Classical particles with spin-possible formulation of many-particle dynamics

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A possible canonical formulation of dynamics for classical particles with spin degrees of freedom is presented. The Klimontovich equation for an exact one-particle distribution function is derived, and its applications are briefly discussed.

In a recent paper, Yang and Hirschfelder discussed the generalization of the classical Poisson brackets for the case of classical particles with the spin (or internal angular momentum) degrees of freedom. As they said in their paper, “there is the possibility that the generalized Poisson bracket we derive may be more general than our formulation.” This is precisely the case we want to illustrate in this Brief Report.

The Yang and Hirschfelder spin Poisson brackets are, in fact, identical to those used originally by Schwinger for the angular momentum, and to the spin Poisson brackets used in the theory of localized magnetism. The field where the Yang and Hirschfelder formulation may be of great use is the kinetic theory of liquids and gases consisting of particles with spin. In spite of obvious interest, for example, in chemical physics applications, the kinetic theory of particles with spin is much less developed as compared with the spinless particle case.

In this paper we present the Klimontovich formulation of the many-particle dynamics which includes spin degrees of freedom. The approach we use follows our previous analysis for a canonical, gauge-invariant formulation of relativistic particle dynamics. The basic quantity in the Klimontovich formulation of many-particle dynamics is the exact one-particle distribution function \( \hat{f}(\mathbf{T}, \mathbf{p}, \mathbf{S}, t) \) defined over, in our case generalized to include spin, one-particle phase space \(-\mu\).

\[
\hat{f}(\mathbf{T}, \mathbf{p}, \mathbf{S}, t) = \sum_{i=1}^{N} \delta(\mathbf{T} - \mathbf{T}_i(t)) \delta(\mathbf{p} - \mathbf{p}_i(t)) \delta(\mathbf{S} - \mathbf{S}_i(t))
\]

(1)

where \( \mathbf{T}_i, \mathbf{p}_i, \) and \( \mathbf{S}_i \) are the \( i \)th particle position, momentum, and spin, respectively. The Poisson brackets of positions and momenta are as usual, while the spin components obey the relation

\[
|S^\alpha, S^\beta|_{PB} = e^{\alpha \beta \rho \sigma} S_\rho S_\sigma
\]

(2)

All the cross Poisson brackets between spin components and the positions and momentum do vanish.

Using these conventional Poisson brackets, together with Eq. (2) one can calculate the Poisson bracket of functions \( \hat{f}(\mathbf{T}, t) \) and \( \hat{f}(\mathbf{Z}, t) \), where \( \mathbf{T} = (\mathbf{T}_1, \mathbf{p}_1, \mathbf{S}_1) \). It reads

\[
\{\hat{f}(\mathbf{T}, t), \hat{f}(\mathbf{Z}, t)\}_{PB} = \left[ \hat{f}(\mathbf{T}_1, \mathbf{p}_2, \mathbf{S}_1, t) - \hat{f}(\mathbf{T}_2, \mathbf{p}_1, \mathbf{S}_2, t) \right] \nabla \cdot \mathbf{s} (\mathbf{T} - \mathbf{Z}) - \mathbf{s} \cdot (\nabla \times \nabla \delta (\mathbf{T} - \mathbf{Z})),
\]

(3)

where \( \tilde{\nabla} = \delta/\delta \mathbf{T}, \mathbf{b} = \delta/\delta \mathbf{p}, \) and \( \nabla \phi = \delta/\delta \mathbf{S} \).

The Poisson bracket Eq. (3) obeys all the necessary conditions, that is, linearity in each argument, antisymmetry, and the Jacobi identity. The function \( \hat{f}(\mathbf{T}, t) \) is now a building block of the theory and, for example, its equilibrium mean value \( \langle \hat{f}(\mathbf{T}, t) \rangle \) is identical to the one-particle distribution function used in the kinetic theory. Averaging \( \langle \hat{f} \rangle \), as usual in the Klimontovich formulation, is carried out over the initial values of particle positions, momenta, and spins. Higher-order correlation functions are obtained by averaging products of the \( \hat{f} \)'s.

For spinless particles \( \hat{f}(\mathbf{T}, t) \) is the classical counterpart of the quantum Wigner distribution function. \( \hat{f} \) also plays the role of a classical “second quantization” operator in phase space dynamics. For particles with spin this relation to the Wigner distributions becomes blurred, since the Wigner functions for spin particles become rather complicated matrix functions.

To illustrate the usefulness of the Poisson bracket Eq. (3) consider a system of particles interacting via the spin-independent potential \( V(\mathbf{T}_i - \mathbf{T}_j) \) and through the spin-dependent part, which, for the sake of definiteness, we use in the Heisenberg form: \( J(\mathbf{T}_i - \mathbf{T}_j) \mathbf{S}_i \cdot \mathbf{S}_j \). Note, however, that now the exchange coupling \( J \) depends on actual positions of the interacting particles. It is via this dependence that the important coupling between the lattice vibrations and magnetic moments enters the theory of the Heisenberg magnets.

The Hamiltonian for our system then reads

\[
H = \sum_{i=1}^{N} \frac{\mathbf{p}_i^2}{2m} + \frac{1}{2} \sum_{i<j} g V(\mathbf{T}_i - \mathbf{T}_j) + \frac{1}{2} \sum_{i} J(\mathbf{T}_i - \mathbf{T}_j) \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{i} U(\mathbf{T}_i) + \sum_{i} \gamma \mathbf{B}(\mathbf{T}_i) \cdot \mathbf{S}_i
\]

(4)

where \( U \) and \( \mathbf{B} \) are the external potential and the magnetic field. \( \gamma \) is the usual coupling constant containing the Bohr magneton and spin value. For simplicity we assume \( \mathbf{S}_i \cdot \mathbf{S}_i = S^2 \). The Hamiltonian (4) can now be rewritten as a functional of \( \hat{f}(\mathbf{T}, t) \):

\[
\hat{H} = \int dT d\mathbf{p} \left[ \frac{\mathbf{p}^2}{2m} + U(\mathbf{p}) + \gamma \mathbf{B}(\mathbf{T}) \cdot \mathbf{S} \right] \hat{f}(\mathbf{T}, t) + \frac{1}{2} \int dT d\mathbf{Z} \left[ V(\mathbf{T}_i - \mathbf{T}_j) + J(\mathbf{T}_i - \mathbf{T}_j) \mathbf{S}_i \cdot \mathbf{S}_j \right] \hat{f}(\mathbf{T}, t) \hat{f}(\mathbf{Z}, t)
\]

(5)
where we have omitted irrelevant for our discussion term \( \sim V(0) \).

The equation of motion for the Klimontovich function \( f(T, t) \), which is in fact the “second quantization” version of the Liouville equation, is now given as

\[
\frac{\partial f(T, t)}{\partial t} = \left[ f(T, t); \mathcal{H}[f] \right]_{PB}. 
\]

On evaluating the Poisson bracket on the right-hand side (RHS) of Eq. (6), using the basic expression Eq. (3), one obtains

\[
\left[ f(T, t); \mathcal{H}[f] \right]_{PB} = - \left\{ \mathbf{F}_T(T) \cdot \mathbf{S}_1, f(T, t) \right\} = - \left\{ \mathbf{F}_T(T) \cdot \mathbf{S}_1, f(T, t) \right\} 
\]

The first term on the right-hand side of Eq. (7) is the tangential derivative of the function \( f \) along one-particle trajectory in the generalized \( m \) space. Explicitly, \( \mathbf{F}_T \) is the force due to the external potential \( U \); \( \mathbf{F}_U = - \nabla U \). \( \mathbf{F}_T(T, s) \) is the force exerted on a particle with the magnetic moment \( s \) moving in an inhomogeneous magnetic field—a Stern-Gerlach force \( \mathbf{F}_S = \gamma_s \mathbf{S} \times \mathbf{B}(r) \).

The \( \mathbf{N}_T \cdot \mathbf{S} \) term is the Bloch torque term, with \( \mathbf{N}_T(T, s) \). The second term on the RHS of Eq. (7) is the collective term arising from the particle interactions. The forces \( \mathbf{F}_T[f] \) are now functions of the distribution \( f \).

\( \mathbf{F}_T \) is the collective force due to potential interactions familiar from conventional Klimontovich theory:

\[
\mathbf{F}_T = - \nabla V(T) - \int d^2 \mathbf{S}_1 \cdot \mathbf{S}_1 \partial_j f(T, t) d^2 \mathbf{S}_1.
\]

The \( \mathbf{F}_S[f] \) term can be interpreted either as a collective Stern-Gerlach force or as a generalized exchange striction one. Indeed,

\[
\mathbf{F}_S[f] = \int d^2 \mathbf{S}_1 \cdot \mathbf{S}_1 \partial_j (T_1 - T_2) f(T_2, t)
\]

can easily be rewritten, in terms of an effective magnetic field

\[
\mathbf{B}_{eff} = \int d^2 \mathbf{S}_1 \times \mathbf{S}_1 \partial_j f(T_2, t)
\]

in a form resembling \( \mathbf{F}_S(T, s) \). On the other hand, if one considers particles sitting on a lattice and vibrating around their equilibrium lattice positions \( c \) with displacements \( u \) then one immediately recognizes in \( \mathbf{F}_S[f] \) the exchange striction interactions used in Refs. 9 and 10. \( \mathbf{N}_T[f] \) is the collective Bloch “torque” term given in terms of a magnetic field \( \mathbf{B}_{eff} \).

\[
\mathbf{N}_T[f] = \int d^2 \mathbf{S}_1 \cdot \mathbf{S}_1 \partial_j f(T_2, t)
\]

Equation (6) is, therefore, a natural generalization of the Klimontovich equation for spinless particles and should be a starting point in analysis of the kinetic theory of particles with spin. A systematic multiplicative and averaging of from Eq. (6) on generates generalized BBGKY hierarchy of equations for many particle distribution functions:

\[
f_n(T, \ldots, T_n; t) = - \left\{ f(T, t); f(T, t); \ldots; f(T, t) \right\}.
\]

For long-range potentials one obtains closure of that hierarchy using the Vlasov equation, which is identical in form to Eq. (6) but with the “operator” \( f \) replaced by a smooth distribution function \( f(T, t) \). Since for spinless particles the Vlasov equation is an exact one in the limit \( g \rightarrow 0, N \rightarrow \infty \), \( gN \rightarrow \text{const} \), where \( g \) is the coupling constant in the Hamiltonian Eq. (4), \( h \) it is plausible that the Vlasov equation is also exact for spin particles when \( J \rightarrow 0, N \rightarrow \infty \), and \( J/N \rightarrow \text{const} \). At the equilibrium level such a system should show similarity to the Hemmer and Imbro model of ferromagnetic fluid.\(^12\) Although our derivations here preclude use of hard-core potentials, it is known, that the Klimontovich equation is valid for such a system, with properly changed potential part of force \( \mathbf{F}_V[f] \). With that modification our Eq. (8) becomes also a starting point for a BBGKY hierarchy for hard-core magnetic particles. Elsewhere we shall discuss the Boltzmann-Lorentz limit of Boltzmann equation for spin particles.\(^13\)

In conclusion, we have shown that the generalized canonical formulation of classical particles with spin degrees of freedom as discussed in Ref. 1 can be reformulated to become a convenient starting point for the Klimontovich formulation of the statistical mechanics for such a system. Possible applications of that formulation have been discussed.

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