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An extension of the dynamical foundation for the statistical equilibrium concept

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Abstract

This paper reviews a recently introduced generalization of dynamical stationarity involving the appearance of stable convolution semigroups in the ultralong time limit. Dynamical stationarity is the basis of the equilibrium concept in statistical mechanics, and the ultralong time limit is a limit in which a discretized time flow is iterated infinitely often while the discretization time step becomes infinite. The new limit is necessary when investigating induced automorphisms for subsets of measure zero. It is found that the induced dynamics on subsets of zero measure is given generically by stable convolution semigroups and not by the conventional translation group. This could provide insight into the macroscopic irreversibility paradox. The induced semigroups are generated by fractional time derivatives of orders less than unity, not by a first-order time derivative as the conventional group. Invariance under the induced semiflows therefore leads to a new form of stationarity, called fractional stationarity. Fractional stationarity provides the dynamical foundation for a generalized equilibrium concept.

1. Introduction

A recent classification theory of phase transitions has paved the way towards a fundamental generalization of the equilibrium concept [1–9]. Such a generalization is needed to describe non-equilibrium systems [10]. Within the generalized classification scheme of Ehrenfest [1–3] a generalized equilibrium concept *at phase transitions* emerges from the discovery of an entirely new class of phase transitions [5,6] whose critical points defy classification within the conventional equilibrium theories[1]. The new generalized

[1] The generalized equilibrium concept was termed "*anequilibrium*" in [5] where the prefix "an-" is an alpha privativum. Unfortunately the prefix conflicts with the indeterminate article. Therefore, I propose alternatively to use the name "*similibrium*" from (self-)similar equilibrium, and in German the term "*Ähnlichgewicht*" instead of the previous "*Ungleichgewicht*".

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equilibrium concept (similibrium or anequilibrium) can be based on a generalization of dynamical stationarity which is defined for a macroscopic observable $X(t)$ through the condition [5,6]

$$\frac{d^{\varpi}}{dt^{\varpi}} X(t) = 0\,, \tag{1.1}$$

where d^{ϖ}/dt^{ϖ} is the fractional Riemann–Liouville derivative with lower limit at 0 of order $0 < \varpi \leqslant 1$. For $\varpi = 1$ this generalization reduces to the familiar stationarity and equilibrium concept.

My objective in this paper is to review recent results concerning the derivation of fractional stationarity from abstract ergodic theory [9,11]. The physical situation corresponds to the critical dynamics at a fluid–solid critical point. Fluid–solid transitions involve ergodicity breaking, i.e. the transition between a large phase space for the fluid and subsets of very small measure describing the structurally arrested solid. They differ in this respect from fluid–fluid phase transitions which show symmetry breaking but no reduction of the underlying phase or state space. In ergodicity breaking phase transition it is necessary to study the dynamics induced on subsets of measure zero of the large phase space corresponding to the fluid.

Despite the fact that the invariant measures guaranteed to exist by the Bogoljubov–Krylov theory [12] may be concentrated on subsets of measure zero, the question of induced transformations on subsets of measure zero appears not to have been studied in ergodic theory [13–17]. It will be seen that pursuing this question from the point of view of the classification theory [5,6] leads not only to a generalized stationarity concept, but turns up in addition some useful new insight into the unresolved macroscopic irreversibility paradox [18].

2. Induced dynamical transformations

Given a dynamical system $(\Gamma, \mathcal{G}, \mu)$ with phase or state space Γ, a σ-algebra $\mathcal{G}$ of measurable subsets of Γ, and a probability measure μ, $\mu(\Gamma) = 1$, the time evolution of the system is generally a *flow* (or semiflow) on $(\Gamma, \mathcal{G}, \mu)$. A flow is defined as a one-parameter family of maps $\widetilde{T}^t : \Gamma \to \Gamma$ such that $\widetilde{T}^0 = I$ is the identity, $\widetilde{T}^{s+t} = \widetilde{T}^s \widetilde{T}^t$ for all $t, s \in \mathbb{R}$. For every $G \in \mathcal{G}$ also $\widetilde{T}G, \widetilde{T}^{-1}G \in \mathcal{G}$ holds. The flow $\widetilde{T}^t$ defines the time evolution of measures through $T^t\mu(G) = \mu(\widetilde{T}^t G)$ as a map $T^t : \Gamma' \to \Gamma'$ on the space Γ' of measures on Γ. Defining as usual [13,16] $\mu(G,t) = \mu((\widetilde{T}^t)^{-1}G)$ shows that

$$T^t \mu(G, t_0) = \mu(G, t_0 - t)\,, \tag{2.1}$$

and thus the flow T^t acts on measures as a translation in time. The existence of the inverse $(T^t)^{-1} = T^{-t}$ for a flow expresses the reversibility of the microscopic time evolution.

Let me briefly recall that the concept of equilibrium appears in ergodic theory as the *invariance* of measures under the time evolution. A measure μ is called *invariant under* *the flow* $\tilde{T}^t$ if $\mu(G) = \mu(\tilde{T}^t G) = \mu((\tilde{T}^t)^{-1}G)$ for all $t \in \mathbb{R}, G \in \mathcal{G}$. The equilibrium (or invariance) concept is closely related to the concept of *ergodicity*. An invariant measure is called *ergodic* if it cannot be decomposed into a convex combination of invariant measures, i.e. if $\mu = \lambda\mu_1 + (1-\lambda)\mu_2$ with μ_1, μ_2 invariant and $0 \leqslant \lambda \leqslant 1$ implies $\lambda = 1, \mu_1 = \mu$ or $\lambda = 0, \mu_2 = \mu$. The invariance of the measure μ implies that

$$T^t\mu(G, t_0) = \mu(G, t_0) \tag{2.2}$$

for all $G \in \mathcal{G}, t \in \mathbb{R}$ and given $t_0 \in \mathbb{R}$. It may also be expressed as $A\mu = -d\mu/dt = 0$, where $A = -d/dt$ is the *infinitesimal generator* of T^t defined as the strong limit

$$A = \lim_{t \to 0^+} \frac{T^t - I}{t} \tag{2.3}$$

with $I = T^0$ denoting the identity.

To define the induced time evolution on a subset $G \subset \Gamma$ it is necessary to discretize the continuous time evolution $\tilde{T}^t$ with $t \in \mathbb{R}$ into the discrete time evolution $\tilde{T}^k$ with $k \in \mathbb{Z}$. The discrete time evolution is generated by the map $\tilde{T} = \tilde{T}^{\Delta t}$ where Δt is the discretization time step. Let $G \subset \Gamma$ be a physically interesting subset on which one wishes to study the induced transformation. A point $x \in G$ is called *recurrent with respect to* G if there exists a $k \geqslant 1$ for which $\tilde{T}^k x \in G$. If μ is invariant under $\tilde{T}$ and $G \in \mathcal{G}$ then almost every point of G is recurrent with respect to G by virtue of Poincaré's recurrence theorem. A set $G \in \mathcal{G}$ is called a *μ-recurrent set* if μ-almost every $x \in G$ is recurrent with respect to G. The transformation $\tilde{T}$ defines an *induced transformation* $\tilde{S}_G$ on subsets G of positive measure, $\mu(G) > 0$, through

$$\tilde{S}_G x(t_0) = \tilde{T}^{\tau_G(x)} x(t_0) = x(t_0 + \tau_G(x)) \tag{2.4}$$

for almost every $x \in G$. The *recurrence time* $\tau_G(x)$ of the point x, defined as

$$\tau_G(x) = \Delta t \min\{k \geqslant 1 : \tilde{T}^k x \in G\}, \tag{2.5}$$

is positive and finite for almost every point $x \in G$. Because G has positive measure it becomes a probability measure space with the induced measure $\nu = \mu/\mu(G)$. If μ was invariant under $\tilde{T}$ then ν is invariant under $\tilde{S}_G$, and ergodicity of μ implies ergodicity also for ν [13].

Poincaré's recurrence theorem guarantees that the induced transformation $\tilde{S}_G : G \to G$ exists for μ-almost every $x \in G$ with $\mu(G) > 0$. To extend the definition to the case of zero measure let $(G, \mathfrak{G}, \nu)$ denote a subspace $G \subset \Gamma$ of measure $\mu(G) = 0$ with σ-algebra $\mathfrak{G}$ contained in $\mathcal{G}$, $\mathfrak{G} \subset \mathcal{G}$, in the sense that $B \in \mathfrak{G}$ for all $B \in \mathcal{G}$. $\mu(B) = 0$ for all $B \in \mathfrak{G}$ while $\nu(B) = \infty$ for all sets $B \in \mathcal{G}$ with $\mu(B) > 0$. Let $0 < \nu(G) < \infty$. If G is ν-recurrent under $\tilde{T}$ in the sense that ν-almost every point (rather than μ) is recurrent with respect to G then the recurrence time $\tau_G(x)$ and the map $\tilde{S}_G$ are defined for ν-almost every point $x \in G$. In the rest of the paper it will be assumed that G is ν-recurrent under $\tilde{T}$, and that $\nu(G \setminus \tilde{S}_G G) = 0$.

The pointwise definition of the induced transformation $\widetilde{S}_G$ is extended to a transformation on measures by averaging over the recurrence times [9,11]. The set

$$G_k = \{x \in G : \tau(x) = k\Delta t\} \tag{2.6}$$

contains the points of G whose recurrence time is $k\Delta t$. The ratio

$$p(k) = \frac{\nu(G_k)}{\nu(G)} \tag{2.7}$$

is the probability to find a recurrence time $k\Delta t$ with $k \in \mathbb{N}$. The numbers $p(k)$ define a discrete (lattice) probability density $p(k)\delta(t - k\Delta t)$ concentrated on the arithmetic progression $k\Delta t, k \in \mathbb{N}$. The action of the induced transformation S_G on measures ϱ on G can now be defined as the mathematical expectation [9,11]

$$S_G\varrho(B, t_0) = \langle T^{\tau_G}\varrho(B, t_0)\rangle = \sum_{k=1}^{\infty} \varrho(B, t_0 - k\Delta t)p(k) , \tag{2.8}$$

where $B \subset G$, and T^t was given in Eq. (2.1). Having defined the induced transformation $S_G : G' \to G'$ on the space G' of measures on G it is of interest to investigate the iterated transformation S_G^N in the long-time limit $N \to \infty$.

3. The ultralong time limit

The induced transformations $\widetilde{S}_G$ and S_G were defined for discrete time. There are three possibilities for removing the discretization in a *long-time limit*. The conventional method assumes $0 < \Delta t < \infty$ (or $\Delta t = 1$). The two other alternatives are $\Delta t \to 0$ and $\Delta t \to \infty$. The first alternative considers the limit $\lim_{\Delta t\to 0, k\to\infty} \widetilde{S}^{k\Delta t}$ in which the discretization step becomes small. This possibility may be called the *short-long-time limit* or *continuous time limit*, and it was discussed in Ref. [9]. The second alternative is to consider the limit $\lim_{\Delta t\to\infty, k\to\infty} \widetilde{S}^{k\Delta t}$ in which the discretization step diverges $\Delta t \to \infty$. This limit has been considered in Ref. [11], and is called the *long-long-time limit* or the *ultralong time limit*. The continuous time and ultralong time limit are analogous to the ensemble limit in the classification of phase transitions [5-7,9].

The induced time transformation S_G (2.8) acts as a convolution operator in time

$$S_G\varrho(B) = \varrho(B) * p. \tag{3.1}$$

Iterating the transformation N times gives

$$S_G^N\varrho(B) = (S_G^{N-1}\varrho(B)) * p = \varrho(B) * \underbrace{p * \ldots * p}_{N \text{ factors}} = \varrho(B) * p_N , \tag{3.2}$$

where the last equation defines $p_N(k)$. If $p_\infty = \lim_{N\to\infty} p_N$ exists, the limiting distribution can be used to define S_G^N in the $N \to \infty$ long-time limit.

The N-fold convolution $p_N(k) = p(k) * \ldots * p(k)$ can be interpreted as the probability density $p_N(k) = \text{Prob}\{\mathcal{T}_N = k\Delta t\}$ of the random sum $\mathcal{T}_N = \tau_1 + \ldots + \tau_N$ of N

independent and identically distributed random recurrence times τ_j with common lattice distribution $p(k) = p_1(k)$ [5,6]. A necessary and sufficient condition for the existence of a limiting density p_∞ for suitably renormalized recurrence times is that the discrete lattice probability density $p(k)$ belongs to the domain of attraction of a stable density [19,20]. Then, because Δt is defined as the maximal value such that all the τ_i are concentrated on the arithmetic progression $k\Delta t$, it follows that for a suitable choice of renormalization constants C_N, D_N

$$\lim_{N\to\infty} \sup_k \left| \frac{D_N}{\Delta t} p_N(k) - h\left(\frac{k\Delta t - C_N}{D_N}; \varpi, \zeta, C, D \right) \right| = 0 , \tag{3.3}$$

where $h(x; \varpi, \zeta, C, D)$ is a limiting stable density whose parameters obey $0 < \varpi \leqslant 2$, $-1 \leqslant \zeta \leqslant 1$, $-\infty < C < \infty$, and $D \geqslant 0$ [19–21]. If $D = 0$ then the limiting distribution is degenerate, $h(x; \varpi, \zeta, C, 0) = \delta(x - C)$ for all values of ϖ and ζ.

The individual recurrence times are positive numbers, $\tau_i \geqslant 0$ for all $i \in \mathbb{N}$. Hence the renormalized recurrence times $\mathcal{T}_N/D_N$ are bounded below, and this gives rise to the constraint $P_\infty(t) = 0$ for $t \leqslant C$ on the possible limiting distributions. The limiting stable distributions compatible with this constraint are given by the distributions whose parameters obey $0 < \varpi \leqslant 1$ and $\zeta = -1$. For $0 < \varpi < 1$ the limiting densities can be written in the form

$$h(x; \varpi, -1, C, D) = \frac{1}{D^{1/\varpi}} h_\varpi \left(\frac{t - C}{D^{1/\varpi}} \right) , \tag{3.4}$$

which expresses the well-known scaling relations for stable distributions [19,20,5,7]. The scaling function $h_\varpi(x)$ is given as

$$h_\varpi(x) = \frac{1}{x\varpi} H^{10}_{11} \left(\frac{1}{x} \,\middle|\, \begin{matrix} (0,1) \\ (0, 1/\varpi) \end{matrix} \right) \tag{3.5}$$

in terms of generalized hypergeometric H-functions. For the definition of $H^{10}_{11}(x)$, the reader is referred to Ref. [22] or Refs. [5,7]. For $\varpi = 1$,

$$h_1(x) = \lim_{\varpi\to 1} h_\varpi(x) = \delta(x - 1) \tag{3.6}$$

is the Dirac distribution. If the limit exists and is non-degenerate, i.e $D \neq 0$, the renormalization constants D_N have the form

$$D_N = (N\Lambda(N))^{1/\varpi\chi} , \tag{3.7}$$

where $\Lambda(N)$ is a slowly varying function. A function $\Lambda(N)$ is called slowly varying at infinity if

$$\lim_{x\to\infty} \frac{\Lambda(bx)}{\Lambda(x)} = 1 , \tag{3.8}$$

for all $b > 0$ [20].

Choosing the centering constants as $C_N = -CD_N$ one finds from Eqs. (3.3) and (3.4) for $N \to \infty$

$$p_N(k) \approx \frac{\Delta t}{D_N} h\left(\frac{k\Delta t - C_N}{D_N}; \varpi, -1, C, D\right) = \frac{\Delta t}{D_N D^{1/\varpi}} h_\varpi\left(\frac{k\Delta t}{D_N D^{1/\varpi}}\right). \tag{3.9}$$

In the traditional long-time limit $N \to \infty$ with $0 < \Delta t < \infty$ it follows that for finite k $\lim_{N\to\infty\, 0<\Delta t<\infty} k\Delta t/(DN\Lambda(N))^{1/\varpi} = 0$ and thus $\lim_{N\to\infty\, 0<\Delta t<\infty} p_N(k) = 0$, unless $D = 0$. Therefore, the conventional long-time limit produces a degenerate limiting distribution if it exists. On the other hand, the ultralong time limit allows Δt to become infinite. If Δt diverges such that

$$\lim_{\substack{N\to\infty \\ \Delta t\to\infty}} \frac{k\Delta t}{D_N} = t \tag{3.10}$$

exists, then this defines a *renormalized ultralong continuous time*, $0 < t < \infty$. In this case $D > 0$ contrary to the conventional limit. It follows that $\lim_{N\to\infty\, \Delta t\to\infty} kp_N(k) = th_\varpi(t/D^{1/\varpi})/D^{1/\varpi}$ and thus from Eq. (3.2) that

$$\begin{aligned} S_\varpi^{t^*}\varrho(B, t_0^*) &= \int_0^\infty \varrho(B, t_0^* - t) h_\varpi\left(\frac{t}{t^*}\right)\frac{dt}{t^*} \\ &= \frac{1}{t^*}\int_0^\infty T^t\varrho(B, t_0^*) h_\varpi(t/t^*)\, dt\,, \end{aligned} \tag{3.11}$$

where the *ultralong time parameter*

$$t^* = D^{1/\varpi} > 0 \tag{3.12}$$

was identified with the width parameter D of the limit law. If τ, τ' are two independent random recurrence times then $D \propto \langle|\tau - \tau'|^\sigma\rangle^{\varpi/\sigma}$ for all $\sigma < \varpi$, where $\langle\ldots\rangle$ is the expectation with respect to the limiting distribution. This shows that $D^{1/\varpi}$ has dimensions of time, and justifies its identification as a new time parameter. The same conclusion follows from (3.6) for $\varpi = 1$ because

$$S_1^{t^*}\varrho(B, t_0^*) = \int_{-\infty}^{\infty} \varrho(B, t_0^* - t)\delta\left(\frac{t}{t^*} - 1\right)\frac{dt}{t^*} = \varrho(B, t_0^* - t^*) = T^{t^*}\varrho(B, t_0^*) \tag{3.13}$$

again identifies $t^* = D^{1/\varpi}$ as an ultralong time parameter.

The results (3.11) and (3.13) imply macroscopic (ultralong time) irreversibility by virtue of (3.12) even if the underlying time evolution $\widetilde{T}^t$ and T^t, respectively, was reversible. This fact is of interest with respect to the irreversibility paradox [18].

4. Fractional stationarity

The induced ultralong time dynamics $S_{\varpi}^{t^*}$ naturally gives rise to a generalized concept of stationarity and equilibrium by requiring invariance of measures ν on G under the induced dynamics $S_{\varpi}^{t^*}$. The invariance condition analogous to (2.2) requires that

$$S_{\varpi}^{t^*}\nu(B,t_0^*) = \nu(B,t_0^*) \tag{4.1}$$

for $t > 0$ and $B \subset G$. For $0 < \varpi < 1$ this condition defines *fractional invariance* or *fractional stationarity* [9,11]. In terms of infinitesimal generators (2.3) the invariance condition becomes

$$A_{\varpi}\nu(B,t) = 0 \tag{4.2}$$

for $t > 0$, where A_{ϖ} is the infinitesimal generator of the induced semigroup $S_{\varpi}^{t^*}$. For $\varpi = 1$ the relation (3.13) implies $A_1\nu(B,t) = -d\nu(B,t)/dt = 0$, which resembles the familiar stationarity concept.

A new and very different stationarity concept arises for $\varpi < 1$. In this case the infinitesimal generators of the stable convolution semigroup $S_{\varpi}^{t^*}$ are obtained [20] by evaluating the generalized function $s_{-}^{-\varpi-1}$ [23] on the time translation group T^s

$$A_{\varpi}\varrho(t) = c^{+}\int_0^{\infty} s^{-\varpi-1}(T^s - T^0)\,ds\,\varrho(t) = c^{+}\int_0^{\infty} s_{-}^{-\varpi-1}T^s\,ds\,\varrho(t)\,, \tag{4.3}$$

where $c^{+} > 0$ is a constant. Comparing (4.3) with the Balakrishnan algorithm [24–26] for fractional powers of the generator of a semigroup T^t

$$(-A)^{\alpha}\varrho(t) = \lim_{t\to 0^+}\left(\frac{I-T^t}{t}\right)^{\alpha}\varrho = \frac{1}{\Gamma(-\alpha)}\int_0^{\infty} s^{-\alpha-1}(I-T^s)\varrho(t)\,ds \tag{4.4}$$

shows that if $A = -d/dt$ denotes the infinitesimal generator of the original time evolution T^t, then $A_{\varpi} = (-A)^{\varpi}$ is the infinitesimal generator of the induced time evolution $S_{\varpi}^{t^*}$. For $0 < \varpi < 1$ the generators A_{ϖ} for $S_{\varpi}^{t^*}$ are *fractional time derivatives* [25,23]. The differential form (4.2) of the fractional invariance condition for ν becomes (Eq. (1.1))

$$\frac{d^{\varpi}}{dt^{\varpi}}\nu(B,t) = 0 \tag{4.5}$$

for $t > 0$, which was first derived in Refs. [5,6]. Its solution is

$$\nu(B,t) = C_0 t^{\varpi-1} \tag{4.6}$$

valid for $t > 0$, with C_0 a constant. This shows that in a fractional stationary dynamical state the volume $\nu(B)$ of regions in phase space shrinks with time. In this sense the generalized concepts of stationarity and equilibrium become applicable to dissipative systems. More generally, (4.5) reads $A_{\varpi}\nu(B,t) = \delta(t)$ with solution $\nu(B,t) = C_0 t_{+}^{\varpi-1}$

for $t \geqslant 0$ in the sense of distributions. The stationary solution with $\varpi = 1$ has a jump discontinuity at $t = 0$, and is not simply constant.

In summary, the study of induced transformations on subsets of measure zero in the ultralong time limit leads to a renormalized ultralong time evolution given by a family of stable convolution semigroups whose generators are fractional time derivatives. Invariance under the ultralong time evolution defines fractional stationarity. Fractional stationarity provides a dynamical basis for generalizing the equilibrium concept of statistical physics into what may be called anequilibrium or similibrium. The special case $\varpi = 1$ recovers the conventional equilibrium concept.

Specific applications of these general results have been discussed elsewhere (see Refs. [5,6,27,28]). These include fractional relaxation [5,6], fractal time random walks [27] and fractional diffusion [28]. While these results suggest a relation with the divergence of relaxation times in solidification and vitrification [29] further theoretical studies are needed to explore all the ramifications of the generalized equilibrium concept.

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