general expression would be:

$$a_0(t) = 1/N\sum_k \cos\omega_k t \tag{36}$$

where:

$$\omega_k = 2|\sin(\pi v_k)|, v_k = k/N \tag{37}$$

$k = -N/2, ., -1, 0, 1, .. N/2$. Since Equation (36) is a dispersion relation, $v's$ will be termed "wave vectors".

4.3. $a_0(t)$ When $N \rightarrow \infty$

If $N \rightarrow \infty$, the sum in Equation (36) may be converted to an integral:

$$rhs\ of\ Equation(36) = 1/2\pi \int_{-\pi}^{\pi} e^{2itsin\theta} d\theta \tag{38}$$

The rhs of Equation (38) is an integral representation of $J_0(2t)$. Hence, $a_0(t) = J_0(2t)$, the same as Equation (18).

It is worth noting here that the zeros of $J_0(2t)$ can thus be obtained from Equation (36) by taking $N \rightarrow \infty$ by the condition:

$$\omega_k t = \pi/2(2n+1), \quad n = 0, 1, 2, .. \tag{39}$$

If we write $J_0(2t) = \Pi(2t - 2t_k)$, by Equation (37):

$$2t_k = \pi(2n+1)/|2sin\pi k/N|, \ k/N = (-1/2, 1/2) \tag{40}$$

Evidently, there are infinitely many zeros in J_0 [30]. This result will be significant in Section 6.

4.4. $\tilde{a}_0(z) = \Psi_N(z)$ When $N \rightarrow \infty$

By Equations (26)–(29),

$$\tilde{\Psi}_N(z) = VcosN\alpha/sinN\alpha \tag{41}$$

where $V = 2sin2\alpha/(z(z^2+4)) = d\alpha/dz \ \ (by\ z = 2isin\alpha)$. Furthermore:

$$cosN\alpha/sinN\alpha = 1/N\ d/d\alpha(logsinN\alpha)$$
$$= 1/N\ d/d\alpha[log(sinN\alpha/sin2\alpha) + logsin2\alpha] \tag{42}$$

The second term on the rhs of Equation (42) may be dropped if $N \rightarrow \infty$. For the first term, by Equations (28) and (29),

$$rhs\ of\ Equation(42) = dz/d\alpha\ d/dz\ \ log\Pi(z-z_k) = dz/d\alpha\ \sum 1/(z-z_k) \tag{43}$$

The prefactor $dz/d\alpha = 1/V$. Since $N \rightarrow \infty$, we can convert the above sum into an integral: writing $\tilde{\Psi} = \tilde{\Psi}_N, N \rightarrow \infty$,

$$\Psi(z) = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} \frac{d\theta}{z - 2isin\theta} = \frac{1}{\sqrt{4+z^2}} \tag{44}$$

The above result is the same as Equation (17).

The asymptotic results Equations (16) and (17) were obtained by taking the $N \rightarrow \infty$ limit first on the hypersurface. What is shown in Section 4 is that the same results are also obtained from finite N solutions for $a_0(t)$.

5. Ergodicity of Dynamical Variable $A = p_0$

If A is a variable of a Hermitian system of N particles, $N \rightarrow \infty$, it is possible to determine whether it is ergodic. According to the ergometric theory of the ergodic hypothesis [31], A is ergodic if $W_A \neq 0$ or ∞, where:

$$W_A = \int_0^{\infty} r_A(t)\ dt \tag{45}$$

where $r_A(t) = (A(t), A)/(A, A) = a_0(t)$, the autocorrelation function of A. By Equation (12),

$$W_A = \tilde{r}_A(z = 0) \tag{46}$$

If $d \to \infty$ as $N \to \infty$, which is the case of HC, $z \to 0$ on Equation (11) yields an infinite product of the following form:

$$W_A = \frac{\Delta_2 \times \Delta_4 \times ... \Delta_{2n}}{\Delta_1 \times \Delta_3 \times ... \Delta_{2n+1}}, \quad n \to \infty \tag{47}$$

Ordinarily, infinite products are difficult to evaluate, as they seem to require product rules that differ from those for finite products. However, they can be determined by Equation (45) or Equation (46) as illustrated below.

5.1. Infinite Harmonic Chain

If $A = p_0$ of HC, we can determine whether A is ergodic by evaluating Equations (45)–(47). If $N \to \infty$, $\sigma = (2, 1, 1, ...)$ (see (16)), and $\Psi(t) = J_0(2t)$ (see Equation (18)). Hence, by Equation (45), $W_A = 1/2$.

It was shown that $\check{\Psi}(z) = 1/\sqrt{z^2 + 4}$; see Equation (17). Hence, by Equation (46), $W_A = 1/2$. Finally, by σ, we can write down the infinite product:

$$W_A = \frac{1 \times 1 \times 1 \times ....}{2 \times 1 \times 1 \times ...} = \frac{1}{2} \tag{48}$$

in agreement with the previous results. As noted above, computing infinite products is a delicate matter. The order of terms in an infinite product may not be altered, nor the terms themselves. In Equation (48), such a nicety did not enter since all elements are one but one. Compare with another example in Section 5.2 below.

5.2. Infinite Harmonic Chain with One End Attached to a Wall

We shall now change HC defined by Equation (13) slightly. Let the coupling between the oscillators at q_{-2} and q_{-1} be cut. Furthermore, let the mass of the oscillator at q_{-1} be infinitely heavy, so that the oscillator at q_0 is attached as if to a wall. The rest of the chain is unchanged. The oscillators in this new configuration are labeled $0, 1, 2..N - 1$, with one end attached to a wall and the other end free. Finally, let $N \to \infty$.

If $A = p_0$, the recurrants are found to have the following form [27,32]:

$\Delta_1 = 2/1, \ \Delta_3 = 3/2, \ \Delta_5 = 4/3, .. \ \Delta_2 = 1/2, \ \Delta_4 = 2/3, \ \Delta_6 = 3/4, ...$

Evidently, they may be put in the form: $\Delta_{2n-1} = (n + 1)/n$ and $\Delta_{2n} = n/(n + 1), \ n = 1, 2, 3, ...$ These recurrants imply that for $A = p_0$ [27,32],

$$a_0(t) = J_0(2t) - J_4(2t) \tag{49}$$

$$\tilde{a}_0(z) = 1/\sqrt{(z^2 + 4)} \ [1 - 1/16 \ (\sqrt{z^2 + 4} - z)^4] \tag{50}$$

By Equation (47),

$$W_A = \frac{1/2 \times 2/3 \times 3/4 \times ... \times n/(n + 1)}{2/1 \times 3/2 \times 4/3 \times ... \times (n + 1)/n}, \quad n \to \infty \tag{51}$$

Each term in the numerator is less than one, while each term in the denominator greater than one. If the terms and the order are preserved, $W_A \to 0$. By Equations (45) and (46), it may be tested using Equations (49) and (50). In both cases, we obtain $W_A = 0$ verifying the infinite product.

Since $W_A = 0$, $A = p_0$ is not ergodic in this chain. For this variable, the phase space is not transitive. If mass at Site 0 is slightly perturbed, the perturbed energy is not delocalized everywhere [33].

6. Harmonic Chain and Logistic Map

The logistic map (LM) is sometimes called the Ising model of chaos for being possibly the simplest model exhibiting chaos [34]. If x is a real number in an interval (0,1), the map is defined by:

$$f(x) = ax(1 - x), \quad x = (0, 1) \tag{52}$$

where a is a control parameter, a real number limited to $1 < a \leq 4$. Thus, the map is real and bounded as x. If there exists $x = x^*$, such that $f(x^*) = x^*$, it is termed a fixed point of $f(x)$. If f^n is an n-fold nested function of f, i.e., $f^n(x) = f(f^{n-1}) = f(f(...f(x)...))$, with $f^1 \equiv f$, there may be fixed points for $f^n : f^n(x^*) = x^*$. The values of the fixed points and the number of the fixed points will depend on the size of the control parameter a.

If $a < 3$, there is only one fixed point for any n. There is a remarkable theorem due to Sharkovskii [35] on $1d$ continuous maps on the interval, such as LM. As applied to this map, this theorem says that if $a \geq 1 + \sqrt{8}$, there are infinitely many fixed points as $n \to \infty$. This implies that a trajectory starting from almost any point in (0,1) is chaotic. At $a = 4$ (the largest possible value), the fixed points fill the interval $x = (0, 1)$ densely with a unique distribution ρ_x, $\int \rho_x dx = 1$. This distribution is known as the invariant density of fixed points, first deduced by Ulam [36,37]:

$$\rho_x = \frac{1}{\pi \sqrt{x(1 - x)}}, \quad 0 < x < 1 \tag{53}$$

The invariant density refers to the spectrum of fixed points in (0,1). The square-root singularity in Equation (53), a branch cut from 0–1, indicates that the spectrum is dense. If μ is a Lebesgue measure, $d\mu(x) = \rho_x dx$. Hence, $\mu = 1$.

We wish to see whether ρ_x, a distribution of fixed points, bears a relationship to ρ_ω, the power spectrum of frequencies in HC. For this purpose, consider the following transformations of variables:

$$x = 1/2 + 1/4 \ \omega \tag{54}$$

and:

$$\rho_x dx = \rho_\omega d\omega \tag{55}$$

By substituting Equation (54) in (53), we obtain by Equation (55):

$$\rho_\omega = \frac{1}{\pi \sqrt{4 - \omega^2}}, \quad -2 < \omega < 2 \tag{56}$$

$$= 0 \text{ if otherwise.}$$

For an infinite HC, $\tilde{a}_0(z = i\omega) = \pi \rho_\omega$. By Equation (17), or Equation (44), the rhs of Equation (56) is precisely the power spectrum for $A = p_0$. Equation (56) shows that the fixed points of LM at $a = 4$ (LM_4) correspond to the frequencies of HC.

Since the frequencies in the power spectrum are positive quantities, let us express Equation (54) as:

$$\omega = 2|1 - 2x|, \quad 0 < x < 1 \tag{57}$$

For LM_4,

$$x = sin^2 \pi y/2 \tag{58}$$

$$y/2 = l/(2N+1), \ l = 1, 2.., N \tag{59}$$

y being the pre-fixed points of *x* the fixed points. If Equation (59) is substituted in Equation (57) and y replaced by $\nu + 1/2$:

$$\omega = 2|sin\pi\nu| \tag{60}$$

The above is identical to Equation (37), the dispersion relation for HC. In the limit $N\rightarrow\infty$, both ν and y lie in the same interval $(-1/2, 1/2)$. This property shows that the pre-fixed points of LM_4 also correspond to the wave vectors of HC.

The correspondence between *x* and ω and also between *y* and ν indicate that the iteration dynamics of LM_4 and the time evolution in HC are isomorphic in their local variables. This implies that if a variable in HC is ergodic, a corresponding variable in LM_4 is also ergodic. If the trajectory of an initial value in LM_4 is chaotic, we must also conclude that the trajectory of a local variable in HC must also be chaotic.

Chaos in HC? Let us first examine chaos in LM_4. According to Sharkovskii, chaos is implied where there are infinitely many periods. By our work, they form a set of uncountable pre-fixed points of Lebesgue measure 1. This results in an aleph cycle, which can never return to the initial point [34]. In an infinite HC, there are also infinitely many periods. See Equation (40). Thus, the HC has the necessary and possibly sufficient property for chaos.

In an infinite HC attached to a wall (see Section 5.2), there is chaos also, as there are infinitely many periods. However, as was already shown, its variables are not ergodic. This indicates that ergodicity is a subtler property than chaos. In a continuous map, there may be chaos, but not ergodicity.

7. Concluding Remarks

In this work, we have dwelt with the dynamics of a monatomic chain with which to illustrate some of the finer points of the dynamics contained in it. This simplest of harmonic chains can be made richer in a variety of ways. One can make one oscillator to have a different mass than its neighbors [25]. It would be a model for an impurity or a defect. One could make it a periodic diatomic chain [8] or even an aperiodic diatomic chain [8]. We are providing a list of recent advances made by the method of recurrence relations on others [38–44]. For related studies on HC by Fokker–Planck dynamics and non-exponential decay, see [7,45,46].

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