Phase-Space Dynamics of Semiclassical Spin-$\frac{1}{2}$ Bloch Electrons

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Following recent interest in a kinetic description of the semiclassical Bloch electron dynamics, we propose a new formulation based on the previously developed Lie-Poisson formulation of dynamics. It includes modifications required to account for the Berry curvature contribution to the electron's equation of motion as well as essential ingredients of a quantum treatment of spin-$\frac{1}{2}$ degrees of freedom. Our theory is also manifestly gauge invariant and thus permits inclusion of the electron interactions. The scope of our formulation extends beyond its solid state physics motivation and includes recently discussed noncommutative generalizations of classical mechanics as well as historically important models from quantum gravity physics.

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Recent theoretical [1] and experimental [2] works have shown that in several important solid state physics applications the motion of charge carriers can be described by semiclassical equations of motion in which the positions of the centers of the localized electron wave function in k and r spaces obey the equations of motion:

$$\dot{\mathbf{k}} = \mathbf{F}/\hbar, \qquad \dot{\mathbf{r}} = \frac{\partial \epsilon(\mathbf{k})}{\hbar \partial \mathbf{k}} + \mathbf{F} \times \mathbf{\Omega}/\hbar. \tag{1}$$

$\mathbf{\Omega}$ is the Berry curvature of the Bloch state $|\mathbf{k}\rangle$, and $\mathbf{F}$ is the net force acting on the carrier (e.g., in the presence of an external electric field $\mathbf{F} = e\mathbf{E}_0 = -e\nabla U$). These equations differ from the "standard" semiclassical equations of motion for Bloch electrons [3] in that they contain the Berry curvature $\mathbf{\Omega}$, defined by [4]

$$\mathbf{\Omega}(\mathbf{k}) = i\langle \nabla_{\mathbf{k}} u_{\mathbf{k}}| \times |\nabla_{\mathbf{k}} u_{\mathbf{k}}\rangle. \tag{2}$$

Here $u_{\mathbf{k}}(\mathbf{r})$ is the periodic part of the Bloch function at wave vector $\mathbf{k}$ for a specific band, and the integral implied by the bracket is over the unit cell of the lattice. Briefly, this term is obtained by carefully following the evolution of the factors involved in constructing a wave packet from Bloch functions [1]. Because $\mathbf{\Omega}$ is gauge invariant, it is potentially observable and is, in general, nonzero for crystals without inversion symmetry [5]. Zak [5], in an extension of Berry's ideas [6], first pointed out that Bloch systems naturally yield geometric phases. Equations (1) assume, for the sake of simplicity, that only a single band with energy $\epsilon(\mathbf{k})$ is important. In what follows we define $\mathbf{p} = \hbar\mathbf{k}$ and incorporate $\hbar$ into the definition of $\mathbf{\Omega}$. Similar equations describe the motion of ultracold atoms in an optical lattice [7].

In our earlier publications we have shown how the dynamics of a variety of interesting physical systems can be formulated in a compact and convenient way using the symplectic Lie-Poisson bracket technique [8]. In this Letter we show how the phase-space dynamics for semiclassical spin-$\frac{1}{2}$ Bloch electrons can be cast into the same form. We begin by writing the symplectic Lie-Poisson brackets for carrier position "$\mathbf{r}$" and momenta "$\mathbf{p}$" in the form

$$\{r_a, r_b\} = \varepsilon_{abc}\Omega_c, \quad \{r_a, p_b\} = \delta_{ab}, \quad \{p_a, p_b\} = 0. \tag{3}$$

Note that in classical dynamics the Poisson brackets between the position components vanish. Equation (3) is the special form of the noncommutative classical mechanics discussed extensively in [9]. It is also interesting to recall that the "noncommutativity" of positions in (3) is analogous to that postulated in early works on quantum gravity [10]. Defining the carrier Hamiltonian as $H(\mathbf{r}, \mathbf{p}) = \epsilon(\mathbf{p}) + eU(\mathbf{r})$, we find that the canonical equations of motion

$$\dot{r}_a = \{r_a, H\}; \qquad \dot{p}_a = \{p_a, H\} \tag{4}$$

are, in fact, identical to the equations of motion (1).

In a recent Letter [1] a kinetic description of carriers and a Boltzmann-like kinetic equation for the carriers' single-particle distribution function were proposed. In this Letter we obtain a more general kinetic equation by following the "second quantized" formulation of kinetic theory developed by Klimontovich [11] and extended for charged, relativistic particles [12] and for classical particles with spin [13].

We begin by developing the formalism for spinless carriers, in which the basic variable describing the state of the system is the single-particle distribution function $f(\mathbf{r}, \mathbf{p}, t)$, and the Hamiltonian is considered to be a functional of f. For noninteracting particles this is the linear functional $H\{f\} = \int d\mathbf{1} H(\mathbf{1}) f(\mathbf{1})$, where $\mathbf{1} \equiv (\mathbf{r}, \mathbf{p})$. The mean value of the physical quantity A is obtained as $\langle A\rangle = \int d\mathbf{1} f(\mathbf{1}) A(\mathbf{1})$. In the semiclassical formulation f possesses all the properties of the classical distribution function; i.e., it is non-negative and normalized. The quantum description can then be obtained by replacing f with the Wigner distribution function $f_{\mathrm{W}}(\mathbf{r}, \mathbf{p})$ [14] and the Lie-Poisson brackets defined below with the properly adapted form of the Moyal brackets [15]. To obtain the kinetic equation governing the evolution of f, one has to (i) define the symplectic bracket for f, and (ii) supplement the resulting Hamiltonian (nondissipative) equation of motion for f with a properly chosen dissipative part (e.g., the collision integral). The symplectic Lie-Poisson bracket for f is ($\vec{\nabla} \equiv \partial/\partial \mathbf{r}$, $\vec{\partial} \equiv \partial/\partial \mathbf{p}$)

$$\{f(\mathbf{1}), f(\mathbf{2})\} = \vec{\nabla} f(\mathbf{1}) \cdot \vec{\partial}\delta(\mathbf{1}-\mathbf{2}) - \vec{\partial} f(\mathbf{1}) \cdot \vec{\nabla}\delta(\mathbf{1}-\mathbf{2}) + \Omega \cdot [\vec{\nabla} f(\mathbf{1}) \times \vec{\nabla}\delta(\mathbf{1}-\mathbf{2})]. \quad (5)$$

The nondissipative kinetic equation for the single-particle distribution function becomes now

$$\frac{\partial}{\partial t} f(\mathbf{1}, t) = \{f(\mathbf{1}), H\{f\}\} = \int d\mathbf{2}\{f(\mathbf{1}), f(\mathbf{2})\}\frac{\delta H\{f\}}{\delta f(\mathbf{2})}. \quad (6)$$

The dissipative equation is obtained by adding to the right-hand side of (6) the proper dissipation operator $W\{f\}$. The choice of $W\{f\}$ depends on the nature of the physical problem discussed. In [1] the relaxation time approximation was used in view of its simplicity. We believe that the collision operator proposed in [16] is more appropriate, because it offers the simple generalization of the Boltzmann-Lorentz [17] collision integral for the lattice gas (tight binding) models. Although our formulation is valid for arbitrary Berry curvature $\mathbf{\Omega}$, in specific applications discussed below we assume that $\mathbf{\Omega}$ is a slowly varying function of the wave vector $\mathbf{k}$ as it traverses the Brillouin zone. This implies that the average value of the Berry curvature $\bar{\mathbf{\Omega}} = \int d\mathbf{p}\mathbf{\Omega}(\mathbf{p})\varphi(\mathbf{p})$ and the average "curvature torque" $\bar{\Xi}_{ab} = \int d\mathbf{p}\Omega_a(\mathbf{p})p_b\varphi(\mathbf{p})/m$ do exist. Here and throughout this work $\varphi(\mathbf{p})$ is the equilibrium momentum distribution for the carriers at "inverse temperature" β defined as $\int d\mathbf{p}\varphi(\mathbf{p})p_i p_j = m\delta_{ij}\beta^{-1}$.

A simple Chapman-Enskog-like approximation assumes that for higher momentum moments of the distribution function [e.g., the stress tensor $P_{ij}(\mathbf{r}, t) = \int d\mathbf{p} p_i p_j f(\mathbf{r}, \mathbf{p}, t)/m$, average Berry curvature $\bar{\mathbf{\Omega}}(\mathbf{r}) = \int d\mathbf{p}\mathbf{\Omega}(\mathbf{p}) f(\mathbf{r}, \mathbf{p})$, etc.] one can make the approximation $f(\mathbf{r}, \mathbf{p}) \approx \varphi(\mathbf{p})\rho(\mathbf{r})$. Using this approximation and the explicit dissipative operator $W\{f\}$ from [16], we obtain the dispersion relation for the density fluctuations $\rho_{\mathbf{q},\omega}$, which replaces Ohm's law for spinless Bloch electrons:

$$[\tilde{\omega}(\mathbf{q}) + iz\Gamma_{\mathbf{q}}][\tilde{\omega}(\mathbf{q}) - iS_{\mathbf{q}}\Gamma_{\mathbf{q}}] = \{\mathbf{q}^2/(m\beta) - e\mathbf{q} \cdot [\mathbf{E}_0 \times (\bar{\mathbf{\Xi}} \cdot \mathbf{q})] + ie\mathbf{E}_0 \cdot \mathbf{q}/m\}. \quad (7)$$

Here $\tilde{\omega}(\mathbf{q}) = \omega - e\mathbf{q} \cdot (\bar{\mathbf{\Omega}} \times \mathbf{E}_0)$, $\Gamma_{\mathbf{q}}$, $S_{\mathbf{q}}$, and z are the scattering amplitude, scatterers' structure factor, and the coordination number, respectively, and $\bar{\mathbf{\Omega}}$, $\bar{\mathbf{\Xi}}$ are the average Berry curvature and curvature torque. Equation (7) shows the frequency shift due to the anomalous Hall drift velocity $e\bar{\mathbf{\Omega}} \times \mathbf{E}_0$.

Next we generalize our model for spin-$\frac{1}{2}$ carriers. In order to do so, we describe the state of the carriers by a spinor distribution function (density matrix) $\hat{f}(\mathbf{r}, \mathbf{p}) = \frac{1}{2} \times \sum_{\alpha=0}^{3} f_\alpha \hat{\sigma}_\alpha$, where $\hat{\sigma}_0$ is the 2×2 unit matrix and $\hat{\sigma}_i$, $i = 1, 2, 3$, are the usual Pauli matrices. The meaning of the spinor components f_α follows from the definition of the mean value of the observable $\hat{A}$, $\langle \hat{A} \rangle = \mathrm{Tr}(\hat{A}\hat{f})$, where Tr denotes the matrix trace in spinor space and integration over the phase-space variables $(\mathbf{r}, \mathbf{p})$. f_0 is the distribution function used for the spinless carriers, and f_α are the particle spin densities: $\langle S_i \rangle = \mathrm{Tr}(\hat{S}_i \hat{f}) = \frac{1}{2}\int d\mathbf{1}\, \mathrm{Tr}(\frac{\hbar}{2}\hat{\sigma}_i \sum_\alpha f_\alpha \hat{\sigma}_\alpha) = \frac{\hbar}{2}\int d\mathbf{1} f_i(\mathbf{1})$. Note that the normalization of f_0 guarantees conservation of the spin length $\langle \mathbf{S}^2 \rangle = \frac{\hbar^2}{4}\int d\mathbf{1} f_0(\mathbf{1})$.

For spinor distribution functions the generalized Lie-Poisson bracket (5) becomes now a functional 4×4 matrix:

$$[\hat{f}(\mathbf{1}), \hat{f}(\mathbf{2})] = \begin{pmatrix} \{f_0(\mathbf{1}), f_0(\mathbf{2})\}, & \{f_0(\mathbf{1}), f_j(\mathbf{2})\} \\ \{f_i(\mathbf{1}), f_0(\mathbf{2})\}, & \{f_i(\mathbf{1}), f_j(\mathbf{2})\} \end{pmatrix}, \quad (8)$$

for $i, j = 1, 2, 3$. The bracket $\{f_0(\mathbf{1}), f_0(\mathbf{2})\}$ is given by (4) and

$$\{f_i(\mathbf{1}), f_0(\mathbf{2})\} = \vec{\nabla} f_i(\mathbf{1}) \cdot \vec{\partial}\delta(\mathbf{1}-\mathbf{2}), \quad \{f_i(\mathbf{1}), f_j(\mathbf{2})\} = \varepsilon_{ijk} f_k(\mathbf{1})\delta(\mathbf{1}-\mathbf{2}). \quad (9)$$

Now the kinetic equation for the density function spinor $\hat{f}$ becomes

$$\frac{\partial \hat{f}(\mathbf{1}, t)}{\partial t} = [\hat{f}(\mathbf{1}), \hat{H}\{\hat{f}\}] + \hat{W}(\hat{f}) \equiv \mathrm{Tr}_2[\hat{f}(\mathbf{1}), \hat{f}(\mathbf{2})]\frac{\delta \hat{H}\{\hat{f}\}}{\delta \hat{f}(\mathbf{2})} + \hat{W}(\hat{f}). \quad (10)$$

Note that the dissipative operator $\hat{W}$ must preserve the length of the spin $\mathbf{S}^2$. The definition of $\{f_i, f_j\}$ in (8) guarantees that the spin length is a Casimir invariant of our Lie-Poisson algebra of spinors $\hat{f}$.

The relaxation of the spin degrees of freedom, accounted for by the dissipative operator $\hat{W}$, was described in [2] by the relaxation time approximation to the collision operator. This approximation can be justified by an analysis of the fully quantum-mechanical collision operator used in the kinetic theory of particles with angular momentum degrees of freedom [18]. This is, however, not the only possible way. The collisions with impurities which change the electron spin direction but preserve the spin magnitude can also be described by a properly tailored version of the Gilbert-Landau spin damping discussed in some models of the dissipative Heisenberg magnet [19]. In this description the damping is described by supplementing the Lie-Poisson bracket by the dissipative bracket, which in our case will read, in the notation of [8],

$$\prec f_i(\mathbf{1}), f_j(\mathbf{2}) \succ = -\lambda[\delta_{ij}\varphi(\mathbf{p_2})\delta(\mathbf{1}-\mathbf{2}) - f_i(\mathbf{1})f_j(\mathbf{2})], \quad (11)$$

where λ is the proper damping coefficient proportional to the transverse inverse relaxation time for spin relaxation. The dissipative operator $\hat{W}$ assumes then the form

$$\hat{W}_{\rm GL}(\hat{f}) = \int d\mathbf{2} \prec \hat{f}(\mathbf{1}), \hat{f}(\mathbf{2}) \succ \frac{\delta H\{\hat{f}\}}{\delta \hat{f}(\mathbf{2})}. \quad (12)$$

It is still possible to add to the dissipative operator (12) the relaxation time collision operator discussed in [1].

The problem of reconciling the Bloch description of an electron in a periodic potential with the usual vector potential description of the magnetic field and the necessity of securing gauge invariance has been the subject of intensive discussion [20]. Here we propose the extension of the phase-space description for charged particles developed in [12,13], which automatically guarantees the gauge invariance of the theory. Thus now the state of the system of semiclassical spin-$\frac{1}{2}$ Bloch electrons is described by a collection of three fields: the defined above spinor field $\hat{f}$ and two vector fields $\mathbf{E}$ and $\mathbf{B}$, the electric and the magnetic field, respectively.

The Lie-Poisson brackets for these variables are defined as follows. The spinor field obeys the bracket relations (8), where now

$$\begin{aligned}\{f_0(\mathbf{1}), f_0(\mathbf{2})\} &= \vec{\nabla} f_0(\mathbf{1}) \cdot \vec{\partial}\delta(\mathbf{1}-\mathbf{2}) - \vec{\partial} f_0(\mathbf{1}) \cdot \vec{\nabla}\delta(\mathbf{1}-\mathbf{2}) \\ &\quad + \Omega \cdot \vec{\nabla} f_0(\mathbf{1}) \times \vec{\nabla}\delta(\mathbf{1}-\mathbf{2}) + e\mathbf{B}(\mathbf{1}) \\ &\quad \cdot \vec{\partial} f_0(\mathbf{1}) \times \vec{\partial}\delta(\mathbf{1}-\mathbf{2}), \end{aligned} \quad (13)$$

and the additional bracket relations are given as

$$\begin{aligned}\{E_i(\mathbf{r}_1), B_j(\mathbf{r}_2)\} &= -\varepsilon_{ijk}\nabla_k \delta(\mathbf{r}_1 - \mathbf{r}_2), \\ \{f_0(\mathbf{1}), \mathbf{E}(\mathbf{2})\} &= -e\vec{\partial} f_0(\mathbf{1})\delta(\mathbf{1}-\mathbf{2}), \\ \{f_\alpha(\mathbf{1}), \mathbf{B}(\mathbf{2})\} &= \{f_i(\mathbf{1}), \mathbf{E}(\mathbf{2})\} = 0 \end{aligned} \quad (14)$$

($\alpha = 0, \ldots, 3$, $i = 1, 2, 3$). The Hamiltonian functional now depends on these three basic fields and reads

$$\begin{aligned} H\{\hat{f}, \mathbf{E}, \mathbf{B}\} &= \int d\mathbf{1} f_0(\mathbf{1})\epsilon(\mathbf{1}) + \gamma \int d\mathbf{1} \sum_{j=1}^{3} f_j(\mathbf{1}) B_j(\mathbf{1}) \\ &\quad + \frac{1}{8\pi}\int d\mathbf{r}(\mathbf{E}^2 + \mathbf{B}^2). \end{aligned} \quad (15)$$

The Hamiltonian (15) is the classical Hamiltonian from [12] supplemented with Zeeman-like coupling terms proportional to $\sum_j f_j B_j$. There is no place here for adding terms which would mimic the Pauli spin-orbit coupling. The latter will follow from a more comprehensive derivation of the equations of motion for spin-charge carriers than that used to establish (1). Issues posed by spin-orbit coupling in combination with Berry phases are important problems for further research.

The equations of motion for state variables $\hat{f}, \mathbf{E}, \mathbf{B}$ are now given by (10) and

$$\frac{\partial \mathbf{E}(\mathbf{r}, t)}{\partial t} = \{\mathbf{E}(\mathbf{r}), H\}, \qquad \frac{\partial \mathbf{B}(\mathbf{r}, t)}{\partial t} = \{\mathbf{B}(\mathbf{r}), H\}. \quad (16)$$

Equations (16) are two of Maxwell's equations for the electromagnetic fields $\mathbf{E}$ and $\mathbf{B}$, containing the spin contribution to the internal magnetic field of the system stemming from the term $\gamma \int d\mathbf{1} \sum_{j=1}^{3} f_j(\mathbf{1}) B_j(\mathbf{1})$ in the Hamiltonian (15). Note that this Hamiltonian is just the sum of the kinetic energies for the corresponding components of the system. The whole interaction is now contained in the Lie-Poisson brackets for the state variables. The full discussion of this point was given in [12].

To see the usefulness of this proposed phase-space description, we apply our formulation to the analysis of the weakly interacting set of semiclassical Bloch electrons in the absence of the magnetic field and neglecting the effect of collisions. It is sufficient then to use the spinless distribution function f. The Maxwell equations (16) reduce then to the Poisson equation for the electric field

$$\vec{\nabla} \cdot \mathbf{E} = 4\pi e \rho, \qquad \vec{\nabla} \times \mathbf{E} = 0, \quad (17)$$

where the particle density ρ is defined as before through the momentum integral of f. Writing now equations for two first moments of f, assuming that the pressure tensor is diagonal, $P_{ij} = \int d\mathbf{p} p_i p_j f(\mathbf{r}, \mathbf{p})/m = \delta_{ij} P(\rho)$, and linearizing them around the state characterized by constant carrier density ρ_0 and constant external electric field $\mathbf{E}_0$, we obtain with the use of (17) the dispersion relation for the system excitations:

$$\begin{aligned}[\omega - e\mathbf{q} \cdot (\bar{\mathbf{\Omega}} \times \mathbf{E}_0)]^2 &\equiv \tilde{\omega}(\mathbf{q})^2 \\ &= \omega_P^2 + c_{ij} q^i q^j + \frac{ie}{m}\mathbf{q} \cdot \mathbf{E}_0. \end{aligned} \quad (18)$$

Here, as usual, ω and $\mathbf{q}$ are the excitation frequency and wave vector, respectively, $\omega_P = \sqrt{4\pi e^2 \rho_0/m}$ is the plasma frequency, $c_{ij} = c^2(\delta_{ij} - \varepsilon_{i\ell k} E_{0\ell} \bar{\Xi}_{kj}/c^2)$, and $c = \sqrt{(\frac{\partial P}{\partial \rho})_0}$ is the speed of sound in the carrier gas. One sees that the excitation group velocity is shifted with respect to that of the usual plasma wave in the frame of reference drifting with the anomalous Hall velocity $\mathbf{v}_D = e\bar{\mathbf{\Omega}} \times \mathbf{E}_0$ and that the sound velocity is anisotropic ($c^2 q^2 \rightarrow c_{ij} q^i q^j$) due to the coupling between the external electric field and the Berry curvature torque $\bar{\Xi}$.

We conclude this Letter with an analysis of the kinetic Eq. (10) using the dissipative operator (12) in the absence of the external electric field and neglecting the internal electric and magnetic fields generated by motion of the charged carriers and described by the solutions of (16). Using the resulting expression for the Hamiltonian (15) and the form of the dissipative operator (12), we derive the conservation equation for the spatial spin density $S_i(\mathbf{r}) = \int d\mathbf{p} f_i(\mathbf{r}, \mathbf{p})$ by integrating (10) over the momenta:

$$\frac{\partial \mathbf{S}(\mathbf{r},t)}{\partial t} + \vec{\nabla} \cdot \mathbf{\Lambda}(\mathbf{r},t) = \gamma \mathbf{S} \times \mathbf{B} - \lambda \mathbf{S} \times (\mathbf{S} \times \mathbf{B}), \quad (19)$$

where the spin current tensor $\Lambda_{ij} = \int d\mathbf{p} p_i f_j(\mathbf{r}, \mathbf{p})$. As it stands, Eq. (19) is the convective version of the Gilbert-Landau equation for the system magnetization widely discussed in the theory of magnetism literature [20]. The absence of the external electric field cancels the Berry curvature contribution to the spin density evolution equation. The Berry curvature will appear if the internal electric field due to carrier dynamics is included in a fashion similar to (18).

The equation of motion for the spin current $\mathbf{\Lambda}$ follows from (10) by multiplication by $\mathbf{p}$ and integration over the momenta. As usual, this will not be a closed equation, because it involves the third-order tensorial current $Q_{ijk} = \int d\mathbf{p} p_i p_j f_k$, for which we would require something like the lowest order Chapman-Enskog assumption $f_j = \varphi(\mathbf{p}) S_j(\mathbf{r})$. Using this approximation we find for the spin current equation

$$\frac{\partial \Lambda_{ij}}{\partial t} + \beta^{-1} \nabla_i S_j = \tau_{ij} + \lambda \Lambda_{ij} \mathbf{S} \cdot \mathbf{B}, \quad (20)$$

where $\tau_{ij} = \gamma \varepsilon_{ilm} \Lambda_{jl} B_m$ is the magnetic torque tensor.

We show in this Letter that the dynamics of an ensemble of the semiclassical spin-$\frac{1}{2}$ Bloch carriers can be described using an algebraic procedure discussed by us before for many other physical models [8], using as building blocks the phase-space distribution spinor and the electric and magnetic fields. We show how the noncommutativity of the position variables, resulting from the Berry curvature contribution to the equations of motion, can be incorporated into the Lie-Poisson brackets for field variables. We outline how the hydrodynamics (moments equations) for the kinetic equations can be formulated in the presence of various different types of dissipative processes. We also show a few explicit examples of how our approach works. For example, we predict Berry curvature-dependent shifts of the plasma frequency and the sound velocity for the semiclassical Bloch electron plasma.

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