Exact Results for the Nonergodicity of *d*-Dimensional Generalized Lévy Walks

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We provide analytical results for the ensemble-averaged and time-averaged squared displacement, and the randomness of the latter, in the full two-dimensional parameter space of the *d*-dimensional generalized Lévy walk introduced by Shlesinger *et al.* [Phys. Rev. Lett. **58**, 1100 (1987)]. In certain regions of the parameter plane, we obtain surprising results such as the divergence of the mean-squared displacements, the divergence of the ergodicity breaking parameter despite a finite mean-squared displacement, and subdiffusion which appears superdiffusive when one only considers time averages.

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In the last decades, Lévy walks [1] have turned out to be a ubiquitous model for the description of complex transport phenomena. Examples are chaotic diffusion generated by nonlinear intermittent iterated maps [2] or low-dimensional nonintegrable Hamiltonian systems [3], where the latter is related to transport of tracer particles in turbulent flows [4] and charged particle motion in magnetized plasmas [5], diffusion of cold atoms in optical lattices [6], photon counting statistics for blinking quantum dots [7], perturbation spreading and anomalous energy diffusion in systems of many interacting particles [8,9], search strategies of animals [10], travel behavior of humans [11], and target search of robots [12]. In addition, there exist various modifications of this basic model [13-17]. The main advantages of the Lévy walk model are that it is flexible enough to describe subdiffusion, normal diffusion, superdiffusion, ballistic transport, and even superballistic diffusion, and that the walker has a well-defined velocity at almost any instant of time [18-21]. As already stated by Shlesinger et al. [18,19], Lévy walks are more physical than the corresponding Lévy flights [22], which consist of sequences of wait and jump events. In the seminal paper of Shlesinger et al. [1], Lévy walks were introduced in a generalized way in which the flight velocities depend on the flight durations in a nonlinear, deterministic way. One motivation was to explain the Richardson law of turbulent dispersion [23,24], i.e., a cubic increase of the meansquared displacement (MSD). Besides its possible application to turbulent flows [1,25], it has been shown that, e.g., integrated Langevin dynamics can be mapped to this generalized Lévy walk model as it was done for the diffusion of cold atoms in optical lattices [26,27]. Furthermore, such nonlinear coupled Lévy walks describe fluid stretching in two-dimensional heterogeneous media [28,29]. In this Letter, we investigate the weakly nonergodic behavior of this generalized Lévy walk model. Weak nonergodicity [30] or also called weak ergodicity breaking in this context means that ensemble averages and time averages do not coincide although the underlying state or phase space is fully accessible [31]. Such a study is motivated by experimental techniques [32-35], where MSDs are either determined by ensemble averages, as in pulsed field gradient nuclear magnetic resonance (PFG-NMR) [36], or alternatively via time averages, as, e.g., in single particle tracking (SPT) experiments [37]. Weak ergodicity breaking has been found experimentally for blinking quantum dots [38], diffusion of lipid granules in living fission yeast cells [39], and diffusion of proteins on the plasma membrane of living cells [40,41]. Many theoretical models of anomalous diffusion have been studied with respect to their ergodic properties [42], among others, fractional Brownian motion [43], subdiffusive continuous time random walks [44,45], diffusion on fractal supports [46], integrated Brownian motion [47], geometric Brownian motion [48], heterogeneous diffusion processes [49], scaled Brownian motion [50], and globally correlated random walks [51]. The weak nonergodicity of Lévy walks, however, has only been investigated for the standard model with constant flight velocities [52-54]. In the following, we precisely define the generalized Lévy walk model and study its weakly nonergodic behavior with respect to the squared displacements. Specifically, we derive analytical results for the ensemble-averaged and time-averaged squared displacement and the randomness of the latter as characterized by the ergodicity breaking parameter. Our calculations are in perfect agreement with numerical simulations, which we cannot show here due to the lack of space. Our findings reveal surprising results, which have not been observed for other models of anomalous diffusion.

The *d*-dimensional generalized Lévy walk [1] consists of a sequence of random flights. The durations T_i of the flights are independent from each other and drawn from a heavy-tailed probability density function $\psi(t) =$ $\gamma/t_0(1 + t/t_0)^{-\gamma-1}, \gamma > 0, t_0 > 0$. The absolute values $|\mathbf{V}_i|$ of the velocities of the flights are constant during one single flight and depend on the flight durations in a nonlinear,

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FIG. 1. Phase diagram for the ensemble-averaged squared displacement (a), the ensemble average of the time-averaged squared displacement (b), and the ergodicity breaking parameter (c). Different ranges of validity of the analytical results are separated by thick black lines in the two-dimensional parameter space. Different kinds of diffusion are color-coded as indicated in the key. The dotted lines in (c) serve as a guide to the eye for a better comparison with the phase diagram in (b).

deterministic way, $|\mathbf{V}_i| = cT_i^{\nu-1}, \nu > 0$, where the directions of the flights are isotropically chosen at random. This model, therefore, is characterized by the two parameters γ and ν . Several equivalent formulations of the model exist. Denoting by $|\mathbf{X}_i|$ the distance travelled during one elementary flight event, one has three defining quantities $|\mathbf{X}_i|$, $|\mathbf{V}_i|$, and T_i . Providing two of them determines the third one, and, therefore, the compound probability of any pair defines the model. In addition, for each pair, one can choose which quantity is given statistically with the other one following deterministically. In Ref. [1], the statistics of the distances $|\mathbf{X}_i|$ was prescribed by $p(\mathbf{x}) \sim$ $|\mathbf{x}|^{-\gamma/\nu-1}(|\mathbf{x}| \to \infty)$, and the velocity was assigned deterministically by $|\mathbf{V}_i| \propto |\mathbf{X}_i|^{1-1/\nu}$. For further details of the generalized Lévy walk including some visualization and its relation to other space-time coupled models see Ref. [55]. For our analytical treatment, we prescribe the durations T_i statistically by $\psi(t)$ with the distances $|\mathbf{X}_i|$ following deterministically; i.e., we consider the distribution $\psi(\mathbf{x}, t)$, where $\psi(\mathbf{x}, t)d^d\mathbf{x}dt$ is the probability that a single flight has duration $T_i \in [t, t + dt]$, and the distance travelled with such a flight lies in an infinitesimal volume around **x**,

$$\psi(\mathbf{x},t) = \frac{1}{S_d(|\mathbf{x}|)} \delta(|\mathbf{x}| - ct^{\nu}) \psi(t), \qquad (1)$$

where $S_d(|\mathbf{x}|) = \{[2\pi^{d/2}]/\Gamma(d/2)\}|\mathbf{x}|^{d-1}$ denotes the surface of the sphere with radius $|\mathbf{x}|$ in *d* Euclidean dimensions, d = 1, 2, ... One also needs the probability $W(\mathbf{x}, t)d^d\mathbf{x}$ of travelling a distance inside an infinitesimal volume around \mathbf{x} in time *t* with a single flight which is longer than *t*, which is determined by

$$W(\mathbf{x},t) = \frac{1}{S_d(|\mathbf{x}|)} \int_t^\infty \delta(|\mathbf{x}| - ct'^{\nu-1}t)\psi(t')dt'$$
$$= \int_1^\infty \lambda^d t \psi(\lambda \mathbf{x}, \lambda t) d\lambda.$$
(2)

 $W(\mathbf{x}, t)$ behaves with respect to the first argument like a probability density and with respect to the second argument like a cumulative distribution. Hence, $\lim_{t\to 0} \int W(\mathbf{x}, t) d^d \mathbf{x} = 1$. We note that the term $\lambda^d t$ of Eq. (2) is missing in the corresponding expression in Ref. [1] although we consider the same model. Therefore, our analytical results for the ensemble-averaged squared displacement deviate from the formulas in Ref. [1] but are in perfect agreement with numerical simulations [57]. The propagator, the conditional probability density $p(\mathbf{x}, t)$ of finding a Lévy walker at position \mathbf{x} at time t under the initial condition $p(\mathbf{x}, t = 0) = \delta(\mathbf{x})$, can be written in Fourier (**k**) and Laplace (*s*) space as [58]

$$p(\mathbf{k},s) = \frac{W(\mathbf{k},s)}{1 - \psi(\mathbf{k},s)}.$$
(3)

From the propagator, one can easily calculate the ensembleaveraged squared displacement (EASD)

$$\begin{split} \langle \Delta \mathbf{x}^{2}(\tau) \rangle_{E} &= \langle [\mathbf{x}(\tau) - \mathbf{x}(0)]^{2} \rangle_{E} = \int_{\mathbb{R}^{d}} \mathbf{x}^{2} p(\mathbf{x}, \tau) d^{d} \mathbf{x} \\ &= \mathcal{L}^{-1} \left\{ -\frac{\partial^{2}}{\partial \mathbf{k}^{2}} p(\mathbf{k}, s) \big|_{\mathbf{k}=\mathbf{0}}; s, \tau \right\}, \end{split}$$
(4)

where \mathcal{L}^{-1} denotes the inverse Laplace transform. In Eq. (4) and in the following, we use the symbols $\langle \cdots \rangle_E$ and $\langle \cdots \rangle_T$ for ensemble and time averages, respectively. One can calculate the asymptotic behavior of $\psi(\mathbf{k}, s)$ and $W(\mathbf{k}, s)$ for $(\mathbf{k}, s) \rightarrow (\mathbf{0}, 0)$, and by inserting the results in Eq. (4), one obtains the long-time behavior $(\tau \rightarrow \infty)$ of the EASD. Our analytical results are illustrated in Fig. 1(a) in the form of a phase diagram. In this Letter, we will concentrate on three unexpected or hitherto unknown phenomena occurring in certain parameter regions. These are (i) the nonexistence of MSDs, (ii) subdiffusion appearing as superdiffusion, and (iii) infinitely strong ergodicity breaking.

(*i*) Nonexistence of the MSD.—Our exact calculations show that in the parameter region $2\nu \ge \gamma + 2$ both, the EASD and the (ensemble averaged) time-averaged squared displacement (TASD), do not exist because they diverge. This area includes the parameter pair $\gamma = 1/2$, $\nu = 3/2$ [black dot in Figs. 1(a) and 1(b)], where according to Ref. [1], a τ^3 increase of the EASD should be found. That this is not the case can be understood from the following argument. The exact EASD is obviously larger than the contribution coming from all trajectories whose duration T_1 of the first flight event is longer than τ , i.e.,

$$\begin{split} \langle \Delta \mathbf{x}^2(\tau) \rangle_E &> \int_{\tau}^{\infty} [v(t_1)\tau]^2 \psi(t_1) dt_1 \\ &\sim \int_{\tau}^{\infty} t_1^{2\nu-\gamma-3} dt_1 = \infty \quad \text{if } 2\nu \ge \gamma+2, \quad (5) \end{split}$$

where we used that for such trajectories the squared displacement after time lag τ is given by $[v(t_1)\tau]^2$ [55]. As a consequence of the divergence of the EASD, the diffusion exponents, i.e., the exponents of the asymptotic increase of the EASD, that can be achieved with this model are strictly smaller than three. Therefore, a cubic increase of the EASD cannot be found in this model. Note, however,

that for instance for the parameter pair $\gamma = 1/2$ and $\nu = 3/2$, the distribution $p_3(D,\tau)$ of the quantity $D_3(\tau) =$ $\Delta \mathbf{x}^2(\tau)/\tau^3$, which we called the distribution of generalized diffusivities in Ref. [59], converges to a limit distribution $p^*(D) \sim D^{-1.5}(D \to \infty)$ with long tails such that its mean value, i.e., the prefactor of the asymptotic increase of the EASD, is infinite [55]. If one determines the EASD for this case numerically from several different finite ensembles, one obtains power laws with random exponents. The divergence of the EASD at the line $2\nu = \gamma + 2$ can most intuitively be attributed to a diverging velocity variance $\langle v^2 \rangle$ of the elementary flight events, which is obtained from Eq. (5) in the limit $\tau \to 0$ by changing variables from t to v. Below the line $2\nu = \gamma + 2$, where the EASD is finite, the same phase diagram is found for the corresponding spacetime coupled Lévy flight [60-63] because there, the character of the diffusion process is only determined by the statistics of the sequences of the endpoints of the elementary events, which are identical for both models, Eq. (1). In contrast, the divergence of the EASD is caused by the continuous connection of the endpoints, Eq. (5), and, therefore, cannot be found for Lévy flights, where the endpoints are connected by one wait and jump event [55].

(ii) Subdiffusion appearing as superdiffusion.—In the triangular region $\gamma < 1$, $\gamma < 2\nu < 1$, where the EASD shows a subdiffusive behavior, the TASD reveals a superdiffusive behavior. To see this, one has to take a closer look at the TASD defined as

$$\langle \Delta \mathbf{x}^2(\tau) \rangle_T = \frac{1}{T - \tau} \int_0^{T - \tau} [\mathbf{x}(t + \tau) - \mathbf{x}(t)]^2 dt.$$
 (6)

For every finite T, this quantity is a random variable. In order to quantify this random variable, we first consider the ensemble average $\langle \langle \Delta \mathbf{x}^2(\tau) \rangle_T \rangle_E$ of the TASD (EATASD). Our starting point for the analytical derivation is the formula [52,64,65], $\langle \Delta \mathbf{x}^2(\tau) \rangle_T =$ Green-Kubo $2\int_0^{\tau} (\tau - t)C_v(t)dt$, where $C_v(t)$ is the autocorrelation function of the velocity process defined as time average, $C_v(t) = 1/(T-t) \int_0^{T-t} v(t') v(t'+t) dt'$. By taking the ensemble average of the Green-Kubo formula, one realizes that the EATASD is essentially determined by the correlation function $\langle \mathbf{v}(t')\mathbf{v}(t'+t)\rangle_E$, which can be calculated by using methods introduced by Godrèche and Luck [66], which were also applied, e.g., in Refs. [54,67]. Eventually, this knowledge allows us to calculate the asymptotic time dependence of the EATASD. More details of the derivation will be published elsewhere [57]. Our analytical results are again illustrated in the form of a phase diagram [see Fig. 1(b)]. Interestingly, these results significantly deviate from the behavior of the EATASD for the space-time coupled Lévy flight, where a linear time dependence was found in the whole parameter plane [62,63]. The reason for this difference is the continuous connection of the sequence of endpoints of the elementary events in the

generalized Lévy walk. The different colors in Figs. 1(a) and 1(b) indicate that the generalized Lévy walk is in general weakly nonergodic. For $\gamma \leq 1$, the mean flight duration, i.e., the typical time scale of the process, is infinite, and, therefore, the measurement time can never be larger than the typical time scale and so weak nonergodicity occurs. As already mentioned, especially in the triangular region $\gamma < 1$, $\gamma < 2\nu < 1$, the EASD shows subdiffusion, but the EATASD indicates superdiffusion. This means, in a NMR experiment, one would measure subdiffusion, but in a SPT experiment, one would measure superdiffusion for the same system. To our knowledge, such a seemingly contradictory behavior has not been recognized before in any model of anomalous diffusion. Details of this phenomenon and its occurrence in other models will be published elsewhere [55,57]. For $\gamma > 1$ and $2\nu < \gamma$, however, the EASD and the EATASD coincide (including the prefactor, i.e., the diffusion coefficient) as expected from normal diffusion. Also for $\gamma > 1$ and $\gamma < 2\nu < \gamma + 1$, the EASD and the EATASD coincide with respect to the diffusion exponent but not with respect to the diffusion coefficient. The reason is that the squared displacements $[\mathbf{x}(t+\tau) - \mathbf{x}(t)]^2$ are nonstationary, but they become stationary for $t \to \infty$. This means that if one determines the EASD after a large enough aging time, i.e., the elapsed time between the beginning of the process and the beginning of the measurement, the EASD and the EATASD coincide. This phenomenon has also been recognized in Refs. [52,68] for the special case $\nu = 1$, i.e., the standard Lévy walk with a constant flight velocity, and was called ultraweak ergodicity breaking. For $\gamma + 1 < 2\nu < \gamma + 2$, we find ballistic diffusion, i.e., a quadratic increase of the EATASD. Interestingly, the transition to the ballistic behavior is connected with the divergence of the second moment of the stationary velocity distribution $p^*(v) =$ $\lim_{t\to\infty} p(v,t)$, where p(v,t) is the probability density of finding a Lévy walker with absolute value v of velocity v at time t. This means $\langle v^2 \rangle = \int v^2 p^*(v) dv = \infty$ if $2\nu \ge \gamma + 1$. For $2\nu > \gamma + 2$, the EATASD diverges. Again, this can easily be explained by only considering the contributions to the EATASD coming from all trajectories whose duration T_1 of the first flight is longer than T. A simple calculation analogous to Eq. (5) shows the divergence.

(iii) Infinitely strong ergodicity breaking.—For the region $2\nu > (\gamma/2) + 2$, the ergodicity breaking becomes infinitely strong in the sense that the square of the relative fluctuation of the TASD captured by the ergodicity breaking (EB) parameter diverges. The EB parameter is defined as variance of the rescaled random variable $\hat{\xi}(\tau) = \langle \Delta \mathbf{x}^2(\tau) \rangle_T / \langle \langle \Delta \mathbf{x}^2(\tau) \rangle_T \rangle_E$ [45], i.e.,

$$\operatorname{EB}(\tau) = \operatorname{Var}(\hat{\xi}(\tau)) = \langle \hat{\xi}^2(\tau) \rangle_E - \langle \hat{\xi}(\tau) \rangle_E^2, \qquad (7)$$

with $\langle \hat{\xi}(\tau) \rangle_E = 1$ due to normalization. The randomness of the TASD is fully captured by the distribution of $\hat{\xi}(\tau)$,

 $p(\xi, \tau) = \langle \delta[\xi - \hat{\xi}(\tau)] \rangle_E$. For an ergodic process, the EB parameter goes to zero if the measurement time T goes to infinity, and the distribution $p(\xi, \tau)$ becomes a delta distribution, $\lim_{T\to\infty} p(\xi,\tau) = \delta(\xi-1)$. For the analytical treatment, we use the method introduced in Ref. [47]. There it was shown by using the Green-Kubo formula that the random variable $\hat{\xi}(\tau)$ is equal in distribution to the random variable $\xi^* = \int_0^T v^2(t) dt / \langle \int_0^T v^2(t) dt \rangle_E$ if $\hat{\xi}(\tau)$ does not depend on τ due to the normalization. In full generality, this equality in distribution holds in the limit for small τ . Therefore, the calculation of the EB parameter essentially reduces to the calculation of $\chi(T) := \langle [\int_0^T v^2(t) dt]^2 \rangle_E$, which is much simpler than the original problem because the velocity process v(t) is piecewise constant. $\chi(T)$ can be calculated by using the methods of Godrèche and Luck [66]. Our analytical results are again illustrated in the form of a phase diagram in Fig. 1(c). For $\gamma < 1$, the EB parameter does not depend on τ , but for $\gamma > 1$, the EB parameter depends on τ , and, therefore, there our analytical results are only valid in the limit $\tau \rightarrow 0$. For the latter region of the parameter plane, where the typical time scale of the process is finite, we observe two essential transitions for the EB parameter. The first one is the transition from a vanishing EB parameter (sector D in Fig. 1(c), where the distribution $p(\xi, \tau)$ is given by the delta distribution what is in agreement with the findings for the special case $\nu = 1$ in [52–54]) to a finite EB parameter (sector $B_{\gamma,\nu}$ and $C_{\gamma,\nu}$, where EB is given by a complicated T dependent expression, which increases with increasing T). This transition can be understood by a violation of the Khinchin theorem [69-72], which states that the EB parameter only asymptotically goes to zero if the correlation function of the quantity to be averaged, in our case the squared displacements, asymptotically goes to zero,

$$\operatorname{Cov}(\Delta \mathbf{x}^{2}(t',\tau),\Delta \mathbf{x}^{2}(t'+t,\tau)) \stackrel{t\to\infty}{\to} 0,$$
(8)

where Cov denotes the covariance function, and we used the abbreviation $\Delta \mathbf{x}^2(t', \tau) = [\mathbf{x}(t' + \tau) - \mathbf{x}(t')]^2$. A simple estimation for the covariance function and the resulting transition of the EB parameter will be presented elsewhere [57]. For $2\nu \ge (\gamma/2) + 2$, the second transition occurs, the EB parameter diverges. Similar to the divergence of the MSDs, also this divergence can easily be understood. The EB parameter is essentially determined by the expectation value $\langle [\langle \Delta \mathbf{x}^2(\tau) \rangle_T]^2 \rangle_E$. We underestimate this quantity by only considering contributions from trajectories whose duration T_1 of the first flight is longer than T. A similar calculation as the one in Eq. (5) gives the above mentioned condition for the divergence of the EB parameter. For $\nu > 1$, the corresponding distribution $p(\xi, \tau)$ is heavy tailed, $p(\xi,\tau) \sim \xi^{-1-\gamma/(2\nu-2)}(\xi \to \infty)$. This also explains the divergence of the EB parameter because the second moment of $p(\xi, \tau)$ diverges for $2\nu \ge (\gamma/2) + 2$. In sector M_{γ}, the EB parameter is given by the variance of the Mittag-Leffler distribution. Furthermore, it is actually numerically confirmed that the distribution $p(\xi, \tau)$ in sector M_{γ} coincides with the Mittag-Leffler distribution. The formula for the EB parameter in sector $A_{\gamma,\nu}$ is very complicated but only depends on γ and ν . Interestingly, for $\nu \rightarrow 1$, the EB parameter goes to zero.

In conclusion, we have seen that the generalized Lévy walk model exhibits surprising phenomena. Ironically, although the Lévy walk was constructed in order to avoid the divergence of the MSD of classical Lévy flights, the MSDs of the generalized Lévy walk diverge for $2\nu > \gamma + 2$. For $\gamma < 1$ and $\gamma < 2\nu < 1$, the EASD shows subdiffusion whereas the TASD indicates superdiffusion. Furthermore, the EB parameter can diverge although the MSDs are finite. Interestingly, Fig. 1 shows that for $\gamma > 3$ and $\gamma > 4$, the EB parameter can become finite or even infinite, respectively, for parameters where the MSDs show normal but non-Gaussian diffusion. The knowledge of these possible scenarios of weak nonergodicity is crucial for the interpretation of single-particle tracking experiments. Note that even if one smooths the discontinuities in the velocity process, all the observed phenomena remain valid.

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