Expectation values of general observables in the Vlasov formalism

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Abstract. Collisionless plasmas in an arbitrary dynamical state are described by the Vlasov equation, which gives the time evolution of the probability density $\rho(x,v)$. In this work we introduce a new analytical procedure to generate particular partial differential equations (PDEs) for an arbitrary macroscopic observable $w(x,v)$ that can be expressed as a function of positions and velocities, without solving the time evolution of the probability itself. This technique, which we will call the “Ehrenfest procedure” (as it produces relations that are analogous to Ehrenfest’s theorem in Quantum Mechanics), is based on the iterative application of the fluctuation-dissipation theorem and the recently proposed conjugate variables theorem (CVT) in order to eliminate the explicit dependence on $\rho$. In particular, we show how this formalism is applied to the Vlasov equation for collisionless plasmas, and derive a general evolution equation for the fluctuations of any macroscopic property $w$ in this kind of plasma.

1. Introduction
The standard treatment of nonequilibrium systems in Statistical Mechanics involves the solution of a partial differential equation (PDE) for the time-dependent probability density of microstates of the system. This is a formidable problem for systems with large number of degrees of freedom, and most of the time it is approximated using numerical methods on a discretized time and space grid. After one solves for the probability density, it is possible to take expectations to compute the nonequilibrium values of macroscopic quantities.

An interesting problem in plasma physics approached from the point of view of Statistical Mechanics is to obtain properties of collisionless plasmas [1] which are described by the Vlasov equation. This equation is a particular case of the Liouville theorem of conservation of the volume of phase space,

$$\frac{\partial \rho}{\partial t} + \{\rho, H\} = 0. \quad (1)$$

where $\rho(x,t)$ is the time-dependent probability density of microstates $x$. In the particular case of collisionless plasma, the Hamiltonian involves kinetic terms and the interaction of charged particles with electromagnetic fields, and Liouville’s theorem becomes the Vlasov equation

$$\frac{\partial \rho}{\partial t} + v \cdot \nabla_x \rho + \frac{q}{m} (E + \frac{1}{c} v \times B) \cdot \nabla_v \rho = 0. \quad (2)$$
This equation is used to model collisionless plasmas out of equilibrium, where the force on each particle is given by the Lorentz force, with time-dependent electric and magnetic fields $E(r,t)$ and $B(r,t)$ respectively, and where those $E$ and $B$ are consistent with Maxwell’s equations.

There is no general analytical solution to this problem for arbitrary electromagnetic fields (or arbitrary charge and current densities) and the numerical methods are extremely expensive in terms of computational cost, as they require the discretization of space and time with a grid size as small as the desired resolution, which depends on the highest frequency of modes of oscillation in the plasma, typically the frequency associated with the electrons [2].

In this work we show a general formalism that allows the construction of the particular PDE associated to an arbitrary, time-dependent macroscopic property $w(r,v,t)$ from the original PDE describing the time evolution of the probability density $\rho$. The development of this procedure, which we will call the “Ehrenfest procedure” (in reference to the Ehrenfest theorem in Quantum Mechanics), requires the application of two mathematical identities of probability theory, namely the fluctuation-dissipation theorem and the conjugate variable theorem, which we will introduce in the next section.

2. Mathematical Tools
As we have explained in the previous section, the objective of this procedure is to move from the problem of solving a PDE for the probability density function to the (usually much simpler) problem of solving a PDE for one of its macroscopic properties. In order to achieve this, we will employ two theorems of probability theory for continuous variables, that are of general validity. These are the Fluctuation-Dissipation Theorem (FDT) and the recently introduced Conjugate Variable Theorem (CVT), which will be used to eliminate the explicit dependence of the probability density function from the PDEs to be solved. In the following we will review the mathematical statement of these theorems.

2.1. Fluctuation-Dissipation Theorem
According to the definition of expectation, any time-dependent macroscopic property $W_t$ can be written as

$$W_t = \langle w(x,t) \rangle_t = \int dx \rho(x,t) w(x,t), \tag{3}$$

where $w(x,t)$ is a macroscopic property, $\rho(x,t)$ is the probability density function and $x = (x^1, x^2, ..., x^n)$ is an instantaneous state of the system. The subindex $t$ in the expectation $< \cdot >_t$ and $W_t$ indicates the temporal dependence of those quantities. Taking partial derivatives of the definition of expectation with respect to time we get

$$\frac{\partial}{\partial t} \langle w(x,t) \rangle_t = \int dx [w(x,t) \frac{\partial}{\partial t} \rho(x,t) + \rho(x,t) \frac{\partial}{\partial t} w(x,t)],$$

and rewriting $\frac{\partial \rho(x,t)}{\partial t}$ as $\rho(x,t) \frac{\partial}{\partial t} \ln \rho(x,t)$ is possible to rewrite each term as an expectation. This leads to the so-called fluctuation-dissipation theorem,

$$\frac{\partial}{\partial t} \langle w(x,t) \rangle_t - \langle \frac{\partial}{\partial t} w(x,t) \rangle_t = \langle w(x,t) \frac{\partial}{\partial t} \ln \rho(x,t) \rangle_t. \tag{4}$$

This identity is valid for any expectation that depends parametrically on variables, as in this case the time $t$. 
2.2. Conjugate Variable Theorem
In a similar way to the FDT, we can construct an identity involving spatial derivatives of an arbitrary observable \( w(x, t) \) and of the probability density \( \rho(x, t) \), the recently introduced conjugate variables theorem \[3\]. Its \( N \)-dimensional version reads
\[
\left\langle \nabla \cdot w(x, t) \right\rangle = -\left\langle w(x, t) \cdot \nabla \ln \rho(x, t) \right\rangle,
\]
where \( \nabla = \frac{\partial}{\partial x_i} \hat{x}_i \) and \( w(x, t) \) is a macroscopic vector property dependent of the state of the system and time.

Both theorems (FDT and CVT) are expectation identities which are valid for states arbitrarily far from equilibrium, and they connect arbitrary expectations involving \( w(x, t) \) and their derivatives, with expectations that include derivatives of \( \ln \rho(x, t) \). In the following we will use this interesting feature of these theorems in order to produce differential equations for the expectation of \( w(r, v, t) \), where we consider the state space as \( x = r \otimes v \).

3. Ehrenfest Procedure
Now we are able to present the analytical procedure that we will call the “Ehrenfest procedure”, first employed in Ref. \[4\]. The idea is to obtain a PDE for the time-dependent expectation \( \left\langle w \right\rangle_t \) of a macroscopic quantity \( w(x, t) \) from the original PDE for the probability density \( \rho(x, t) \).

In order to fix ideas, we will demonstrate the procedure on the Vlasov equation, which is a PDE for \( \rho(r, v, t) \) of the form
\[
\frac{\partial \rho}{\partial t} + v \cdot \nabla_r \rho + \frac{F}{m} \cdot \nabla_v \rho = 0,
\]
where \( \rho = \rho(x, t) \) with \( x = r \otimes v \) and \( F \) is the Lorentz force, given by \( F = q(E + \frac{1}{c}v \times B) \).

The procedure is divided in three stages. First, we rewrite the PDE for \( \rho \) as a PDE for \( \ln \rho \) by using the relations
\[
\frac{\partial}{\partial t} \rho = \rho \frac{\partial}{\partial t} \ln \rho,
\]
\[
\nabla_x \rho = \rho \nabla_x \ln \rho.
\]

Once we have put the original PDE in logarithmic form,
\[
\rho \frac{\partial}{\partial t} \ln \rho + \rho v \cdot \nabla_x \ln \rho + \rho \frac{F}{m} \cdot \nabla_v \ln \rho = 0.
\]
we introduce expectations by applying the operator \( \int d\text{d}r\text{d}v w \cdot \) with the test function \( w(x, v, t) \) defined over the state space) and using the definition of expectation,
\[
\left\langle w(r, v, t) \right\rangle_t = \int d\text{d}r\text{d}v w(r, v, t) \rho(r, v, t),
\]
we obtain
\[
\int d\text{d}r\text{d}v \rho \left[ w \frac{\partial}{\partial t} \ln \rho + wv \cdot \nabla_x \ln \rho + w \frac{F}{m} \cdot \nabla_v \ln \rho \right] = 0,
\]
that is,
\[
\left\langle w \frac{\partial}{\partial t} \ln \rho + wv \cdot \nabla_x \ln \rho + w \frac{F}{m} \cdot \nabla_v \ln \rho \right\rangle = 0.
\]
Finally, we use CVT and FDT to eliminate \( \ln \rho \) from each expectation, in order to reduce them to expectations involving derivatives (spatial or temporal) of \( w \). More precisely, we eliminate \( \partial_t \ln \rho \) using the FDT, and \( \nabla \ln \rho \) using CVT. In this case, we obtain

\[
\frac{\partial}{\partial t} \langle w \rangle_t = \left\langle \frac{\partial w}{\partial t} + \partial_x (w v) + \partial_v (w \frac{F}{m}) \right\rangle,
\]

which can be expanded as

\[
\frac{\partial}{\partial t} \langle w \rangle_t = \left\langle \frac{\partial w}{\partial t} \right\rangle_t + \left\langle v \partial_x w + w \partial_v v \right\rangle_x + \left\langle \frac{F}{m} \partial_v w + w \partial_v \frac{F}{m} \right\rangle_v.
\]

(12)

Here we notice that we can simplify this result even further. As \( v \) is not dependent of \( x \) (\( \nabla_x v = 0 \)) and for the case of the Lorentz force \( \nabla_v \cdot F = 0 \), we arrive at our main result, which is a PDE for an arbitrary property \( \langle w \rangle_t \),

\[
\frac{\partial}{\partial t} \langle w \rangle_t = \left\langle \frac{\partial w}{\partial t} \right\rangle_t + \left\langle v \cdot \partial_x w \right\rangle_t + \left\langle \frac{F}{m} \cdot \partial_v w \right\rangle_t.
\]

(13)

This resembles a classical analog of Ehrenfest’s theorem in Quantum Mechanics [5],

\[
\frac{d}{dt} \langle \hat{\Omega} \rangle = \left\langle \frac{\partial \hat{\Omega}}{\partial t} \right\rangle - \frac{i}{\hbar} \left\langle \left[ \hat{\Omega}, \hat{H} \right] \right\rangle.
\]

(14)

where the Poisson bracket has to be used instead of the quantum-mechanical commutator.

**4. Results**

Using the main result of this work, namely Eq. 13, it is possible to obtain the PDE for the fluctuations of an arbitrary quantity \( w(r, v, t) \). We will illustrate this by considering the velocity fluctuations \( \langle (\delta v)^2 \rangle_t \), and for this we will use \( v = v \) and \( w = v^2 \) separately in Eq. 13. First, we obtain the time evolution of \( v \) as

\[
\frac{\partial}{\partial t} \langle v \rangle_t = \left\langle \frac{\partial v}{\partial t} \right\rangle_t + \left\langle v \partial_x v \right\rangle_t + \left\langle \frac{F}{m} \partial_v v \right\rangle_t,
\]

(15)

but \( \partial_t v = 0 \) and \( \partial_x v = 0 \), so we simplify it as

\[
\frac{\partial}{\partial t} \langle v \rangle_t = \left\langle \frac{F}{m} \right\rangle_t.
\]

(16)

This has a clear meaning: the change in the mean value of the velocity is given by the mean acceleration. Now, we obtain the evolution equation for \( w = v^2 \),

\[
\frac{\partial}{\partial t} \langle v^2 \rangle_t = \frac{2}{m} \left\langle F \cdot v \right\rangle_t.
\]

(17)

We can join Eqs. 16 and 17 by taking

\[
\frac{\partial}{\partial t} \langle (\delta v)^2 \rangle_t = \frac{\partial}{\partial t} \langle v^2 \rangle_t - 2 \langle v \rangle_t \cdot \frac{\partial}{\partial \langle v \rangle_t} \langle v \rangle_t,
\]

(18)

and we can write a PDE for \( \langle (\delta v)^2 \rangle_t = \langle v^2 \rangle_t - \langle v \rangle_t^2 \) of the form

\[
\frac{\partial}{\partial t} \langle (\delta v)^2 \rangle_t = \frac{2}{m} \left\{ \langle q E \cdot v \rangle_t - \langle v \rangle_t \langle qE \rangle - \frac{q}{c} \langle v \times B \rangle \langle v \rangle_t \right\}.
\]

(19)

Here is interesting to note that, for the case where electromagnetic fields \( E \) and \( B \) are spatially homogeneous, the right-hand side vanishes and we have that the size of the velocity fluctuations is kept constant in time.
5. Concluding remarks

We have shown the application of our “Ehrenfest procedure” to the Vlasov equation for collisionless plasmas. Our main result here was a general relation, Eq. 13, which gives the time evolution of any macroscopic property in a Vlasov system. From the general Ehrenfest relation we have derived the partial differential equation for the velocity fluctuations, Eq. 19, which indicates that for a collisionless plasma under spatially homogeneous electromagnetic fields, its initial velocity distribution does not widen with time. We can see that the Ehrenfest procedure is a general tool applicable whenever we have a system that follows a continuity equation for probability. It allows to quickly obtain dynamical evolution equations for particular properties, and thus appears as a powerful addition to the study of dynamical systems and non-equilibrium Statistical Mechanics.

Testing of Eq. 13 and 19 on different configurations of fields remains as future work, to be connected with numerical simulations of Vlasov systems.

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