Weak Disorder Strongly Improves the Selective Enhancement of Diffusion in a Tilted Periodic Potential

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The diffusion of an overdamped Brownian particle in a tilted periodic potential is known to exhibit a pronounced enhancement over the free thermal diffusion within a small interval of tilt values. Here we show that weak disorder in the form of small, time-independent deviations from a strictly spatially periodic potential may further boost this diffusion peak by orders of magnitude. Our general theoretical predictions are in excellent agreement with experimental observations.

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Diffusion plays a key role for mixing and homogenization but also for particle selection and separation tasks [1]. A particularly simple and common way to manipulate the force-free diffusion of a Brownian particle is by means of a spatially periodic force field [2] with a nonvanishing systematic component [3–12]; i.e., the force derives from a tilted or biased periodic potential. Such dynamics arise in a large variety of different physical systems [7–10], for example, colloidal particles in optical potentials [3–6] cold atoms in optical lattices [11], or globular DNA in microstructures [12]. While the force-free thermal diffusion of an overdamped Brownian particle is always reduced when switching on an unbiased periodic potential [2], the diffusion coefficient as a function of an additional bias exhibits a pronounced peak [7–9] in a small vicinity of the so-called critical tilt, i.e., the threshold bias at which deterministic running solutions set in. This theoretical prediction has recently been confirmed by several experimental works [4–6]. However, for many experimental realizations of the above mentioned large variety of systems involving a tilted periodic potential [3–12], small, time-independent deviations of the potential from strict spatial periodicity are practically unavoidable. The objective of our present Letter is a detailed theoretical understanding of such weak disorder effects. An immediate first guess is that they will somehow ‘‘wash out’’ the diffusion peak around the critical tilt. For instance, one might argue that enhanced diffusion requires a tilt close to criticality [9] and this fine-tuning will unavoidably be spoiled by the random variations superimposed to the original periodic potential. Here, we show that exactly the opposite is the case: Tiny deviations from spatial periodicity result in an even more pronounced peak of the diffusion coefficient. Hence, the often unavoidable weak disorder is not an experimental nuisance but rather a new tool for sorting particles by way of a very strong and selective diffusion enhancement for certain species within a mixture. We remark that diffusion in the presence of temporal rather than spatial disorder represents a related but still different case. It also may result in accelerated diffusion, but, in contrast to our present case, already without a bias [13].

Our starting point is the usual overdamped Brownian motion in 1D [2–10]:

$$\eta \dot{x}(t) = -U'(x(t)) + \sqrt{2\eta kT}\,\xi(t), \tag{1}$$

where η is the viscous friction coefficient, and thermal fluctuations are modeled by unbiased, δ-correlated Gaussian noise $\xi(t)$ with thermal energy kT. The potential $U(x)$ consists of a tilted periodic part $V(x)$ and ‘‘random’’ deviations $W(x)$ (quenched disorder),

$$U(x) = V(x) + W(x), \qquad V(x) = V_0(x) - xF, \qquad V_0(x+L) = V_0(x), \tag{2}$$

where F is a tilting force (static bias) and L the spatial period. Without loss of generality we focus on potentials ‘‘tilted to the right’’, i.e. $F \geq 0$. The quantities of main interest are drift (average velocity) and diffusion,

$$v := \lim_{t\to\infty} \frac{\langle x(t)\rangle_\xi}{t}, \qquad D := \lim_{t\to\infty} \frac{\langle x^2(t)\rangle_\xi - \langle x(t)\rangle_\xi^2}{2t}, \tag{3}$$

where $\langle\cdot\rangle_\xi$ indicates an average over the noise $\xi(t)$ in (1). While many of the following considerations can be generalized to other types of disorder $W(x)$, we focus on the analytically most convenient case of unbiased, homogeneous Gaussian disorder. In other words, considering x as ‘‘time’’, $W(x)$ is a stationary, Gaussian stochastic process with mean value $\langle W(x)\rangle = 0$ and correlation

$$c(x-y) := \langle W(x)W(y)\rangle. \tag{4}$$

For simplicity only, we further assume that the correlation $c(x)$ is monotonically decreasing for $x \geq 0$ from

$$\sigma^2 := \langle W(x)^2\rangle = c(0) \tag{5}$$

to $c(x\to\infty) = 0$. A simple example is the critically damped harmonic oscillator

$$\lambda^2 W''(x) = -2\lambda W'(x) - W(x) + 2\sigma\lambda^{1/2}\gamma(x) \tag{6}$$

driven by δ-correlated Gaussian noise $\gamma(x)$, yielding a Gaussian $W(x)$ with $c(x) = \sigma^2(1 + |x|/\lambda)e^{-|x|/\lambda}$; see Fig. 1.

Without the disorder $W(x)$, the following rigorous results are known (see [9] and references therein)

$$v = D_0[1 - e^{-LF/kT}]/A, \qquad D = D_0 B/A^3, \tag{7}$$

where $D_0 := kT/\eta$ is the force-free diffusion coefficient according to Einstein and

$$A = \int_0^L \frac{dx}{L} \int_0^L dy\, e^{[V(x)-V(x-y)]/kT}, \tag{8}$$

$$B = \int_0^L \frac{dx}{L} \int_0^L dy \int_0^L dp \int_0^L dq\, e^{g/kT}, \qquad g = V(x) - V(x-y) - V(x-p) + V(x+q), \tag{9}$$

see also [7,8,10,14] for related findings. In particular, for $F = 0$ one recovers the result [2]

$$D(F=0) = \frac{D_0}{C_+ C_-}, \qquad C_\pm = \int_0^L \frac{dx}{L} e^{\pm V(x)/kT}. \tag{10}$$

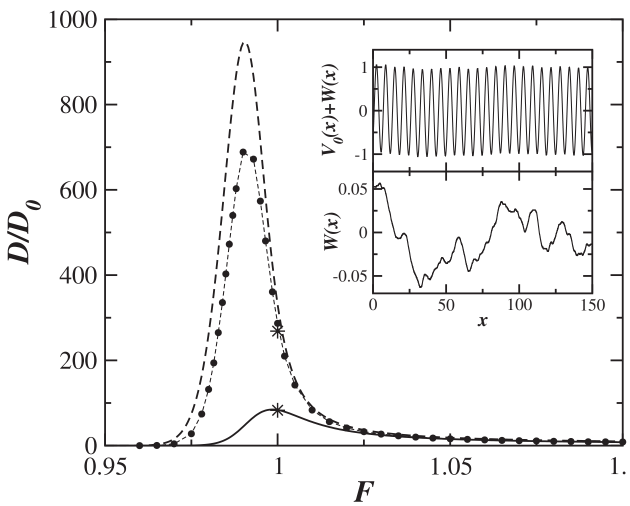

FIG. 1. Diffusion D from (3) versus tilt F for the dynamics (1) and (2) with $V_0(x) = \sin(x)$ (i.e., $L = 2\pi$, $F_c = 1$), $\eta = 1$, $kT = D_0 = 0.001$ (dimensionless units). The disorder $W(x)$ is a stationary Gaussian process satisfying (6) with $\sigma = 0.03$ and $\lambda = L$. The insets illustrate $U(x, F = 0) = V_0(x) + W(x)$ (randomness hardly visible) and $W(x)$ (randomness alone) from (2). Filled dots (connected by short dashes): Numerically exact results. Dashed line: Analytical approximation (7), (15), and (17), with (23) and (24), and $a = b = 0$. Solid line: Exact analytical result (7)–(9) in the absence of disorder ($\sigma = 0$). Lower and upper stars: analytical approximations (22) (no disorder) and (25) (with disorder), respectively. For large and small F (not shown) all curves monotonically approach $D(F \to \infty) = D_0$ and $D(F = 0) \ll D_0$. Main conclusion: the purely periodic potential leads to a maximal diffusion enhancement by about a factor of 70 (solid line) while a tiny amount of disorder (insets) further boosts the peak by a factor of 10 (dots).

Next we include the disorder $W(x)$ in (2). In a first step we assume that $W(x + NL) = W(x)$ for some integer N. Hence, $U(x)$ in (2) is a tilted periodic potential with period NL. Accordingly, (7)–(10) remain valid after replacing L by NL and $V(x)$ by $U(x)$. Exploiting (2), one can rewrite (8) after some manipulations as

$$A = \int_0^L \frac{dx}{L} \int_0^L dy\, e^{[V(x)-V(x-y)]/kT} \tilde{A}(x, y), \tag{11}$$

$$\tilde{A}(x, y) := \sum_{n=0}^{N-1} \langle e^{[-nLF + W(x) - W(x-y-nL)]/kT} \rangle, \tag{12}$$

where $\langle f(x) \rangle := N^{-1} \sum_{\nu=0}^{N-1} f(x + \nu L)$. Next, we let $N \to \infty$ and adopt the usual tacit assumption [14,15] that this limit commutes with the limit $t \to \infty$ in (3). Exploiting that the Gaussian process $W(x)$ is ergodic and satisfies $\langle e^W \rangle = e^{\langle W^2 \rangle /2}$ yields

$$\tilde{A}(x, y) = \sum_{n=0}^{\infty} e^{[-nLF + \tilde{c}(y+nL)]/kT}, \tag{13}$$

$$\tilde{c}(x) := [\sigma^2 - c(x)]/kT. \tag{14}$$

From the monotonicity of $c(x)$ [see above (5)] one can infer upper and lower bounds for (13) and thus for (11). Finally, one recovers the same formula for v as in (7) but now with the relevant A given for any $F \geq 0$ by

$$A = (1 + a) \int_0^L \frac{dx}{L} \int_0^L dy\, e^{[V(x)-V(x-y)+\tilde{c}(y)]/kT}, \tag{15}$$

$$a = e^{-LF/kT}[e^{\vartheta(\sigma/kT)^2} - 1] \tag{16}$$

with some (unknown) $\vartheta \in [0, 1]$. Note that a and $\tilde{c}(y)$ are non-negative and that both quantities vanish (for all y) if and only if there is no disorder. In the latter case, (15) reproduces (8), otherwise the disorder always reduces the velocity v. This conclusion in fact applies to much more general types of disorder $W(x)$, as can be inferred by applying Jensen's inequality to (12). Finally, it follows from (15) that $v \to F/\eta$ for $F \to \infty$, independently of $V(x)$ and $W(x)$. For related findings see also [15].

An analogous calculation yields the same formula for the diffusion as in (7) with A given by (15) and B by

$$B = (1 + b) \int_0^L \frac{dx}{L} \int_0^L dy \int_0^L dp \int_0^L dq\, e^{[g+h]/kT} \tag{17}$$

for any $F \geq 0$, where g is defined in (9) and

$$h = \tilde{c}(y) + \tilde{c}(p) - \tilde{c}(q) - \tilde{c}(y-p) + \tilde{c}(y+q) + \tilde{c}(p+q), \tag{18}$$

$$b = [1 - (1 - e^{-LF/kT})^3][e^{\kappa(\sigma/kT)^2} - 1] \tag{19}$$

with some (unknown) $\kappa \in [-2, 5]$. One readily sees that $1 + b > 0$ and that (9) is recovered in the absence of $W(x)$. However, whether the disorder enhances or reduces the diffusion is not immediately obvious, with the following exceptions: From (7), (15), and (17) one finds that

$$D(F \to \infty) = D_0 \tag{20}$$

and from (10)—analogous to the derivation of (15)—that

$$D(F = 0) = (D_0/C_+C_-)e^{-(\sigma/kT)^2}. \tag{21}$$

With the Cauchy-Schwartz inequality it follows [16] that $D(F = 0) \leq D_0$ and with (10) and (21) that the disorder always reduces the diffusion for $F = 0$.

As exemplified in Fig. 1 and discussed in detail in [9], without disorder, the diffusion D, considered as a function of the tilt F, develops a pronounced peak near $F_c := \max_x V_0'(x)$. The critically tilted potential $V(x) = V_0(x) - xF_c$ thus exhibits a strictly negative slope ($V' < 0$) apart from plateaux ($V' = V'' = V_0'' = 0$, $V''' = V_0''' < 0$) at $x_c + nL$ for a generically unique $x_c \in [0, L)$ and arbitrary integers n. In other words, in the noiseless dynamics (1), F_c marks the transition from locked to running deterministic solutions. For finite but weak noise, the peak of $D(F)$ about F_c satisfies [9]

$$D(F_c, W = 0) \simeq 0.021 D_0 L^2 |V_0'''(x_c)/kT|^{2/3}. \tag{22}$$

With our findings $D(F = 0) \leq D_0$ and $D(F \to \infty) = D_0$ we thus can conclude that the peak height of $D(F)/D_0$ scales like $T^{-2/3}$, and similarly for its width [9].

Next we consider the influence of the disorder $W(x)$ in the above most interesting regime of small $F - F_c$ and kT. As intuitively expected and confirmed by closer inspection, in this regime the integrals in (15) and (17) are dominated by small values of $x - x_c$ y, p, q, thus admitting the following approximate expansions

$$V(x_c + \delta) \simeq V(x_c) - (F - F_c)\delta + V_0'''(x_c)\delta^3/6, \tag{23}$$

$$\tilde{c}(x) \simeq \tilde{c}''(0)x^2/2. \tag{24}$$

Further, we henceforth neglect a and b in (15) and (17) [17]. The main virtues of these approximations are: (i) They still reproduce the correct limiting behavior for $F \to \infty$ and also qualitatively capture the small F behavior, namely, extremely small values of drift and diffusion. In other words, they are expected to reasonably work for all $F \geq 0$, as confirmed by Fig. 1. (ii) The main effects of $V_0(x)$ and $W(x)$ are already captured by F_c, $V_0'''(x_c)$, and $\langle W'(x)^2 \rangle = -c''(0)$. (iii) For $F = F_c$ and sufficiently small kT, the integrands in (15) and (17) exhibit very pronounced maxima and thus can be evaluated by means of saddle point approximations, yielding the "universal scaling law"

$$D(F_c) \simeq D(F_c, W = 0)(1 + 1.9 Q e^{416 Q^3/3}), \tag{25}$$

$$Q := \langle W'(x)^2 \rangle / [|V_0'''(x_c)|^{2/3}(kT)^{4/3}]. \tag{26}$$

The general analytical results (20), (21), and (25) represent the main findings of our present Letter: Already a small amount of disorder typically leads to a much more pronounced peak of $D(F)$ than without disorder. An illustration is provided by Fig. 1.

As an application of our general theory, we finally address the experiment from Ref. [4]: A colloidal sphere with diameter 1.48 μm and $D_0 = kT_{\mathrm{room}}/\eta \simeq 0.19\ \mu\mathrm{m}^2/\mathrm{s}$ moves along a ring of light. The particle feels $N = 80$ potential minima with period $L \simeq 0.33\ \mu$m due to spatial variations of the light intensity and a torque due to orbital angular momentum transfer by the photons from two superimposed optical vortices [4,18], whose relative strengths are controlled by an experimental parameter $\alpha \in [0, 1]$. The resulting equation of motion takes the form (1) [18] with a potential (2) corresponding to the total circumferential force from Eq. (4) in [4], namely,

$$-U'(x) = F_0[\Phi(\alpha) + \Psi(\alpha)\cos(2\pi x/L)] - W'(x) \tag{27}$$

with $\Phi(\alpha) := (1 - \alpha)/(1 + \alpha)$ and $\Psi(\alpha) := 2[\alpha(\epsilon^2\Phi^2 + \zeta^2)]^{1/2}/(1 + \alpha)$. Further, F_0, ϵ, and ζ are fit parameters, accounting for the laser intensity and the particle's shape, size, and composition (light scattering and absorption properties). The torque being proportional to the light intensity gives rise to the first term on the right hand side of (27) (fit parameter F_0) and also to part of the second term [18] (fit parameter ϵ). Additionally, the second term accounts for the polarizable particle's coupling to the gradient of the light intensity (fit parameter ζ). Finally, $W(x)$ in (27) accounts for random imperfections of the experimental optics [4]. Its variance is fixed by observing that $-W'(x)/F_0$ corresponds to the function $\eta(\theta)$ in [4] and that $\langle |\eta(\theta)|^2 \rangle \approx 0.01$ according to [4]. Further statistical properties of $W(x)$ cannot be quantitatively related to those of the bare intensity reported in [4] since both the intensity and the intensity gradient contribute—after suitably averaging over the particle volume—to $W(x)$. For this reason, we model $W(x)$ as Gaussian process (6) with periodicity $W(x + NL) = W(x)$ and $\langle W'(x)^2 \rangle = \sigma^2/\lambda^2 = 0.01 F_0^2$. Regarding the correlation length λ, we found that its exact quantitative value hardly matters and we have chosen $\lambda = 2L$, in accordance with both Figure 1 from [4] and the given particle size. Figure 2 depicts our fit to the experimental results with parameter values $F_0 = 1.37$ pN, $\epsilon = 0.38$, and $\zeta = 0.25$. [19]. In view of the periodicity $W(x + NL) = W(x)$ we used the exact analytics (7) with A from (11) and similarly for B. The remaining dependence of the results on the realization of $W(x)$ is still notable for $N = 80$. In the absence of more than one experimental realization, we have selected also in the theory a well fitting, but still representative single realization $W(x)$. The minor differences between theory and experiment can be naturally attributed to the fact that this $W(x)$ is still not exactly the one realized in the experiment and to oversimplifications of the theoretical model (1) *per se*. Once $W(x)$ and all fit parameters are fixed in (27), it is possible to approximately estimate the underlying bare

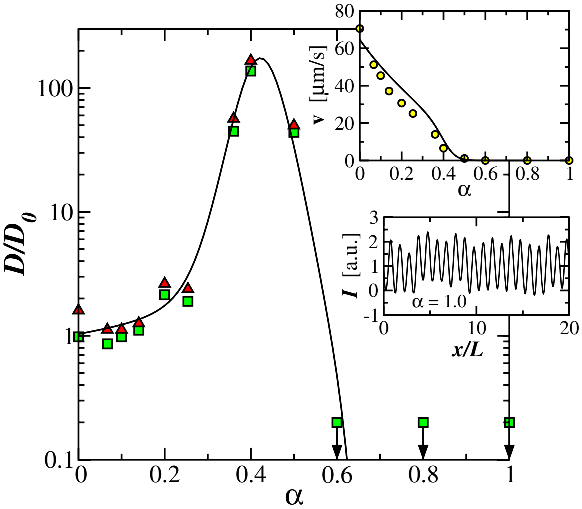

FIG. 2 (color online). Symbols: Experimentally measured diffusion D and velocity v (upper inset), adopted from Fig. 3 of Ref. [4]. Solid lines: Theoretical fit. Lower inset: Approximate intensity profile in arbitrary units for $\alpha = 1.0$ and $x \in [0, 20L]$.

intensity $I(x)$. The resulting $I(x)$ in Fig. 2 indeed agrees quite well with Fig. 1 from [4]. All in all, our theory thus agrees in every respect very well with the experiment from [4]. An analogous comparison with the experiments from [5,6] is prohibited by their small N values.

In conclusion, our main finding consists in the general analytical results (20), (21), and (25), implying that even a tiny amount of disorder superimposed to the (dominating) periodic potential may further boost the previously known sharp diffusion peak near the critical tilt by orders of magnitude; see Fig. 1. A further main point of our analytical findings is the universality of this very selective and very strong diffusion enhancement close to the critical tilt. Considering that different species of particles typically couple differently to the periodic and random potential and/or to the bias force we expect different values of the critical tilt for each species. This opens the possibility of sorting particles by way of selectively enhancing the diffusion for certain species within a mixture. The experimentally often unavoidable weak disorder quite unexpectedly improves rather than deteriorates the effectivity of the selection mechanism. Experiments along these lines for a mixture of different DNA-fragments in a periodically structured microfluidic device analogous to those from [12] are presently in preparation in the labs of D. Anselmetti at the University of Bielefeld.

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