ac-driven phase-dependent directed diffusion

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We study directed diffusion of a particle in a periodic symmetric potential under the influence of a time-periodic external field. The field lowers the symmetry of the phase space flow which results in directed diffusion even if the potential and the field are reflection symmetric. We analyze the interplay between broken symmetry and dynamical chaos.

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Nonlinear transport processes in a spatially periodic potential $U(x+2\pi)=U(x)$ are of interest for such topics as stochastic diffusion in nonlinear systems [1], transport in randomly driven systems [2], and in solid state physics [3], to name a few. Chaotic transport in a nonlinear dynamical system implies the possibility to travel in phase space if the initial conditions of the particle belong to the chaotic layer of the system. The chaotic layer can appear in some vicinity of the separatrix of the unperturbed motion when a perturbation is applied to an integrable system. A weak time-periodic field $E(t)$ can serve as such a perturbation generating a variety of stochastic diffusive regimes in spatially periodic systems [4,5]. A prominent example for directed transport in such systems is ratchet transport, i.e., a (colored) noise-induced macroscopic current in a periodic potential with or without space reflection symmetry. Ratchet transport was extensively studied for different situations, including chaotic dissipative systems and overdamped regimes [6]. Possible experimental manifestations of ratchet diffusion can be expected, e.g., for the phase diffusion in Josephson junctions and the motion of proteins along biopolymers. Recently, the effect of an ac field on directed diffusion in reflection symmetric and nonsymmetric periodic potentials was also studied in Ref. [7]. There it has been shown that the breaking of the time reflection symmetry of the force $E(t)$ plays the same role as the breaking of the space reflection symmetry of the potential $U(x)$ leading to directed diffusion controlled by an ac field.

In this paper we study phase-dependent directed transport in systems without breaking reflection symmetries in time or space. This transport mechanism results from the specific symmetry of the equations of motion combined with the presence of nonlinear processes. We investigate the simplest case of the harmonically driven mathematical pendulum with the Hamiltonian

$$H = \frac{p^2}{2} + U(x) - x E(t) , \quad U(x) = \sin(x) , \quad E(t) = \varepsilon \sin(\omega t + \phi) .$$

(1)

Here $(x,p)$ are canonically conjugated dimensionless variables, $\varepsilon,\omega,\phi$ are, respectively, the amplitude, frequency, and phase of the time-dependent field, which we consider to be a (strong) perturbation of the unperturbed motion of the particle in the potential $U(x)$. Eq. (1) corresponds to a dipole interaction between an oscillator and an external perturbation field [1] in the long wave length limit. The combined action of the ac field $E(t)$ and periodic potential $U(x)$ results in a nonintegrable type of dynamics with either quasiperiodic or stochastic trajectories. Using the model Hamiltonian (1) we show that the ac field lowers the symmetry of the dynamical system. This results in a phase-dependent directed diffusion, even if the potential $U(x)$ and the field $E(t)$ are reflection symmetric. We will analyze the interplay between broken symmetry and dynamical chaos.

Let us start with some unexpected results of numerical studies of Eq. (1). Simulations were performed in the following way: take a large ensemble of initial conditions ($N \sim 10^6$) at $t=0$ with energies randomly chosen in a thin layer beyond the unperturbed separatrix, $1-\Delta < E(t=0) < 1; \Delta \ll 1$, and coordinates uniformly distributed over the unit cell of the potential $-3\pi/2 < x(t=0) < \pi/2$. Thus all particles would be trapped in the chosen cell for the unperturbed dynamics. The ac field induces dynamical chaos allowing for an escape of the particles. The small value of $\Delta$ must satisfy the Chirikov overlap criterion so that (almost) all particles in the ensemble perform stochastic motion [8]. Such a choice of the initial positions presents a (quasi) microcanonical distribution for the unperturbed dynamical system. Nonzero values of $\Delta$ ensure better averaging. By means of numerical integration of the equations of motion we obtain the average escape times $\tau_0$ and $\tau_1$ of a particle to the neighboring right and left cells of the potential. The averaging is performed over the full ensemble with integration times being of the order of $10^3$ time units, which is much larger than the maximum time to reach the neighboring cell. The results are shown in Fig. 1. We observe a substantial asymmetry of the particle flux to the right and to the left, respectively. This asymmetry indicates the existence of directed diffusion in the system. The asymmetry vanishes only for some specific values of the phase $\phi = \phi_0 + k\pi$, where $k$ is an integer. For small amplitudes $\varepsilon < 0.05$ or for large frequencies $\omega > 3$, i.e., in the limit of a very narrow layer of the stochastic motion, we find $\phi_0 \to \pi/2$.

To understand these results we start with the consideration of the limit of large energies, and neglect the potential in zeroth order: $U(x)=0$. The velocity of a particle in the ac field then reads

$$V(t) = C_0 - \varepsilon/\omega \cos(\omega t + \phi) , \quad V(0) = V_0 .$$

(2)
Here $\langle \cdots \rangle$, means time averaging. It follows from Eq. (2) that

$$C_0 = V_0 + e/\omega \cos(\phi).$$

(3)

Given a distribution of initial conditions $p(X_0, V_0)$ with symmetry $p(X, V) = p(X, -V)$, the mean time-averaged velocity per particle is not equal to zero:

$$\bar{V} = e/\omega \cos(\phi).$$

(4)

The ac field lowers the previous symmetry of the phase space flow $\{+ V_0 \rightarrow -V_0\}$ into $\{+ V_0 \rightarrow -V_0; \phi \rightarrow -\phi + \pi\}$ (this is one reason for the macroscopic transport observed in the short-time simulations in Fig. 1; we come back to the case of transport in a potential below).

Next we study the case when the initial energy is large compared to the potential $U(x) = E_0 \geq V_0^2/2 + \sin(x_0) > 1$. To simplify the analytical calculations we put $\omega \gg 1$ and assume that the initial distribution is uniform in space: $p(X, V) = \delta(|V| - V_0)$. After averaging we obtain

$$\bar{V} = \frac{\pi}{K(\kappa^{-1})} \frac{\text{sgn}[V_0 + (e/\omega) \cos(\phi)]}{\kappa}.$$

$$\kappa^2 = \frac{1}{2} + \left(1 + \frac{V_0^2}{\epsilon \cos(\phi)}\right)^2 + \sin\left(X_0 + \frac{\epsilon \sin(\phi)}{\omega^2}\right) \equiv 1,$$

(5)

$$\bar{V} = \langle \bar{V} \rangle_{X_0, V_0} = \frac{1}{4\pi} \int_0^{2\pi} \{\bar{V}(+V_0, X_0) + \bar{V}(-V_0, X_0)\} dX_0.$$

(6)

Here $K$ is the elliptic integral of first type. Avoiding cumbersome analytical formulas, numerically calculated average velocities $\bar{V}$ for micronanoeletronics with different initial energies $E_0$ are presented in Fig. 2. The estimated upper boundary of the stochastic layer is $E_{\text{st}} = 1.1$. For $E_0 \gg E_{\text{st}}$ the function $\bar{V}(\phi)$ approaches the form of $\cos(\phi)$. With decreasing $E_0$, the maximum value of $\bar{V}_{\text{max}}$ increases (see upper inset). It passes through a maximum and subsequently decreases with further lowering $E_0$. This behavior is connected to the sticking of a trajectory to the vicinity of the unperturbed hyperbolic fixed point. The numerically obtained symmetric phase $\phi_0$ defined through the equality $\bar{V}(\phi_0) = 0$, is $\pi/2$ at $E_0 \approx E_{\text{st}}$ (see lower inset).

The situation drastically changes when $E_0$ is crossing the boundary of the chaotic part in phase space ($E_0 < E_{\text{st}}$). After crossing there is a nonzero probability for a trajectory to be trapped by partly destroyed KAM tori [1] as well as to travel in arbitrary direction in the manner of Lévy flights [4,11]. These processes reduce the amplitude $\bar{V}_{\text{max}}$. In addition, as shown in the lower inset for a finite realization length $T$ (i.e., the time of averaging), the symmetric point $\phi_0$ is abruptly shifted from $\pi/2$: $\phi_0 = \pi/2 + \delta(\phi_0)$. With increasing time $T$ one finds $\bar{V}_{\text{max}} \sim 1/T$ and the mean velocity tends to zero for infinite $T$. This is shown in Fig. 3. The power law

$$\langle \bar{V} \rangle_{X_0, V_0} = \frac{1}{4\pi} \int_0^{2\pi} \{\bar{V}(+V_0, X_0) + \bar{V}(-V_0, X_0)\} dX_0.$$
behavior reflects the superdiffusive nature of the motion inside the stochastic layers, i.e., it results from the fast anomalous stochastic diffusion, which is analogous to the quasibalistic regime and does not obey usual laws of diffusive motion [9]. Such a regime is possible in any time-dependent system having regions of bounded and unbounded motion at different sides of the unperturbed separatrix [4,10]. Simultaneously, a power law decay always implies the absence of localization and the notion of a localization length is meaningless. The function $V_{\text{max}}(T)$ tends slowly to zero with increasing $T$; therefore the directed diffusion predicted can be detected for finite values of $T$. Note that there are two competitive mechanisms of the long-time self-averaging of $V_{\text{max}}$ in the stochastic layer. The first one is connected to the ergodicity and mixing of chaotic dynamics itself while the second one results from the weak noise of numerical and real experiments. The role of noise is discussed below.

It is interesting to note that for a fixed value of the phase $\phi$, the escape time to the right or to the left is practically independent on the amplitude of perturbation for $0.1 < \epsilon < 0.4$, implying that the probability for a trajectory to cross the unperturbed separatrix is almost constant. This fact was mentioned in Ref. [10] and was attributed to the anomalous diffusion in phase space. A detailed analysis of this phenomenon is beyond the scope of the present paper.

The observed directed diffusion depends periodically on the phase $\phi$ of the driving field. After additional averaging over $\phi$ the effect of a macroscopic current vanishes:

$$\langle \dot{V} \rangle_{\phi} = 0.$$  \hfill (7)

Here we discuss three important situations when this averaging occurs.

The first one corresponds to an average over initial times, i.e., when we inject given particle distributions at random initial times. Averaging over initial times equals averaging over the phase. However, if the injection times are correlated (e.g., the injection times are triggered and spaced by a multiple of the period of the field) then directed current will be reinforced. Since even quasiperiodic injection time-sequences will ultimately average over the phase, in reality we simply need finite samples where traveling along the sample takes finite time.

The second example is a spatially inhomogeneous wave [11], for instance,

$$E(t) = \epsilon \sin(kx - \omega t + \phi).$$  \hfill (8)

If we consider two particles with same initial positions and opposite velocities, the average velocity will still be nonzero. However, if we consider a distribution of initial positions, averaging over the initial positions equals averaging over the phase of the individual particle pairs: $\langle \cdot \cdot \cdot \rangle_s = \langle \cdot \cdot \cdot \rangle_{\phi}$. Again the specific asymmetry in the chaotic regime can be detected only for finite samples when the long wave limit is valid.

The third example of complete averaging is a noisy driving force:

$$E(t) = \epsilon \sin(\omega t + \phi) + \epsilon_1 \xi(t),$$  \hfill (9)

where $\xi(t)$ is a white noise with intensity $\epsilon_1$ [12]. The noise also induces an averaging over the phase $\phi$. The larger $\epsilon_1$ the faster is the averaging due to the noise. To avoid that, the characteristic time of the directed diffusion $\tau_D$ must be much smaller than the time scale of the thermal diffusion $\tau_\xi$. In a sample of size $L$ the simplest estimate thus reads

$$\tau_D \approx L/v \ll \tau_\xi.$$  \hfill (10)

Consequently, phase-dependent directed diffusion manifests itself only for finite samples on finite times.

To refine our explanation of the property (7), let us return to the question of the symmetry in the equations of motion. Given a trajectory

$$X(t, x_0, V_0), \ P(t, x_0, V_0)$$  \hfill (11)

of system (1), one more trajectory can be successively generated by the transformations

$$t \to -t: \ X(-t - 2\phi/\omega, x_0, V_0), \ P(-t - 2\phi/\omega, x_0, V_0).$$  \hfill (12)

The absolute value of the time-averaged velocity is the same for both trajectories. For $\phi = \phi_s$, these trajectories ["original" (11) and "generated" (12)] would belong to the above described microcanonical distribution and would cancel each other. For $\phi \neq \phi_s$ the compensation of contributions from different trajectories no longer takes place and we detect directed transport. This is the main reason for the effects described. We need further averaging over $\phi$ in order to ensure cancellation of the contributions coming from Eqs. (11) and (12). If we wish to overcome Eq. (7), we have to break the corresponding symmetry, e.g., by taking either an ac field without reflection symmetry:

$$E(t)_{\text{asym}}(x) = \epsilon \sin(\omega t + \phi) + \beta_x \sin(2[\omega t + \phi] + \nu_x),$$

$$\beta_x < 1; \ \ \ \nu_x \neq \pm \pi k/2$$  \hfill (13)

or combining it with a potential without reflection symmetry [7]

$$U(x)_{\text{asym}} = \sin(x) + \beta_u \sin(2x + \nu_u),$$

$$\beta_u < 1; \ \ \ \nu_u \neq \pm \pi k/2.$$  \hfill (14)

The case of the ac field and the potential without reflection symmetry represents a deterministic counterpart to the stochastic ratchets [6,7], where directed transport is not zero in spite of self-averaging over the phase due to the action of a noisy force. A detailed study of the properties of the field (13) and of the potential (14) can be found in [13].

There exist also examples of quantum particles in tight-binding potentials, for which directed currents do not vanish after averaging over infinitely long time. Consider a tight-binding Hamiltonian in semiclassical approximation

$$H_{\text{tb}} = -\cos(p) - x E(t),$$  \hfill (15)

with the same field $E(t)$ as in Eq. (1). Equation (15) accounts for a periodic potential $U(x)$ via the periodic dispersion relation of quasiparticles $\varepsilon(p) = -\cos(p)$ [3]. Since the
Hamiltonian (15) corresponds to a nonlinear but completely integrable system, we have an explicit expression for the velocity
\[ \dot{x}(t) = \frac{\partial V}{\partial p} = \sin[p_0 + \epsilon \omega (\cos(\phi) - \cos(\omega t + \phi))]. \]
(16)
\[ \langle V(t + p_0) + V(t - p_0) \rangle / 2 = J_0(\epsilon \omega \cos(p_0) \sin(\epsilon \omega \cos(\phi))). \]
(17)
Assuming a Boltzmann distribution for the particles \( F_B = \text{const} \times \exp[-\epsilon(p_0) \beta] \) and integrating over \( p_0 \), the averaged current in the ballistic regime reads [3]
\[ \langle j \rangle = \langle n I_1(\beta) / I_0(\beta) \rangle J_0(\epsilon \omega \sin(\epsilon \omega \cos(\phi))). \]
\[ \langle j \rangle \beta = 0. \]
(18)
Here \( \beta \) is the dimensionless inverse temperature, \( n \) is the particles density, \( I_{0,1} \) are the modified Bessel functions and \( J_0 \) is the Bessel function of zeroth order. At \( \phi = \pi/2 \) we have \( \langle j \rangle = 0 \) as expected [3]. Note that directed currents in similar systems (for fixed \( \phi = \phi_0 \)) have been also found due to dynamical chaos in the selfconsistent evolution or due to mixing of different harmonics of the driving field [14,15], while the current in Eq. (18) is supported by regular dynamics under the action of the one-dimensional field.

To summarize, we have studied directed diffusion in a spatially periodic symmetric potential under the action of a symmetric time-periodic external field. We have shown that the ac field leads to phase-dependent macroscopic transport in finite samples by lowering the dynamical symmetry, even if the potential and the field themselves are reflection symmetric. This flux is fully controlled by the phase of the ac field. For a given amplitude of the ac field the amplitude of the flux is maximized for particle energies closely above the unperturbed separatrix. We have also demonstrated that in sufficiently short samples the dynamical asymmetry is amplified due to chaos, leading to a shift in the phase values where zero current occurs. The maximum of the mean velocity decays as inverse time.

An additionally applied (white) noise gives rise to averaging over the phase resulting in zero currents in the long time limit. However, for a finite sample [see Eq. (10)] one can construct a source of colored noise, which would periodically inject particles into the system. If the injection is in phase with the driving field, it would allow for an experimental observation. Moreover, additional breaking of space- and/or time-reflection symmetry may counteract the self-averaging which otherwise leads to a vanishing mean velocity.

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[9] Anomalous diffusion can be described in the framework of the fractional kinetic equation, which must be used instead of the usual diffusion equation, see, for instance, A.I. Saichev and G.M. Zaslavsky, Chaos 7, 753 (1997).


[12] In general a dissipation term should be included together with the noise to exclude heating. The dissipation has to be rather weak to satisfy the Melnikov criterion [8] so that the chaotic layer persists.

