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Gauge-free Hamiltonian structure of the spin Maxwell–Vlasov equations

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ABSTRACT

We derive the gauge-free Hamiltonian structure of an extended kinetic theory, for which the intrinsic spin of the particles is taken into account. Such a semi-classical theory can be of interest for describing, e.g., strongly magnetized plasma systems. We find that it is possible to construct a generalized noncanonical Poisson bracket on the extended phase space, and discuss the implications of our findings, including stability of monotonic equilibria.

High energy density plasma physics has become a popular subject (see, e.g., [1] and references therein). In such systems, quantum mechanical effects, such as wave function dispersion and/or statistical effects, can become important (for a recent experimental example, see [2]), and much of these plasmas can be rightly termed *quantum plasmas*. Much of the early literature on quantum plasmas has focused on condensed matter systems with a background lattice structure and the linear effects that follows (see, e.g., [3]). However, recent developments show a different direction, where the nonlinear aspects of such systems are in focus [4, 5]. Examples of recent results include quantum ion-acoustic waves [6], Jeans instabilities in quantum plasmas [7], trapping effects [8], magnetization by photons [9] and relativistic effects [10,11]. Typically, the quantum hydrodynamic equations are derived by starting from the Schrödinger equation and making the Madelung ansatz [12]. However, a method that more closely resembles the classical case is to use kinetic equations as a starting point (see Ref. [12] for a comparison between the different approaches). The field of quantum kinetic theory [13] in many ways started with the ambitions of Wigner, as presented in Ref. [14], to bridge the gap between classical Liouville theory and statistical quantum dynamics [15–17]. Thus, the development of quantum kinetic theory was partly due to an interest in obtaining a better understanding of the quantum-to-classical transition [18] (see also [19]). However, another important aspect of quantum kinetic theory is as a computational tool for, e.g., quantum plasmas [5], condensed matter systems [20,21], and, in general, quantum systems out of equilibrium [22], and in that respect shares many commonalities with quantum optics [23]. As shown in [24–28], spin is such an effect, the one of particular interest here.

When developing new models it can be important to show that they are Hamiltonian – all of the most important models of physics have this property, when phenomenological or other dissipation is neglected. If this is not the case, the non-Hamiltonian nature of these models gives rise to spurious dissipation that may not be readily identifiable or quantifiable. Thus, one role of Hamiltonian or action principle formulations is to filter out deficient models, a role that is not straightforward to play for matter models given in terms of Eulerian or spatial variables. Such models possess noncanonical Hamiltonian form, i.e. they are Hamiltonian but the conventional variables are not a canonically conjugate set and consequently the Poisson bracket possesses noncanonical form – yet it retains its Lie algebraic properties of antisymmetry, bilinearity, and the Jacobi identity. (See e.g. [29–32]. Also see [33,34] for recent work applicable to plasmas.)

For the kinetic theory of interest here we show it has a noncanonical Hamiltonian structure that is a generalization of that given in [30,35,36]. (See also [37].) We present the noncanonical Poisson bracket, prove directly that it satisfies the Jacobi identity, find Casimir invariants for the theory, and present an energy-like theorem that demonstrates that all equilibria with monotonically decreasing distributions are stable.

We consider the nonrelativistic spin Maxwell–Vlasov equation for $f(\mathbf{x}, \mathbf{v}, \mathbf{s}, t)$, an electron phase space density:

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$$\frac{\partial f}{\partial t} = -\mathbf{v}\cdot\nabla f + \left[\frac{e}{m}\left(\mathbf{E} + \frac{\mathbf{v}}{c}\times\mathbf{B}\right) + \frac{2\mu_e}{m\hbar c}\nabla(\mathbf{s}\cdot\mathbf{B})\right]\cdot\frac{\partial f}{\partial \mathbf{v}} + \frac{2\mu_e}{\hbar c}(\mathbf{s}\times\mathbf{B})\cdot\frac{\partial f}{\partial \mathbf{s}} \qquad (1)$$

where m and $e > 0$ are the electron mass and charge, respectively, $2\pi\hbar$ is Planck's constant, $\mu_e = g\mu_{\mathbf{B}}/2$ is the electron magnetic moment in terms of $\mu_{\mathbf{B}}$, the Bohr magneton, and the electron spin g-factor. Eq. (1) is coupled to the dynamical Maxwell equations,

$$\frac{\partial \mathbf{B}}{\partial t} = -c\nabla\times\mathbf{E}, \qquad (2)$$

$$\frac{\partial \mathbf{E}}{\partial t} = c\nabla\times\mathbf{B} - 4\pi\mathbf{J} \qquad (3)$$

through the current $\mathbf{J} = \mathbf{J}_f + c\nabla\times\mathbf{M}$, which has "free" and spin magnetization parts:

$$\mathbf{J}_f := -e\int d^3v\, d^3s\, \mathbf{v} f, \qquad (4)$$

$$\mathbf{M} := -\frac{2\mu_e}{\hbar}\int d^3v\, d^3s\, \mathbf{s} f. \qquad (5)$$

Extension to multiple species is straightforward.

Note, Eqs. (1), (2), and (3), with (4) and (5), are to be viewed classically and consequently a full nine-dimensional phase space integration, $d^9z = d^3x\, d^3v\, d^3s$, is considered for f. Later we will see how a spin quantization constraint can be applied.

The Hamiltonian functional for the theory is

$$H[\mathbf{E},\mathbf{B},f] = \int d^9z\left(\frac{m}{2}v^2 + \frac{2\mu_e}{\hbar c}\mathbf{s}\cdot\mathbf{B}\right)f + \frac{1}{8\pi}\int d^3x\left(E^2 + B^2\right) \qquad (6)$$

which can be shown directly to be conserved, but this will become obvious after the Hamiltonian structure is given. Similarly, it can be shown that the total momentum,

$$\mathbf{P} = \int d^9z\, f m\mathbf{v} + \frac{1}{4\pi c}\int d^3x\, \mathbf{E}\times\mathbf{B}, \qquad (7)$$

is conserved, whence it is evident that spin carries no linear momentum.

The noncanonical spin Maxwell–Vlasov bracket is composed of several parts:

$$\begin{aligned}\{F,G\}_{sMV} = \int d^9z\, f\Big(&[F_f,G_f]_c &(8)\\ &+ [F_f,G_f]_B &(9)\\ &+ [F_f,G_f]_s &(10)\\ &+ \frac{4\pi e}{m}(F_E\cdot\partial_v G_f - G_E\cdot\partial_v F_f)\Big) &(11)\\ &+ 4\pi c\int d^3x\,(F_E\cdot\nabla\times G_B - G_E\cdot\nabla\times F_B), &(12)\end{aligned}$$

where

$$[f,g]_c := \frac{1}{m}(\nabla f\cdot\partial_v g - \nabla g\cdot\partial_v f), \qquad (13)$$

$$[f,g]_B := -\frac{e\mathbf{B}}{m^2c}\cdot(\partial_v f\times\partial_v g), \qquad (14)$$

$$[f,g]_s := \mathbf{s}\cdot(\partial_s f\times\partial_s g), \qquad (15)$$

with standard partial derivatives denoted by $\partial_v := \partial/\partial\mathbf{v}$ and functional derivatives by $F_f := \delta F/\delta f$, etc. Term (10) of $\{\,,\}_{sMV}$ is new and accommodates the spin; it is not surprising that it has an inner bracket based on the $so(3)$ algebra [38]. The remaining terms (8), (9), (11), and (12) produce the usual Vlasov–Maxwell theory [30,35–37,39]. It is a simple exercise to show that Eqs. (1), (2), and (3) are given as follows:

$$\frac{\partial f}{\partial t} = \{f,H\}_{sMV},$$

$$\frac{\partial \mathbf{B}}{\partial t} = \{\mathbf{B},H\}_{sMV},$$

$$\frac{\partial \mathbf{E}}{\partial t} = \{\mathbf{E},H\}_{sMV}.$$

This is facilitated by the identity $\int d^9z\, f[g,h] = -\int d^9z\, g[f,h]$, which works for all three brackets of (13), (14), and (15).

There are two approaches to obtaining a Hamiltonian description. The usual one is by constructing an action principle by postulating a Lagrangian density with the desired observables and symmetry group, and then effecting a Legendre transformation, when possible, to obtain a Hamiltonian theory. Alternatively one can postulate an energy functional and Poisson bracket as we have done here. When exploring new territory with this latter approach, one must prove directly the Jacobi identity $\{\{F,G\},H\} + \{\{G,H\},F\} + \{\{H,F\},G\} \equiv 0$ for all functionals F, G, and H. With the former approach this is guaranteed if the action principle and Legendre transform exist and one can perform a chain rule calculation to obtain a bracket in terms of the desired observables. This was done for the Maxwell–Vlasov bracket in [36], where it is necessary to assume the existence of a vector potential. However, with the bracket approach one need not assume the existence of a vector potential, and one can proceed in a self-contained gauge-free manner to show that the Maxwell–Vlasov bracket satisfies

$$\big\{\{F,G\}_{MV},H\big\}_{MV} + \text{cyc} = \frac{e}{m^2c}\int d^6z\, f\nabla\cdot\mathbf{B}\left[\left(\frac{\partial F_f}{\partial\mathbf{v}}\times\frac{\partial G_f}{\partial\mathbf{v}}\right)\cdot\frac{\partial H_f}{\partial\mathbf{v}}\right]. \qquad (16)$$

This result was quoted in [30] (details of this early explicit (and tedious) calculation will be given elsewhere). Thus, although the Maxwell–Vlasov Hamiltonian theory is gauge-free, it requires $\nabla\cdot\mathbf{B} = 0$.

One can construct an action principle for the spin Maxwell–Vlasov theory of the form of [40–42] and then proceed to the bracket $\{F,G\}_{sMV}$ (see e.g. [43]), but we find it easier to prove the Jacobi identity directly. Writing $\{F,G\}_{sMV} = \{F,G\}_{MV} + \{F,G\}_s$ and using :=: to denote the cyclic sum we have

$$\begin{aligned}\big\{\{F,G\}_{sMV},H\big\}_{sMV} &:=: \big\{\{F,G\}_{MV},H\big\}_{MV} + \big\{\{F,G\}_s,H\big\}_{MV}\\ &\quad + \big\{\{F,G\}_{MV},H\big\}_s + \big\{\{F,G\}_s,H\big\}_s\\ &:=: \big\{\{F,G\}_s,H\big\}_{MV} + \big\{\{F,G\}_{MV},H\big\}_s, \end{aligned} \qquad (17)$$

where the second equality follows because of (16) (assuming solenoidal $\mathbf{B}$) and the fact that $\{F,G\}_s$ is a Lie–Poisson bracket (see e.g. [31,44]). Thus it only remains to show that the cross terms cancel, which is facilitated by a theorem in [30]; viz., when functionally differentiating $\{F,G\}_{MV}$ and $\{F,G\}_s$, which are needed when constructing the cross terms, one can ignore the second functional derivative terms. These cancel by virtue of the symmetry of the second variation and antisymmetry of the bracket. Using the symbol $\doteq$ to denote equivalence modulo the second variation terms, we obtain

$$\frac{\delta\{F,G\}_{MV}}{\delta f} \doteq [F_f,G_f]_c + [F_f,G_f]_B + \frac{4\pi e}{m}(F_E\cdot\partial_v G_f - G_E\cdot\partial_v F_f), \qquad (18)$$

$$\frac{\delta\{F,G\}_s}{\delta f} \doteq [F_f,G_f]_s, \qquad (19)$$

while all other needed functional derivatives vanish. Thus

$$\big\{\{F,G\}_{MV},H\big\}_s := \int d^9z\bigg(f\big[[F_f,G_f]_c+[F_f,G_f]_B,H_f\big]_s + \frac{4\pi e}{m}f[F_E\cdot\partial_v G_f - G_E\cdot\partial_v F_f, H_f]_s\bigg), \tag{20}$$

$$\big\{\{F,G\}_s,H\big\}_{MV} := \int d^9z\bigg(f\big[[F_f,G_f]_s,H_f\big]_c + f\big[[F_f,G_f]_s,H_f\big]_B - \frac{4\pi e}{m}f\,H_E\cdot\partial_v[F_f,G_f]_s\bigg). \tag{21}$$

The first line of (20) and the first two lines of (21) cancel by virtue of the Jacobi identities for the brackets $[\,,\,]_{c,B,s}$ on functions, while the second line of (20) and the last term of (21) cancel upon permutation.

Having established the Jacobi identity, we search for Casimir invariants, functionals that commute with all other functionals. Using the equations obtained from $\{C,F\}=0$ for all F, we obtain

$$C^{fs} = \int d^9z\,\mathscr{C}\big(f,s^2\big), \tag{22}$$

$$C^E = \int d^3x\,\kappa_E(\mathbf{x})\bigg(\nabla\cdot\mathbf{E}+4\pi e\int d^3v\,d^3s\,f\bigg), \tag{23}$$

$$C^B = \int d^3x\,\kappa_B(\mathbf{x})\nabla\cdot\mathbf{B}, \tag{24}$$

where $\mathscr{C}$, κ_E, and κ_B are arbitrary functions of their arguments. The Casimir C^{fs} is a consequence of the fact that the solution to (1) is a volume preserving rearrangement, i.e. that the solution can be written as the initial condition on the characteristics. It is not difficult to see that (1) can be written in conservation form on the full nine-dimensional space. The s^2 dependence of the Casimir C^{fs} is the lift of the $so(3)$ spin Casimir to the kinetic theory. Such inner Casimirs always give rise to Casimirs of the field theory. The Casimir C^E clearly implies Poisson's equation, an initial condition that would remain preserved should we change the Hamiltonian functional. It is a local Casimir because of the arbitrary function $\kappa_E(\mathbf{x})$, which is used here to make the point that it is conserved point-wise. The local quantity C^B is technically not the same as the others because its vanishing is required for the Jacobi identity. However, this is only technical because $\{C^B,F\}=0$, for all F, whether or not $\nabla\cdot\mathbf{B}=0$.

A consequence of the Casimir C^{fs} is that s^2 is constant on level sets (contours) of f, which can be viewed as a classical prequantization property. If we suppose f has the from $f = c(s^2)f_c(\mathbf{x},\mathbf{v},\mathbf{s},t)$, then it follows that if f_c satisfies (1) then f does. Choosing

$$f = \delta\big(|\mathbf{s}|-\hbar/2\big)f_c(\mathbf{x},\mathbf{v},\mathbf{s},t) \tag{25}$$

we enforce the usual quantization condition and our integrals reduce from integrations over d^9z to $d^3x\,d^3v\,d\Omega$, where $d\Omega$ denotes the spin sphere as in e.g. [27]. Because of the pure antisymmetry of the $so(3)$ structure constants, Liouville's theorem on characteristics follows immediately; however, for general cosymplectic forms, J, i.e. for brackets of the form $[f,g]=\partial f/\partial w^i J^{ij}(w)\partial g/\partial w^j$, one can insert a factor of $\sqrt{\det J}$ restricted to symplectic leaves to define a proper 'volume' measure (see e.g. [31]).

Having found the Casimir invariants we can write down a variational principle for equilibria and then proceed to investigate stability by the technique introduced in [45] (see also [46]), which has become known as the energy-Casimir method (see e.g. [31,47,48]). First we seek extrema of the quantity $\mathscr{F} := H + C^{fs} + C^E + C^B$, which must give rise to equations for equilibria:

$$\frac{\delta\mathscr{F}}{\delta f} = \mathscr{K} + 4\pi e\kappa_E + \mathscr{C}_f\big(f,s^2\big) = 0, \tag{26}$$

$$\frac{\delta\mathscr{F}}{\delta\mathbf{E}} = \mathbf{E} - 4\pi\nabla\kappa_E = 0, \tag{27}$$

$$\frac{\delta\mathscr{F}}{\delta\mathbf{B}} = \mathbf{B} - 4\pi\nabla ka_B = 0, \tag{28}$$

where $\mathscr{C}_f := \partial\mathscr{C}/\partial f$, $\mathscr{K} := mv^2/2 + 2\mu_e\mathbf{s}\cdot\mathbf{B}/\hbar c$ and we define the 'particle energy' by $\mathscr{E} := \mathscr{K} + 4\pi\kappa_E$. Evidently $-4\pi\kappa_E$ is the electrostatic potential and $\mathbf{B}$ must be an external field, i.e. $\mathbf{J} = \nabla\times\mathbf{B} = 0$ (cf. the results for the Maxwell–Vlasov case [49,50]). Assuming $\mathscr{C}_f$ has an inverse, we obtain the following for the equilibrium distribution function:

$$f_e(\mathscr{E}) = \mathscr{C}_f^{-1}\big(-\mathscr{E},s^2\big). \tag{29}$$

If we chose $\mathscr{C}$ to be proportional to the usual entropy expression $f\ln f$, neglect the dependence on s^2, and assume $\mathbf{E}=0$, an acceptable choice, then we obtain the Maxwell–Boltzmann-like equilibrium of [27]. Proceeding to the second variation we obtain

$$\delta^2\mathscr{F} = \frac{1}{2}\int d^9z\,\mathscr{C}_{ff}(\delta f)^2 + \frac{1}{8\pi}\int d^3x\big((\delta E)^2+(\delta B)^2\big) = -\frac{1}{2}\int d^9z\,\frac{(\delta f)^2}{\partial f_e/\partial\mathscr{E}} + \frac{1}{8\pi}\int d^3x\big((\delta E)^2+(\delta B)^2\big), \tag{30}$$

where the second equality of (30) follows upon differentiating the condition $\mathscr{E}+\mathscr{C}_f=0$ with respect to f. From (30) we immediately draw the formal conclusion that equilibria that are monotonically decreasing functions of $\mathscr{E}$ are stable, because $\delta^2\mathscr{F}$ serves as a Lyapunov functional. More rigorous versions of this have been proved for the Vlasov equation in both the plasma and astrophysical contexts (see e.g. [51]).

Only a limited class of equilibria come from $\delta\mathscr{F}=0$, *viz.* current free equilibria. Such equilibria minimize the total magnetic field energy subject only to the constraint $\nabla\cdot\mathbf{B}=0$. Similarly, the need for invertibility of $\mathscr{C}_f$ selects out only monotonic $f_e(\mathscr{E})$, which follows from minimizing the total 'particle' energy at fixed volume-preserving rearrangement constraint (see e.g. [49,50,52]). Thus the limited class of equilibria contains minimally constrained equilibria, and their stability assures us that these 'vacuum' states are stable, a notion consistent with and akin to thermodynamic stability. This serves as a check that our spin theory is reasonable, but does not imply that these are the only stable equilibrium states. For example, in the context of the Vlasov–Poisson system multi-bumped equilibria can be stable by the Penrose criterion (see e.g. [53]) and similar stability analyses can be addressed for a variety of equilibria of our system. We also point out that the complete set of equilibria can be gotten from a constrained variational principle with 'dynamically accessible variations' [31], but this will not be considered further here.

In summary, the formulation of an extended kinetic theory for electrons, taking into account the intrinsic spin and the relevant magnetization effects, was considered. In particular, the semiclassical limit, valid for length scales large compared to the size of the electron wave function was given. Based on the extended phase space, the Hamiltonian structure was discussed, and a noncanonical Poisson bracket was found that satisfies the Jacobi identity. Furthermore, we obtained the related Casimir invariants and showed the stability of all equilibria with monotonically decreasing distributions. Our findings could act as a guiding tool for further extended Hamiltonian theories, including quantum effects from Pauli or Dirac theory, for which a gauge-line has to be included in the phase of the definition of the corresponding Wigner function

[54,55]. Moreover, the stability of the equilibria can be an important principle in future numerical studies of strongly magnetized systems.

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