Space-Time Velocity Correlation Function for Random Walks

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Space-time correlation functions constitute a useful instrument from the research toolkit of continuous-media and many-body physics. Here we adopt this concept for single-particle random walks and demonstrate that the corresponding space-time velocity autocorrelation functions reveal correlations which extend in time much longer than estimated with the commonly employed temporal correlation functions. A generic feature of considered random-walk processes is an effect of velocity echo identified by the existence of time-dependent regions where most of the walkers are moving in the direction opposite to their initial motion. We discuss the relevance of the space-time velocity correlation functions for the experimental studies of cold atom dynamics in an optical potential and charge transport on micro- and nanoscales.

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Introduction.—Finiteness of velocity is a fundamental property of any physical process taking place in space and time. This concept was incorporated in the framework of random-walk theory [1], a formalism that is particularly successful in describing diffusion phenomena [2]. If the speed of a walking particle is constant, the coupling between the distance traveled and the time it takes leads to the confinement of the spreading process to a casual cone. Within the cone the density of particles is described by the phenomenological diffusion equation [3]. The space-time coupling also regularizes fast superdiffusion by removing possibly unphysical divergences from the momenta of the corresponding processes [4,5].

The velocity of a random-walk process can be treated as an additional dynamical variable whose evolution is itself a random process. The Green-Kubo relation [6] highlights the importance of the corresponding temporal autocorrelation function by connecting its integral to the diffusion constant [7]. It is evident, however, that the velocity autocorrelations of a random walk cannot last longer than the time between two consecutive reorientation events.

Following this premise, we next ask whether more extended correlations can be detected by unfolding the velocity correlation function into the *spatial* domain. Here, we answer this question positively by introducing a characteristic that reveals hitherto unnoticed properties of random-walk processes. We define the space-time (s-t) velocity autocorrelation function for single-particle random walks by adopting a concept widely used in fluid dynamics [8], gas, and plasma kinetics [9]. For models yielding normal and superdiffusive dynamics, we show that this function helps to uncover long-lived correlations that extend beyond the horizon dictated by the standard temporal correlation function. Furthermore, the unfolding into the spatial domain allows for a meaningful description of velocity correlations when the temporal correlation function simply does not exist. We argue that the process-specific generalized correlation function can be accessed experimentally. Thus it can serve as a tool to determine stochastic processes underlying macroscopic diffusion phenomena observed in experiments.

Continuous-time random walks and s-t velocity autocorrelation function.—We consider single-particle processes that belong to a class of continuous-time random walks (CTRWs) [2]. In its simplest one-dimensional realization, such a walk is performed by a particle moving ballistically with a fixed velocity v_i between two turning events. The duration of the ith "flight," that is the time interval between two consecutive turnings, $\tau_i = t_{i+1} - t_i$, is governed by a probability density function (PDF) $\psi(\tau)$. At the end of each flight the particle changes its velocity to a new random value v_{i+1}, sampled from the PDF $h(v)$, and then starts a new flight. Two random variables, τ_i and v_i, are statistically independent, but the spatial and temporal evolution of the walker during the flight is coupled, $x_{i+1} - x_i = v_i \tau_i$. This general setup is able to reproduce normal and anomalous diffusion regimes [10,11], and there is a multitude of real-life systems and processes whose dynamics can be described by this model [12–16].

The key property of the described CTRW model is a well-defined velocity of a walker at any instant of time. It allows us to introduce a space-time velocity autocorrelation function for a single-particle process by redefining the conventional expression [8,9]

$$\mathcal{C}_{vv}(x,t) = \langle v(0,0)v(x,t)\rangle. \tag{1}$$

That is, we assume that the particle starts its walk with initial velocity $v(x=0,t=0) = v_0$. After a time t the particle is found at the point x with some velocity $v(x,t)$. To estimate $\mathcal{C}_{vv}(x,t)$, an observer at time t averages the product of the actual and the initial velocities of all particles that are located within a bin $[x, x + dx]$. The so-measured quantity can be formalized as

$$\mathcal{C}_{vv}(x, t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} v v_0 \frac{P(v, x, v_0, t)}{P(x, t)} dv_0 dv, \quad (2)$$

where $P(v, x, v_0, t)$ is the joint PDF for a particle to start with velocity v_0 and to be in the point x at time t with velocity v [17]. Since the particle has first to arrive to the point x for the measurement to occur, we use the formula for the conditional probability and divide the joint density by the spatial PDF $P(x, t)$. The latter is a well-studied characteristic of the CTRW processes [2]. In contrast, a challenging quantity to tackle is the joint probability of particles' positions and velocities. To focus on its role, we introduce the spatial density of the velocity correlation function,

$$C(x, t) = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} v v_0 P(v, x, t|v_0) h(v_0) dv_0 dv. \quad (3)$$

Here we split the joint PDF, $P(v, x, v_0, t) = P(x, v, t|v_0)h(v_0)$, in order to factorize the averaging with respect to initial velocities [18]. There are two noteworthy features of this new quantity. First, after the integration over x, Eq. (3) yields the standard temporal velocity autocorrelation function $C(t) = \langle v(0)v(t)\rangle$. Second, to return to the original s-t velocity autocorrelation function, Eq. (1), $C(x, t)$ has to be normalized with the spatial density $P(x, t)$,

$$\mathcal{C}_{vv}(x, t) = C(x, t)/P(x, t). \quad (4)$$

Therefore, our further analysis is restricted to the function $C(x, t)$, while the obtained results can be immediately mapped onto $\mathcal{C}_{vv}(x, t)$ by virtue of Eq. (4).

We are now set to derive an equation for $P(v, x, t|v_0)$. We first introduce the frequency of velocity changes, $\nu_{v_0}(x, t)$, with $\nu_{v_0}(x, t)dxdt$ counting the number of particles whose flights ended in the interval $[x, x + dx]$ during the time interval $[t, t + dt]$. The additional subscript v_0 tracks the history of particles and denotes only those which had velocity v_0 at $t = 0$. The balance equation for ν_{v_0} assumes the form of an integral equation, reading

$$\nu_{v_0}(x, t) = \int_{-\infty}^{+\infty} dv \int_0^t \nu_{v_0}(x - v\tau, t - \tau)h(v)\psi(\tau)d\tau + \psi(t)\delta(x - v_0 t). \quad (5)$$

A particle changes its velocity at the end of the flight of duration τ that was initiated at the point $x - v\tau$. Multiplication by $\psi(\tau)d\tau$ and $h(v)dv$ yields the probability of having a flight time τ and velocity v. We also assume that all particles start their random walks at $t = 0$ and $x = 0$. The last term on the right-hand side accounts for the particles that finish their very first flight at the given instant of time t. Correspondingly, $P(v, x, t|v_0)$ is

$$P(v, x, t|v_0) = \int_0^t \nu_{v_0}(x - v\tau, t - \tau)h(v)\Psi(\tau)d\tau + \Psi(t)\delta(x - v_0 t)\delta(v - v_0). \quad (6)$$

A particle has a velocity v at point (x, t) if it has previously changed its velocity at time $t - \tau$ and still is in the process of flight with velocity v. The probability to stay in the flight until time t is given by $\Psi(t) = 1 - \int_0^t \psi(\tau)d\tau$. The second term on the right-hand side of Eq. (6) accounts for the particles that are still in their first flight. The above two equations can be resolved by using a combined Fourier-Laplace transform with respect to x and t which turns convolution-type integrals into algebraic products. We use $\mathcal{L}[\cdots]$ and a hat to denote the Laplace and Fourier transforms, and a tilde for a combination of the two, whereas k and s denote coordinates in the Fourier and Laplace spaces. We find $\tilde{P}(v, v_0, k, s)$, and by using Eq. (3), obtain the general expression for the velocity correlation density in the Fourier-Laplace space,

$$\tilde{C}(k, s) = \frac{\mathcal{L}[\int_{-\infty}^{\infty}\Psi(\tau)e^{-ikv\tau}vh(v)dv]\mathcal{L}[\int_{-\infty}^{\infty}\psi(\tau)e^{-ikv_0\tau}v_0h(v_0)dv_0]}{1 - \mathcal{L}[\hat{h}(k\tau)\psi(\tau)]} + \mathcal{L}\left[\int_{-\infty}^{\infty}\Psi(t)e^{-ikv_0\tau}v_0^2h(v_0)dv_0\right]. \quad (7)$$

Equation (7) constitutes the central result of this Letter. When integrating this function over x, the first term, describing the contribution from the particles that have changed their velocities several times, vanishes. It is only the particles remaining in their first flight that contribute to $C(t)$. This implies that $C(t) = \langle v^2\rangle\Psi(t)$. Below we consider several regimes of diffusion which are possible in the current random-walk model, ranging from the standard diffusion to ballistic superdiffusion.

Lévy walks: From normal to ballistic superdiffusion.—The Lévy-walk process [2] is a particular case with a bimodal choice of the velocity PDF, $h(v) = [\delta(v - u_0) + \delta(v + u_0)]/2$, and the PDF of flight time

$$\psi(\tau) = \frac{\gamma}{\tau_0}\frac{1}{(1 + \tau/\tau_0)^{1+\gamma}}, \quad (8)$$

where τ_0 sets the time scale of the process. The positive scaling exponent $\gamma > 0$ plays a key role in defining the type of the diffusion. If $\gamma > 2$, then the mean square of the flight time is finite and the process reproduces normal, Brownian-like diffusion, with the linear scaling of the mean squared displacement, $\langle x^2(t)\rangle \propto t$ [2]. The mean squared flight time diverges for $1 < \gamma < 2$, which leads to anomalously fast spreading, $\langle x^2(t)\rangle \propto t^{3-\gamma}$ [4,19]. In the extreme case of $0 < \gamma < 1$, the first moment of the flight time diverges. The anomaly is strong and dominates evolution leading to the ballistic scaling of the mean squared displacement, $\langle x^2(t)\rangle \propto t^2$. In all cases, however, the density of particles $P(x, t)$ is confined to the ballistic cone, $x \in [-u_0 t, u_0 t]$.

When $\gamma > 2$, inside of the casual cone and in the asymptotic limit, the density of particles obeys the standard diffusion equation [3],

$$\frac{\partial P(x,t)}{\partial t} = D\Delta P(x,t); \qquad D = \frac{u_0^2\tau_0}{\gamma - 2}. \tag{9}$$

In this case, the first term of Eq. (7) in normal coordinates reduces to a simple result,

$$C_{\mathrm{centr}}(x,t) = \frac{u_0^2 D\tau_0}{\gamma - 1}\Delta P(x,t) = \frac{u_0^2\tau_0}{\gamma - 1}\frac{\partial P(x,t)}{\partial t}. \tag{10}$$

It reveals an interesting relation between the PDF of the process and the corresponding correlation density function, namely, that $C(x, t)$ is proportional to $\partial P(x, t)/\partial t$ and, according to Eq. (4), the normalized s-t correlation function $\mathcal{C}_{vv}(x, t) \propto \partial \ln P(x, t)/\partial t$. Note that the contribution of the second term in Eq. (7) corresponds to the ballistic delta peaks, running with the speed u_0 and decaying in time according to $\Psi(t)$. Ballistic peaks are the hallmark of Lévy walks [20]. Their contribution is typically considered to be asymptotically vanishing in the regime of standard diffusion. However, only these peaks contribute to the temporal correlation function $C(t)$ and therefore cannot be neglected. By taking into account that the number of particles in the peaks also decays as $\Psi(t)$, it immediately follows from Eq. (4) that the normalized s-t correlation function, Eq. (1), remains constant at the ballistic fronts, $\mathcal{C}_{vv}(x = \pm u_0 t, t) = u_0^2$.

The results presented by Eqs. (9) and (10) are valid for an arbitrary choice of $\psi(t)$ that has finite second moment, $\int_0^\infty \tau^2\psi(\tau)d\tau < \infty$, including the case of the exponential PDF $\psi(\tau) = e^{-\tau/\tau_0}/\tau_0$. In this case, $C(t) = u_0^2 e^{-t/\tau_0}$, while $C(x, t)$, for example, at $x = 0$, scales like $t^{-3/2}$. This example highlights the fact that the s-t velocity correlation functions provide access to long-lived correlations and therefore increase the chance of their detection.

For $1 < \gamma < 2$, the mean squared flight time diverges. It induces a superdiffusive behavior with the density of particles obeying a generalized diffusion equation [21],

$$\frac{\partial P(x,t)}{\partial t} = -K(-\Delta)^{\gamma/2}P(x,t), \tag{11}$$

where $K = \tau_0^{\gamma-1}u_0^{\gamma}(\gamma - 1)\mathbf{\Gamma}[1-\gamma]\cos(\pi\gamma/2)$ and $\Delta^{\gamma/2}$ is the fractional Laplacian operator [22]. Note that this description is valid in the inner part of the casual cone only. In there, $C(x, t)$ is proportional to the fractional Laplacian of the density of particles,

$$C_{\mathrm{centr}}(x,t) = -\frac{u_0^2 K\tau_0}{\gamma - 1}(-\Delta)^{\gamma/2}P(x,t) = \frac{u_0^2\tau_0}{\gamma - 1}\frac{\partial P(x,t)}{\partial t}, \tag{12}$$

or, by virtue of Eq. (11), to the time derivative of this density. Therefore, the velocity autocorrelations are negative near the point $x = 0$; see Fig. 1. Upon the departure from the origin, the correlation density becomes positive and produces two local maxima.

By setting $\gamma < 1$ in Eq. (8), one can enhance the anomalous character of the process. The average flight time diverges and this implies a ballistic scaling for the density of particles. Again, $C(x, t)$ can be evaluated in the Fourier-Laplace space. As an illustration, we consider the case $\gamma = 1/2$ where both quantities, $P(x, t)$ and $C(x, t)$, can be expressed in terms of analytic functions [10,11]. The density exhibits a U-shaped profile, diverging at the ballistic fronts: $P(x, t) = \theta(u_0 t - |x|)/[\pi(t^2u_0^2 - x^2)^{1/2}]$. The correlation density function behaves similarly,

$$C(x,t) = u_0^2\tau_0^{1/2}\left[\frac{\delta(x-u_0t)}{t^{1/2}} + \frac{\delta(x+u_0t)}{t^{1/2}} - \frac{\theta(u_0t-|x|)}{2t^{3/2}u_0}\right]. \tag{13}$$

From this result it follows that velocity correlations are negative and nearly constant inside the ballistic cone. The relative decay rate $P(x, t)/C(x, t)$ is of the order $t^{1/2}$ now. The profiles evaluated via direct numerical simulations of the random walk, cf. Fig. 2(a), perfectly match the analytical prediction.

Velocity-induced superdiffusion.—Regimes of diffusion described by the Lévy-walk model are bound by the ballistic propagation so that no particles can cross the front $|x| = u_0 t$. One possible way to overcome this limitation is

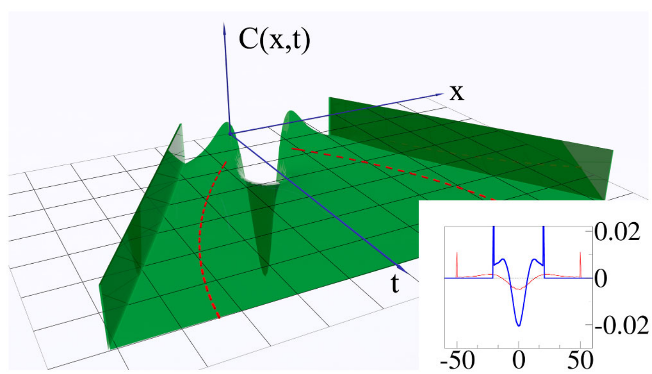

FIG. 1 (color online). Density of the space-time velocity correlation function for the superdiffusive Lévy walk, Eq. (12), with $\gamma = 3/2$ as a function of x and t. The red dashed lines indicate the positions of local maxima $x_m^{\pm}$ on the x-t plane which follow the power-law scaling $x_m^{\pm} \propto \pm t^{1/\gamma}$, while the height of the maxima decays as $t^{-1-1/\gamma}$. The inset depicts spatial profiles of $C(x, t)$ for two different instants of time, $t = 20$ (thick blue line) and 50 (thin red line).

to allow the flight speed to have a broad distribution. Assume that $h(v)$ is a Lorentz distribution, $h(v) = (\pi u_0)^{-1}(1 + v^2/u_0^2)^{-1}$, a velocity PDF frequently employed in plasma and kinetic theories [23]. For such velocity PDF, the density of particles is independent of the flight-time distribution and also possesses the Lorentz shape in the asymptotic limit [11]: $P(x, t) = u_0 t/[\pi(u_0^2 t^2 + x^2)]$. The expression for the correlation density function then acquires the form

$$C(x, t) = u_0^2\left[-\frac{u_0 t}{\pi(u_0^2 t^2 + x^2)} + \frac{1}{u_0 t}\Psi(t)\right]. \tag{14}$$

The first term is proportional to the density but with the opposite sign and the second depends on the flight-time distribution. Note that the integral of $C(x, t)$ with respect to x diverges when $\Psi(t) \neq 0$, meaning an infinite $C(t)$. In clear contrast, the density of the velocity correlation function is well defined; see Fig. 2(b).

Discussion.—In all considered regimes there is a region of negative correlations at the vicinity of the starting point. This means that the majority of particles found there are flying in the direction opposite to that of their initial motion, which we call an *echo effect*. The shape of the echo region and the time scaling of its width are model-specific characteristics. Simulations of a stochastic process described by a system of Langevin equations (see the Supplemental Material [24]) show analogous results, which suggests that our findings are applicable to a broad class of stochastic transport processes characterized by finite velocity of moving particles.

Perhaps the best candidate for the analog simulation of superdiffusive continuous-time random walks is a cold atom moving in a periodic optical potential. There are strong evidences, both theoretical [13] and experimental

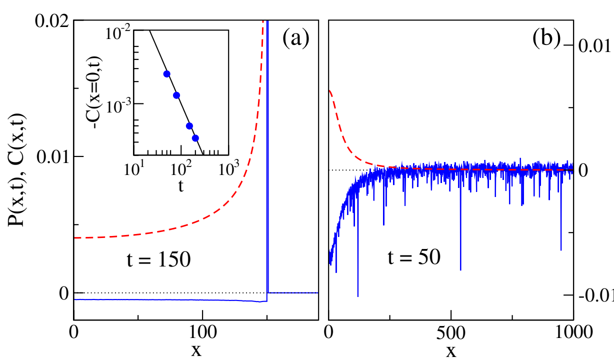

FIG. 2 (color online). Densities of particles, $P(x, t)$ (dashed red lines), and the spatial density of velocity correlations, $C(x, t)$ (solid blue lines) for (a) the Lévy walk in the regime of ballistic superdiffusion ($\gamma = 1/2$), Eq. (13), and (b) the case of Lorentzian velocity PDF, Eq. (14), with $\psi(\tau) = \delta(\tau - 1)$. Correlation functions were obtained by averaging over 10^8 realizations of the corresponding process. The inset shows $C(0, t)$ at four different instants of time. Solid line corresponds to the power law $t^{-3/2}$. All other parameters are set to 1.

[25,26], that the diffusion of the atom along the potential is anomalous and can be reproduced with Lévy-walk models [26,27]. We suggest that the velocity correlation function can be measured in experiments and thus will help to build a proper microscopic model. It is possible to prepare a strongly localized ensemble with all atoms having near equal velocities, either by sudden release of atoms from a ballistically moving deep optical well or by using more exotic setups [28,29]. For such initial states, the measurement of $C(x, t)$ is equivalent to finding the PDF $P(v, x, t)$; see Eq. (3). The PDF of instantaneous velocities, $P(v, t)$, can be measured with the routine time-of-flight technique [30], when velocity of an atom is transformed into the atom position, which is then recorded by using the florescence effect. It is also feasible to measure the spatial distribution of atoms, $P(x, t)$, by using the florescence image of the cloud [30]. A measurement of the space-dependent velocity PDF requires the implementation of the time-of-flight technique combined with a consecutive deconvolution procedure [31]. By knowing the spatial distribution of the cloud at time t (obtained from another experiment under the same conditions), the deconvolution transform can be performed numerically on the fluorescent snapshot of the time-of-flight experiment to reconstruct $P(x, v, t)$ and, consequently, to calculate $C(x, t)$. More sophisticated measurement protocols can also be developed [32].

The negative velocity echo, being a distinctive footprint of CTRWs, can be used as a benchmark to judge the validity of random-walk approaches to the charge transport on nanoscale. The velocity echo can be detected by measuring the current-current s-t correlations after a local injection of electrons into a nanotube [33]. A recently developed terahertz time-domain measurement technique [34] can be used for the readout. This noninvasive method is capable to resolve the electron dynamics on picosecond time scale, thus providing an insight into the real-time propagation of electrons along the nanotube [35]. Another type of system, where short injection pulses of charge carriers are routinely used to probe charge transport, is slabs of semiconductors [36]. It is noteworthy that recent experiments have revealed a good agreement between the dynamics of holes in a bulk of n-doped InP slab and a Lévy-walk model [37].

Conclusions.—The spatial dependence of the s-t density of velocity autocorrelations, Eq. (3), can be decomposed into two contributions. The first is produced by the particles which have performed several flights before the observation time. The second originates from the particles that are still in their first flight. For any random walk with finite average flight times, the central part of the velocity correlation pattern can be calculated as the time derivative of the particle's density.

We believe that the concept developed here can be utilized for any process that can be described as a continuous-time random walk, where finite velocities can be attributed to the diffusing entities at any instant of time [38–40]. It is possible to generalize the spatiotemporal velocity autocorrelation functions to the case of two-dimensional random walks (see the Supplemental Material [24]), thus reaching another level of detail in the analysis of the complex transport phenomena [12,14–16,25,41–43].

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