

Ergodic Theory, Infinite Products, and Long Time Behavior in Hermitian Models

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Ergodic theory has been approached from the side of the time averages with correlation functions from many-body models. The condition for ergodic behavior is formulated in terms of infinite products of certain numbers associated with time evolution. Physical properties that make a model ergodic are identified.

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1. *Introduction.*—Ergodicity is a fundamental concept in statistical mechanics [1(a)]. Very roughly and narrowly put, it says that the time averages of dynamic functions are the same as the ensemble averages of the same. Most papers on this subject discuss this equality or equivalence in the context of classical ergodic theory, many in highly abstract terms [1(b),1(c)]. It is difficult to discern from them the specific physical properties that make a many-body model ergodic.

The approach of Khinchin, adapted by Kubo, is to do the time averages on correlation functions from quantum many-body models [2]. These correlation functions describe dynamic processes, which are measurable by inelastic scattering [3]. This approach very naturally takes us to the dynamic processes therein to look for the physical basis of ergodic behavior. Suppose an isolated body is made to interact with a small time-dependent external field $h(t)$, gradually turned on from a remote past. Denote the process by $H'(t) = H + V(t)$, where H is the energy of the isolated body and $V(t) = Ah(t)$ the interaction energy, A a dynamical variable such that $[H, A] \neq 0$. Let $\chi(t, t')$ be the response function of this body to $h(t)$ [4(a)]. Suppose the same body is now subjected to a small time-independent field h , the process denoted by $H' = H + V$, $V = Ah$. Let χ be the response function, i.e., the static susceptibility at $h = 0$ [4(b)].

For these linear response functions, the ergodic hypothesis would say that

$$\frac{1}{T} \int_0^T \int_0^t \chi(t, t') dt' dt = \chi, \quad (1)$$

where $T \rightarrow \infty$, to be taken after the thermodynamic limit [5]. Since the right-hand side of (1) is assumed finite and well behaved, the ergodic hypothesis cannot hold if the left-hand side (lhs) contains divergent or singular terms. If the lhs of (1) were equal to $\tilde{\chi}(\omega = 0)$ the zero frequency limit of the dynamic susceptibility, the ergodic hypothesis could be tested by calculating χ and $\tilde{\chi}(0)$ specifically for a given many-body model. In fact, whether $\tilde{\chi}(0) = \chi$ (Kubo's condition) has been studied for several models, but the results have been ambiguous [6]. To be able to address ergodicity in Hermitian models, we believe that there must be given two *necessary* conditions: (a) the thermo-

dynamic limit (although implicit already, it's needed to exclude finite systems satisfying the equality) and (b) another limit given below, related to irreversibility. Then, Kubo's condition can be replaced with another more explicitly connected with the time evolution.

2. *Dynamic response functions.*—Linear response theory says that for a *stationary* system $\chi(t, t') = \chi(t - t') = i\langle [A(t), A(t')] \rangle_H$ if $t > t'$ and $= 0$ if otherwise. Also, $\chi(t) = -R(t)$, $t > 0$, where $R(t) = (A(t), A)$, $A \equiv A(0)$, and the inner product means the Kubo scalar product (KSP) in H [3]. Since $\chi = (A, A)$, $\chi = R(0)$ also. Thus both χ and $\chi(t)$ flow from $R(t)$, which for a Hermitian H can be obtained by the recurrence relations method [7], briefly sketched below.

We obtain $A(t)$ by solving Heisenberg's equation, $\dot{A}(t) = i[H, A(t)]$, on a *realized* inner product space of d dimensions, space \mathbf{S} realized by KSP. Let $A(t)$ be a vector in space \mathbf{S} , spanned by d basis vectors f_0, f_1, \dots, f_{d-1} , satisfying $(f_m, f_{m'}) = 0$ if $m' \neq m$. Thus, formally,

$$A(t) = \sum_{m=0}^{d-1} a_m(t) f_m, \quad (2)$$

where a_m 's are basis functions which denote the amplitudes of the projections of $A(t)$ onto the basis vectors f_m 's at time t . If (2) is to be the solution of the Heisenberg equation on space \mathbf{S} , these basis vectors and functions must satisfy certain model-dependent recurrence relations (RR1 and RR2).

Starting with $f_0 \equiv A$, we can obtain by RR1 the basis vectors one by one, thereby d also. If $f_0 = A$, $a_m(t = 0) = 1$ or 0 if $m = 0$ or not (boundary conditions), and $a_0(t) = R(t)/\chi$, $\chi = (A, A) < \infty$. The basis functions are connected by RR2,

$$\Delta_{m+1} a_{m+1}(t) = -\dot{a}_m(t) + a_{m-1}(t), \quad (3)$$

$$0 \leq m \leq d - 1,$$

where $\Delta_m = (f_m, f_m)/(f_{m-1}, f_{m-1})$, m th *recurrent*. The complete set of the recurrants, $\sigma = (\Delta_1, \Delta_2, \dots, \Delta_{d-1})$, is made up of the (model dependent) lengths of the basis vectors. Thus it describes the shape of \mathbf{S} [8].

If $m = 0$ in (3), with $a_{-1} \equiv 0$,

$$\Delta_1 a_1(t) = -\dot{a}_0(t). \quad (4)$$

Since $a_0(t) = R(t)/\chi$, the lhs of (4) is $\chi(t)/\chi$. Let $\tilde{a}_m(z) = T[a_m(t)]$, $\text{Re} z > 0$, where T is the Laplace transform operator. Then, (4) becomes

$$\tilde{\chi}(z)/\chi = 1 - z\tilde{a}_0(z). \quad (5)$$

If $z = i\omega + 0$, where ω is the frequency, (5) states the fluctuation dissipation theorem [3]. In addition it contains a basis for Kubo's ergodicity condition. If $z \rightarrow 0$ in (5), $\tilde{\chi}(z=0) = \chi$ if $\tilde{a}_0(z \rightarrow 0) = \text{const}$. Excluded are $\tilde{a}_0(z) \rightarrow 0$ and ∞ as $z \rightarrow 0$ [9].

Now apply T on (3). Setting $m = 1$, we can obtain an expression for \tilde{a}_1/\tilde{a}_0 , which may be used in (5). Successively doing so we obtain (noting $\Delta_m = 0$ if $m \geq d$ for a d -dimensional \mathbf{S}),

$$\tilde{a}_0(z) = 1/z + \Delta_1/z + \Delta_2/z + \cdots + \Delta_{d-1}/z, \quad (6)$$

a continued fraction of order $d - 1$. If $d < \infty$ as in some models, $\tilde{a}_0(z)$ is a meromorphic function. Thus, $\text{Im}\tilde{\chi}(\omega)$ consists of a finite number of resonant frequencies and $R(t)$ is not irreversible [10]. To obtain $R(t)$ that is irreversible, a model must have a state of $d = \infty$ [condition (b)] [11(a)].

3. *Infinite products and models.*—If $d \rightarrow \infty$, (6) becomes an infinite continued fraction of Stieltjes in the s -fraction form. By taking $z \rightarrow 0$ therein (after $d \rightarrow \infty$ if allowed) we can write it as

$$\tilde{a}_0(z \rightarrow 0) = \frac{\Delta_2\Delta_4\Delta_6\cdots}{\Delta_1\Delta_3\Delta_5\cdots} \equiv W, \quad (7)$$

an infinite product, said to be the *canonical* form of W . The numbers appearing in (7) are the structural details of space \mathbf{S} . W probably cannot be calculated directly from the canonical form except in trivial cases [11(b)]. But it can be calculated indirectly by two equivalent ways: (a) taking the $z = 0$ limit if $\tilde{a}_0(z)$ is known and (b) evaluating $\int_0^\infty a_0(t) dt$ if $a_0(t)$ is known. Returning to (5), we can now state the necessary and sufficient condition for ergodic behavior. If $0 < W < \infty$, a model is ergodic with respect to variable A . If $W = 0$ or ∞ , it is not.

We first illustrate the evaluation of W through the hyperbolic secant memory $a_0(t) = \text{sech}t$, used in dynamics of certain liquids [12]. This form of memory derives from space \mathbf{S} of $\sigma = (1^2, 2^2, 3^2, \dots)$. For this σ we obtain $W = \pi/2 \equiv W(\text{Wallis})$ from the canonical form, first given by Wallis many years ago. On the other hand $\int_0^\infty \text{sech}t dt = \pi/2$. Also, $\tilde{a}_0(z) = T[\text{sech}t] = 1/2\{\psi(z/4 + 3/4) - \psi(z/4 + 1/4)\}_{z=0} = \pi/2$, $\psi(z) = d \log \Gamma(z)/dz$. We now evaluate W in three other simple models to see what makes them ergodic and how they may be broken.

A. *Harmonic oscillator chains:* For a nearest-neighbor (nn) coupled classical harmonic oscillator (HO) chain of $2N$ atoms with periodic boundary conditions, let the masses be the same m except one m' (tagged atom), parameterized by $\lambda \equiv m/m'$ (the coupling constants the same). If $A = p'$ the momentum of the tagged atom, space \mathbf{S} has $d = 2N + 1$ and $\sigma = (2\lambda, 1, 1, \dots, 2)$. If

$N \rightarrow \infty$, $d \rightarrow \infty$, and $\sigma \rightarrow (2\lambda, 1, 1, \dots)$ [13(a),13(b)]. In this trivial case of σ , we obtain $W = 1/(2\lambda)$ from the canonical form, also by setting $z = 0$ in $\tilde{a}_0(z) = 1/\{(1 - \lambda)z + \lambda(z^2 + 4)^{1/2}\}$ [13(a)]. If λ is finite, W is finite and the model is ergodic with respect to p' . If the tagged atom is perturbed, the perturbed energy is delocalized throughout the chain. Time averaging of this dynamic process singles out the $\omega = 0$ mode (coherent translation) as the "ergodic mode."

If $\lambda \rightarrow \infty$, the tagged atom appears as if attached to walls on both sides. The perturbed energy is reflected by the walls. The translation mode is lost and ergodic mode is destroyed (*localization* limit $W = 0$). If $\lambda \rightarrow 0$, the tagged atom becomes a Brownian particle, moving along little affected by the vibrations of the little masses. The translation mode exists but is incoherent and the ergodic mode is again destroyed (*ballistic* limit $W = \infty$).

Let m' now denote any one of the HOs on a Bethe lattice of q coordination number (but $m' = m$). If $N \rightarrow \infty$, $d \rightarrow \infty$ also and $\sigma \rightarrow (q, 1, q - 1, 1, q - 1, 1, q - 1, \dots)$ [14]. By the canonical form, $W = 0$ if $q \geq 3$, also by $\tilde{a}_0(z \rightarrow 0) = Cz$, where $C = (q - 1)/(q(q - 2))$. It is at the localization limit. A Bethe lattice has no translation mode.

If a chain is of diatomic masses m_1 and m_2 regularly alternated, space \mathbf{S} for p_1 (of any one with m_1) has $\sigma = (2\lambda, 1, 1, \lambda, \lambda, 1, 1, \lambda, \lambda, \dots)$, where now $\lambda = m_2/m_1$. We find $W = \tilde{a}_0(z = 0) = 1/\sqrt{2\lambda(\lambda + 1)}$ [15]. If λ is finite, there exists a coherent translation mode in the chain, i.e., ergodic with respect to p_1 just as in a monatomic chain ($\lambda = 1$). This structure is a rich source of infinite products.

B. *Spin-1/2 XY chains:* For $H = -J \sum_i (s_i^x s_{i+1}^x + s_i^y s_{i+1}^y)$, $s_{N+1} = s_1$, $a_0(t)$ is known for the x and z components of a single spin at high temperatures and $N \rightarrow \infty$ [16,17(a)]. If $A = s^x$ (a spin at any site), space \mathbf{S} has $\sigma = (1, 2, 3, \dots)$ with $2J^2 \equiv 1$ [16(b)]. Thus $W = \sqrt{W(\text{Wallis})} = \sqrt{\pi/2}$, also by the integration of $a_0(t) = \exp(-t^2/2)$ and by setting $z = 0$ in $\tilde{a}_0(z) = T[\exp(-t^2/2)] = \sqrt{\pi/2} \exp(z^2/4) \text{erfc}(z/\sqrt{2})$. Since W is finite, the model is ergodic with respect to spin component s^x or s^y . The $\omega = 0$ mode corresponds to a coherent rotation in the xy plane of the interaction in spin space.

If $A = s^z$ (at any site), then $a_0(t) = [J_0(t)]^2$, now with $J \equiv 1$ [17(a)]. Also, $\tilde{a}_0(z) = T\{[J_0(t)]^2\} = 1/z F(1/2, 1/2, 1, -4/z^2)$. Thus $W = \tilde{a}_0(z = 0) = -\frac{1}{\pi} \log z$, $z \rightarrow 0+$, attaining the ballistic limit, meaning that the model is nonergodic with respect to spin component s^z . The log divergence of W is also seen from $a_0(t \rightarrow \infty) \sim 0(1/t)$. The equation of motion of the z component of a spin at site 0 is $\dot{s}_0^z = i(s_0^y s_0^x - s_0^x s_0^y)$, $0' = \pm 1$. The motion resembles a vortex line moving in the direction perpendicular to the plane of spin interaction. It is analogous to an incoherent translation [17(b)].

C. *3D Electron gas:* For an electron gas at the ground state, let $A = \rho_k$, the density operator at wave vector k , measured in units of the Fermi wave vector $k_F \equiv 1$. If $k > 1$ and the electronic density $r_S \approx 3.5$, space \mathbf{S} is given by

$\sigma = (2s, 2.1, 2(s+1), 2.2, 2(s+2), 2.3, \dots)$, where $s = 3k^2/16x$, $x = \langle KE \rangle_H$, where KE is the kinetic energy. At $r_S = 3.5$, $s = 0.2568k^2$; and $s \approx 1$ if $k = 2$ [18].

For this space, $a_0(t) = M(s, 1/2, -t^2/2) \sim \Gamma(1/2)/\Gamma(1/2 - s)(t/2)^{-2s}$ as $t \rightarrow \infty$, where M is the Kummer function. If, e.g., $s = 1/2$, $W = \sqrt{\pi/2}$, obtained from $\int M dt$, another source of infinite products. From the canonical form we can see that $W \rightarrow 0$ (localization) if $s \rightarrow \infty$ (i.e., $k \rightarrow \infty$). At very short wavelengths, the density fluctuations resulting from inelastic scattering take place over very small regions of space; and they cease to be ergodic when the inelastic scattering is at its deepest.

4. *Long time behavior.*—The long time behavior of $a_0(t)$ may be deduced as a *metrical* property of $A(t)$ in space \mathbf{S} . In addition to $a_0(0) = 1$ (boundary condition), $|a_0(t)| \leq 1$ by the Schwarz inequality. Let $\delta(t) = \|A(t) - A(0)\|$, where $\|A\|^2 = (A, A) < \infty$, $A \equiv A(0)$. If H is Hermitian, there is an invariance property $\|A(t)\| = \|A\|$ [7(a)]. Hence,

$$\delta^2(t) = 2\|A\|^2[1 - a_0(t)]. \quad (8)$$

If $d \rightarrow \infty$ (first), by the orthogonality (2) and the invariance property $\delta(t \rightarrow \infty) = \delta_{\max} = \sqrt{2}\|A\|$. By (8), for space \mathbf{S} of $d = \infty$,

$$a_0(t \rightarrow \infty) = 0. \quad (9)$$

This irreversibility is only a necessary condition for ergodicity [19]. The sufficient condition is that

$$a_0(\rightarrow \infty) \sim t^{-x}, \quad x > 1, \quad (10)$$

if $a_0(t)$ is monotonically decreasing. Then, $d/dt a_0(t) = 0$, $d^2/dt^2 a_0(t) = 0, \dots, d^k/dt^k a_0(t) = 0$, $k < \infty$, all evaluated at $t = \infty$. It follows from RR2 that $a_1(t) = 0$, $a_2(t) = 0, \dots, a_k(t) = 0$, $k < \infty$, at $t = \infty$. They imply that the projections of $A(t)$ onto $\{f_k\}$ vanish, i.e., $(A(t), f_k) = 0$ for $0 \leq k < \infty$, as $t \rightarrow \infty$. As a result, the trajectory of $A(t)$ on \mathbf{S} is irreversible if $d \rightarrow \infty$. For those nonmonotonically decreasing, e.g., $J_0(t)$, $j_0(t)$, the derivatives of the basis functions also vanish for all finite orders as $t \rightarrow \infty$.

5. *Concluding remarks.*—We shall now examine the ergodic hypothesis more grossly. Equation (1) may be expressed as [by dividing both sides by χ and recalling $R(t)/\chi = a_0(t)$] [20]

$$\tilde{\chi}(0)/\chi + a_0(T) - W/T = 1, \quad (T \rightarrow \infty). \quad (11)$$

The irreversibility, i.e., $a_0(\infty) = 0$ has often been thought to be a sufficient condition [2,6(a)]. But as (11) shows, it is evidently insufficient by itself to weigh the hypothesis. Our model analysis also has shown that the irreversibility in a Hermitian model is a metrical property of space \mathbf{S} only. The hypothesis is tested sufficiently by W .

In our analysis d (dimensionality of space \mathbf{S}) is a fundamental parameter. If $d < \infty$, the spectrum of $\tilde{a}_0(z)$ is discrete, thus $a_0(t)$ periodic. If $d \rightarrow \infty$, the spectrum becomes continuous, whereupon $a_0(t)$ is irreversible and ergodic behavior possible. This parameter d brings to mind

something similar in the analysis of 1D iterative maps, e.g., logistic map [21]. In the bifurcation of stable fixed points on route to chaos, the distribution of iterates is discrete after a finite number of iterations (corresponding to a finite d), where the Lyapunov exponent is nonpositive. The distribution becomes dense in a chaotic region reached after an infinite number of iterations, where the Lyapunov exponent is positive and ergodic behavior said to exist.

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- [4] (a) $\chi(t, t')$ is defined through $\langle A(t) \rangle_{H'(t)} = \langle A(t) \rangle_H + \int_{-\infty}^t \chi(t, t') h(t') dt'$, where, e.g., $\langle \dots \rangle_H$ denotes an average over states of H; see [3]. (b) The static response function is defined by $\langle A \rangle_{H'} = \langle A \rangle_H + \chi h$. See Ref. [3].
- [5] In classical ergodic theory, $\langle Q_t \rangle_{\text{time}} = \langle Q \rangle_{\text{ens}}$, Q phase function. Since $\langle \langle Q_t \rangle_{\text{time}} \rangle_{\text{ens}} = \langle \langle Q_t \rangle_{\text{ens}} \rangle_{\text{time}}$ [see Ref. 1(b), p. 123], $\langle \langle Q_t \rangle_{\text{ens}} \rangle_{\text{time}} = \langle Q \rangle_{\text{ens}}$. In quantum analog, Q is to be replaced by \hat{Q} , an equivalent operator. Thus, $\langle \langle \hat{Q}_t \rangle_{\text{ens}} \rangle_{\text{time}} = \langle \hat{Q} \rangle_{\text{ens}}$, in parallel to the classical form, exemplified by (1). If one can do the time average on $\langle \hat{Q}(t) \rangle_{\text{ens}}$, doing so would seem a simple way to test the ergodic hypothesis.
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- [8] Because of RR2 [Eq. (3)], a_m 's are not arbitrary functions. They must be linearly independent and must satisfy the Bessel equality $\sum [a_m(t)]^2 (f_m, f_m) = (f_0, f_0)$ or $\sum [a_m(t)]^2 \Delta_1 \Delta_2 \dots \Delta_m = 1$, an invariance property in space \mathbf{S} . See Ref. [7a]; also M. H. Lee, *Phys. Rev. Lett.* **51**, 1227 (1983). Admissible solutions of RR2 depend on d and σ . Hence they reflect the shape of space \mathbf{S} as illustrated through the following two simple (but

- model realized) examples: (i) If $d = 2$ and $\sigma = (\mu^2)$, $a_0(t) = \cos\mu t$ and $a_1(t) = \sin\mu t/\mu$. (ii) If $d = \infty$ and $\sigma = (2x, x, x, x, \dots)$, $a_m(t) = 2^m J_m(\mu t)/\mu^m$, $m \geq 0$, $\mu = 2x^{1/2}$. The invariance property is given in (i) by a trigonometric identity, and in (ii) by an addition theorem of the Bessel functions. The shape of space \mathbf{S} in (ii) is almost a hypersphere if $x = 1$. This shape and the Bessel function solutions are one to one. Different shapes, e.g., hyperellipsoids imply different admissible forms of the basis functions. See M.H. Lee, Phys. Rev. E **61**, 3571 (2000), especially App. E.
- [9] If $\tilde{a}_0(0) = 0$, the zero frequency mode is absent, i.e., localized states only. More generally since $\tilde{a}_0(z) = 1/\{z + \tilde{\varphi}(z)\}$, $\tilde{\varphi}(z)$ the memory function [7(a)], a vanishing \tilde{a}_0 means a divergent memory function. If the memory function vanishes, the zero frequency refers to incoherent translation. Both limits bring about nonergodic behavior.
- [10] From (6), $\tilde{a}_0(z \rightarrow 0) = \alpha z$ or β/z (α and β constants) if d is an even or an odd number. Thus, $\tilde{\chi}(0) = \chi$ if d even and $\tilde{\chi}(0) < \chi$ if d odd. This accounts for the results of Ref. [6(b)] since for the Ising models $d = q + 1$, where q is the coordination number. In these models are realized the spaces of finite d even after the thermodynamic limit [condition (a)]. See J. Florencio, S. Sen, and M.H. Lee, Braz. J. Phys. **30**, 725 (2000). If N is finite, similar results are also obtained [excluded by condition (a)].
- [11] (a) The state of $d = \infty$ in (6) may not be reached from a state of finite d , even or odd. See Ref. [10] also. As shown later through the HO models, a state of $d = \infty$ is a state of broken symmetry in σ . The numbers in this state are so great that they may not be said to be even or odd integers. The state of $d = \infty$ is in fact a state of high symmetry. (b) Infinite products do not necessarily obey the basic rules governing finite products, e.g., the rule of commutativity. To be computable, infinite products must have a regular sequence. The computation may still depend delicately on the sequence and on the meaning of the canonical form.
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- [18] J. Hong and M. H. Lee, Phys. Rev. Lett. **70**, 1972 (1993).
- [19] The classical form of (9) is $\langle A(t)A \rangle - \langle A \rangle^2 = 0$, $t \rightarrow \infty$, an oft-discussed condition in ergodic theory. See Ref. [2], Eq. (3.19), and Ref. [6(a)].
- [20] With the stationarity property, (1) can be integrated by parts. The result looks similar to the mean-square displacement fluctuations going over into the Green-Kubo formula. [See, e.g., M. H. Lee, Phys. Rev. Lett. **85**, 2422 (2000), Eq. (13); also Ref. [2], Eq. (9.2).] After replacing $\chi(t)$ with $-\dot{R}(t)$, another partial integration brings it to (11).
- [21] See, e.g., H. G. Schuster, *Deterministic Chaos* (Physik-Verlag, Weinheim, 1984).