BIRKHOFF THEOREM AND ERGOMETER: RELATIONSHIP BY AN EXISTENCE ASSUMPTION*

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By means of the recently developed ergometer, Birkhoff's theorem is made physically useful. In particular, the conditions of the theorem are given an interpretation through a many-body model which exhibits both ergodic and nonergodic behavior depending on the range of a certain parameter of the model. To our knowledge these illustrations are the first known examples of the use of Birkhoff's theorem in many-body theory.

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1. Introduction

In 1931 the mathematician G.D. Birkhoff proved a theorem on Boltzmann's ergodic hypothesis (EH). It is a profound theorem, stated in abstract terms. Perhaps due to its abstractness, it is not well understood by most in statistical mechanics. It is thus no surprise to find that the theorem has never been applied to a many-body model to determine whether ergodicity exists in it and, if so, what is that which makes it ergodic. For over some 70 years the theorem has languished in the mathematics realm, not where it was probably originally intended by Birkhoff since it was meant to solve a physics problem [1, 2].

While the abstract nature might be a reason for this state of affairs, one could also suggest another possibility endemic to purely mathematical theorems. As an analogy take, for example, the Pythagorean theorem, perhaps

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the most famous of all mathematical theorems. But only a subset of triangles meet the condition of the theorem. What is more, what if we had no devices to measure an angle, where would this theorem be found?

To a degree, this analogy may perhaps be apt to the situation in which Birkhoff's theorem finds itself. This theorem says that EH is valid under certain conditions. Like all mathematical conditions, they are universal, that is, they transcend systems. However we do not *a priori* know whether anyone of physical systems would pass, let alone how many of them. Plainly we need a device with which to measure different physical models for Birkhoff's conditions on the time averages in a measure preserving phase space.

Fortuitously this device now exists, called an ergometer. It is a product of a physical theory on EH recently developed by us. A physical theory is per force not universal, but system dependent or system specific. It "measures" the ergodicity system by system.

The ergometer can determine whether and why a system is ergodic with respect to a dynamical variable say A [3–5]. If it determines that A is not ergodic, we can see how Birkhoff's conditions are not being met. By this process the work of the ergometer makes the abstract theorem a useful, even practical means to understand ergodicity.

2. Orthogonal approaches to EH

If A is a dynamical variable in a many-body system in thermal equilibrium, EH asserts that the time average of A is equal to the ensemble average of A. More precisely put,

$$\lim_{T\to\infty} \frac{1}{T} \int_0^T \langle A(t)\rangle dt = \langle A\rangle \,, \tag{1}$$

where the brackets on the l.h.s. are meant to average over all initial values of $A(t)$. This averaging insures that both sides are being compared at the same temperature at which the system is in equilibrium. The original version of EH was intended for classical systems. We extend it to include quantum systems since EH is just as necessary here. It is in the belief that EH has to be a foundation of statistical mechanics for *all* systems.

Birkhoff proves (1) by seeking a condition or conditions under which the time average exists. We, however, regard (1) as a physical entity in a system, which is amenable to a measurement. Evidently the two approaches go about in an orthogonal manner, the former universally and the latter specifically. Can they be combined? Suppose the time average in a specific system is assumed to exist but without the attendant universal conditions. What would this partially combined approach yield?

Turning to the l.h.s. of (1), we regard $A(t)$ to be accessible by a time dependent external probe $h(t)$ say. It is sufficient to consider a linear response to such a probe.

Let the total energy at time t be given by

$$H'(t) = H(A) + h(t)A\,, \tag{2}$$

where $H(A)$ denotes the internal energy and $h(t)$ the external field.

Then in the framework of linear response theory [6],

$$\langle A(t)\rangle_{H'(t)} = \langle A\rangle_H + \int_{-T}^{t} h(t')\chi_A(t,t')dt'\,, \tag{3}$$

where $\chi_A(t,t')$ is the linear response function defined by

$$\chi_A(t,t') \;=\; \frac{i}{\hbar}\langle[A(t),A(t')]\rangle_H \tag{4a}$$

$$\;=\; 0 \text{ if otherwise}\,, \tag{4b}$$

where $A(t) = \exp(itH)A\exp(-iHt)$ with $\hbar = 1$. To take the simplest case we let the response function be stationary in addition to being causal.

After Birkhoff, we shall assume that the time average of the causal stationary linear response function *exists*: $0 < I_{\rm ta} < \infty$, where

$$I_{\rm ta} = \lim \frac{1}{T}\int_0^T\int_0^t \chi_A(t-t')dt'dt\,. \tag{5}$$

But we make no other assumptions on the time average (which Birkhoff brings in). We should note here that the response function which is being time averaged in (5) depends on the internal energy $H(A)$ only since the probe field is factored in linear response theory. Thus this is in the spirit of Birkhoff's time average which, being a mathematical theory, does not refer to an external probe.

Assuming that $I_{\rm ta}$ exists, we now proceed as follows: In linear response theory the most basic function is $R_A(t) = (A(t),A),\ t \geq 0$, the autocorrelation function of A, also known as the relaxation function. The inner product of A and B is defined by

$$(A,B) = \frac{1}{\beta}\int_0^\beta du\langle A(u)B^\star\rangle - \langle A\rangle\langle B^\star\rangle\,, \tag{6}$$

where β is the inverse temperature, $\langle \ldots \rangle$ means an ensemble average with respect to H and $A(u) = \exp(uH)A\exp(-uH)$, and * Hermitian conjugation. This inner product is sometimes known as the Kubo scalar product. Thus, $(A, A) = R_A(0) = \chi_A$ the static susceptibility.

Now we use the well known relation found in linear response theory

$$\frac{d}{dt}R_A(t) = -\chi_A(t), \qquad t > 0\,. \tag{7}$$

Substituting (7) on the r.h.s. of (5), we obtain readily

$$I_{\mathrm{ta}} = \chi_A - \lim \frac{1}{T}\int_0^T R_A(t)dt\,. \tag{8}$$

First, for the r.h.s. of (8) to exist, which we assume after Birkhoff, we must fix the temperature away from any anomalous points, so that χ_A is a finite constant. Second, the integral of $R_A(t)$ must also remain finite as $T \to \infty$, so that it is removed by the action of the prefactor $1/T$. It is possible that the integral may vanish *identically.* This possibility must also be excluded since, if otherwise, it is no longer the time average of EH.

Thus if I_{ta} is to exist, $0 < \int_0^\infty R_A(t)dt < \infty$, provided that χ_A is also finite. If it is finite, we may replace in the integral $R_A(t)$ by $r_A(t) = R_A(t)/R_A(0)$ since $R_A(0) = \chi_A$ is finite if it is not at an anomalous point (*e.g.* critical temperature). Thus we arrive at the conclusion that the existence assumption implies that

$$I_{\mathrm{ta}} = \chi_A \tag{9}$$

provided that $0 < W < \infty$, where

$$W = \int_0^\infty r_A(t)dt\,. \tag{10}$$

We have already shown that proving (9) is equivalent to proving (1), that is EH. But notice that the above W condition is exactly the same one for EH that we have earlier derived independently, now referred to as an ergometer [1–3]. It is reassuring to recover the ergometer from another approach. Perhaps more far reaching is: The ergometer is recovered without Birkhoff's secondary conditions (metrical transitivity and almost everywhereness). It must mean that these secondary conditions are contained in the ergometer.

It should also be noted that while Birkhoff's theorem should apply strictly to classical systems only, our above analysis by the existence assumption does not rely on any classical properties. Hence the ergometer applies to a system whether quantum or classical or a quantum system in the classical domain. Thus the ergometer encompasses the entire domain. By our analysis, it seems reasonable to conclude also that the concepts of Birkhoff's theorem are applicable to the same entire domain.

Finally the ergometry is about the autocorrelation function and its long time behavior. It is a function perhaps most central in nonequilibrium statistical mechanics. From it one can obtain the memory function and the structure factor [7]. As t grows, the autocorrelation function must vanish if W is to be finite. Asymptotically vanishing is termed *irreversible*. We have shown elsewhere that according to the ergometer, irreversibility is a necessary but not sufficient condition for ergodicity [8]. Irreversible behavior is also important to self diffusion in determining whether it is normal or anomalous [9–11]. Thus the ergometer is not an ad hoc quantity but one that is deeply rooted in many-body dynamics. It is amenable to analysis by the recurrence relations method as illustrated below.

3. Ergometer

To see how Birkhoff's secondary conditions are contained in the ergometer, we need to evaluate W by obtaining the normalized autocorrelation function $r(t)$ in a many-body model. For a Hermitian model, $r(t)$ may be obtained by the recurrence relations method which has now been successfully and widely applied [14–16].

As an illustration, we shall consider a $1d$ linear nn coupled chain of $2N$ harmonic oscillators in periodic boundary conditions. We shall let the mass of one of the oscillators be M and the masses of the rest m each. It is a model known sometimes as one impurity harmonic oscillator chain model. If the impurity mass M is much lighter than m, it becomes a vacancy model. If M is much heavier than m, it becomes a Brownian model. Thus the dynamics of a one impurity model is of considerable physical interest in nonequilibrium statistical mechanics [16].

The Hamiltonian is given by

$$H = \sum_j \frac{p_j^2}{2m_j} + \frac{k}{2}\sum_j (x_{j+1} - x_j)^2 \,, \tag{11}$$

where p_j and x_j are the momentum and position of j-th oscillator, $m_j = M$ if $j = 0$ and $m_j = m$ if $j = \pm 1, \pm 2, \ldots \pm N$, and k the Hookes constant. We will impose periodic boundary conditions such that *e.g.* $x_{-N} = x_N$. That is, the chain is in the form of a ring of $2N$ oscillators, in which the impurity mass is at site 0. We introduce a mass ratio parameter $\lambda = m/M$, where $\lambda = (0, \infty)$. In this work we will be concerned primarily with the Brownian limit $\lambda \to 0$.

If $A = p_0$ (the momentum of the impurity mass), the autocorrelation function of p_0 is obtained by the recurrence relations method [12]. In particular, for $0 < \lambda < \frac{1}{2}$,

$$r(t) = \frac{1}{\sqrt{\pi}} \frac{\lambda}{1-2\lambda} \sum_{n=1} b^n \Gamma\left(n+\tfrac{1}{2}\right) \frac{J_n(ut)}{(ut/2)^n}\,, \tag{12}$$

where $b = (1-2\lambda)/(1-\lambda)^2$, J_n is the Bessel function, and $u = 2\sqrt{k/m}$. Observe that $0 < b < 1$ if $0 < \lambda < \frac{1}{2}$.

While (12) appears complicated, it can be shown that if $\lambda = \frac{1}{2}$, it reduces to the well known solution $J_1(ut)/(ut/2)$. The solution is also known if $\lambda \to \frac{1}{2}$, but we will not show it since it is not germane to our ergodicity analysis intended here.

We shall now evaluate the ergometer W by (12):

$$W = \int_0^\infty r(t)dt = \frac{1}{\sqrt{\pi}} \frac{\lambda}{1-2\lambda} \sum_n b^n \Gamma(n+\tfrac{1}{2}) \int_0^\infty \frac{J_n(ut)}{(ut/2)^n} dt\,. \tag{13}$$

By using the known result [17],

$$\int_0^\infty J_n(x)/x^n dx = \Gamma(\tfrac{1}{2})/2^n \Gamma(n+\tfrac{1}{2})\,, \tag{14}$$

in (13) we obtain

$$W = 1/u\lambda\,. \tag{15}$$

Thus, W is finite as long as $\lambda \neq 0$. That is, p_0 is ergodic if λ is finite. But as $\lambda \to 0$, $W \to \infty$ meaning that p_0 ceases to be ergodic. The process of the loss of ergodicity as $\lambda \to 0$ may be understood in terms of Birkhoff's conditions: As long as λ is finite, there is only one dynamical domain. If mass M is perturbed, the delocalization of the perturbation energy takes place over the entire body of the chain. In the language of Birkhoff, thee is but one invariant and everywhere is metrically transitive.

But as $\lambda \to 0$, a perturbation on mass M makes it to respond singly by itself, not totally nor collectively, and causes it to move ballistically, in which the rest of the body simply accompanies it. The perturbation energy does not get delocalized to this part of the body. There are thus two invariants and the ergodicity is lost.

The structure of the ergometer (15) is suggestive. If, for example, $\lambda \to \infty$, $W \to 0$, which is the other end of the W spectrum, where ergodicity vanishes. If (15) is applicable at this limit, there is also the loss of ergodicity, indicating a duality between the two ends of the W spectrum. As we show in Appendix A, (15) turns out to be in fact valid for all values of λ. Since the ergodicity is lost at $\lambda = \infty$, according to Birkhoff there must be at least two invariants. If the impurity mass is perturbed as $\lambda \to \infty$, the dynamics becomes simpler. It is as if the impurity mass is attached to a wall on both sides. As a result, the perturbed energy is localized within, whose dynamics is that of an oscillatory motion. The rest of the body is effectively unperturbed, resulting in two invariants.

There are however subtler differences in spite of this duality in the loss of ergodicity. If $\lambda \to 0$ (heavy impurity limit), the autocorrelation (12) can be expressed as follows [18]:

$$\lim_{\lambda\to 0} r(t) = 1 - \lambda p(t)\,, \tag{16}$$

where $p(t) > 0$ is some regular function of t. Thus as $\lambda \to 0$, irreversibility is lost. The dynamics becomes ballistic. On the other hand

$$\lim_{\lambda\to\infty} r(t) = D\cos\mathit{\Omega} t + \lambda^{-1} g(t)\,, \tag{17}$$

where $D = 2(1-1/\lambda)/(2-1/\lambda) = 1 - 1/2\lambda + \ldots$, $\mathit{\Omega} = u\lambda/\sqrt{2\lambda-1} = \sqrt{2k/M}(1+1/4\lambda+\ldots)$ and $q(t)$ is another regular function of t [12]. In the limit $\lambda \to \infty$, irreversibility is also lost. But the dynamics becomes periodic instead.

4. Concluding remarks

We have shown that Birkhoff's theorem, which has long languished in the mathematical realm, can provide a deep understanding into the physics of ergodicity. This possibility has been brought about by the development of the ergometer, a physical device with which ergodicity in a many-body model can be assayed. By this relationship we also point out that the concepts due to Birkhoff should also be applicable in the quantum domain since the ergometer is applicable in both the classical and quantum domain. Making Birkhoff's theorem a physically useful tool will further help develop ergometry, the mapping of the ergodic landscape.

Appendix A

General proof of equation (15)

There are several ways to prove that Eq. (15) is valid for all values of λ. We give below perhaps the simplest proof.

$$W = \lim_{z\to 0}\int_0^\infty e^{-zt} r(t)dt = \hat{r}(z\to 0)\,, \tag{A.1}$$

where $\hat{r}(z)$ means the Laplace transform of $r(t)$. We have shown that

$$\hat{r}(z) = \left[\lambda\left\{pz + \sqrt{(z^2+u^2)}\right\}\right]^{-1} , \tag{A.2}$$

where $p = 1/\lambda - 1$. See [12], Eq. 7 therein. Eq. (A.2) is valid for all values of λ. If $z \to 0$ in (A.2), we obtain $W = 1/u\lambda$. *q.e.d.*

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