Supplementary Material for "Space-time velocity correlation function for random walks."

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I. A CASE OF LANGEVIN DYNAMICS

The Langevin equation (LE) is another fundamental model, complementary to random walks, used for microscopic description of diffusive transport. A close relationship between the LE and random walk models suggests that the results obtained for the last should stay valid for the former (and vice versa). It is natural, therefore, to test the concept of the space-time velocity correlation function on the standard one-dimensional Langevin process, which is governed by the following pair of linear differential equations:

$$\dot{x} = v \tag{1}$$

$$\dot{v} = -\gamma v + \xi(t). \tag{2}$$

Here $\xi(t)$ is white Gaussian noise and $\langle \xi(t)\xi(t')\rangle = D_v\delta(t-t')$. Similar to the considered random walks, the key feature of the LE process is a finite velocity of a diffusing particle at each moment of time. In the asymptotic regime, the spatial PDF of the particles obeys the standard diffusion equation with $D = D_v/(2\gamma^2)$. There is also no problem with derivation of the corresponding velocity auto-correlation function, $C(t)$, see Ref. [1]. However, we were unable to obtain analytic expression for the s-t correlation function, $C(x,t)$; its derivation for the case of LE remains an open problem worth of further investigation [2].

In Fig. 1 we present the results of numerical simulations obtained by propagating equations (1-2) in time. As expected, the calculated space-time velocity correlation function fits with the analytic prediction, see Eq.(6) in the main text. Namely, the function $C(x,t)$ is given by the first time derivative of the spatial PDF, obtained from the corresponding diffusion equation.

II. GENERALIZATIONS TO HIGHER DIMENSIONS

The concept of the s-t velocity correlation function can be extended to higher dimensions in a straightforward manner.

In the case when velocity directions at each step of a random walk are isotropic and independent random variables, general expressions retain their form with the only modification that the corresponding velocity and coordinates, see Eqs.(3-5)in the main text, have to be replaced by the corresponding vector quantities, $x, k, v \to \mathbf{r}, \mathbf{k}, \mathbf{v}$.

The increase of the dimensionality has certain consequences though; even for the regime of standard diffusion the asymptotic analysis is more cumbersome. However, this does not affect the qualitative outcome. Fig.2 depicts the results of simulations together with analytical expresiions for a two-dimensional random walk in the regime of normal diffusion. As its one-dimensional predecessor, the velocity correlation function is given here by the time derivative of the radial particle PDF, $P(r,t)$.

Two- and three-dimensional random walks are key ingredient of the random coil model, simple yet powerful concept popular in polymer physics [3, 4]. The random coil model assumes that each monomer –which is a step of a random walk– has a length l and is randomly oriented in space, see the inset on Fig. 2. Therefore each configuration of the polymer corresponds to some realization of a random walk of a fixed step length l with the directions of consequent steps being uncorrelated. The length of the polymer $L = n \cdot l$ corresponds to the duration of the corresponding random walk process. Remarkably, our results allow to find correlations between the directions of monomers which are separated by a distance s along the backbone of the polymer (see green shaded path on the inset of Fig. 2) while being separated in real space by a distance $|\mathbf{r}|$. This information might be useful for

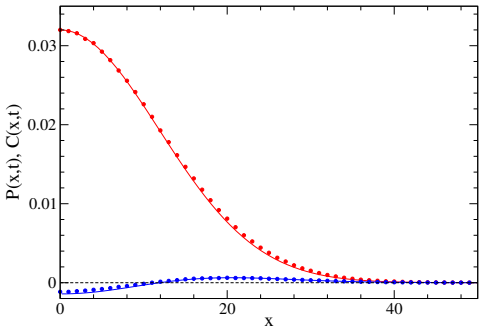

FIG. 1. Spatial density $P(x,t)$ (red dots) and space-time velocity auto-correlation function $C(r,t)$ (blue dots) obtained by sampling evolution of the system (1 - 2) for $t = 40$. The parameters are $\gamma = 0.1$ and $D = 0.05$. The blue line corresponds to the PDF obtained from the corresponding diffusion equation, the red line is given by the time derivative of the PDF, see Eq. (6) in the main text.

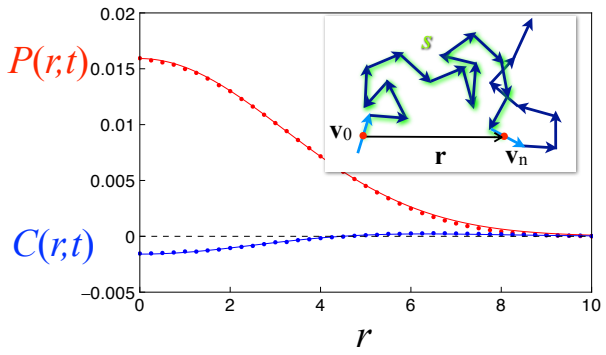

FIG. 2. Radial density $P(r,t)$ (red line) and space-time velocity auto-correlation functions $C(r,t)$ (blue line) for the two-dimensional diffusion. Dots show the results on numerical simulations. Speed and average flight time in the exponential distribution are set to unity, $t = 10$.

the estimation of monomer-monomer interactions whose strength depends on the alignment of monomers; one example is the homologous recombination of chromosomes [5] during meiosis.

[1] G. E. Uhlenbeck and L. S. Ornstein, Phys. Rev. **36**, 823D841 (1930).

[2] This problem, in principle, can be approached from the opposite end, by using the Fokker-Planck equation. This equation governs the evolution of the PDF $P(x,v,t)$, which process is parametrized by the initial conditions including v_0. The averaging of the product $v(x,t)\cdot v_0$ with the PDF $P(x,v,t)$, weighted by the Maxwellian distribution $h(v_0)$, will yield $C(x,t)$.

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