ON THE METRIPECTIC DYNAMICS FOR SYSTEMS WITH INTERNAL DEGREES OF FREEDOM

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Following an earlier discussion of the mixed canonical and dissipative description of the many-particle dynamics we present a variant approach to the dynamics of a system with internal degrees of freedom. This is illustrated on the example of classical particles equipped with classical spin.

Following the revival of interest in the behavior of classical, nonlinear systems, a variety of new theoretical tools was developed to allow for a description of the essential properties of those systems. One of the most powerful mathematical methods developed recently is the Lie–Poisson bracket technique [1], the use of which has led to considerable progress in our understanding of conservative relativistic fluid and plasma dynamics [2–6]. On the other hand it has been appreciated since quite a time that the nonlinear dissipative systems are of predominant applied interest [7,8]. The phase transformation physics should serve here as an important example.

Quite recently it has been argued that one can describe the irreversible or dissipative processes by means of the dissipative bracket technique [9,10]. It has also been demonstrated that one can unify both Lie–Poisson and dissipative brackets into a technique called either mixed canonical–dissipative or metriplectic one [11]. That technique has been employed implicitly in refs. [12–14] to study the nonrelativistic Navier–Stokes fluid and magnetic systems. Recently we have discussed metriplectic dynamics of relativistic plasma kinetics [15].

In this Letter we present a generalization of the metriplectic dynamics for the case of many-particle systems when the particles are equipped with internal degrees of freedom. Previously we have outlined the Lie–Poisson formulation for such a system [16]. The dynamics we shall study here shares similarity with the one called DCB1 in ref. [10].

Consider a system of classical, nonrelativistic particles possessing additional degrees of freedom lumped together into a vector S which we shall call spin. We shall assume that spin components obey the usual Poisson bracket relations for the angular momentum generators, that is

\[ \{ S^i; S^j \} = \epsilon^{ij\beta} S^\beta \delta_{ij}, \]

where \( i, j \) label the particle and \( \alpha, \beta, \ldots \) are the cartesian tensor indices. \( r_i \) and \( p_i \) denote the particle position and momentum, respectively, and their Poisson brackets have the usual form. Assume now that the dynamics of the system is governed by the hamiltonian \( H(\{ r_i \}, \{ p_i \}, \{ S_i \}) \), which we write in the form

\[ H(\{ r_i \}, \{ p_i \}, \{ S_i \}) = H(\{ r_i \}, \{ p_i \}) + H_s(\{ r_i \}, \{ S_i \}), \]

where \( H(\{ r_i \}, \{ p_i \}) \) is the particle hamiltonian involving the translational degrees of freedom, and \( H_s(\{ r_i \}, \{ S_i \}) \) is the spin hamiltonian. Guided by the possible applications we assume that \( H_s \) preserves the spin length. Indeed it is convenient, although not essential, to think about \( H_s \) as being the Heisenberg ferromagnet-like hamiltonian

\[ H_s(\{ r_i \}, \{ S_i \}) = \frac{1}{2} \sum_i J(r_i, r_j) S_i \cdot S_j, \]
where the exchange coupling $J(r_i, r_j)$ depends on the actual particle positions.

There are several important physical models which are described by the Hamiltonian (1). With the Kac–Uhlenbeck–Hemmer-like Hamiltonian it was used in Ref. [17] for a description of ferromagnetic fluids. Restricting spin degrees of freedom to Ising-like spin and with free-particle-like $H$, it was used for studying certain aspects of line shapes [18]. Identifying $\{r_i\}$ with the displacements of particles from corresponding lattice sites we obtain the frequently used model of compressible magnets [19]. Our Hamiltonian can also be viewed as a simplification of those used in the orientational order theories of freezing transition [20]. Finally, one can speculate on a possible relation of the Hamiltonian (1) to those used in gluon plasma dynamics [21].

On evaluating the Poisson brackets with the Hamiltonian (1) we obtain the particle equation of motion. The important one is the spin equation, which we can write as

$$\dot{S}^a = \{S^a, H\} = \epsilon^{a b c} \frac{1}{\hbar} \Delta_{b c}^\alpha$$

(2)

where $\beta$ is the effective magnetic field equal to $-\delta H/\delta S^\alpha$. Note, that the force felt by the particle will contain now also the Stern–Gerlach force [15].

In order to describe our system in a more convenient way we follow Ref. [15] and introduce the one-particle Klimontovich distribution function $f \{r, p, S\}$,

$$f(r, p, S) = \sum_i \delta(r-r_i) \delta(p-p_i) \delta(S-S_i)$$

(3)

The Lie–Poisson structure of the theory is now reflected in the following bracket relations $(1 = \{(r, p, S)\})$:

$$\{f(1); f(2)\} = (f(r_1, p_1, S_1) - f(r_2, p_2, S_2)) \mathcal{V} \cdot \delta(1-2)$$

$$-S^a \left( \mathcal{D}(1) \times \mathcal{D}(1-2) \right),$$

(4)

where $\mathcal{V} = \partial/\partial r, \mathcal{D} = \partial/\partial p$ and $\mathcal{D} = \partial/\partial S$.

The Hamiltonian $H$ is now the functional of the Klimontovich function $H = H\{f\}$, cf. Refs. [15,16]. The equation of motion for $f$ follows from $\partial f/\partial t = \{f, H\}$ and has the form of the modified Vlasov equation [16]. New terms appearing in that equation correspond with the collective Stern–Gerlach force and collective Bloch torque.

Now, let us consider the damping of the spin degrees of freedom. Recall that due to the degenerate character of the symplectic form defined by the spin-component Poisson brackets the length of spin $S^2 = S^\alpha S^\alpha$ becomes the Casimir function [1,3,11]. On physical grounds the damping should also preserve the length of the spin, therefore we shall use the transverse damping of the spin motion, the so-called Gilbert damping [14]. The damping force on a spin has now the form

$$F = -\lambda S \times (S \times B),$$

(5)

where again $B$ is the effective magnetic field. We can now write the damped equation of motion for the spin variables as

$$\partial_t S^a = \{S^a, H\} + \{\{S^a, H\}; H\},$$

(6)

where the double curly bracket denotes the metric, or dissipative bracket, defined as

$$\{\{S^\alpha; S^\beta\} = -\lambda \delta^{\alpha \beta} \frac{1}{\hbar} \Delta_{\alpha \beta}$$

$$-\lambda \delta^{\alpha \beta} \Pi^{\alpha \beta}$$

(7)

The dissipative bracket of two functionals $A$ and $B$ is now defined with the help of eq. (7) as

$$\{\{A; B\} = \sum_i \delta A \frac{\delta B}{\delta S^\alpha} \{\{S^\alpha; \} \} \frac{\delta B}{\delta S^\beta}.$$  

(8)

The metriplectic dynamics is now defined by combining the Lie–Poisson brackets with the dissipative one. The equation of motion for a dynamical variable $A = A\{r, p, S\}$ reads now $\partial_t A = \{A; H\}$, where $\{:\} = \{\} + \{\{\}\}$. Using eqs. (7), (8) we can evaluate the metric bracket for the Klimontovich function $f\{r, p, S\}$:

$$\{\{f(1); f(2)\} = -\lambda S^a \Pi^{\alpha \beta} \frac{\delta f(1)}{\delta p^\beta} \delta(1-2).$$

(9)

We are now prepared to write down the exact Klimontovich equation for the distribution $f(1, t)$. As usual $f$ should be considered as the classical phase space operator in the “second quantization” approach to classical statistical mechanics. Averaging $f(1, t)$ over the initial ensemble we obtain the smooth one-particle distribution function. As in the Vlasov plasma theory we can adopt the canonical and met-
ric brackets defined by eqs. (4), (9) as the fundamental bracket relations valid also for smooth functions. With that in mind we write the fundamental equation of motion in our theory as

$$\partial_t f(1, t) = \{ f(1, t); \mathcal{H}[f] \}$$

$$= \{ f(1, t); \mathcal{H}[f] \} + \int d^2 Q^{ab}(1, 2)$$

$$\times (S_2^2 f(2, t) \partial^a f(1, t) - S_2^a f(1, t) \partial^a f(2, t)), \quad (10)$$

where the canonical bracket gives rise to reversible Vlasov-like terms discussed in ref. [16], and the tensor $Q^{ab} = -\lambda S_2^a S_2^b \mathcal{F}(r_1, r_2)$. Although eq. (10) looks like the kinetic equation, in fact it is quite a different equation from, say, the Boltzmann kinetic equation for particles with spin [22]. It does not conserve energy. Indeed $\mathcal{H} = [\mathcal{H}, \mathcal{H}] \leq 0$ as it should be, since we are dealing with a dissipative system. As in the model DCB1 from ref. [10] the generating function for both simplectic and dissipative bracket is the hamiltonian $\mathcal{H}[f]$.

In order to develop a consistent statistical mechanics of our system we should now supplement the right-hand side of eq. (10) with a fluctuating force $l(1, t)$ and consider eq. (10) as the Langevin equation for the distribution function $f$. The r.h.s. of eq. (10) defines then the “systematic force” and it can be rewritten as $\mathcal{F} \cdot \text{grad}(f)$ where grad is the tangential derivative along the orbit in the $(r, p, S)$ space. This allows one to write the Fokker–Planck equation for the probability distribution $\mathcal{P}[f, t]$ with the diffusion matrix given by the Langevin force correlation

$$\langle l(1, t) l(2, t) \rangle = \mathcal{F}(1, 2) \delta(t_1 - t_2).$$

The entropy of the system is now given in terms of $\mathcal{P}[f]$,

$$\mathcal{S}[\mathcal{P}] = -\int \mathcal{P} \log \mathcal{P} \, Df.$$
M. Barma, Phys. Rev. B 7 (1975) 2710;  