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

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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 non-zero 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.

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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 non-Newtonian liquid [9], two-dimensional conducting electron gas in arrays of triangular shaped quantum dots [10], to name a few. For more information we refer the interested reader to [11].

The model Hamiltonian of a particle of unit mass and its dynamical equation of motion can be written as:
\[ H = \frac{p^2}{2} + U(x) - xE(t) \ , \ \ddot{x} = -U'(x) + E(t) \ . \]  

(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 non-zero 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 \([5]\)):

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

(2)

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

(3)

Here the constants \( \mathcal{X} \) and \( \tau \) 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 been also 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

\[ \gamma \ddot{x} + U'(x) + E(t) = 0 \ , \]

(4)

may possess an additional symmetry
\[
\mathbf{S}_c \left[ \begin{array}{c}
 x(t; x_0, p_0) \\
 p(t; x_0, p_0)
\end{array} \right] = 
\left[ \begin{array}{c}
 x(-t + \tau; x_0, p_0) + \mathcal{X} \\
 -p(-t + \tau; x_0, p_0)
\end{array} \right],
\]

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 \( \mathbf{S}_c \) 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 will 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])

\[
\hat{\mathcal{L}} f \equiv \partial_t f + \dot{x} \partial_x f + \dot{p} \partial_p f = \mathcal{J}(f, F),
\]

\[
\dot{x} = p, \quad \dot{p} = -U'(x) + E(t).
\]

Here \( f \equiv f(t, x, p) \) is an unknown distribution function, \( F \equiv F(x, p) \) is some equilibrium distribution function chosen as:

\[
F(x, p) \equiv F_x(x)F_p(p) = \frac{e^{-p^2/2} e^{-U(x)}}{\sqrt{2\pi} L}, \quad L = \int_0^{2\pi} e^{-U(x)} dx,
\]

and \( \mathcal{J}(f, F) \) is a collision integral. Here we apply the momentum independent single relaxation time approximation (also known as “\( \tau \)-approximation”) [13]. Thus, the collision integral should be written as

\[
\mathcal{J}(f, F) = -\nu(f - F)
\]

where \( \nu \) is the dissipation constant or the characteristic relaxation frequency (\( 1/\nu \) is the relaxation time to the equilibrium state). This is the simplest form of a collision integral which
includes 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 dynamical symmetry breaking. Note that for any finite $\nu$ time reversal symmetry
is broken, so that we are concerned with $\hat{S}_a$ only. The limit of $\nu \to 0$ 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 $\nu \to \infty$ will also induce a symmetry $\hat{S}_c$.

We start with a perturbative description of the overdamped case when $1/\nu$ is the smallest
time scale in the system (formally, we put $\nu \gg 1$). We rewrite Eq. (6) in the following form

$$f(x,p,t) = F(x,p) - \frac{1}{\nu} \hat{L} f(x,p,t). \quad (10)$$

Since $1/\nu$ is a small parameter here, we expand the unknown function $f$ into a series in
terms of $1/\nu$:

$$f(x,p,t) = F(x,p) + \sum_{i=1}^{\infty} (-1)^i \frac{\hat{f}_i(x,p,t)}{\nu^i}. \quad (11)$$

Collecting terms of the same order, we successively find the increments $f_i$. The average
value of the dc current is calculated using

$$j_{dc} = \langle j(t) \rangle_t, \quad j(t) = \langle p f(t,x,p) \rangle_{x,p}, \quad (12)$$

where $\langle ... \rangle_{x,p,t}$ stands for averaging over the phase space coordinates $(x,p)$ and time
correspondingly. 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 $[3]$, we will observe this fact by analysing the increments $f_i$. We
show this using the following model

$$U(x) = U_0 \left\{ 1 - \cos x + \frac{v_2}{2} [1 - \cos(2x + \theta)] \right\}, \quad (13)$$

$$E(t) = E_1 \cos \omega t + E_2 \cos(2\omega t + \alpha). \quad (14)$$
As it was already shown in the previous work \cite{5}, this choice of the potential and external force can break both 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 \cite{14}. In both cases the appropriate time-space symmetries are broken except for specific values of $\theta$ and $\alpha$. As already explained, we need to break only $\hat{S}_a$ since time reversal and thus $\hat{S}_b$ are already violated for nonzero $\nu$. We find (a more detailed description of these calculations will be reported elsewhere) that the lowest order increment which yields a non-zero dc current in case (i) is proportional to $1/\nu^5$ and to the square of the external field $E(t)$:

$$j_{dc} = -\frac{3}{\nu^5} \langle E^2(t) \rangle \langle U''(x)F''_x(x) \rangle_x = -\frac{3}{2\nu^5} E_1^2 \int_0^{2\pi} U'''(x)e^{-U(x)} dx . \quad (15)$$

The integral in the above formula cannot be computed analytically. Yet we find that it is non-zero 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 non-zero contribution to the current appears in seventh order of the perturbation theory. As a result we obtain the following expression for the dc current

$$j_{dc} = -\frac{15}{\nu^7} \langle E^3(t) \rangle \langle U''(x)F''''_x(x) \rangle_x = -\frac{45}{4\nu^7} \frac{I_1(U_0)}{I_0(U_0)} E_2 E_1^2 \cos \alpha . \quad (16)$$

Here $I_n(z)$ is the modified Bessel function of $n$th order \cite{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. (3)]. 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 $\nu$ 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 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 of $\nu \to 0$.

The limit of small dissipation appears to be difficult to be treated analytically. We have used 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 w.r.t. $p$:

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

(17)

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

$$F(x, p) = \frac{|0\rangle}{2^{1/4} \pi^{1/4}} \sum_{m=-\infty}^{\infty} F_m e^{imx} , \quad U(x) = \sum_{m=-\infty}^{\infty} U_m e^{imx} , \quad C_n(t, x) = \sum_{m=-\infty}^{\infty} A_{n,m}(t)e^{imx}.$$  

(18)

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

$$\dot{A}_{0,m} + \frac{1}{\sqrt{2}} E(t)A_{1,m} - \frac{i}{\sqrt{2}} \sum_l lU_l A_{n,m-l} + \frac{i}{\sqrt{2}} mA_{1,m} = -\nu(A_{0,m} - F_m)$$

(19)

and $n > 0$

$$\dot{A}_{n,m} + \frac{1}{\sqrt{2}} E(t)(\sqrt{n+1}A_{n+1,m} - \sqrt{n}A_{n-1,m}) + \frac{i}{\sqrt{2}} m(\sqrt{n+1}A_{n+1,m} + \sqrt{n}A_{n-1,m}) -$$

$$\frac{i}{\sqrt{2}} \sqrt{n+1} \sum_l lU_l A_{n+1,m-l} + \frac{i}{\sqrt{2}} \sqrt{n} \sum_l lU_l A_{n-1,m-l} = -\nu A_{n,m}.$$  

(20)

The resulting ODEs for the time-dependent coefficients $A_{n,m}(t)$ are integrated numerically. After a sufficiently large integration time $\gg 1/\nu$ the system will relax into a time-periodic attractor. On this attractor the induced current is given by
\[
\langle p \rangle_{p,x} = 3\sqrt{2\pi}^{1/4}\sum_{n=0}^{\infty} A_{2n+1,0}\frac{\sqrt{(2n)!}}{2^n n!} \sqrt{2n + 1}
\]

which can be further averaged over time. Actual computation requires cutoffs in \(n\) and \(m\). Results presented below are checked to be independent on the chosen cutoff values. For the following results the cutoff values were \(n_{\text{max}} = 60\) and \(m_{\text{max}} = 30\).

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

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

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 also \(t_0 = 0\). Since the underlying dynamical system is non-integrable we have to find the characteristics numerically. We choose a large random ensemble of initial conditions with \(|p_0| < |p_{\text{max}}|\) and use them directly to generate an approximation of \(f(x, p, t)\) in accordance with Eq. (22). 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 \(\sim 10 - 20\%\) for large relaxation parameter \(\nu\) or large dc current \(j_{dc}\) after averaging of 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 \((\Delta j_{dc} \sim |j_{dc}| = 0.002\) at \(\nu = 0.001\) and \(E_2 = 0\)). In order to achieve the accuracy of the order of \(\Delta j_{dc}/j_{dc} \sim 1/3 \div 1/2\) 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 \( \nu \to 10^{-3} \). Both methods give nearly identical results for \( \nu \geq 10^{-2} \div 10^{-1} \).

Fig. 1 displays the dependence of the full time-dependent current on time on the attractor of the kinetic equation computed with the help of method II for \( \nu = 0.01 \). We observe the expected periodic variation in time, with a nonzero time averaged dc current indicated 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 percent.

![Graph showing time dependence of j(t) on the attractor of the kinetic equation.](image)

**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: \( \nu = 0.01, \alpha = 1.5, \nu_2 = 0, U_0 = 6, E_1 = -2.6, E_2 = -2.04, \omega = 0.85 \). The dashed line denotes the reference of \( j = 0 \).

In Fig. 2 we show the dependence of the averaged dc current on the dissipation parameter \( \nu \). Results from both above described methods are presented. They show data which are similar qualitatively and quantitatively (see the caption for details).
FIG. 2. Dependence of the averaged dc current \( J_{dc} \), on the dissipation parameter \( \nu \), computed for the case of broken time symmetry using numerical methods I (\( \diamond \)) and II (\( * \)) with parameters as in Fig. 1 except \( \alpha = 1 \). The inset shows a log-log plot of this dependence with parameters as in Fig. 1 except \( \alpha = 0 \) (\( \circ \)) and \( E_2 = 0, v_2 = 0.8, \theta = 2 \) (\( + \)).

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 \( \nu \) 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 non-zero 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 non-zero 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 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 a restoring of \( \hat{S}_b \). This leads to a 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 \( \nu \) including \( \nu \rightarrow 0 \).
In Fig. 3 we show the dependence of the averaged dc current on the “phase difference” \( \alpha \) for three different values of the dissipation parameter \( \nu = 4, 1, 0.3 \), computed with the help of 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 restoral. With increasing \( \nu \) the dc current becomes zero for \( \alpha = \pm \pi/2 \) which is a consequence of restoring of \( \hat{S}_c \) symmetry. With decreasing \( \nu \) we observe a vanishing of the current at \( \alpha = 0, \pi \) which is a consequence of restoring of the \( \hat{S}_b \) symmetry.

FIG. 3. Dependence of the averaged dc current on the phase delay parameter \( \alpha \) for different values of \( \nu \): \( \nu = 0.3 \) (filled circles), \( \nu = 1 \) (squares) and \( \nu = 4 \) (triangles). Note that the current values are scaled by a factor of 4.86 (\( \nu = 1 \)) and 181.6 (\( \nu = 4 \)). The lines connecting the data are splines. Other parameters are as in Fig. 1.

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 current due to nonlinear mixing of harmonics takes
place in agreement with previous symmetry consideration [5]. In particular, it follows that in the limit of small $\nu$ the attractor of the Boltzmann equation (6-7) 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 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 gives zero current in the $\nu \to 0$ limit and $\cos \alpha$ dependence [cf. (16)] for all $\nu$ due to the presence of an additional symmetry of the $\nu = 0$ case. Details will be published elsewhere.