# Weak Ergodicity Breaking in the Continuous-Time Random Walk

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The continuous-time random walk (CTRW) model exhibits a nonergodic phase when the average waiting time diverges. Using an analytical approach for the nonbiased and the uniformly biased CTRWs, and numerical simulations for the CTRW in a potential field, we obtain the nonergodic properties of the random walk which show strong deviations from Boltzmann-Gibbs theory. We derive the distribution function of occupation times in a bounded region of space which, in the ergodic phase recovers the Boltzmann-Gibbs theory, while in the nonergodic phase yields a generalized nonergodic statistical law.

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The ergodic hypothesis is a cornerstone of statistical mechanics. It states that ensemble averages and time averages are equal in the limit of infinite measurement time. Starting with the work of Bouchaud, there has been growing interest in weak ergodicity breaking, which finds applications in a wide range of physical systems: phenomenological models of glasses [1], laser cooling [2,3], blinking quantum dots [4,5], and models of atomic transport in optical lattices [6]. Weak ergodicity breaking is found for systems whose dynamics is characterized by power law sojourn times, with infinite average waiting times. In such systems the microscopical time scale diverges, for example, the average trapping time of an atom in the theory of laser cooling [2,3]. The relation between ergodicity breaking and diverging sojourn times can be briefly explained by noting that one condition to obtain ergodicity is that the measurement time is long, compared with the characteristic time scale of the problem. However this condition is never satisfied if the microscopical time scale, i.e., the average trapping time, is infinite. It is important to note that the concept of trapping time probability density function (PDF) $\psi(t)$, with a diverging first moment, is widespread and found in many fields of physics [2,7–10]. It was introduced into physics by Scher and Montroll in the context of continuous-time random walk (CTRW) [11]. This well known model [8–10] exhibits anomalous subdiffusion $\langle x^2\rangle \propto t^\alpha$ with $\alpha < 1$, and aging behaviors [12] which are related to ergodicity breaking.

Clearly if the CTRW is nonergodic, Boltzmann-Gibbs statistics is not valid, in a way defined precisely later. The goal of this Letter is to obtain a generalization of Boltzmann-Gibbs statistical mechanics for CTRW models. In addition to its theoretical importance, this goal is timely due to recent observations on the single level of the CTRW type of dynamics [13,14], for example, anomalous diffusion of a single magnetic bead in a polymer network with a well defined temperature $T$ [14]. In single particle experiments, the many particle averaging, i.e., the problem of ensemble averaging, is removed [15]. Hence a fundamental question is whether time averages of single particle trajectories yield information identical to ensemble averages. The large number of applications of the CTRW model, e.g., in the context of chaos theory [10], and related models like the trap model and the comb model, make us believe that constructing a general nonergodic theory for such systems is worthy.

In this Letter we classify nonergodicity in terms of statistics of occupation times [16]. Consider a random walk process, with some dynamical rules, on a one dimensional lattice, with lattice points $x = -L, -L + 1, \ldots, 0, \ldots L$. The total time a particle occupies a lattice point $x$ is denoted with $t_x$ and is called the occupation time. The fraction of occupation time is $\bar{p}_x = t_x/t$ where $t$ is the measurement time. The investigation of nontrivial distributions of occupation times has a long history in the mathematics community (see [16] for references). More recently, it was a topic for physical interest, for example, the distribution of occupation times of random walks on random walks (the Sinai model) was considered in [17], and in the context of the persistence of the diffusion equation [18] (see also [16] and references therein). The questions addressed in this Letter are: what is the distribution of $\bar{p}_x$ for CTRW models? And how is this distribution related to the equilibrium of an ensemble of noninteracting random walkers, in particular, to Boltzmann-Gibbs statistics?

*Model 1.*—We consider a one dimensional unbiased CTRW on a lattice. Let $\psi(t)$ be the PDF of waiting times at the sites. The particle starts at site $x = 0$; it will wait there for a period $t_1$ determined from $\psi(t)$, then jump with a probability $1/2$ to the left, and with probability $1/2$ to the right. After the jump, say to lattice point 1, the particle will pause for a period $t_2$, whose statistical properties are determined by $\psi(t)$. It will then jump either back to point $x = 0$ or to $x = 2$. Then the process is renewed. Reflecting boundary conditions on $\pm L$ are used. We consider the generic case [8–10], where

$$\psi(t) \sim \frac{A t^{-(1+\alpha)}}{|\Gamma(-\alpha)|}, \tag{1}$$

when $t \to \infty$ and $0 < \alpha < 1$, $A > 0$. Specific values of $\alpha$ for a wide range of physical systems and models are given in [7–12,14]. In this case the average waiting time is infinite.

 

To obtain the distribution of fraction of occupation time we introduce a state function $\theta_x(t)$ which is equal to 1 when the particle is on $x$, otherwise it is zero. Thus $\theta_x(t)$ follows a two state process: jumping between the value 1 (called state $+$) and zero (state $-$) and vice versa. The PDF of times when the particle occupies state $+[-]$ is denoted with $\psi_+(t)[\psi_-(t)]$, respectively. In the CTRW model $\psi_+(t) = \psi(t)$. To obtain $\psi_-(t)$, note that after the particle leaves lattice point $x$ it is either on $x+1$ or on $x-1$. Let $t_{\rm R}(t_{\rm L})$ be the random time it takes the particle starting on $x+1(x-1)$ to return to $x$, and $f_{\rm R}(t_{\rm R})[f_{\rm L}(t_{\rm L})]$ the corresponding PDF of the first passage time, respectively. Then the PDF of times in state $-$ is $\psi_-(t) = [f_{\rm R}(t) + f_{\rm L}(t)]/2$. To find the first passage time PDFs $f_{\rm R}(t)$ and $f_{\rm L}(t)$ we used an important property of the CTRW [19]. Let $S_{\rm R}(N)$ be the probability of survival after $N$ steps, in the presence of an absorbing boundary on $x$, for a particle starting on $x+1$ and a reflecting boundary on $x = L$. Let $\tilde{S}_{\rm R}(z) = \sum_{N=0}^{\infty} z^N S_{\rm R}(N)$ be the moment generating function for the $R$ random walk. Then the Laplace transform of $f_{\rm R}(t)$ is [19]

$$\hat{f}_{\rm R}(u) = \frac{1-\hat{\psi}(u)}{u}\tilde{S}_{\rm R}[\hat{\psi}(u)] \tag{2}$$

where $\hat{\psi}(u)$ is the Laplace transform of $\psi(t)$. A similar equation holds for left random walks, which yields $\hat{f}_{\rm L}(u)$. To calculate $\tilde{S}_{\rm R}(z)$ we consider the discrete time random walk, namely, a binomial random walk, using a transfer matrix method (details left for future publication). We then use Eq. (2) and the Tauberian theorem to find the long time behavior of $f_{\rm R}(t)$ and $f_{\rm L}(t)$, which in turn yield

$$\psi_-(t) \sim \frac{A(2L-1)t^{-(1+\alpha)}}{|\Gamma(-\alpha)|}. \tag{3}$$

From Eqs. (1) and (3) we see that the function $\theta_x(t)$ follows a two state process, jumping between state $+$ and $-$, with power law waiting times in both states. We apply now a known limit theorem of Lamperti [20] and find that the PDF of the fraction of times $\bar{p}_x$ is

$$\lim_{t\to\infty} f(\bar{p}_x) = \delta_\alpha((2L-1)^{-1}, \bar{p}_x), \tag{4}$$

where $\delta_\alpha(\mathcal{R}_x, \bar{p}_x)$

$$\equiv \frac{\sin\pi\alpha}{\pi}\frac{\mathcal{R}_x\bar{p}_x^{\alpha-1}(1-\bar{p}_x)^{\alpha-1}}{\mathcal{R}_x{}^2(1-\bar{p}_x)^{2\alpha} + \bar{p}_x^{2\alpha} + 2\mathcal{R}_x(1-\bar{p}_x)^\alpha\bar{p}_x^\alpha\cos\pi\alpha}. \tag{5}$$

Equations (4) and (5) show that for unbiased CTRWs $\mathcal{R}_x$ equals $1/(2L-1)$ and is independent of the position of the observation point $x$, as expected from an unbiased random walk. For $\mathcal{R}_x = 1$ and $\alpha = 1/2$ Eq. (5) is the familiar arcsine PDF.

Now consider a large ensemble of noninteracting particles. The probability that a member of the ensemble will occupy lattice point $x$, for reflecting boundary conditions, in equilibrium is $P_x^{\rm eq} = 1/(2L)$. In an ergodic phase $P_x^{\rm eq} = \bar{p}_x$ in statistical sense, and in the limit of long measurement times. Indeed, as can be seen from Eq. (5) when $\alpha \to 1$ we have $f(\bar{p}_x) = \delta(\bar{p}_x - P_x^{\rm eq})$, namely $\delta_{\alpha=1}()$ is Dirac's delta function. Thus, when the average waiting time is finite we get an ergodic behavior.

On the other hand Eq. (4) shows that when $\alpha < 1$, we have a nontrivial distribution of $\bar{p}_x$ even in the long time limit. We notice that we can rewrite our solution in a more elegant form

$$\lim_{t\to\infty} f(\bar{p}_x) = \delta_\alpha\left(\frac{P_x^{\rm eq}}{1-P_x^{\rm eq}}, \bar{p}_x\right). \tag{6}$$

This equation will turn out to be rather general, and not limited to the unbiased CTRW model. The importance of the formula is that it relates the statistics of occupation times with the equilibrium $P_x^{\rm eq}$ of the system obtained from an ensemble of particles.

*Model 2.*—We now consider the biased CTRW. This well known model yields anomalous diffusion with a drift [8,9,11]. Now the probability of jumping left (right) is $0 < q < 1$ $(1-q)$, respectively. The special case $q = 1/2$ is the unbiased walk. Similar to the unbiased case, we calculate the first passage time problem using the waiting time PDF equation (1). We then prove that Eq. (6) is still valid; however, now

$$P_x^{\rm eq} = \frac{(\frac{1-q}{q})^x}{Z}, \tag{7}$$

and on the boundaries $P_L^{\rm eq} = (1-q)[(1-q)/q]^{L-1}/Z$ $P_{-L}^{\rm eq} = q[(1-q)/q]^{-L+1}/Z$, and $Z$ is the normalization obtained from $\sum_{x=-L}^{L} P_x^{\rm eq} = 1$.

The biased and unbiased CTRW are used to model a large number of physical processes. An important subclass of CTRWs are thermal CTRWs, used to model systems where the particle is in contact with a heat bath, e.g., [9,11,13,14,21]. For such cases, the equilibrium state for an ensemble of particles is Boltzmann's equilibrium. Then, the standard condition of detailed balance is imposed on the dynamics (see mathematical details below). In what follows we assume that Boltzmann statistics is valid for ensembles of particles.

The biased CTRW is used to model anomalous diffusion under the influence of a constant external driving force $\mathcal{F}$, e.g., [11]. The potential energy at each point $x$, excluding the reflecting boundaries due to the interaction with the external driving force is $V_x = -\mathcal{F}ax$ and $a$ is the lattice spacing. The well known condition of detailed balance then relates the probability of making a jump left to the temperature $T$:

$$q = \frac{1}{1+\exp(\frac{\mathcal{F}a}{T})}. \tag{8}$$

Using Eqs. (7) and (8) we can rewrite the PDF of occupation fraction in an elegant form

$$f(\bar{p}_x) = \delta_\alpha\left(\frac{P_x^B}{1-P_x^B}, \bar{p}_x\right), \tag{9}$$

where $P_x^B = \exp(-\mathcal{F}ax/T)/Z$, is the canonical Boltzmann probability. When the external force is zero we have $P_x^B = 1/Z$ and $Z = 2L$. Equation (9) is a generalization of Boltzmann-Gibbs ergodic theory, for systems satisfying a CTRW type of dynamics. For the case $\alpha = 1$ we recover the Boltzmann-Gibbs theory, since then $\bar{p}_x = P_x^B$.

*Model 3.*—We consider a CTRW in an external nonlinear potential field. We define a potential profile for the system $\{V_{-L}, V_{-L+1}, \ldots V_{x,} \ldots\}$. The main goal is to check if our main result, Eq. (6), is valid also for thermal random walks in more complicated energy profiles than the linear field. Then at each lattice point $x$ the particle has a probability of jumping to the left $Q_L(x)$ and a probability of jumping right $Q_R(x) = 1 - Q_L(x)$. These probabilities are related to the potential field according to the detailed balance condition

$$\frac{Q_L(x)}{1 - Q_L(x-1)} = \exp\left(-\frac{V_{x-1} - V_x}{T}\right), \qquad (10)$$

implying that the equilibrium of an ensemble of particles is the Boltzmann equilibrium. What is the distribution of the fraction of occupation time in this case? We claim that Eq. (6) is still valid however now

$$P_x^{\rm eq} = P_x^B = \frac{\exp(-\frac{V_x}{T})}{Z} \qquad (11)$$

is the Boltzmann equilibrium and $Z$ is the partition function. Thus, a general relation between the partition function of the problem, the basic tool of statistical physics, and the distribution of occupation times characterizing the ergodicity breaking is found. While we were able to prove this relation for the biased and unbiased random walk, for the more general case we use numerical simulations to check our theory.

We use the example of a random walk in a harmonic potential. The problem of anomalous diffusion in a harmonic field was considered in the context of fractional Fokker-Planck equations [21] and in single protein experiments [13]. As a by-product, our work shows that fractional Fokker-Planck equations [9] can be used to describe the density of many particles and not time average quantities, in this sense the fractional kinetic framework is very different than the standard Fokker-Planck equations.

The potential field we choose is $V_x = Kx^2$, with $K = 1$, and $T = 3$. Equation (10) and the symmetry condition $Q_L(0) = 1/2$ define the set of transition probabilities $\{Q_L(x)\}$ for the problem. In the simulations the particle starts at the origin, it waits there for a random time determined by the normalized waiting time PDF $\psi(t) = \alpha t^{-(1+\alpha)}$ for $t > 1$, it then jumps left or right according to the probability laws $Q_L(x)$, which in turn depends on the external potential field and temperature via the detailed balance condition. First in Fig. 1 we check that our simulations yield Boltzmann equilibrium in the harmonic field for an ensemble of particles. This means that we plot histograms of the position of many particles after a long simulation time.

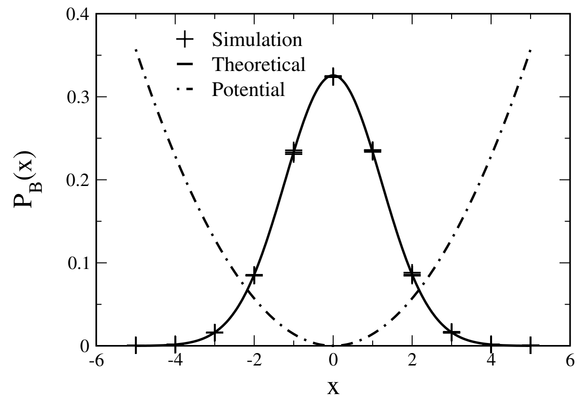


FIG. 1. Boltzmann's equilibrium for an ensemble of CTRW particles, in a harmonic potential field, and fixed temperature $T = 3$. In simulations (cross) we use $\alpha = 0.3$, 0.5, 0.8, the results being indistinguishable. The figure illustrates that for an ensemble of particles standard equilibrium is obtained. Ergodicity breaking is found only when long time averages of single particle trajectories are analyzed. The scaled potential (dot dash curve) is the harmonic potential field, and the solid curve is Boltzmann's equilibrium distribution.

To investigate nonergodicity we then consider one trajectory at a time. We obtain from the simulations, the total time $t_x$ spent by a particle on the lattice point $x = 0$, namely, at the minimum of the potential, and then construct histograms of the occupation fraction $\bar{p}_x = t_x/t$.

We consider the case $\alpha = 0.3$ in Fig. 2 and show an excellent agreement between our nonergodic theory Eqs. (9) and (11) and numerical simulations. The figure

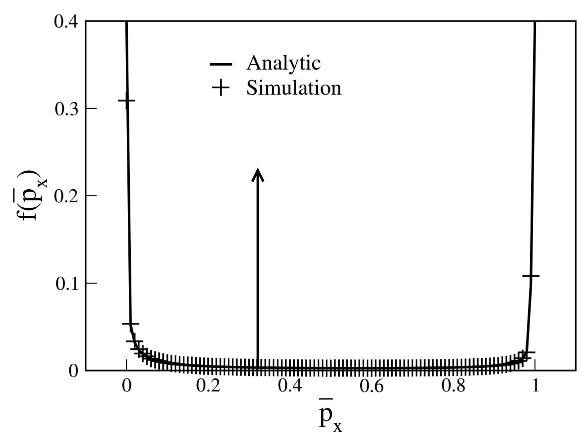


FIG. 2. The PDF of occupation fraction $\bar{p}_x = t_x/t$ where $t_x$ is the occupation time on lattice point $x = 0$. The random walk is in a harmonic potential field, the point $x = 0$ being the minimum of energy. For an ergodic process satisfying detailed balance, the PDF $f(\bar{p}_x)$ would be narrowly centered around the value predicted by Boltzmann which is given by the arrow. In a given numerical experiment, it is unlikely to obtain the value of $\bar{p}_x$ predicted using Boltzmann-Gibbs ergodic theory. The solid curve is the analytical formula Eq. (9) without fitting and with $\alpha = 0.3$ and $T = 3$.

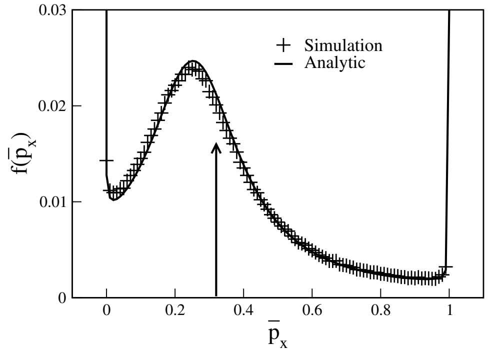


FIG. 3. Same as Fig. 2, however, now $\alpha = 0.8$. Instead of the $U$ shape found in Fig. 2 we find a distorted $W$ shape of the PDF. A peak close to Boltzmann's value for $\bar{p}_x$, i.e., the arrow on $P_x^B$, is an indication that as $\alpha$ is increased the ergodic phase is approached.

exhibits a $U$ shaped PDF. To understand this behavior, note that for $\alpha \ll 1$ we expect that the particle will get stuck on one lattice point during a very long period, which is of the order of the measurement time $t$. This trapping point can be either the point of observation (e.g., $x = 0$ in our simulations) or some other lattice point. In these cases we expect to find $\bar{p}_x \simeq 1$ or $\bar{p}_x \simeq 0$, respectively. Hence the PDF of $\bar{p}_x$ has a $U$ shape. This behavior exhibits large deviations from ergodic behavior, in the sense that we have a very small probability for finding the occupation fraction close to the value predicted by Boltzmann's ergodic theory (the arrow).

When we increase $\alpha$ we anticipate a "more ergodic" behavior, in particular, in the limit $\alpha \to 1$. An ergodic behavior means that the occupation fraction $\bar{p}_x$ is equal to Boltzmann's probability (i.e., the arrows in the figures). In Fig. 3 we set $\alpha = 0.8$ and observe a peak in the PDF of $\bar{p}_x$ centered in the vicinity of the ensemble average value. Note, however, that the PDF $f(\bar{p}_x)$ still attains its maximum on $\bar{p}_x = 0$ and $\bar{p}_x = 1$.

Why does the PDF of the occupation fraction Eq. (6) have such a general validity, at least within CTRW models? According to the limit theorem Eq. (5), the PDF of an occupation fraction depends on two parameters, $\alpha$ and $\mathcal{R}_x$. As mentioned, the nonuniversal exponent $\alpha$ is the anomalous diffusion exponent in the relation $\langle x^2 \rangle \propto t^\alpha$, obtained in previous works, for different types of models [8,9]. The parameter $\mathcal{R}_x$, seems difficult to obtain from microscopical models, and first principles. To solve this difficulty, we notice that using Eq. (5), we find the ensemble average

$$\langle \bar{p}_x \rangle = \int_0^1 \bar{p}_x \delta_\alpha(\mathcal{R}_x, \bar{p}_x) \mathrm{d}\bar{p}_x = \frac{\mathcal{R}_x}{1 + \mathcal{R}_x}. \qquad (12)$$

On the other hand, the ensemble average must be equal also to $\langle \bar{p}_x \rangle = P_x^{\mathrm{eq}}$. Hence, $\mathcal{R}_x = P_x^{\mathrm{eq}}/(1 - P_x^{\mathrm{eq}})$ as we indeed found in all the three CTRW models we investigated. In particular when detailed balance conditions hold $P_x^{\mathrm{eq}} = P_x^B$. This very general argument might mean that the nonergodic distribution of the occupation fraction, and its relation to Boltzmann-Gibbs statistical mechanics, is more general than the domain of CTRW type of models under investigation in this Letter.

To summarize, Eq. (6) yields the nonergodic statistical mechanical theory of the CTRW, both for thermal and nonthermal models. For thermal CTRWs, our theory gives the distribution of $\bar{p}_x$, while the ergodic Boltzmann-Gibbs theory states $\bar{p}_x = P_x^B$. The mathematical foundation of the theory is the limit theorem (5) related to the arcsine law. The physical input is the anomalous diffusion exponent $\alpha$. A connection between the nonergodic dynamics and the partition function was found, which enables us to find nontrivial ergodicity breaking properties of the underlying random walk, in particular, the random walk in a potential field.

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