

Rectification of current in ac-driven nonlinear systems and symmetry properties of the Boltzmann equation

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Abstract. – We study rectification of a current of particles moving in a spatially periodic potential under the influence of time-periodic forces with zero mean value. If certain time-space symmetries are broken, a nonzero directed current of particles is possible. We investigate this phenomenon in the framework of the kinetic Boltzmann equation. We find that the attractor of the Boltzmann equation completely reflects the symmetries of the original one-particle equation of motion. Especially, we analyse the limits of weak and strong relaxation. The dc current increases by several orders of magnitude with decreasing dissipation.

In recent years, a lot of efforts have been devoted to the study of a directed current of particles in a spatially periodic potential under the simultaneous action of an external time-dependent field with zero mean [1]. Most of the previously done work was connected with transport in the presence of a stochastic external field (noise) [2–4]. Another set of problems concerns systems driven by a deterministic periodic force [5–7] with applications to current generation in semiconductor superlattices [8], a free particle moving in a nonNewtonian liquid [9], two-dimensional conducting electron gas in arrays of triangular shaped quantum dots [10], to name a few. For more information, we refer an interested reader to [11].

The model Hamiltonian of a particle of unit mass and its dynamical equation of motion can be written as

$$H = p^2/2 + U(x) - xE(t), \quad \ddot{x} = -U'(x) + E(t). \quad (1)$$

Here U is a spatially periodic potential $U(x) = U(x + 2\pi)$, E is an ac field $E(t) = E(t + T)$ with zero mean value and frequency $\omega = 2\pi/T$.

A recent approach to the problem of current rectification [5] was based on the analysis of symmetries of the dynamical equations of motion with and without additional dissipation. Consider trajectories generated from an ensemble of initial conditions in phase space. A dc current can be calculated by averaging over initial conditions and time. To generate a nonzero

dc current, it is necessary to break all relevant symmetries which are responsible for transforming a trajectory with $x(t; x_0, p_0)$, $p(t; x_0, p_0)$, $x(t_0; x_0, p_0) = x_0$ and $p(t_0; x_0, p_0) = p_0$ into another one with a momentum of the opposite sign. Note that the generated trajectory must belong to the same statistical ensemble. These symmetries can be expressed via combinations of shifts and reflections in time and space (see [5]):

$$\hat{S}_a \begin{bmatrix} x(t; x_0, p_0) \\ p(t; x_0, p_0) \end{bmatrix} = \begin{bmatrix} -x(t + T/2; x_0, p_0) + 2\mathcal{X} \\ -p(t + T/2; x_0, p_0) \end{bmatrix}, \quad (2)$$

$$\hat{S}_b \begin{bmatrix} x(t; x_0, p_0) \\ p(t; x_0, p_0) \end{bmatrix} = \begin{bmatrix} x(-t + 2\tau; x_0, p_0) \\ -p(-t + 2\tau; x_0, p_0) \end{bmatrix}. \quad (3)$$

Here the constants \mathcal{X} and τ are defined by the shape of functions $U(x)$ and $E(t)$ and are in correspondence with the discrete symmetry groups of the Hamiltonian (1). If $U'(x + \mathcal{X}) = -U'(-x + \mathcal{X})$ and $E(t) = -E(t + T/2)$, the dynamical equations of motion are invariant under the symmetry operation \hat{S}_a (this symmetry has also been observed and discussed by Ajdari *et al.* [12] for the overdamped case). On the other hand, if $E(t + \tau) = E(-t + \tau)$, they have \hat{S}_b symmetry (dissipationless case provided). Both symmetries (2)-(3) may be broken by choosing appropriate functions $U(x)$ and $E(t)$.

In the overdamped case, the corresponding dynamical equation $\gamma\dot{x} + U'(x) + E(t) = 0$ may possess the additional symmetry

$$\hat{S}_c \begin{bmatrix} x(t; x_0, p_0) \\ p(t; x_0, p_0) \end{bmatrix} = \begin{bmatrix} x(-t + \tau; x_0, p_0) + \mathcal{X} \\ -p(-t + \tau; x_0, p_0) \end{bmatrix}, \quad (4)$$

provided that $U(x)$ and $E(t)$ possess the following properties: $U'(x) = -U'(x + \mathcal{X})$ and $E(t) = -E(-t + \tau)$. Note that the symmetry \hat{S}_c , if realized, is based on time reversal in the overdamped limit, which is quite unexpected. An independent discovery of this symmetry has been done in [11] (coined ‘‘supersymmetry’’).

The model analysis in [5] does not account for more realistic statistical properties of an ensemble of particles (like thermalization of the distribution). Still, it provides one with a good intuitive understanding of current rectification. On the other hand, a lot of solid-state applications require a more rigorous statistical description of transport properties. The aim of the present paper is to show that the symmetry approach can be applied as well to the classical kinetic Boltzmann equation. We shall show in particular that the attractor of the Boltzmann equation completely reflects the symmetries of the original equation of motion for one particle. The kinetic Boltzmann equation reads (see, for example, [13])

$$\hat{\mathcal{L}}f \equiv \partial_t f + \dot{x}\partial_x f + \dot{p}\partial_p f = \mathcal{J}(f, F), \quad \dot{x} = p, \quad \dot{p} = -U'(x) + E(t). \quad (5)$$

Here $f = f(t, x, p)$ is an unknown distribution function, $F = F(x, p)$ is some equilibrium distribution function chosen as $F(x, p) \equiv F_x(x)F_p(p) = [\exp[-p^2/2]/\sqrt{2\pi}][\exp[-U(x)]/L]$, $L = \int_0^{2\pi} \exp[-U(x)]dx$, and $\mathcal{J}(f, F)$ is a collision integral. Here we apply the momentum-independent single relaxation time approximation (also known as ‘‘ τ -approximation’’) [13]. Thus, the collision integral should be written as $\mathcal{J}(f, F) = -\nu(f - F)$, where ν is the dissipation constant or the characteristic relaxation frequency (ν^{-1} is the relaxation time to equilibrium). This is the simplest form of a collision integral which includes the relaxation to the equilibrium distribution and breaks time-reversal symmetry. We do not intend to discuss its validity for specific physical realizations. Rather, we consider the resulting kinetic equation

as a treatable case which allows us to demonstrate the qualitative features of the dynamical symmetry breaking. Note that for any finite ν , time reversal symmetry is broken, so that we are concerned with \hat{S}_a only. The limit of $\nu \rightarrow 0$ will lead to a restoring of time reversal symmetry (see below) and consequently to a necessary consideration of \hat{S}_b as well. Interestingly, the opposite limit $\nu \rightarrow \infty$ will also induce the symmetry \hat{S}_c .

We start with a perturbative description of the overdamped case when ν^{-1} is the smallest time scale in the system (formally, we put $\nu \gg 1$). We rewrite eq. (5) in the following form:

$$f(x, p, t) = F(x, p) - \nu^{-1} \hat{\mathcal{L}} f(x, p, t). \quad (6)$$

Since ν^{-1} is a small parameter, we expand the unknown function f into a series of ν^{-1} :

$$f(x, p, t) = F(x, p) + \sum_{i=1}^{\infty} (-1)^i \frac{f_i(x, p, t)}{\nu^i}. \quad (7)$$

Collecting terms of the same order, we successively find the increments f_i . The average value of the dc current is calculated using $j_{\text{dc}} = \langle j(t) \rangle_t$, $j(t) = \langle pf(t, x, p) \rangle_{x, p}$, where $\langle \dots \rangle_{x, p, t}$ stands for averaging over the phase space coordinates (x, p) and time, respectively. We expect the attractor of the Boltzmann equation to possess the same symmetries as the corresponding dynamical equations of motion which should be reflected in the vanishing or nonvanishing of j_{dc} . In other words, if the relevant symmetries are broken in the equations of motion [5], we shall observe this fact by analysing the increments f_i . We show this using the model

$$U(x) = U_0 \{1 - \cos x + v_2 [1 - \cos(2x + \theta)]/2\}, \quad (8)$$

$$E(t) = E_1 \cos \omega t + E_2 \cos(2\omega t + \alpha). \quad (9)$$

As already shown in [5], this choice of the potential and external force can break both the symmetries (2)-(3). We apply the perturbation analysis for two specific cases: i) $v_2 \neq 0$, $E_2 = 0$ and ii) $v_2 = 0$, $E_2 \neq 0$. A related overdamped case was discussed in terms of harmonic mixing in [14]. In both the cases, the appropriate time-space symmetries are broken except for specific values of θ and α . As already explained, we need to break only \hat{S}_a , since time reversal and thus \hat{S}_b are already violated for nonzero ν . We find (a more detailed description of these calculations will be reported elsewhere) that the lowest-order increment, which yields a nonzero dc current in the case i), is proportional to ν^{-5} and to the square of the external field $E(t)$:

$$j_{\text{dc}} = -\frac{3}{\nu^5} \langle E^2(t) \rangle_t \langle U'(x) F_x''(x) \rangle_x = -\frac{3}{2\nu^5 L} E_1^2 \int_0^{2\pi} U'''(x) e^{-U(x)} dx. \quad (10)$$

The integral in the last formula cannot be computed analytically. Yet, we find that it is nonzero only when $v_2 \neq 0$ and $\theta \neq 0, \pi$ because otherwise the symmetry of the potential function enforces the vanishing of the above expression. For the case ii) this term equals zero and the first nonzero contribution to the current appears in the seventh order of the perturbation theory. As a result, we obtain the following expression for the dc current:

$$j_{\text{dc}} = -\frac{15}{\nu^7} \langle E^3(t) \rangle_t \langle U'(x) F_x'''(x) \rangle_x = -\frac{45}{4\nu^7} \frac{I_1(U_0)}{I_0(U_0)} E_2 E_1^2 \cos \alpha. \quad (11)$$

Here $I_n(z)$ is the modified Bessel function of n -th order [15]. Note that the averaged current is proportional to $\cos \alpha$ in this case. The symmetry which causes the vanishing of the dc current

for $\alpha = \pm\pi/2$ is \hat{S}_c (see eq. (4)). The above considered case ii) with $\alpha = \pm\pi/2$ satisfies exactly this symmetry. To conclude the consideration of $\nu \gg 1$, we find perfect agreement between the symmetry properties of the dynamical equations of motion and the symmetry properties of the used kinetic equation, resulting in a vanishing or appearance of a dc current.

Let us now investigate the case of intermediate $\nu \sim 1$ and weak $\nu \ll 1$ dissipation. When the characteristic relaxation frequency ν approaches zero, the solution of the kinetic equation is expected to adequately describe the properties of the (microcanonical) ensemble of trajectories in the phase space of the underlying dynamical system. Especially, we expect that if allowed by the choice of the functions $U(x)$ and $E(t)$, the symmetry \hat{S}_b described in detail in [5] should be restored on the attractor of the kinetic equation in the limit $\nu \rightarrow 0$.

The limit of small dissipation appears to be difficult for analytical treatment. We have performed numerical simulations to calculate the dc current in this case. Two independent numerical methods have been used.

The first one (method I) is based on the expansion of the unknown distribution function $f(t, x, p)$ into Hermitian polynomials in p - and Fourier series in x -space. First, we expand f into a series with respect to p :

$$f(t, x, p) = \sum_{n=0}^{\infty} C_n(t, x) |n\rangle, \quad |n\rangle = \frac{H_n(p)}{\pi^{1/4} \sqrt{2^n n!}} e^{-p^2/2}, \quad (12)$$

where $H_n(p)$ are the Hermitian polynomials of the n -th order. Since $U(x)$ and $F(x, p)$ are periodic functions in x , we may expand

$$F(x, p) = \frac{|0\rangle}{\sqrt{2\sqrt{\pi}}} \sum_{m=-\infty}^{\infty} F_m e^{imx}, \quad U(x) = \sum_{m=-\infty}^{\infty} U_m e^{imx}, \quad C_n(t, x) = \sum_{m=-\infty}^{\infty} A_{n,m}(t) e^{imx}. \quad (13)$$

Using $\langle n|n'\rangle = \delta_{n,n'}$ we arrive at the following infinite set of coupled ordinary differential equations for $n \geq 0$:

$$\begin{aligned} \dot{A}_{n,m} + \frac{1}{\sqrt{2}} E(t) (\sqrt{n+1} A_{n+1,m} - \sqrt{n} A_{n-1,m}) + \frac{i}{\sqrt{2}} m (\sqrt{n+1} A_{n+1,m} + \sqrt{n} A_{n-1,m}) - \\ - \frac{i}{\sqrt{2}} \sqrt{n+1} \sum_l l U_l A_{n+1,m-l} + \frac{i}{\sqrt{2}} \sqrt{n} \sum_l l U_l A_{n-1,m-l} = -\nu (A_{n,m} - \delta_{0,n} F_m). \end{aligned} \quad (14)$$

The resulting ODEs for the time-dependent coefficients $A_{n,m}(t)$ are integrated numerically. After a sufficiently large integration time $t \gg \nu^{-1}$, the system will relax into a time-periodic attractor. On this attractor, the induced current is given by

$$\langle p \rangle_{p,x} = 3\sqrt{2}\pi^{1/4} \sum_{n=0}^{\infty} A_{2n+1,0} \frac{\sqrt{(2n)!}}{2^n n!} \sqrt{2n+1}, \quad (15)$$

which can be further averaged over time. Actual computation requires cut-offs in n and m . The results presented below are checked to be independent of the chosen cut-off values. For the following results the cut-off values were $n_{\max} = 60$ and $m_{\max} = 30$.

The second approach (method II) is based on the method of characteristics. Taken an equilibrium distribution at zero time, the solution of the linear kinetic equation with the constant relaxation time can be expressed through the equilibrium distribution function and

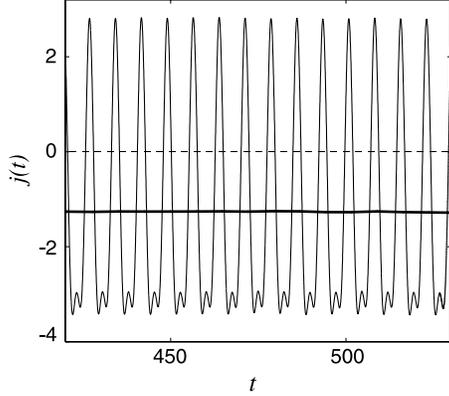


Fig. 1

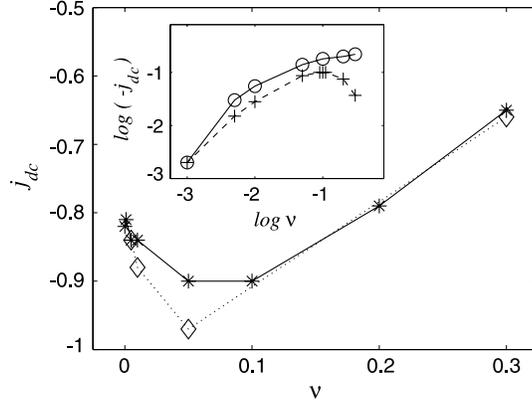


Fig. 2

Fig. 1 – Time dependence of $j(t)$ on the attractor of the kinetic equation (thin solid line). The thick solid horizontal line shows the value of the dc part of $j(t)$. Parameters: $\nu = 0.01$, $\alpha = 1.5$, $v_2 = 0$, $U_0 = 6$, $E_1 = -2.6$, $E_2 = -2.04$, $\omega = 0.85$. The dashed line denotes the reference of $j = 0$.

Fig. 2 – Dependence of the averaged dc current (see text) on the dissipation parameter ν , computed for the case of broken time symmetry using numerical methods I (\diamond) and II ($*$) with parameters as in fig. 1, except for $\alpha = 1$. The inset shows a log-log plot of this dependence with parameters as in fig. 1, except for $\alpha = 0$, (\circ) and $E_2 = 0$, $v_2 = 0.8$, $\theta = 2$ ($+$).

a statistically weighted contribution of the trajectories in the phase space [16]:

$$f(x, p, t) = F \left[\eta_x^{(0)}(t, t_0, x, p), \eta_p^{(0)}(t, t_0, x, p) \right] e^{-\nu(t-t_0)} + \nu \int_{t_0}^t e^{-\nu(t-t')} F \left[\eta_x(t', x, p), \eta_p(t', x, p) \right] dt'. \quad (16)$$

We remind that the functions $\eta_{x,p}^{(0)}$ stand for the inverted equation of a trajectory, *i.e.*, they denote the dependence of the point on a trajectory $\{x, p, t\}$ on its initial conditions; characteristics $\eta_{x,p}$ correspond to the trajectory which passes through the point $\{x, p, t'\}$ in the phase space. For brevity, we put $t_0 = 0$. Since the underlying dynamical system is nonintegrable, we have to find the characteristics numerically. We choose a large random ensemble of initial conditions with $|p_0| < |p_{\max}|$ and use them directly to generate an approximation of $f(x, p, t)$ in accordance with eq. (16). The accuracy of the approximation is controlled by the number of trajectories (initial conditions) used. We used up to 10^5 trajectories to gain good averaging statistics. The net error of calculations was estimated as ~ 10 – 20% for the large relaxation parameter ν or the large dc current j_{dc} , after averaging the current $j(t)$ over several periods T of the field $E(t)$. The maximal error has been detected in those cases when the average dc current tends to zero, for example, when we put $\nu = 0.001$ and $E_2 = 0$ (see inset of fig. 2). In this case the fluctuations of the mean value of the current averaged over several periods T were of the order of residual value of the dc current ($\Delta j_{\text{dc}} \sim |j_{\text{dc}}| = 0.002$ at $\nu = 0.001$ and $E_2 = 0$). In order to achieve the accuracy of the order of $\Delta j_{\text{dc}}/j_{\text{dc}} \sim 1/3$ – $1/2$, we had to perform averaging over hundreds of periods T . Note that method II has some analogy to the direct sampling in classical Monte Carlo simulations.

Method I is an optimal tool for not too small relaxation $\nu \geq 0.01$, while method II shows up with larger errors in calculations, but covers nevertheless the limit of $\nu \rightarrow 10^{-3}$. Both the methods give nearly identical results for $\nu \geq 10^{-2}$ – 10^{-1} .

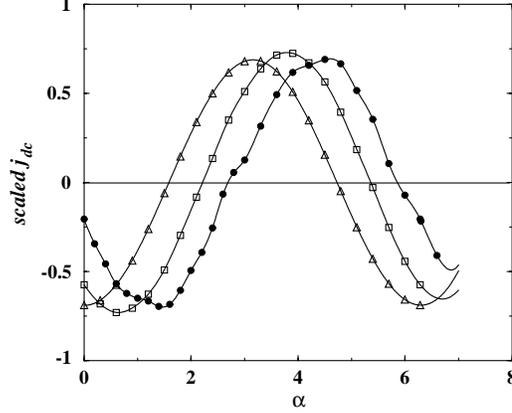


Fig. 3 – Dependence of the averaged dc current on the phase delay parameter α for different values of ν : $\nu = 0.3$ (\bullet), $\nu = 1$ (squares) and $\nu = 4$ (\triangle). Note that the current values are scaled by the factors 4.86 ($\nu = 1$) and 181.6 ($\nu = 4$). The lines connecting the data are splines. Other parameters are as in fig. 1.

Figure 1 displays the time dependence of the full time-dependent current on the attractor of the kinetic equation computed using method II for $\nu = 0.01$. We observe the expected periodic variation in time with a nonzero time-averaged dc current shown by the thick horizontal line. Note that in this case the dc current is of the order of the time-dependent current amplitude (only three times less). This implies that the underdamped case may serve as an ideal testing ground in various applications, since the rectification effect is of the order of 30%.

In fig. 2 we show the dependence of the averaged dc current on the dissipation parameter ν . Results from both the above-described methods are presented. They show data which are similar qualitatively and quantitatively (see the caption for details). Consider the case of $E_2 \neq 0$, $\alpha \neq 0$, $v_2 = 0$. Directed current appears due to a violation of the \hat{S}_a symmetry. When the dissipation ν reaches zero, this symmetry is still broken, however, the dynamical equations of motion may restore a second symmetry, \hat{S}_b . But for the above set of parameters, \hat{S}_b is also violated, and a nonzero dc current should persist down to zero dissipation. This is observed in fig. 2. Suppose now we choose $\alpha = 0$, then \hat{S}_a is still violated, and $j_{dc} \neq 0$ for nonzero dissipation (see inset of fig. 2). However, in the limit of zero dissipation \hat{S}_b is restored: $E(t) = E(-t)$ and our numerical simulations show that the current tends to zero as predicted by symmetry considerations. The same happens in the case of a “ratchet potential”, $v_2 \neq 0$ and without harmonic mixing ($E_2 = 0$). For $\nu \neq 0$ both \hat{S}_a and \hat{S}_b are violated, resulting in a nonzero dc current. Again, the limit of zero dissipation leads to restoring \hat{S}_b . This leads to disappearance of the average dc current at $\nu = 0$ (see inset of fig. 2). Thus, the numerical simulations confirm our expectation that the attractor properties of the kinetic equation reflect the symmetries \hat{S}_a , \hat{S}_b of the underlying dynamical equations for all ν including $\nu \rightarrow 0$.

In fig. 3 we show the dependence of the averaged dc current on the “phase difference” α for three different values of the dissipation parameter $\nu = 4, 1, 0.3$, computed using method I. Note that the currents for $\nu = 4$ and $\nu = 1$ are scaled with factors 181.6 and 4.86, respectively. Consequently, we observe an enhancement of the maximum dc current value by more than two orders of magnitude when going from the overdamped case ($\nu = 4$) to the underdamped one ($\nu = 0.3$). Besides this observation, fig. 3 displays again the consequences of symmetry breaking or restoration. With increasing ν the dc current becomes zero for $\alpha = \pm\pi/2$ which

is a consequence of restoring of \hat{S}_c symmetry. With decreasing ν , we observe the vanishing of the current at $\alpha = 0, \pi$ which is a consequence of restoring the \hat{S}_b symmetry.

Conclusions. – In this paper we extend the symmetry approach for explanation of a dc current in driven nonlinear systems to the framework of the classical kinetic Boltzmann equation. We have analysed separately the cases of large and small dissipation and have demonstrated that the rectification of the current due to nonlinear mixing of harmonics takes place in agreement with the previous symmetry considerations [5]. In particular, it follows that in the limit of small ν , the attractor of the Boltzmann equation (5) reflects the dynamical symmetries of the Newtonian equations of motion [17]. Finally, we observe that a proper choice of the system parameters in the underdamped case ensures the value of the dc current to be of the order of the ac current amplitude. The underdamped case leads to an enhancement of the dc current by several orders of magnitude as compared to the overdamped one.

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- [17] Note that the consideration of a tight-binding model [8] gives zero current in the limit $\nu \rightarrow 0$ and the $\cos \alpha$ dependence (cf. eq. (16)) for all ν due to the presence of an additional symmetry of the case with $\nu = 0$. Details will be published elsewhere.