Anisotropic diffusion in square lattice potentials: Giant enhancement and control

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received 8 December 2011; accepted in final form 22 February 2012
published online 20 March 2012

PACS 05.45.-a - Nonlinear dynamics and chaos
PACS 05.40.-a - Fluctuation phenomena, random processes, noise, and Brownian motion
PACS 05.60.-k - Transport processes

Abstract – The unbiased thermal diffusion of an overdamped Brownian particle in a square lattice potential is considered in the presence of an externally applied ac driving. The resulting diffusion matrix exhibits two orthogonal eigenvectors with eigenvalues \( D_1 > D_2 > 0 \), indicating anisotropic diffusion along a “fast” and a “slow principal axis”. For sufficiently small temperatures, \( D_1 \) may become arbitrarily large and at the same time \( D_2 \) arbitrarily small. The principal diffusion axis can be made to point into (almost) any direction by varying either the driving amplitude or the coupling of the particle to the potential, without changing any other property of the system or the driving.

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Introduction. – Thermal diffusion plays a key role in many physical, chemical, and biological processes. At thermal equilibrium, the free diffusion as considered, e.g., by Einstein [1], is generically reduced by an additional periodic potential [2], and —at least for the most common periodic lattice structures— remains spatially isotropic (see below). Out of equilibrium, the main focus has so far been on periodic potentials in one-dimension, perturbed by either a static “bias force” (tilted washboard potentials) [3–5] or by an unbiased, time-dependent driving [6]. The most remarkable finding in both cases is that the diffusion coefficient \( D \) may exhibit a giant enhancement over the free (Einsteinian) diffusion coefficient \( D_0 \). More precisely, for asymptotically small \( D_0 \), the ratio \( D/D_0 \) diverges, while \( D_0 \) itself still tends to zero, apart from certain fine-tuned (non-analytical) potential shapes and system parameters, for which \( D \) may remain finite.

Another topic of considerable recent interest concerns the effect of disorder (random deviations from a strictly periodic potential), which may give rise to a further diffusion enhancement or even to anomalous diffusion [7].

Works on genuine new phenomena in higher dimensions are scarce: Guantes and Miret-Artés [8] studied biased diffusion induced by an asymmetric external driving. Sancho et al. and Lacasta et al. [9] put their main focus on (possibly transient) anomalous diffusion effects. Experimentally, Tierno et al. observed giant transversal diffusion of paramagnetic particles on an uniaxial garnet film in the presence of an oscillating magnetic field [10].

Here, we reconsider the prototypical situation of Brownian motion in a more than one-dimensional periodic potential and we demonstrate that a simple ac driving generically results in anisotropic diffusion, whose direction and magnitude depend in quite an intriguing way on the potential, the driving, and the particle properties.

Model. – To keep things as simple as possible, we specifically focus on a square lattice in two dimensions and on a square-wave (rectangular) driving. Yet, our main results readily carry over to various other drivings and more general lattice potentials in two as well as in three dimensions.

Our starting point is the the Langevin dynamics

\[
M\ddot{\vec{r}}(t) + \eta\dot{\vec{r}}(t) = -\nabla U(\vec{r}(t)) + \vec{F}(t) + \sqrt{2\eta kT}\vec{\xi}(t),
\]

where \( M \) is the mass of the Brownian particle, \( \eta \) its friction coefficient, and \( \vec{r} = x\vec{e}_x + y\vec{e}_y \) its position in the \( x-y \)-plane, with \( \vec{e}_x \) and \( \vec{e}_y \) being the unit vectors in the \( x \)- and \( y \)-direction. Further, \( U(\vec{r}) \) stands for the spatially periodic potential, \( \nabla U(\vec{r}) \) its gradient, and \( \vec{F}(t) \) the temporally periodic force. The last term in (1) accounts for thermal noise as usual [2–4,6,8,9]: \( T \) is the temperature, \( k \) Boltzmann’s constant, and \( \vec{\xi}(t) = \xi_x(t)\vec{e}_x + \xi_y(t)\vec{e}_y \) consists of two independent, delta-correlated, Gaussian noises \( \xi_x(t) \), \( \xi_y(t) \).

As announced, we specifically address the case that the periodic potential \( U(\vec{r}) \) is composed of rotation-symmetric
on-site potentials $U_1(\vec{r})$ on a square lattice with period $L$, 

$$U(\vec{r}) = \sum_{m,n=-\infty}^{\infty} U_1(\vec{r} - [m\vec{e}_x + n\vec{e}_y]L). \tag{2}$$

As illustrated by fig. 1, our standard example will be the Yukawa potential 

$$U_1(\vec{r}) = Q \exp\{-|\vec{r}|/4L\}/|\vec{r}|, \tag{3}$$

where $Q \geq 0$ quantifies the coupling of the particle to the potential (e.g. the particle charge in the case of a screened electrostatic potential).

Likewise, the announced square-wave driving is formally given by 

$$\vec{F}(t) = \vec{e}_\alpha A \sin[\sin(\omega t)] \tag{4}$$

with amplitude $A$, frequency $\omega$, and direction $\vec{e}_\alpha := \vec{e}_z \cos \alpha + \vec{e}_y \sin \alpha$. In other words, it switches between $A$ and $-A$ every half-period $\pi/\omega$, and $\alpha$ represents the angle between the driving force and the $x$-axis, see fig. 1.

Yet, as already said, our main qualitative findings turn out to be largely independent of the above particular choice of on-site potential, lattice structure, and driving.

To further reduce the number of model parameters, we can and will choose the units of length, time, energy, and temperature so that 

$$L = 1, \quad \omega = 1, \quad \eta = 1, \quad k = 1, \tag{5}$$

and we focus on the simplest and most important case [2–4,6] that inertia effects are negligible (overdamped limit), i.e. $M \to 0$ in (1), yielding 

$$\dot{\vec{r}}(t) = -\nabla U(\vec{r}(t)) + \vec{F}(t) + \sqrt{2\eta \xi(t)}. \tag{6}$$

We remark that in the presence of an additional, externally applied static bias force, a quite interesting response behavior in the form of a directed net particle motion arises [11,12]. In the following, our main focus will be on a quite different issue, namely the unbiased diffusion of a Brownian particle in the absence of any further perturbation.

**Diffusion matrix.** – For symmetry reasons, the above specified dynamics rules out any systematic particle transport, i.e. we are dealing with a purely diffusive, unbiased Brownian motion, characterized by a $2 \times 2$ diffusion matrix $D$ with matrix elements 

$$D_{ij} = \lim_{t \to \infty} \frac{\langle r_i(t) r_j(t) \rangle}{2t}, \tag{7}$$

where $r_i, r_j \in \{x, y\}$ (see below (1)) and where $\langle \cdot \rangle$ indicates the ensemble average over many realizations of the stochastic dynamics. For ergodicity reasons and due to the long-time limit in (7), the initial conditions are irrelevant and we can without loss of generality focus on 

$$\vec{r}(0) = \vec{0}. \tag{8}$$

Since $D$ is symmetric and positive, there are two orthogonal eigenvectors with eigenvalues 

$$D_1 \geq D_2 > 0. \tag{9}$$

Essentially, a statistical ensemble of (non-interacting) Brownian particles, all starting from the origin at time $t = 0$, thus evolves in the course of time into a bigger and bigger “particle cloud” of ellipsoidal shape, see fig. 2. For large times $t$, and neglecting local details on the scale of the spatial period $L$, this cloud is quantified by a Gaussian probability density [4,13] of variance $2D_1 t$ along some “fast principal axis” $\bar{\vec{e}}_o := \bar{\vec{e}}_z \cos \Theta + \bar{\vec{e}}_y \sin \Theta$, and of variance $2D_2 t$ along the orthogonal “slow principal axis”.

The angle $\Theta$ between “fast direction” and $x$-axis is thus $180^\circ$-periodic, i.e. 

$$\Theta \text{ and } \Theta + 180^\circ \text{ are equivalent.} \tag{10}$$

Free diffusion (vanishing $U(\vec{r})$ and $\vec{F}(t)$) according to Einstein [1] amounts to $D_1 = D_2 = D_0$ with $D_0 = kT/\eta$ for the original dynamics (1) and $D_0 = T$ for the rescaled dynamics (6).

Including the periodic potential $U(\vec{r})$, but still without oscillating force $\vec{F}(t)$, the system (2)–(6) is still invariant under rotations by $90^\circ$, implying isotropic diffusion ($D_1 = D_2$).

Including also the driving $\vec{F}(t)$, this symmetry is broken, implying anisotropic diffusion ($D_1 > D_2$) in the generic case. The remaining two symmetry arguments are: i) It is sufficient to consider $\alpha \in [0^\circ, 45^\circ]$. ii) If the driving direction $\vec{e}_\alpha$ coincides with a symmetry axis of the square lattice (i.e. $\alpha = 0^\circ$ or $\alpha = 45^\circ$) then $\bar{\vec{e}}_o$ will be parallel or orthogonal to $\vec{e}_\alpha$. In any other case ($0^\circ < \alpha < 45^\circ$) it is impossible to predict $\bar{\vec{e}}_o \text{ a priori.}$
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Fig. 2: (Color online) Typical examples of diffusive “particle clouds”. The corresponding (unbiased) Gaussian probability densities are completely characterized by the variance $2D_1t$ along the long principal axis and by the variance $2D_2t$ along the short principal axis of the ellipsoidal clouds. In other words, the plot must simply be rescaled by $\sqrt{t}$ in the course of time. Quantitatively, every single depicted point represents a numerical solution at time $t = 10^5$ of the stochastic dynamics (2)–(6) with initial condition (8) and parameters $Q = 1, \alpha = 35^\circ, T = 5 \cdot 10^{-3}$, and $A = 6$ (blue), $A = 7.84$ (green).

After a couple of unsuccessful attempts one furthermore realizes that analytical progress is quite hopeless. Therefore we now turn to the presentation of our numerical results (next section), followed by a brief account of the underlying basic physical mechanisms (section “Discussion”).

Results. – We first exemplify the most interesting regime of the parameters $Q, A, \alpha$ and later provide a more systematic exploration: fig. 3 depicts the “fast” and “slow” diffusion coefficients $D_1$ and $D_2$ together with their ratio $D_1/D_2$ and the “fast direction” $\Theta$. A pronounced anisotropy of the diffusion is indicated by the fact that $D_1 \gg D_2$. The corresponding “particle cloud” (see fig. 2 and below eq. (9)) thus actually resembles a very narrow “particle beam”. Its orientation $\Theta$ may assume any value between $0^\circ$ and (almost) $-180^\circ$ upon variation of the driving amplitude $A$ for the specific choice of the remaining parameters used in fig. 3. For other such choices, an even larger range of $\Theta$-values can be covered. Since $\Theta$ and $\Theta + 180^\circ$ are equivalent (see (10)), we can conclude that essentially any possible orientation of the “fast” diffusion direction can be realized upon variation of $A$, without changing any other property of the system or the driving, see fig. 2.

Decreasing the temperature $T$ yields larger $D_1/D_2$ ratios for practically all amplitudes $A$ in fig. 3 for which the long time limit in (7) could be numerically reached, i.e. the diffusion anisotropy gets more pronounced. Whereas $D_2$ always decreases upon lowering the temperature, $D_1$ increases within certain “$A$-windows” around $A = 7.4, A = 7.8, A = 8.2$ etc., and decreases otherwise.

According to fig. 4, analogous findings are recovered upon variation of the potential strength $Q$ from (3). Hence, particles with different “charges” $Q$ can be diffusively “beamed” into different directions very “fast” and with very high precision. In other words, a periodic “surface potential” can act as a very efficient particle sorting device.

A more detailed low-temperature asymptotics of $D_i$ ($i = 1, 2$) is provided by fig. 5, evidencing an Arrhenius-type behavior

$$D_i \sim \exp\{-E_i/T\} \quad (11)$$

with certain “effective energies” $E_1 < 0 < E_2$. The same behavior is recovered within all of the above-mentioned
"A-windows". For all other A-values, one finds (as expected and hence not shown) the same asymptotics as in (11), but now with $0 < E_1 < E_2$.

We thus can conclude that the diffusive particle motion can become arbitrarily “fast” and anisotropic for sufficiently small temperatures $T$. Likewise, in comparison to the free diffusion coefficient $D_0 = T$, the ratio $D_1/D_0$ diverges and $D_2/D_0$ approaches zero for asymptotically small $T$.

**Discussion.** – For an intuitive understanding of what is going on, we first focus on the dynamics (2)–(6) in the deterministic limit ($T = 0$). Without driving ($A = 0$) the particle readily settles down into one of the local minima of the periodic potential (2), (3), see also fig. 1. Upon increasing $A$, all those point attractors evolve via a complicated sequence of bifurcations into (possibly coexisting) periodic, quasi-periodic, or chaotic attractors, whose quite intricate details also depend on the values of $Q$ and $\alpha$ [11,12]. As might not have been immediately anticipated, but in fact is rather plausible at second glance, some of the so emerging deterministic attractors give rise to a permanent directed particle motion, see fig. 6. For symmetry reasons, such “transporting attractors” always appear in pairs with opposite transport velocities by way of spontaneous symmetry breaking. Besides such a pair, there may or may not coexist additional (transporting or non-transporting) attractors. The actual occurrence of those transporting attractors and the concomitant quantitative transport velocities $\bar{v}$ are only accessible by
rates $\gamma_x$ and $\gamma_y$, respectively. Since the driving $\vec{F}(t)$ predominantly acts along the $x$-direction for $0 < \alpha < 45^\circ$, it seems plausible that $\gamma_x > \gamma_y$. Hence one can infer that

$$D_1 \approx L^2 \gamma_x / 2,$$

$$D_2 \approx L^2 \gamma_y / 2.$$  

Therefor, we can conclude that $\Theta \approx 0^\circ$. From the usual Boltzmann-Arrhenius temperature dependence of the rates $\gamma_{x,y}$ one finally recovers (11) with $0 < E_1 < E_2$. For the rest, the rates $\gamma_{x,y}$ and hence $D_{1,2}$ from (12,13) may still depend on $A$ (and likewise on $Q$ and $\alpha$) in a very complicated way. Altogether, these considerations explain the main features of fig. 1 up to about $A = 6$.

Next we focus on the “red stripes” in fig. 7, indicating two symmetric attractors with spontaneous transport in the $y$-direction at certain velocities $\pm v$. Denoting by $\gamma_y$ the rate of noise induced transitions between them, a similar calculation as in refs. [5,14] yields for the diffusion coefficient in the $y$-direction the approximation

$$D_1 \approx v^2 / (2 \gamma_y),$$

whereas in the $x$-direction one obtains similarly as in (12) the approximation

$$D_2 \approx L^2 \gamma_x / 2.$$  

Hence, one can conclude that $\Theta \approx \pm 90^\circ$. This provides an explanation of eq. (11) with $E_1 < 0 < E_2$, an explanation of fig. 3 within the above mentioned “$A$-windows”, and an explanation of fig. 5. Moreover, we recognize that these “$A$-windows” are in fact the descendants of the “red stripes” in fig. 7.

So far, we tacitly neglected the possibility that besides the transporting attractors there may still coexist further non-transporting attractors. Numerically, one finds that this is indeed the case within a subset of the colored regions in fig. 7 (not shown). In such a case, the noise-induced transitions between the various attractors are governed by several different rates, resulting in similar but more complicated estimates for $D_{1,2}$ than in (12)–(15).

Analogous generalizations apply for the small parameter regions in fig. 7 which are colored differently from red, corresponding to a spontaneous deterministic transport into a direction substantially different from $\phi = 90^\circ$.

Coming back to the remaining $A$-values in fig. 3—namely those larger than about $A = 6$ but not contained in one of the $A$-windows— it turns out that, essentially, again thermal hopping prevails, but now predominantly in steps of $\sqrt{2}L$ along the bisectrix $y = x$, hence $\Theta \approx -135^\circ$. Occasionally, one also encounters more complicated types of motion, resulting in even smaller $\Theta$-values.

As expected, with increasing temperature $T$, all these feature become more and more “washed out” in fig. 3. Especially, this applies to the neighborhood of $A = 6.5$, in accordance with the tightly nested red and white stripes in the corresponding region of fig. 7.
Analogous considerations apply to fig. 4. Overall, we thus can conclude that for sufficiently low temperatures \(T\), giant anisotropic diffusion arises within all colored parameter regions in fig. 7, and that pronounced variations of the principal diffusion axes are expected whenever crossing a border between colored and white regions.

The entire pertinent parameter regions in fig. 7 are not very large as far as their measure is concerned, but still very appreciable for instance from the following viewpoint: For (almost) any given amplitude \(A\) it is possible to find angles \(\alpha\) and coupling strengths \(Q\) for which all those effects can be observed [12].

Finally, it also seems worth mentioning that in contrast to giant diffusion enhancement in one-dimensional periodic potentials [3,6], in our present case i) not only the ratio \(D_1/D_0\), but also \(D_1\) itself diverges for asymptotically small temperatures, and ii) the pertinent parameter regions are of finite measure.

**Conclusions.**—Starting with Einstein’s ground-breaking work on Brownian motion [1], the subject of diffusion has attracted a lot of attention due to its practical relevance in numerous specific systems, but also due to its theoretical interest as a fundamental form of transport per se. Here, we reconsidered diffusion in a particularly simple “minimal model”: a spatially periodic system, driven out of equilibrium in one of the experimentally most natural and common ways, namely by an oscillating driving force. Our first main finding is an extreme anisotropy of the diffusion, whose “speed” in one direction may grow exponentially fast as temperature decreases, while the perpendicular “speed” approaches zero exponentially fast. Our second main finding is that the principal axes of the anisotropic diffusion can be made to point into (practically) any direction by solely varying, e.g., the ac driving amplitude or the coupling of the particle to the periodic potential, but without changing any other property of the system or the driving.

The indispensable prerequisites for those diffusion effects are very weak and ubiquitous: Brownian motion in a spatially periodic lattice potential under the action of an oscillating driving force is a paradigmatic scenario in a large variety of different contexts, e.g., diffusion on the surface [8] but also in the bulk of a crystal under the action of electromagnetic perturbations, migration in periodic arrays of laser traps, or in periodically structured micro- or nano-fluidic systems, to name but a few [9,10,12].

One reason why those very fundamental diffusion phenomena have not been discovered earlier may be the fact that the underlying key mechanisms of spontaneous symmetry breaking has not been naturally associated with such systems up to now. A second reason is that a very careful numerical exploration is required with a clear idea of what one is actually looking for. In turn, once the quantitative numerical predictions for a specific experimental system are available, verifying and exploiting the predicted effects seems quite feasible and worthy to us.

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This work was supported by Deutsche Forschungsgemeinschaft under SFB 613 and RE1344/5-1.

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