ERGODIC CONDITION FOR HERMITIAN MANY-BODY PROBLEMS*

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The ergodic hypothesis due to Boltzmann represents a foundation of statistical mechanics. In spite of its importance, whether the hypothesis is really valid, or even to what extent it is valid, is still not established. To help make the ergodic hypothesis more amenable to physical tests, we need to develop a workable ergodic condition. If a system is Hermitian, it is possible to formulate an ergodic condition using a dynamical response function appearing in inelastic scattering processes. The ergodic condition is expressed in terms of the relaxation function. It describes when the hypothesis is valid and when it can break down. As an application we show that a system ceases to be ergodic when the critical temperature is approached.

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1. Introduction

Statistical mechanics is built on two important foundations: Gibbs' ensemble theory and Boltzmann's ergodic hypothesis. The ensemble theory is used almost exclusively in statistical mechanical calculations, so that its validity is beyond question. The ergodic hypothesis (EH) is generally assumed to be valid but it rests on much less firm ground. In many places one reads that it is not universally valid [1]. There have been shown that in certain models it actually fails based on the arguments of inequalities [2, 3]. These uncertainties make it all the more necessary that we need to put the study of the validity of EH in the forefront of our attention.

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The difficulty of proving or disproving EH in a many body system in thermal equilibrium is well known [4]. One would need to know how to solve the equations of motion *e.g.* Heisenberg equation. One must still face an infinite time integral which may not be easy to handle. For these reasons the study of EH has not been undertaken until very recent times. Advances in solving the Heisenberg equation or its analog the generalized Langevin equation have encouraged many workers to re-examine EH from a variety of different perspectives [5–17].

In statistical mechanics we deal with models of infinitely many degrees of freedom. What is needed is a kind of measurer or even a meter with which one could determine whether a given model is ergodic in a certain physical domain such as high temperatures, or whether such a model can cease to be ergodic upon entering a different domain like the critical region. A workable ergodic condition could provide an answer if one could be found. Our study is premised on finding an ergodic condition with which one can say that this one is ergodic and why it is so, or that one is not and why it fails to be ergodic. Arguments based on inequalities cannot readily adduce physical underpinnings although they might in some cases determine whether a system is ergodic or not [2,3]. These arguments are also not general enough to go beyond those which may be adapted to this approach. We shall see that it is possible to obtain a general ergodic condition if a system is Hermitian.

2. What to time average

In the ergodic theory, which is a study in pure mathematics concerned with EH in classical statistical mechanics, almost any dynamical function may be considered provided that it is an integrable function [18]. We depart from this practice and look for a particular dynamical function which plays a significant role in inelastic scattering processes. In such a function we may find a link between EH and energy absorption by scattering. When a many-body system is inelastically scattered, the scattered energy must delocalize in that system in some manner. The delocalization process means a time evolution. Since time averaging is taken over the time of evolution, it seems clear that there has to be a connection between EH and energy delocalization [19].

For these reasons, we shall consider the time dependent susceptibility $\chi(t,t')$ from linear response theory. Let $\langle A(t)\rangle = TrA\rho(t)$, where A is a dynamical variable (*e.g.* a density or spin density) at time t and ρ the density matrix with $H'(t)$, where

$$H'(t) = H(A) + h(t)A\,, \tag{1}$$

where $h(t)$ is an external field and H denotes a system which may be an interacting system like a Coulomb gas. We shall assume H to be Hermitian. Then, the time dependent susceptibility is defined through [20]

$$\langle A(t)\rangle = \int_{-\infty}^{t} h(t')\chi(t-t')dt' \,. \tag{2}$$

We assume that the susceptibility is causal. According to linear response theory [21, 22] which we adopt in this scattering formulation,

$$\chi(t-t') = \begin{cases} i/\beta \ \langle [A(t),\ A(t')]\rangle \\ 0 \text{ if otherwise} \end{cases} \,, \tag{3}$$

where the brackets are now an ensemble average with the density matrix ρ with H, not $H'(t)$. We shall time average over this quantity to see whether we can recover the time independent susceptibility χ as EH would assert.

3. Time averaging and EH

We shall time average the time dependent susceptibility over a long time. Consider the following time integral

$$I_{\mathrm{ta}} = \lim_{T\to\infty} \frac{1}{T}\int_0^T \int_0^t \chi(t,t')dt'dt \,. \tag{4}$$

A homogeneous macroscopic system always enjoys a stationarity property: $\chi(t,t') = \chi(t-t')$. We shall take advantage of this property and change $t - t' \to t'$. This change of the variables helps to reduce the double integral into a single one. Also, we shall henceforth suppress $\lim(T \to \infty)$, but this limit is always implied when T appears anywhere in an expression. Introduce a new function $\varphi(t)$ defined by

$$\varphi(t) = \int_0^t \chi(t')dt' \,. \tag{5}$$

Evidently $\varphi(t = 0) = 0$ and $d\varphi(t)/dt = \chi(t)$. Consider the integral of φ by partial integration:

$$\int_0^T \varphi(t)dt = T\varphi(T) - \int_0^T t\chi(t)dt \,. \tag{6}$$

From linear response theory, $\chi(t) = -d/dt R(t)$, $t > 0$. If this is used in (6), by yet another partial integration, we obtain for rhs of (6)

$$= T \int_0^T \chi(t)dt + T\,R(T) - \int_0^T R(t)dt\,. \tag{7}$$

Thus the time average I_{ta}(see Eq. (4)) becomes

$$I_{\mathrm{ta}} = \int_0^T \chi(t)dt + R(T) - \frac{1}{T}\int_0^T R(t)dt\,. \tag{8}$$

The above expression can be made to look simpler if we adopt the Laplace transform expression, implicit with $T \to \infty$ as stated earlier. Let $\tilde{\chi}(z) = \int_0^\infty e^{-zt}\chi(t)dt$, Re $z > 0$, and similarly for $\tilde{R}(z)$. Then,

$$I_{\mathrm{ta}} = \tilde{\chi}(0) + R(\infty) - \frac{1}{T}\tilde{R}(0)\,. \tag{9}$$

Evidently (9) looks a lot tidier. By EH, $I_{\mathrm{ta}} = \chi$, where χ is the static susceptibility. Thus by EH, we conclude that

$$\tilde{\chi}(0) + R(\infty) - \frac{1}{T}\tilde{R}(0) = \chi\,. \tag{10}$$

But is (10) really correct? Thus testing the correctness of (10) is equivalent to testing EH itself. We restate EH on the susceptibilities:

$$\lim_{T\to\infty} \int_0^T \int_0^t \chi(t-t')dt'dt = \chi\,. \tag{11}$$

In Appendix A, we give another view showing how it might arise.

4. Relaxation function

Equation (10) shows that the validity of EH may rest on the behavior of the relaxation function $R(t)$ at least as far as EH on the susceptibilities is concerned. The relaxation function is originally given by linear response theory but it may also be defined independently, simply as an amplitude in an inner product space realized by the Kubo scalar product [23],

$$R(t) = (A(t), A),\ \ t \ge 0\,, \tag{12}$$

where $A(t) = e^{iHt}Ae^{-iHt}$, $A = A(t=0)$, and $\hbar = 1$. It has the following important properties needed for our analysis:

(a) $R(0) = \chi$, where χ is the time independent susceptibility.

(b) $dR(t)/dt = -\chi(t)$, $t > 0$.

(c) $dR(t = 0)/dt = 0$.

If we Laplace transform property-b, together with properties-a and -c, we obtain

$$\tilde{\chi}(z) + z\tilde{R}(z) = \chi\,. \tag{13}$$

Evidently it is also true if $z = 0$. Thus,

$$\tilde{\chi}(0) + z\tilde{R}(z)\,|_{z=0} = \chi\ . \tag{14}$$

Now we must recognize that (14) is an *exact* statement since it follows from the definition of $R(t)$. It may or may not possess any physical content but it is an exact relationship. Let us compare (10) obtained by EH against this exact one (14). We at once see that they do not agree. One must conclude that EH cannot generally be valid!

But can it be valid in some special situations? It can happen if $\tilde{R}(0)$ is finite. If it is finite, it implies that $R(t = \infty) = 0$. Also it is possible that $\tilde{R}(0)$ is identically zero. We must remove this possibility since if otherwise it becomes independent of $T \to \infty$. Thus we arrive at a condition

$$0 < \tilde{R}(z = 0) < \infty\,. \tag{15}$$

If (15) is satisfied, EH on the susceptibilities is valid. It would appear at this stage that EH is of limited validity. If $R(0) = \chi$ is finite, we introduce $r(t) = R(t)/R(0)$. We restate (15) as

$$0 < W < \infty\,, \tag{16}$$

referred to as the *ergodic condition*, where

$$W = \tilde{r}(z = 0) \tag{17a}$$

$$= \int_0^\infty r(t)dt\,. \tag{17b}$$

We shall show below that W may be expressed in an infinite product of certain static quantities called *recurrants.* The English mathematician J. Wallis studied infinite products in 1655(!) and our W is named after him.

5. Recurrence relations method

The recurrence relations method has proved to be a powerful technique for solving dynamical properties of Hermitian many body systems [23–26]. This method has now been widely applied to a variety of such models very successfully [27–38]. According to this method $\tilde{r}(z)$ is expressible in a continued fraction as:

$$\tilde{r}(z) = 1/z + \Delta_{1/Z} + \Delta_{2/Z} + \cdots \Delta_{d-1/Z}\,, \tag{18}$$

where d denotes the dimensions of the inner product space of A. It can range from 2 to ∞. Also Δ_1, Δ_2, *etc.* are known as *recurrants*, the norms of basis vectors spanning the space of A.

If d is finite, $r(t)$ is periodic, thus $r(t = \infty) \neq 0$. It means that a system which is spanned by a finite set of basis vectors in an inner product space realized by the Kubo scalar product is *never* ergodic.

If $d \to \infty$, its amplitude can decay to $r(\infty) = 0$, termed *irreversible* [16]. We are thus interested in an inner product space with indefinitely many dimensions. We now take the limit $d \to \infty$ first, and limit $z \to 0$ second on $\tilde{r}(z)$ of (18):

$$W = \lim(z \to 0) \lim(d \to \infty) \tilde{r}(z) \tag{19}$$

$$= \frac{\Delta_2 \Delta_4 \Delta_6 \cdots}{\Delta_1 \Delta_3 \Delta_5 \cdots} \tag{20}$$

an infinite product. The ergodic condition can thus be defined by (17a,b) or (20). All three are equivalent, but on occasion one is easier to evaluate than the others. Below we illustrate them by one example. Suppose $\Delta_n = n^2$ in some suitable dimensionless units, realized in a certain fluid model [39]. For this form of the recurrants, $r(t) = \operatorname{sech} t$. Thus

$$W = \int_0^\infty \operatorname{sech} t\, dt = \pi/2\,. \tag{21}$$

If these recurrants are substituted in (19), it becomes Wallis' infinite product, recovering (21). This system, having $r(t) = \operatorname{sech} t$ and $r(\infty) = 0$, is ergodic.

6. Ergodicity and self diffusion

If $W = 0$ or ∞, it fails to satisfy the ergodic condition. A system that gives either one of the end values of the W spectrum is not ergodic. When $W = 0$, it is referred to as the localization limit. It occurs when the energy delocalization is incomplete due to the energy flow being locally prevented. When $W = \infty$, the energy delocalization is also incomplete. But in this case it is globally localized, whose motion is akin to a ballistic motion.

In the case of $W = 0$, a system will behave irreversibly, *i.e.* $r(t = \infty) = 0$. But the perturbation that is generated by an external probe will result in a standing wave. The perturbation energy is not distributed over the nodal positions of a standing wave. This leads to a failure of EH. In the case of $W = \infty$, $r(t = \infty) \neq 0$. This is typical of how a Brownian particle behaves in a sea of small masses. The time average is over the path of a Brownian particle ignoring the internal degrees of freedom, again leading to a failure of EH.

EH can be given different physical interpretation if A denotes the velocity of a particle. If particles in a system are all identical, $W = D$ the self diffusion constant [40]. Thus ergodicity means self diffusivity. When EH does not hold, self diffusion is either zero or becomes anomalous [41]. In many cases one can understand the validity of EH through the physically accessible self diffusivity.

7. Critical region

We will make one important application to the critical region. If a system behaves ergodic when T is above T_c (critical temperature), does it remain ergodic as T approaches T_c? This is a question that is particularly relevant to experiment. To our knowledge there is no definitive theoretical understanding on it.

Let us assume that a system is ergodic when $T > T_\mathrm{c}$. It means that the isothermal susceptibility or compressibility χ is finite. When T is approached T_c, we assume that it will diverge owing to an onset of critical fluctuations. According to the structure of W given in an infinite product, see (20), all recurrants are finite when $T > T_\mathrm{c}$ including $\Delta_1 = (\dot{A}, \dot{A})/(A, A)$. As $T \to T_\mathrm{c}$, $(\dot{A}, \dot{A})$ remains finite, but $(A, A) = \chi \to \infty$. Thus $W \to \infty$, attaining the ballistic limit. Thus according to our ergodic condition, a system ceases to be ergodic in the critical region.

The physical reason behind the loss of ergodicity in the critical region is as follows: When scattered in the critical region, the critical fluctuations subsume all the scattered energy leaving noncritical fluctuations essentially unaffected. This behavior is much like a Brownian particle being scattered, becoming independent of the internal degrees of freedom.

8. Concluding remarks

Boltzmann's ergodic hypothesis represents a foundation of statistical mechanics. But to our knowledge there have been no theories providing an explicit workable ergodic condition with which to establish the validity of the hypothesis in a many-body problem. We have derived an explicit condition (16), denoted by W, an infinite integral of the relaxation function given by linear response theory. By the recurrence relations method W is shown to be expressible in an infinite product, first studied 350 years ago by Wallis. To our knowledge our work represents a first application of infinite products in physical theory.

One immediate conclusion is that EH does not hold in the critical region. EH can be interpreted in physical terms via self diffusion. EH fails when self diffusion vanishes or becomes anomalous. This link suggests a possible avenue to re-examine the ergodic theory from a physical perspective. In particular it might be possible to approach Birkhoff's theorem on EH via the legs of self diffusivity. This work will be consider in the future.

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Appendix A

Origin of equation (4)

We follow linear response theory and use Eq. (2), identifying $< A(t) >= M(t)$, where $M(t)$ is the magnetization at time t. It may refer to a paramagnet or a simple ferromagnet above T_{c}. EH would asserts that

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

where M is the magnetization by an applied static field h, that is, $M = \chi h$, where h is the applied static field and χ the static susceptibility. If (2) is substituted in lhs of (A1), we obtain (suppressing the *lim* sign, which is implied),

$$\frac{1}{T}\int_0^T \int_0^t h(t')\chi(t-t')dt'dt = M\,. \tag{A.2}$$

Now we assume that $h(t) = h$, a constant external field. Then

$$h\frac{1}{T}\int_0^T \int_0^t \chi(t-t')dt'dt = M\,. \tag{A.3}$$

But $M = \chi h$ by linear response theory. Hence under EH it follows that

$$\frac{1}{T}\int_0^T\int_0^t \chi(t-t')dt'dt = \chi\,, \tag{A.4}$$

recovering Eq. (4).

One might argue that the lower limit on the integral in Eq. (2) should be not zero but $-\infty$. That is, the field $h(-\infty) = 0$, which is gradually turned on. This is a usual statement of linear response theory. In our treatment we set $h(t=0) = 0$, which turns out to be a little more convenient. If necessary, it is possible to start with $h(t = -\infty)$. In this case, EH would assert that

$$\lim_{T\to\infty}\frac{1}{2T}\int_{-T}^{T} M(t)dt = M\,. \tag{A.5}$$

Now the same analysis yields

$$\tilde{\chi}(0) + R(\infty) - \frac{1}{2T}\tilde{R}(0) = \chi\,. \tag{A.6}$$

If this is compared with (9), we see that the only change is $T \to 2T$. Hence there is no fundamental change by using $h(0) = 0$ in place of $h(-\infty) = 0$. We have adopted the form of (4) this being customary in the ergodic theory.

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