Variational formulation of the Vlasov equation

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Abstract. A new variational framework for the Liouville equation is presented. The Vlasov equation is obtained from the complete factorisation of the trial distribution function, while the linearised Vlasov equation arises from the additional assumption of small oscillations around an equilibrium state. It is stressed that the definition of this state does not necessarily require minimisation of the free energy. The classical energy-weighted sum rule is derived.

1. Introduction

The Vlasov equation, since its initial formulation in 1938 [1], has been extensively applied in plasma physics. Recently it has been introduced into nuclear physics, after the recognition that the main features of collective motions, such as nuclear vibrations and deep inelastic reactions, could be suitably described within a classical phase space [2]. It is well known that the Vlasov equation corresponds to a one-particle reduction of the Liouville dynamics.

We have proposed in [3] a variational approach to the quantum mechanical Liouville-von Neumann equation. Our method contrasts with that proposed by Balian and Veneroni [4, 5] in that it does not aim to obtain the best expectation value of a given observable at a certain time but only pretends to approach variationally the Liouville-von Neumann equation. Therefore, instead of having both density matrices and observables as variational objects—a procedure which in the most general situation gives rise to redundant dynamics (Liouville-von Neumann and backward Heisenberg equations of motion)—we concentrate solely on density matrices. We believe this less ambitious approach helps the quantum statistical variational principle to become more transparent.

Balian and Veneroni have stated in [5] that their formalism, using two variational operators which are duals of each other, has an obvious translation in classical statistical mechanics. In the present work we discuss the classical counterpart of the simpler formulation presented in [3], where the variations are restricted to density matrices. Nevertheless, this cannot be directly obtained by a mapping of the Wigner-Kirkwood type from the Lagrangian of [3], some modification of the action principle being required.

Starting from a convenient action principle, we derive in this work the Liouville equation for the distribution function of a general many-particle system.

The technique of Lagrange multipliers is involved, in a very similar way to the general process of constructing variational principles discussed in [6]. The procedure used in [6] relies on incorporating defining equations through the use of generalised Lagrange multipliers, which may be functions or operators.

Restrictions in the variational family of distribution functions lead to manageable approximations to the classical many-body dynamics. The Vlasov equation, corresponding to uncorrelated single-particle motion, is readily obtained in our framework, as well as its linearised version. We sketch the main steps of the derivation, since we believe this is useful to illustrate the role of the generalised Lagrange multipliers.

We remark that the derivation presented is, in principle, independent of any quantal formalism and holds whether a quantal treatment is relevant or not.

In § 2 we introduce the general formalism. The static solution and the small-amplitude oscillations around it are considered in particular.

In § 3, the independent-particle approximation is shown to lead to the Vlasov equation for the single-particle distribution function. The linear response around equilibrium is treated just for the sake of completeness, although the result is known. The nature of equilibrium is discussed. The static solution, which should be associated with the so-called 'passive states' of quantum statistical mechanics [7, 8], does not need to be a thermal equilibrium state, since the static limit of our procedure is more general than the usual minimisation of a thermodynamical potential. The classical energy-weighted sum rule is derived at the end of this section.

The conclusions are collected in § 4, where possible applications are also referred to.

2. General formalism

2.1. Variational approach to the Liouville equation

It is well known that the time-dependent Schrödinger equation for a system described by the Hamiltonian H may be obtained from the variational principle

$$\delta \int_{t_1}^{t_2} L \, dt = 0 \tag{2.1}$$

where the Lagrangian L is given by

$$L = \langle \Psi | i \, d/dt - H | \Psi \rangle \tag{2.2}$$

$|\Psi\rangle$ denoting the time-dependent state vector.

For physical situations requiring the use of mixed states we accept that the evolution of the density matrix is adequately described by the Liouville–von Neumann equation

$$\dot{D} = -i[H, D]. \tag{2.3}$$

As we have shown in [3], this equation may be derived from a variational principle (2.1), provided the Lagrangian is given by

$$L = -i \, \mathrm{Tr}(U D_0 \dot{U}^+) - \mathrm{Tr}(U D_0 U^+ H) \tag{2.4}$$

where D is a fixed (time-independent) density matrix and $U = U(t)$ a time-dependent unitary operator. We may write U in the form $U = \exp(iS)$, $S = S(t)$ being a time-dependent Hermitian operator.

The manipulations required to derive (2.3) from (2.1) and (2.4) rely heavily on the expression of the trial density matrix D

$$D(t) = U(t) D_0 U(t)^+. \tag{2.5}$$

The time dependence of $D(t)$ is introduced through the unitary operator $U(t)$.

In the classical case it is not convenient to use the classical counterpart of the operator U as a variational field, so that the variational formulation should be modified in order to describe the evolution in phase space.

At this point we introduce the set Λ of all distribution functions $F = F(x_1, p_1, \ldots, x_N, p_N)$ of a given N-particle system, which may be obtained from a particular distribution function F_0 by a canonical transformation

$$\Lambda = \left\{ F \colon F = F_0 + \{S, F_0\} + \frac{1}{2!}\{S, \{S, F_0\}\} + \ldots \right\} \tag{2.6}$$

with $S = S(x_1, p_1, \ldots, x_N, p_N)$ a real function. Here $\{A, B\}$ denotes the Poisson bracket between the functions A and B. Let $F = F(x_1, p_1, \ldots, x_N, p_N, t)$ be a trial distribution function belonging to the set Λ for each value of t. Then there exists a generator G such that

$$\dot{F} = \{G, F\}. \tag{2.7}$$

From (2.6) we conclude that the generator G is conveniently given by the following expression:

$$G = \dot{S} + \frac{1}{2!}\{S, \dot{S}\} + \frac{1}{3!}\{S, \{S, \dot{S}\}\} + \ldots. \tag{2.8}$$

The following Lagrangian is considered:

$$L = \int FG \, d\Gamma_{1-N} - \int FH \, d\Gamma_{1-N} \tag{2.9}$$

where

$$d\Gamma_{1-N} = d\Gamma_1 \ldots d\Gamma_N = d^3x_1 \, d^3p_1/(2\pi)^3 \ldots d^3x_N \, d^3p_N/(2\pi)^3$$

is the integral element in phase space and H is the classical Hamiltonian of the system.

We restrict the variations of F to the set Λ and impose (2.7) as a subsidiary condition using the technique of Lagrange multipliers.

We shall show in the following that an action principle based on the Lagrangian (2.9) leads to the Liouville equation

$$\dot{F} = \{H, F\} \tag{2.10}$$

that is, that the exact generator G coincides with the Hamiltonian H (see (2.7)).

The variations δF and δG are not independent of each other, due to the relation indicated by (2.7) which must be satisfied at all times. This constraint is imposed with the aid of a generalised Lagrange multiplier $A = A(x_1, p_1, \ldots, x_N, p_N, t)$, which is a real function of all the phase-space variables and of the time.

The following generalised action is therefore considered:

$$I = \int_{t_1}^{t_2} dt \left(L - \int d\Gamma_{1-N} A(\dot{F} - \{G, F\}) \right) \tag{2.11}$$

where L is given by (2.9). This action should be made stationary with respect to arbitrary variations of F and G at intermediate instants of time between t_1 and t_2.

The variation of (2.11) yields

$$\delta I = \int_{t_1}^{t_2} dt \int d\Gamma_{1-N} [\delta FG + F\delta G - \delta FH - A(\delta\dot{F} + \{\delta F, G\} + \{F, \delta G\})] = 0. \tag{2.12}$$

The term involving $\delta\dot{F}$ may be integrated by parts, giving

$$-\int_{t_1}^{t_2} dt \int d\Gamma_{1-N}(A\delta\dot{F}) = -\int d\Gamma_{1-N}(\delta F A)\Big|_{t_1}^{t_2} + \int_{t_1}^{t_2} dt \int d\Gamma_{1-N}(\dot{A}\delta F). \qquad (2.13)$$

We impose the following condition at the endpoints:

$$\int d\Gamma_{1-N}(\delta F(t_1)A(t_1)) = \int d\Gamma_{1-N}(\delta F(t_2)A(t_2)) \qquad (2.14)$$

in order that the first term of (2.13) vanishes.

Since the variations δF and δG are arbitrary for intermediate times $(t_1 < t < t_2)$, we arrive at the following Euler-Lagrange equations:

$$G - H + \dot{A} - \{G, A\} = 0 \qquad (2.15)$$

$$F - \{A, F\} = 0. \qquad (2.16)$$

From (2.15) we obtain

$$\{F, G - H + \dot{A} - \{G, A\}\} = 0. \qquad (2.17)$$

We observe that $\{F, \{G, A\}\}$ may be transformed, using the Jacobi identity, (2.7) and (2.16), to give

$$\{F, \{G, A\}\} = -\{G, \{A, F\}\} - \{A, \{F, G\}\}$$
$$= -\{G, F\} + \{A, \dot{F}\}$$
$$= -\dot{F} + \{A, \dot{F}\}. \qquad (2.18)$$

Thus

$$\{F, G - H\} + (\{F, \dot{A}\} + \dot{F} - \{A, \dot{F}\}) = 0. \qquad (2.19)$$

From (2.16) it follows that

$$\dot{F} - \{\dot{A}, F\} - \{A, \dot{F}\} = 0 \qquad (2.20)$$

and therefore (2.19) leads to

$$\{F, G - H\} = 0. \qquad (2.21)$$

Inserting (2.21) in (2.7), (2.10) is obtained as desired.

A comment about the condition (2.14) is appropriate here. This condition enables us to disregard the endpoint contribution to the variation of the action.

Since we are only considering an action integral with the purpose of obtaining an equation of motion for the distribution function and the actual value of the action is irrelevant, we may add to the Lagrangian a term which is a total time derivative. The term

$$\frac{d}{dt}\int d\Gamma_{1-N}(A(t)F(t)) \qquad (2.22)$$

will cancel the endpoint contribution represented by the first term on the RHS of (2.13). The condition (2.14) may be imposed without any loss of generality, since in our formalism it is innocuous. On the contrary, the boundary conditions discussed by Balian and Veneroni in [5] are physically relevant. That there are two boundary conditions is related to the fact that two equations of motion arise in their formulation, duplicating the dynamical description when no limitations on the variations are made.

We emphasise the essential conceptual difference between the goal of our variational principle and that of Balian and Veneroni, which has a price to pay for being more ambitious, namely boundary conditions must be incorporated in the Lagrangian. Although with $G = H$ (2.9) looks similar to the classical image of equation (3.1) of [5], we should note that in the present work A does not correspond to a physical observable but is only a convenient mathematical object. Moreover, we do not *a priori* identify G with H.

2.2. Static case

From the Liouville equation (2.10) it follows that a state of equilibrium, characterised by a time-independent distribution function F_0, occurs only if we have

$$\{F_0, H\} = 0. \tag{2.23}$$

However, this equation alone does not ensure the existence of stable equilibrium, which is expressed by the following condition:

$$E_0 = \int d\Gamma_{1-N}(F_0 H) \leqslant \int d\Gamma_{1-N}(FH) \tag{2.24}$$

for all $F \in \Lambda$ (see (2.6)).

If at $t = 0$ the distribution function $F(0) = F(t)|_{t=0}$ does not satisfy $\{F(0), H\} = 0$, then $F(t)$ is not stationary, i.e. $F(t)$ may oscillate. Around which state does $F(t)$ oscillate? $F(t)$ may oscillate around the state F_0 satisfying (2.24) (the distribution function F_0 is the classical image of the quantal 'passive states' discussed in [7, 8]). Henceforth it seems natural to assume that short-term dynamics applies before statistical equilibrium sets in. We discuss this issue in more detail in [9].

It is possible to derive (2.23) from (2.24). We have

$$\delta E = \int d\Gamma_{1-N}(\delta FH) = \int d\Gamma_{1-N}(\{S, F_0\}H) = \int d\Gamma_{1-N}(S\{F_0, H\}) = 0 \tag{2.25}$$

from which, S being an arbitrary real function, (2.23) follows. We remark that the variation principle expressed by (2.25) corresponds to the static limit of (2.12).

2.3. Linear response

Let us now consider the linear response to a small external perturbation of a system initially in equilibrium. At all instants after the disturbance, the function is described by a distribution function, which differs only infinitesimally from the stationary one. The fact that the function S is infinitesimal allows us to neglect terms of higher order than the second in S in the expansion $F = F_0 + \{S, F_0\} + \frac{1}{2}\{S, \{S, F_0\}\} + \ldots$ and in (2.8). In the following, F_0 denotes the state of stable equilibrium satisfying (2.24).

We now replace the Lagrangian (2.9) by its leading order expression, which is quadratic in S,

$$L^{(2)} = \frac{1}{2} \int d\Gamma_{1-N} F_0(\{S, \dot{S}\} - \{S, \{H, S\}\}). \tag{2.26}$$

The linear terms do not appear since they do not contribute to the final result in view of the stationarity condition (2.23) and of the condition (2.14) at the endpoints.

The variation of the action corresponding to (2.26) yields

$$\int d\Gamma_{1-N} F_0(\{\delta S, \dot{S}\} - \{\delta S, \{H, S\}\}) = 0 \tag{2.27}$$

so that

$$\int d\Gamma_{1-N} \delta S(\{\dot{S}, F_0\} - \{\{H, S\}, F_0\}) = 0. \tag{2.28}$$

As the variations δS are arbitrary, we finally obtain

$$\{\dot{S}, F_0\} = \{H, \{S, F_0\}\} \tag{2.29}$$

where use has been made of the stationarity condition (2.23) and of the Jacobi identity for Poisson brackets. The last equation should be understood as expressing the exact classical linear response to small perturbations.

In the study of the linear response no use has been made of a Lagrange multiplier, since a truncation of (2.8) has been introduced directly in (2.9).

3. Independent-particle approximation

3.1. Vlasov equation

In general, the exact description of many-body systems of physical relevance requires rather complex distribution functions. We must therefore resort to some approximation scheme, based on an adequate choice of the variational family of distribution functions. The distribution function is supposed to have a form specified *a priori*, which is guessed on the basis of physical arguments. Simplicity of the subsequent treatment is usually invoked in this choice.

The independent-particle approximation consists in choosing right from the outset the following many-particle distribution function:

$$F_N(x_1, p_1, \ldots, x_N, p_N, t) = \frac{1}{N!} \exp(-\bar{N}) \bar{N}^N \prod_{i=1}^{N} d(x_i, p_i, t) \tag{3.1}$$

where $\bar{N}$ is the average particle number. The function d is normalised to unity at all instants

$$\int d\Gamma_i d(x_i, p_i, t) = 1 \tag{3.2}$$

so that

$$\sum_N \int d\Gamma_{1-N} F_N = 1.$$

The approximation (3.1) means that correlations due to two-particle collisions are neglected.

To obtain the Lagrangian adequate to the approximation (3.1) we begin by generalising (2.9) to the case of a variable number of particles. We consider the following Lagrangian:

$$L = \sum_N \left(\int F_N G \, d\Gamma_{1-N} - \int F_N H \, d\Gamma_{1-N} \right). \tag{3.3}$$

Since the particles are identical, the energy may be written as

$$E = \sum_N \int HF_N \, d\Gamma_{1-N} = \sum_N \int d\Gamma_{1-N} \left(\sum_{i=1}^N \frac{p_i^2}{2m} + \tfrac{1}{2} \sum_{i \neq j=1}^N v(ij) \right) F_N$$

$$= \sum_N N \int d\Gamma_{1-N} \frac{p_1^2}{2m} F_N + \sum_N \tfrac{1}{2} N(N-1) \int d\Gamma_{1-N} v(12) F_N$$

$$= \int \frac{p_1^2}{2m} f(1) \, d\Gamma_1 + \tfrac{1}{2} \int\int v(12) f(1) f(2) \, d\Gamma_1 \, d\Gamma_2 \qquad (3.4)$$

where

$$f(i) = f(x_i, p_i, t) = \bar{N} d(x_i, p_i, t). \qquad (3.5)$$

If the distribution function F should retain the structure exhibited by (3.1), then the generator of its time derivative is of the form

$$G = \sum_{i=1}^N g(x_i, p_i, t) \qquad (3.6)$$

where the function $g(x, p, t)$ is such that

$$\dot{d}(x, p, t) = \{g(x, p, t), d(x, p, t)\}. \qquad (3.7)$$

The Lagrangian of the independent-particle approximation is finally obtained:

$$L = \int g(1) f(1) \, d\Gamma_1 - \int \frac{p_1^2}{2m} f(1) \, d\Gamma_1 - \tfrac{1}{2} \int\int v(12) f(1) f(2) \, d\Gamma_1 \, d\Gamma_2. \qquad (3.8)$$

This Lagrangian is supplemented by the subsidiary condition

$$\dot{f}(1) = \{g(1), f(1)\} \qquad (3.9)$$

which is equivalent to (3.5). The condition (3.9) is implemented with the aid of a Lagrange multiplier $a(x, p, t)$ which is a real function of the phase-space variables of a single particle and of the time. The derivation of the Euler–Lagrange equations corresponding to the Lagrangian (3.8), with the constraint (3.9), proceeds along similar steps to those leading from (2.11) to (2.21) and (2.10). One finds

$$\dot{f} = \{h, f\} \qquad (3.10)$$

with

$$h = h[f] = p^2/2m + \int v(x, x') f(x', p', t) \, d\Gamma'. \qquad (3.11)$$

Equation (3.10) is precisely the Vlasov equation. It is possible in principle, but difficult in practice, to improve the distribution function given by (3.1). This problem is related to the non-existence of a safe criterion to truncate the Bogoliubov–Born–Green–Yvon–Kirkwood chain of equations, which incorporates in a systematic fashion correlations absent in the mean-field approximation [10].

3.2. Temperature-dependent Thomas-Fermi theory

The stationary limit of (3.10)

$$\{h_0, f_0\} = 0 \tag{3.12}$$

where $h_0 = h[f_0]$, can be derived from the minimum principle for the energy, expressed in (2.25), assuming as variational space the set of distribution functions of the form (3.1), such that the single-particle distribution functions are obtainable by canonical transformations from any one of these functions.

In particular, the well known Thomas-Fermi result for finite temperatures [11] corresponds to minimising the energy, keeping the entropy fixed. The solution of this problem is

$$f_0(\mathbf{x}, \mathbf{p}) = \{1 + \exp[\beta(h_0(\mathbf{x}, \mathbf{p}) - \lambda)]\}^{-1} \tag{3.13}$$

where β is the inverse temperature and λ is the chemical potential necessary to guarantee the normalisation condition (3.2).

We point out that the solution (3.13) is determined by a supplementary requirement about the entropy of the system. We may however fix the equilibrium distribution function by a different condition, envisaging the description of situations different from the standard thermal equilibrium.

3.3. Linearised Vlasov equation and associated sum rule

We are especially interested in the analysis of small-amplitude motion near equilibrium.

We may obtain from the variation of (2.26), in the framework of the independent-particle approximation (3.1), the linearised Vlasov equation, which represents the classical limit of the quantal random phase approximation:

$$\{f_0(1), \dot{s}(1)\} + \{\{h_0(1), s(1)\}, f_0(1)\} + \int d\Gamma_2 f_0(2)\{\{v(12), s(2)\}, f_0(1)\} \tag{3.14}$$

with f_0 satisfying (3.12).

This equation has been applied in nuclear physics to account for small-amplitude vibrational modes [12-14]. Solutions of (3.14) at zero temperature are able to reproduce the giant resonances characteristic of the nuclear fluid, if allowance is made for deformations of the Fermi sphere in the variational function. If this ansatz is enlarged by including local distortions of the Fermi sphere, it is possible to describe low-lying modes, which are a continuation in the quantal region of the classical capillary waves. In fact, these excitations exist due to the absence of Landau damping, a kind of damping which can be accounted for in a phase-space description. At finite temperatures, we expect a redistribution of strength between low- and high-lying modes.

We note that the linearised Vlasov equation is a sum rule conserving theory, so that any redistribution of strength presented in a quantal description should also be apparent from a classical treatment.

In the remainder of this section we will prove that the classical random phase approximation does preserve the energy-weighted sum rule at any temperature.

The normal modes of (3.14) are obtained postulating the following ansatz for the time dependence of the function s:

$$s = s(\mathbf{x}, \mathbf{p}, t) = \sum_n (s_n \exp(-i\omega_n t)\alpha_n^*(\mathbf{x}, \mathbf{p}) + \text{CC}). \tag{3.15}$$

The collective frequencies ($\omega_n > 0$) are the eigenvalues of the equation

$$i\omega_n\{f_0(1), \alpha_n^*(1)\} = \{\{h_0(1), \alpha_n^*(1)\}, f_0(1)\}$$

$$+ \left\{\int d\Gamma_2(f_0(2)\{v(R), \alpha_n^*(2)\}), f_0(1)\right\} \tag{3.16}$$

while the transition amplitudes s_n are given by

$$s_n = i \int d\Gamma_1 f_0(1)\{\alpha_n(1), s(1)\} \tag{3.17}$$

provided the following normalisation is adopted:

$$i \int d\Gamma_1 f_0(1)\{\alpha_n(1), \alpha_m^*(1)\} = \delta_{nm}. \tag{3.18}$$

We observe that

$$\int d\Gamma_1 f_0(1)\{\alpha_n(1), \alpha_m(1)\} = 0. \tag{3.19}$$

From (2.28), with δS replaced by S, we obtain

$$\int d\Gamma_1 f_0(1)\{\dot{s}(1), s(1)\}$$

$$= \int d\Gamma_1 f_0(1)\{\{h_0(1), s(1)\}, s(1)\}$$

$$+ \int\int d\Gamma_1 d\Gamma_2 f_0(1)f_0(2)\{\{v(12), s(2)\}, s(1)\}$$

$$= \sum_N \int d\Gamma_{1-N} F_0\{S, \{S, H\}\}. \tag{3.20}$$

The first member can be evaluated, giving

$$\int d\Gamma_1 f_0(1)\{s(1), \dot{s}(1)\} = -2 \sum_n \omega_n |s_n|^2 \tag{3.21}$$

where use has been made of (3.15), (3.18) and (3.19). Thus

$$\sum_n \omega_n |s_n|^2 = \tfrac{1}{2} \sum_N \int d\Gamma_{1-N} (F_0\{S, \{S, H\}\}) \tag{3.22}$$

where the second member should be evaluated in the independent-particle framework. Clearly, (3.22) is the classical analogue of the quantal energy-weighted sum rule, which is valid for arbitrary temperatures [15].

4. Conclusions

We have developed a variational formulation to the Liouville equation, which in particular is appropriate to the derivation of the Vlasov theory in the independent-particle approximation. We have pointed out that the stationary limit encompasses

statistical equilibrium as described by the thermal Thomas-Fermi theory, but is more general than that, since we may choose trial distribution functions which do not need to be canonically equivalent to the distribution function describing statistical equilibrium. The Vlasov equation may be linearised around any static solution.

Among the physical situations in which our variational method should be useful we sketch an example taken from nuclear physics.

The recent experimental discovery of giant resonances in 'hot' nuclei [16] has motivated the extension of semiclassical techniques from zero to finite temperature. The giant dipole resonance in compound nuclei was the first observed collective mode built up on a statistical excitation of the particle degrees of freedom. Recent work along the lines of the present paper [17] seems to support the view that the semiclassical methods already tested successfully for $T = 0$ are also adequate to the consideration of thermal excited systems.

Acknowledgments

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