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Spin dynamics with non-Abelian Berry gauge fields as a semiclassical constrained Hamiltonian system

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Abstract
The dynamics of observables which are matrices depending on $\hbar$ and taking values in classical phase-space is defined by retaining the terms up to the first order in $\hbar$ of the Moyal bracket. Within this semiclassical approach a first-order Lagrangian involving gauge fields is studied as a constrained Hamiltonian system. This provides a systematic study of spin dynamics in the presence of non-Abelian Berry gauge fields. We applied the method to various types of dynamical spin systems and clarified some persisting discussions. In particular employing the Berry gauge field which generates the Thomas precession, we calculated the force exerted on an electron in the external electric and magnetic fields. Moreover, a simple semiclassical formulation of the spin Hall effect is accomplished.

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1. Introduction

In [1], the intrinsic spin Hall effect was studied considering the Abelian and non-Abelian Berry gauge fields [2] arising from the adiabatic transport. After this seminal work, there has been a great effort to employ Berry gauge fields to acquire a better understanding of spin-dependent dynamics semiclassically [3–17]. Although similar phenomena were treated letting coordinates and/or momenta be noncommuting, they appear to be disconnected. We would like to present a formulation which embraces these approaches. In our formulation keeping track of the semiclassical approximation is easy and interactions between different gauge fields can be introduced in a simple manner.

To present our approach we need to recall the Weyl–Wigner–Groenewold–Moyal (WWGM) method of quantization [18] as well as the Dirac formulation of constrained Hamiltonian systems [19].

Quantum dynamics of particles without spin is usually provided by operators depending on the quantum phase-space variables $(\hat{p}_\mu, \hat{x}_\mu)$ satisfying the Heisenberg algebra: $[\hat{p}_\mu, \hat{x}_\nu] = -i\hbar\delta_{\mu\nu}, [\hat{p}_\mu, \hat{p}_\nu] = 0$ and $[\hat{x}_\mu, \hat{x}_\nu] = 0$. However, there is an alternative approach due to WWGM where one introduces symbols of operators and their star product: observables are functions of classical phase-space variables and the operator product is replaced with the star product [18]. The WWGM method works well for observables possessing a classical limit. However, it is not clear how it should be generalized to embrace spin degrees of freedom. Spin may be incorporated into classical mechanics considering the semiclassical approximation as well as the nonrelativistic limit of the Dirac Hamiltonian. The latter is given in terms of operator-valued matrices. Hence, we consider observables which are matrices whose elements are the functions of classical phase-space variables but depend on $\hbar$. Dynamical equations of these matrix-valued symbols will be given by a semiclassical bracket acquired from the Moyal bracket.

When there are some different types of gauge fields, they can be incorporated into the Hamiltonian formalism by considering an enlarged Lagrangian system which leads to second class constraints. Indeed, to embed Berry gauge fields in the semiclassical scheme, a constrained Hamiltonian dynamics will be presented starting from an appropriate matrix-valued Lagrangian. We adopt the Dirac formulation of constrained Hamiltonian dynamics by replacing the Poisson bracket with the proposed semiclassical bracket. This furnishes us with a systematic formulation of dynamics when non-Abelian Berry gauge fields are present.

Once this formulation of matrix-valued observables coupled to gauge fields is accomplished, we can employ it to investigate dynamical properties of diverse spin systems. The semiclassical dynamics of Bloch electrons in the adiabatic approximation where interband interactions are neglected was discussed in [8, 11]. We study the same problem within our approach. We achieved the correct phase-space measure and noncommutativity of phase-space variables. Unitary transformations which generate Berry gauge fields are also considered. We derived the equations of motion which can be used in topological spin transport [12]. In [15] was shown that when an electric field is applied to an electron, a transverse force on the spin current occurs. This force resulted in the Heisenberg equation of motion of velocity, considering the nonrelativistic limit of the Dirac Hamiltonian. We show that it can easily be derived within our formulation. On the other hand, the nonrelativistic limit of the Dirac Hamiltonian can also be obtained by a momentum-dependent Berry gauge field which generates the Thomas precession [20]. We calculate the force acting on an electron in the electric and magnetic fields in the presence of this gauge field. The same transverse force on the spin current occurs, which depends only on the electric field. However, the terms depending on both the magnetic and electric fields do not concur. Experiments may settle this disagreement. The intrinsic spin Hall effect was envisaged in [21] analyzing the spin current due to the Rashba Hamiltonian [22]. Investigating the Rashba Hamiltonian is still attractive, although when the vertex corrections are taken into account the originally proposed universal behavior of a spin Hall conductivity does not survive [23] (for a review see [24]). We study the Rashba spin–orbit coupling within our semiclassical approach to attain a very simple formulation of the spin Hall conductivity. It is inspired by the derivation of the Hall conductivity by demanding that the force acting on electrons vanish.

In section 2 we present the semiclassical bracket of matrix-valued observables and its basic properties. The semiclassical constrained Hamiltonian formulation which leads to a systematic approach of analyzing dynamical systems with different sorts of non-Abelian gauge fields is given in section 3. An application of the formalism to various dynamical spin systems is considered in section 4. We clarified some persisting discussions and also gave a simplistic formulation of the spin Hall conductivity. The obtained results and other possible applications are discussed in the concluding section.

2. Semiclassical symbols and the Moyal bracket

Let us deal with the classical canonical variables (p_μ, x_μ) corresponding to the quantum phase-space $(\hat{p}_\mu, \hat{x}_\mu)$; $\mu = 1, \ldots, M$. In the WWGM method of quantization one considers the symbol map [18]

$$\mathcal{S}(\hat{f}(\hat{p}, \hat{x})) = f(p, x), \tag{1}$$

where $f(p, x)$ is the c-number function corresponding to the operator $\hat{f}(\hat{p}, \hat{x})$.

Let the operator product of the quantum observables $\hat{f}$ and $\hat{g}$ be

$$\hat{f}(\hat{p}, \hat{x})\hat{g}(\hat{p}, \hat{x}) = \hat{h}(\hat{p}, \hat{x}).$$

The symbol map should respect the operator product, so that we should introduce a (star) product satisfying

$$\mathcal{S}(\hat{f}(\hat{p}, \hat{x})\hat{g}(\hat{p}, \hat{x})) = \mathcal{S}(\hat{h}(\hat{p}, \hat{x})) = \mathcal{S}(\hat{f}(\hat{p}, \hat{x})) \star \mathcal{S}(\hat{g}(\hat{p}, \hat{x})). \tag{2}$$

Obviously, the symbol map as well as the star product depends on the operator ordering adopted. We deal with the Weyl ordering where the associative star product is

$$\star = \exp\left[\frac{\mathrm{i}\hbar}{2}\left(\frac{\overleftarrow{\partial}}{\partial x^\mu}\frac{\overrightarrow{\partial}}{\partial p_\mu} - \frac{\overleftarrow{\partial}}{\partial p^\mu}\frac{\overrightarrow{\partial}}{\partial x_\mu}\right)\right]. \tag{3}$$

The arrows on the derivatives indicate the direction in which they should be applied. We adopt the Einstein convention, hence the repeated indices are summed over. To imitate the commutator of operators, we define the Moyal bracket of two arbitrary observables $f(p, x)$ and $g(p, x)$ as

$$[f(p, x), g(p, x)]_\star \equiv f(p, x) \star g(p, x) - g(p, x) \star f(p, x). \tag{4}$$

Hence, the classical phase-space variables satisfy the Moyal bracket

$$[p_\mu, x^\nu]_\star = -\mathrm{i}\hbar\delta_\mu^\nu, \tag{5}$$

analogous to the canonical commutation relations. The classical limit of the Moyal bracket (4) is the Poisson bracket:

$$\lim_{\hbar\to 0}\frac{-\mathrm{i}}{\hbar}[f(p, x), g(p, x)]_\star = \{f(p, x), g(p, x)\} \equiv \frac{\partial f}{\partial x^\nu}\frac{\partial g}{\partial p_\nu} - \frac{\partial f}{\partial p_\nu}\frac{\partial g}{\partial x^\nu}. \tag{6}$$

When one considers the Dirac Hamiltonian or higher spin formalisms, it is still possible to define a symbol map. Now observables are matrices which take values in the classical phase-space [25, 26]. The Moyal bracket of the matrices $M_{ab}(p, x)$ and $N_{ab}(p, x)$ can be defined as

$$([M(p, x), N(p, x)]_\star)_{ab} = M_{ac}(p, x) \star N_{cb}(p, x) - N_{ac}(p, x) \star M_{cb}(p, x). \tag{7}$$

However, the classical limit (6) of (7), in addition to the Poisson brackets of matrices, yields a commutator of matrices which is singular. Generally the observables in a block-diagonal form are taken into account for getting rid of the matrix commutator. As far as observables possessing a direct classical interpretation are considered, this restriction seems necessary for a semiclassical study [26]. Indeed, we will relax this condition. When interactions are considered, the nonrelativistic limit of the Dirac Hamiltonian may include the spin. Then there will be terms depending on $\hbar$ whose classical limit is not direct. We would like to study the semiclassical spin dynamics. Thus, although we deal with the classical phase-space we let the symbols depend on $\hbar$. Therefore, instead of the classical limit (6) we deal with the limit obtained from the Moyal bracket (7) by retaining the terms up to $\hbar$:

$$\{M(p,x), N(p,x)\}_C \equiv \frac{-\mathrm{i}}{\hbar}[M,N] + \frac{1}{2}\{M(p,x), N(p,x)\} - \frac{1}{2}\{N(p,x), M(p,x)\}. \tag{8}$$

We would like to emphasize that the first term is the commutator of matrices; it is not the quantum-mechanical one. Hence, it is not an attempt to combine the quantum commutator and the Poisson bracket[1]. Although we keep terms up to $\hbar$ order in the Moyal bracket (7), remember that M and N can depend on $\hbar$. In fact, (8) is an expansion in powers of $\hbar$ where only the first two lowest nonvanishing terms are retained.

Multiplication of observables is still given by the star product (3). Hence the Jacobi identity which should be satisfied is given by

$$\begin{aligned}\{M,\{N,L\}_C\}_\star &+ \{N,\{L,M\}_C\}_\star + \{L,\{M,N\}_C\}_\star \\ &= [M,\{N,L\}] - [M,\{L,N\}] + \{M,[N,L]\} - \{[N,L],M\} - \frac{\mathrm{i}}{\hbar}[M,[N,L]] \\ &\quad + (\text{cyclic permutations of } M, N, L) + \mathcal{O}(\hbar) = 0.\end{aligned}$$

In fact one can show that it is fulfilled up to the $\hbar$ order. Moreover, one can observe that the Leibniz rule defined as

$$\{M\star N, L\}_C = \{M,L\}_C \star N + M \star \{N,L\}_C \tag{9}$$

is also satisfied at the $\hbar$ order.

To define semiclassical dynamical equations, we propose to replace the Poisson bracket in classical dynamical equations with the semiclassical bracket (8). Let the symbol of the Dirac Hamiltonian or its nonrelativistic approximation be the matrix $H(p,x)$. Thus, we consistently establish

$$\dot{M}(p,x) = \{M(p,x), H(p,x)\}_C \tag{10}$$

as the time evolution of the semiclassical observable $M(p,x)$. It is worth recalling that, as is elucidated above, in this equation of motion one retains the lowest two nonvanishing terms in $\hbar$.

3. A semiclassical constrained Hamiltonian system

When a classical system is described with a Lagrangian, the definition of canonical momenta can yield some relations between coordinates and momenta which are called primary constraints. Preserving these constraints in time may produce some other constraints [19]. Once all the constraints are derived each one can be classified as first or second class due to their Poisson bracket relations. A method of treating second class constraints is to introduce Dirac brackets which effectively set the constraints equal to zero. We will consider a constrained Hamiltonian system utilizing the semiclassical bracket (8) and the dynamical equation (10).

Let us consider the first-order Lagrangian which is a $N \times N$ matrix:

$$\mathcal{L} = \dot{r}^\alpha\left(\tfrac{1}{2}Iy_\alpha + \rho\mathcal{A}_\alpha(r,y) + \eta a_\alpha(r,y)\right) - \dot{y}^\alpha\left(\tfrac{1}{2}Ir_\alpha - \xi\mathcal{B}_\alpha(r,y)\right) - \mathcal{H}_0(r,y). \tag{11}$$

[1] For the attempts of combining the Poisson and quantum brackets, see [27] and references given therein.

Here, $\alpha = 1, \ldots, n$, and for the nonrelativistic case the dot over the variables indicates the derivative with respect to time t and for the relativistic formalism it is the derivative with respect to an evolution parameter $\tau.\rho, \xi$ and η are coupling constants corresponding to the gauge fields $\mathcal{A}$, $\mathcal{B}$ and a, respectively, which are $N \times N$ matrices. I is the unit matrix. Observe that in (11) generally one cannot get rid of $\mathcal{A}$, $\mathcal{B}$ and a terms by redefining the coordinates r_α or y_α. The definition of canonical momenta

$$\Pi_r^\alpha = \frac{\partial \mathcal{L}}{\partial \dot{r}_\alpha}, \qquad \Pi_y^\alpha = \frac{\partial \mathcal{L}}{\partial \dot{y}_\alpha}$$

leads to vanishing of the relations

$$\psi^{1\alpha} \equiv \left(\Pi_r^\alpha - \tfrac{1}{2} y^\alpha\right) I - \rho \mathcal{A}^\alpha - \eta a^\alpha, \tag{12}$$

$$\psi^{2\alpha} \equiv \left(\Pi_y^\alpha + \tfrac{1}{2} r^\alpha\right) I - \xi \mathcal{B}^\alpha, \tag{13}$$

which are called primary constraints. In terms of the canonical Hamiltonian $\mathcal{H}_0$, we need to introduce the extended Hamiltonian

$$\mathcal{H}_e = \mathcal{H}_0 + \lambda_z^\alpha \psi_\alpha^z, \tag{14}$$

where λ_z^α are Lagrange multipliers and $z = 1, 2$. To employ the semiclassical approach of section 2, we identify the canonical variables as $p^\mu = \left(\Pi_y^\alpha, \Pi_r^\alpha\right)$ and $x_\mu = (y_\alpha, r_\alpha)$. The semiclassical brackets between the constraints can be shown to be

$$\begin{aligned}
\left\{\psi_\alpha^1, \psi_\beta^1\right\}_C &= \rho F_{\alpha\beta} + \eta f_{\alpha\beta} - \frac{\mathrm{i}\rho\eta}{\hbar}[\mathcal{A}_\alpha, a_\beta] - \frac{\mathrm{i}\rho\eta}{\hbar}[a_\alpha, \mathcal{A}_\beta], \\
\left\{\psi_\alpha^2, \psi_\beta^2\right\}_C &= \xi G_{\alpha\beta}, \\
\left\{\psi_\alpha^1, \psi_\beta^2\right\}_C &= -g_{\alpha\beta} + \xi \frac{\partial \mathcal{B}_\beta}{\partial r^\alpha} - \rho \frac{\partial \mathcal{A}_\alpha}{\partial y^\beta} - \eta \frac{\partial a_\alpha}{\partial y^\beta} - \frac{\mathrm{i}\xi\rho}{\hbar}[\mathcal{A}_\alpha, \mathcal{B}_\beta] - \frac{\mathrm{i}\xi\eta}{\hbar}[a_\alpha, \mathcal{B}_\beta],
\end{aligned}$$

where $g^{\alpha\beta}$ is the flat metric, and field strengths are defined as

$$f_{\alpha\beta} = \frac{\partial a_\beta}{\partial r^\alpha} - \frac{\partial a_\alpha}{\partial r^\beta} - \frac{\mathrm{i}\eta}{\hbar}[a_\alpha, a_\beta], \tag{15}$$

$$F_{\alpha\beta} = \frac{\partial \mathcal{A}_\beta}{\partial r^\alpha} - \frac{\partial \mathcal{A}_\alpha}{\partial r^\beta} - \frac{\mathrm{i}\rho}{\hbar}[\mathcal{A}_\alpha, \mathcal{A}_\beta], \tag{16}$$

$$G_{\alpha\beta} = \frac{\partial \mathcal{B}_\beta}{\partial y^\alpha} - \frac{\partial \mathcal{B}_\alpha}{\partial y^\beta} - \frac{\mathrm{i}\xi}{\hbar}[\mathcal{B}_\alpha, \mathcal{B}_\beta]. \tag{17}$$

Therefore, constraints (12) and (13) are second class and the condition of preserving them in time,

$$\left\{\psi_\alpha^z, \mathcal{H}_e\right\}_C \approx 0, \tag{18}$$

where $\approx$ indicates that the equality is valid up to vanishing of constraints, will determine λ_α^z. In fact, in terms of

$$C_{\alpha\beta}^{zz'} = \left\{\psi_\alpha^z, \psi_\beta^{z'}\right\}_C, \qquad C_{\alpha\gamma}^{zz''} C_{z'z''}^{-1\gamma\beta} = \delta_\alpha^\beta \delta_{z'}^z, \tag{19}$$

one can show that (18) leads to

$$\lambda_z^\alpha = -\left\{\psi_\beta^{z'}, H_0\right\}_C C_{zz'}^{-1\alpha\beta}. \tag{20}$$

To set effectively the second class constraints (12) and (13) equal to zero, we introduce the semiclassical Dirac bracket

$$\{M, N\}_{CD} \equiv \{M, N\}_C - \{M, \psi^z\}_C C_{zz'}^{-1} \{\psi^{z'}, N\}_C. \tag{21}$$

Now, in dynamical equations the semiclassical bracket of observables (8) should be substituted with the semiclassical Dirac bracket (21). Observe that the coordinates satisfy

$$\{r^\alpha, r^\beta\}_{CD} = C_{11}^{-1\alpha\beta}, \tag{22}$$

$$\{y^\alpha, y^\beta\}_{CD} = C_{22}^{-1\alpha\beta}, \tag{23}$$

$$\{r^\alpha, y^\beta\}_{CD} = C_{12}^{-1\alpha\beta}. \tag{24}$$

We omitted the unit matrix I on the left-hand sides. Obviously, $C_{12}^{-1\alpha\beta} = -C_{21}^{-1\alpha\beta} = g_{\alpha\beta} + \cdots$, thus one should consider r_α as coordinates and y_α as the corresponding momenta.

The equation of motion of an observable $\mathcal{O}(r, y)$ is given with the extended Hamiltonian as

$$\dot{\mathcal{O}}(r, y) = \{\mathcal{O}(r, y), H_e\}_C, \tag{25}$$

in accord with the constrained dynamical systems. Plugging solution (20) into (14) yields

$$\mathcal{H}_e = \mathcal{H}_0 - \left\{\psi_\beta^{z'}, H_0\right\}_C C_{zz'}^{-1\alpha\beta}\psi_\alpha^z.$$

The inverse matrix elements $C_{zz'}^{-1\alpha\beta}$ will be obtained as a power series in the coupling constants ρ, ξ which may be identified with $\hbar$. Then in the equation of motion (25) we will retain the lowest two nonvanishing terms in $\hbar$.

4. Spin dynamics

Within the formulation of the previous section, we will focus on some different approaches of studying semiclassical dynamics of electrons in terms of Berry gauge fields. Before considering specific systems let us present the general formulation where $a_\alpha = a_\alpha(r)$ is an Abelian gauge field and the coupling constants are $\eta = e/c, \xi = \hbar$ and $\rho = -\hbar$. In our notation $e < 0$ for an electron. The matrix $C_{\alpha\beta}^{zz'}$ defined in (19) reads

$$C_{\alpha\beta}^{zz'} = \begin{pmatrix} \frac{e}{c} f_{\alpha\beta} - \hbar F_{\alpha\beta} & -g_{\alpha\beta} + \hbar M_{\alpha\beta} \\ g_{\alpha\beta} - \hbar M_{\beta\alpha} & \hbar G_{\alpha\beta} \end{pmatrix}, \tag{26}$$

where

$$M_{\alpha\beta} = \frac{\partial \mathcal{B}_\beta}{\partial r^\alpha} + \frac{\partial \mathcal{A}_\alpha}{\partial y^\beta} + \mathrm{i}[\mathcal{A}_\alpha, \mathcal{B}_\beta]. \tag{27}$$

Obviously, $M_{\alpha\beta}$ does not possess any symmetry or antisymmetry with respect to the indices, so that one should distinguish $M_{\alpha\beta}$ from $M_{\beta\alpha}$. The inverse of (26) can be calculated at the first order in $\hbar$ as

$$C_{11\alpha\beta}^{-1} = \hbar G_{\alpha\beta}, \tag{28}$$

$$C_{12\alpha\beta}^{-1} = g_{\alpha\beta} + \hbar M_{\beta\alpha} - \frac{e}{c}\hbar (Gf)_{\alpha\beta}, \tag{29}$$

$$C_{21\alpha\beta}^{-1} = -g_{\alpha\beta} - \hbar M_{\alpha\beta} + \frac{e}{c}\hbar (fG)_{\alpha\beta}, \tag{30}$$

$$C_{22\alpha\beta}^{-1} = \frac{e}{c} f_{\alpha\beta} - \hbar F_{\alpha\beta} + \frac{e\hbar}{c}(Mf)_{\alpha\beta} - \frac{e\hbar}{c}(Mf)_{\beta\alpha} - \frac{e^2\hbar}{c^2}(fGf)_{\alpha\beta}. \tag{31}$$

The equations of motion of the phase-space variables can be obtained as

$$\dot{r}^\alpha = \hbar\left(\frac{\partial H_0}{\partial r^\beta} + \mathrm{i}[\mathcal{A}_\beta, H_0]\right) G^{\alpha\beta} + \left(\frac{\partial H_0}{\partial y^\beta} - \mathrm{i}[\mathcal{B}_\beta, H_0]\right)\left(g^{\alpha\beta} + \hbar M^{\beta\alpha} - \frac{e\hbar}{c}(Gf)^{\alpha\beta}\right), \tag{32}$$

$$\dot{y}^\alpha = \left(\frac{\partial H_0}{\partial r^\beta} + \mathrm{i}[\mathcal{A}_\beta, H_0]\right)\left(-g^{\alpha\beta} - \hbar M^{\alpha\beta} + \frac{e\hbar}{c}(fG)^{\alpha\beta}\right) + \left(\frac{\partial H_0}{\partial y^\beta} - \mathrm{i}[\mathcal{B}_\beta, H_0]\right)$$
$$\times\left(\frac{e}{c}f^{\alpha\beta} - \hbar F^{\alpha\beta} + \frac{e\hbar}{c}(Mf)^{\alpha\beta} - \frac{e\hbar}{c}(Mf)^{\beta\alpha} - \frac{e^2\hbar}{c^2}(fGf)^{\alpha\beta}\right), \tag{33}$$

at the first order in $\hbar$, employing definition (25).

4.1. Phase-space measure

In [8, 11], the Berry phase emerges because of keeping only lower band effects in studying the semiclassical dynamics of Bloch electrons. To understand this formalism let $a_\alpha = a_\alpha(r)$ be the electromagnetic gauge field with the coupling constant $\eta = e/c$ and the Berry gauge fields be $\mathcal{A}_\alpha = 0$ and $\mathcal{B}_\alpha = \mathcal{B}_\alpha(y)$ with $\xi = \hbar$. Although, in [8, 11] only the Abelian gauge field was considered, we let $\mathcal{B}_\alpha$ be non-Abelian. Hence, the matrix C is given as in (26) with $F_{\alpha\beta} = M_{\alpha\beta} = 0$, and at the first order in $\hbar$ the following semiclassical Dirac brackets result,

$$\{r_\alpha, r_\beta\}_{CD} = \hbar G_{\alpha\beta}, \tag{34}$$

$$\{r_\alpha, y_\beta\}_{CD} = g_{\alpha\beta} - \frac{e\hbar}{c}(Gf)_{\alpha\beta}, \tag{35}$$

$$\{y_\alpha, r_\beta\}_{CD} = -g_{\alpha\beta} + \frac{e\hbar}{c}(fG)_{\alpha\beta}, \tag{36}$$

$$\{y_\alpha, y_\beta\}_{CD} = \frac{e}{c}f_{\alpha\beta} - \frac{e^2\hbar}{c^2}(fGf)_{\alpha\beta}. \tag{37}$$

Similar relations were obtained in [28] by studying the electromagnetic interactions of anyons. Now, the equations of motion of r_α and y_α can be straightforwardly derived from (32) and (33), respectively.

Adopting the formalism of the usual constrained Hamiltonian systems [29, 30], the semiclassical phase-space volume element in the presence of second class constraints is given by

$$\left(\prod_\alpha \mathrm{d}\Pi_r^\alpha\, \mathrm{d}\Pi_y^\alpha\, \mathrm{d}y_\alpha\, \mathrm{d}r_\alpha\right)\det{}^{1/2}C\,\delta(\psi_1)\delta(\psi_2).$$

After eliminating Π_r and Π_y by employing constraints (12) and (13), and using (26) with $F_{\alpha\beta} = M_{\alpha\beta} = 0$, the phase-space volume element becomes

$$\left(\prod_\alpha \mathrm{d}y_\alpha\, \mathrm{d}r_\alpha\right)\det{}^{1/2}C = \left(\prod_\alpha \mathrm{d}y_\alpha\, \mathrm{d}r_\alpha\right)\left(1 - \frac{f_{\gamma\beta}G^{\gamma\beta}}{2}\right). \tag{38}$$

This is the phase-space volume element discussed in [8, 11]. Although in a different context in [8] the role of second class constraints in defining the phase-space volume element (38) was noted.

4.2. Unitary transformations

The nonrelativistic approximation of the Dirac Hamiltonian interacting with external fields can be obtained in terms of the Foldy–Wouthuysen unitary transformation U. In [1, 13] Foldy–Wouthuysen transformations were engaged to introduce Berry gauge fields. In [13] a projector on the positive energy space $\mathcal{P}$ is employed to define

$$B_i = \mathcal{P}U\frac{\partial U^\dagger}{\partial y^i}. \tag{39}$$

Here, y_i are the components of the 3-vector $\boldsymbol{y}$ and the flat metric is $g_{ij} = \delta_{ij}; i, j = 1, 2, 3$. The Berry gauge field can be shown to be [13]

$$B_i = \frac{c^2\epsilon_{ijk}y_j\sigma_k}{2\left(E_p^2 + mc^2E_p\right)}, \tag{40}$$

where $E_p^2 = (\boldsymbol{y}\cdot\boldsymbol{y})c^2 + m^2c^4$ and σ_i are the Pauli matrices. This is a non-Abelian gauge field. Using (40) in the general approach (22)–(24), (28)–(31) with $\mathcal{A} = 0$, $a = 0$ and $\xi = \hbar$, yields

$$\{y_i, y_j\}_{CD} = 0, \tag{41}$$

$$\{y_i, r_j\}_{CD} = -\delta_{ij}, \tag{42}$$

$$\{r_i, r_j\}_{CD} = -\mathrm{i}\epsilon_{ijk}\frac{c^4}{2E_p^3}\left(m\sigma^k + \frac{y^k(\boldsymbol{y}\cdot\sigma)}{E_p + mc^2}\right). \tag{43}$$

These coincide with the noncommutativity relations obtained in [13].

On the other hand, in [12] a unitary transformation $U = U(r, y)$ which diagonalizes the initial matrix-valued Hamiltonian was introduced. Generally $U = U(r, y)$ depends on all phase-space variables. Hence one can define the gauge fields which are non-Abelian as $\mathcal{A}_i^G = -U\frac{\partial U^\dagger}{\partial r^i}, \mathcal{B}_i^G = U\frac{\partial U^\dagger}{\partial y^i}$, with $\xi = \hbar, \rho = -\hbar$. Because of being pure gauge fields their field strengths vanish: $F_{ij}^G = 0$, $G_{ij}^G = 0$. However, in the adiabatic approximation one deals with

$$\mathcal{A}_i^{(ad)} \equiv \mathrm{diag}\left(U\frac{\partial U^\dagger}{\partial r^i}\right), \qquad \mathcal{B}_i^{(ad)} \equiv \mathrm{diag}\left(U\frac{\partial U^\dagger}{\partial y^i}\right). \tag{44}$$

Though these are Abelian gauge fields, their field strengths

$$F_{ij}^{(ad)} = \frac{\partial\mathcal{A}_j^{(ad)}}{\partial r^i} - \frac{\partial\mathcal{A}_i^{(ad)}}{\partial r^j}, \qquad G_{ij}^{(ad)} = \frac{\partial\mathcal{B}_j^{(ad)}}{\partial y^i} - \frac{\partial\mathcal{B}_i^{(ad)}}{\partial y^j}$$

do no longer vanish.

The equations of motion of the phase-space variables can be read directly from (32) and (33) as

$$\dot{r}_i = \hbar\frac{\partial H_0}{\partial r_j}G_{ij}^{(ad)} + \frac{\partial H_0}{\partial y_j}\left(\delta_{ij} + \hbar M_{ij}^{(ad)} - \frac{e\hbar}{c}(G^{(ad)}f)_{ij}\right),$$

$$\dot{y}_i = \frac{\partial H_0}{\partial r_j}\left(-\delta_{ij} - \hbar M_{ij}^{(ad)} + \frac{e\hbar}{c}(fG^{(ad)})_{ij}\right)$$
$$+ \frac{\partial H_0}{\partial y_j}\left(\frac{e}{c}f_{ij} - \hbar F_{ij}^{(ad)} + \frac{e\hbar}{c}(M^{(ad)}f)_{ij} - \frac{e\hbar}{c}(M^{(ad)}f)_{ij} - \frac{e^2\hbar}{c^2}(fG^{(ad)}f)_{ij}\right),$$

where f_{ij} is the electromagnetic field strength, $\eta = e/c$ and

$$M_{ij}^{(ad)} = \frac{\partial\mathcal{B}_j^{(ad)}}{\partial r^i} + \frac{\partial\mathcal{A}_i^{(ad)}}{\partial y^j}.$$

In terms of these equations of motion one can study topological spin transport.

4.3. Transverse spin force

We would like to discuss the spin-dependent dynamics obtained in [15] within our approach by using the equations of motion (32) and (33). For this purpose we choose the canonical Hamiltonian to be

$$H_0 = \frac{1}{2m}\boldsymbol{y}^2 + V + \mu_B\sigma\cdot\boldsymbol{B}, \tag{45}$$

where $\mu_B = -e\hbar/2mc$ and at the first order in $\hbar$ we take $V_{\text{eff}} = V(\boldsymbol{r}) + \frac{\hbar^2}{8m^2c^2}\frac{\partial^2 V(\boldsymbol{r})}{\partial r_i^2} \approx V. B_i = \frac{1}{2}\epsilon_{ijk} f^{jk}$ is the external magnetic field and σ_i are the Pauli matrices. In accord with [15] we let $\mathcal{B} = 0$ and the other Berry connection be

$$\mathcal{A}_i = \frac{\epsilon_{ijk}\sigma_j}{4mc^2}\frac{\partial V}{\partial r_k}. \tag{46}$$

Moreover, we set $\eta = e/c$ and $\rho = -\hbar$. We would like to emphasize that r_i and y_i are the coordinates and momenta in the restricted phase-space. When we plug the gauge field (46) and the canonical Hamiltonian (45) into the equations of motion (32), (33) we obtain

$$\dot{r}_i = \frac{\partial H_0}{\partial y_i} = \frac{y_i}{m}, \tag{47}$$

$$\dot{y}_i = -\frac{\partial H_0}{\partial r_i} - \mathrm{i}[\mathcal{A}_i, H_0] + \frac{\partial H_0}{\partial y_j}\left(\frac{e}{c} f_{ij} - \hbar F_{ij}\right). \tag{48}$$

The force can directly be read from (48) in terms of the velocity $\boldsymbol{v} \equiv \dot{\boldsymbol{r}}$ given by (47) as

$$\begin{aligned}\mathcal{F}_i = \dot{y}_i = m\ddot{r}_i = &-\frac{\partial}{\partial r_i}(V + \mu_B\sigma\cdot\boldsymbol{B}) + \frac{e}{c}\epsilon_{ijk}v_j B_k \\ &+ \frac{\hbar}{4mc^2}\left(\epsilon_{ijk}\sigma^j v_l\frac{\partial^2 V}{\partial r_l\partial r_k} + \epsilon_{jkl}\sigma^j v^k\frac{\partial^2 V}{\partial r_l \partial r_i}\right) + \frac{\mu_B}{2mc^2}\left(\sigma_i B_l\frac{\partial V}{\partial r_l} - B_i\sigma_l\frac{\partial V}{\partial r_l}\right) \\ &+ \frac{\hbar}{8m^2c^4}\epsilon_{ijk}\sigma_l\frac{\partial V}{\partial r_l}v_j\frac{\partial V}{\partial r_k}.\end{aligned} \tag{49}$$

Indeed, this is the force obtained in [15]. The last term is the transverse spin force on the spin current quadratic in the electric field.

Equations of motion following from the nonrelativistic approximation of the Dirac Hamiltonian can be derived in electrodynamics employing the Thomas precession [31] without referring to the Dirac Hamiltonian. The relation between the nonrelativistic limit and the Thomas precession was clarified in [20] by showing that the latter should be considered as a Berry phase when the external electric potential is smooth. The related gauge field can be obtained in the nonrelativistic limit from (40). Hence, to obtain the force acting on an electron in the external electric and magnetic fields, it should be possible to consider either the gauge field $\mathcal{A}$ given in (46) or the gauge field $\mathcal{B}$ obtained from (40) in the nonrelativistic limit: let $\mathcal{A} = 0$ and deal with the electrodynamic gauge field $a_i(r)$, $\eta = e/c$ and the nonrelativistic limit of the non-Abelian gauge field (40)

$$\mathcal{B}_i = \frac{1}{4m^2c^2}\epsilon_{ijk}y^j\sigma^k. \tag{50}$$

Field strength of this gauge field can be calculated to be

$$G_{ij} = \frac{-1}{2m^2c^2}\epsilon_{ijk}\sigma^k + \frac{1}{8m^4c^4}\epsilon_{ijk}y_k(\sigma\cdot\boldsymbol{y}), \tag{51}$$

where we used $\xi = \hbar$.

By ignoring the fG terms in (32) and (33), the equations of motion are

$$\dot{y}_i = -\frac{\partial(V + \mu_B\sigma\cdot\boldsymbol{B})}{\partial r^i} + \frac{e}{mc}\epsilon_{ijk}y_j B_k, \tag{52}$$

$$\dot{r}_i = \frac{y_i}{m} + \hbar G_{ij}\frac{\partial V}{\partial r_j} + \frac{\mu_B}{2m^2c^2}(B_i(\boldsymbol{y}\cdot\sigma) - \sigma_i(\boldsymbol{B}\cdot\boldsymbol{y})). \tag{53}$$

Now, by keeping the terms linear in the velocity v_i one can show that

$$m\ddot{r}_i = m\{\dot{r}_i, H_e\}_C = -\frac{\partial}{\partial r_i}(V + \mu_B\sigma\cdot\boldsymbol{B}) + \frac{\hbar}{2mc^2}\epsilon_{ijk}\sigma^j v_l \frac{\partial^2 V}{\partial r_l \partial r_k} + \frac{e}{c}\epsilon_{ijk}v_j B_k$$
$$+ \frac{\mu_B}{2mc^2}\left(\sigma_i B_l \frac{\partial V}{\partial r_l} - B_i\sigma_l\frac{\partial V}{\partial r_l}\right) + \frac{\hbar}{8m^2c^4}\epsilon_{ijk}\sigma_l\frac{\partial V}{\partial r_l}v_j\frac{\partial V}{\partial r_k}. \quad (54)$$

Up to some $\partial^2 V/\partial r_i \partial r_j$ terms this coincides with (49). In fact, the latter approach is valid for potentials changing slowly. However, neglecting the fG terms in (32) and (33) is not justified, due to the fact that they may give contributions of the μ_B/mc^2 order to the force. Indeed, retaining the fG terms in (32) and (33) and using $\mu_B = -e\hbar/2mc$, the equations of motion of the $\hbar$ order are

$$\dot{y}_i = -\frac{\partial(V + \mu_B\sigma\cdot\boldsymbol{B})}{\partial r^i} + \frac{e}{mc}\epsilon_{ijk}y_j B_k - \frac{\mu_B}{mc^2}\left(\frac{\partial V}{\partial r^i}\sigma_j B^j - \sigma_i B_j\frac{\partial V}{\partial r_j}\right), \quad (55)$$

$$\dot{r}_i = \frac{y_i}{m} + \hbar G_{ij}\frac{\partial V}{\partial r_j} - \frac{\mu_B}{2m^2c^2}(B_i(\boldsymbol{y}\cdot\sigma) + \sigma_i(\boldsymbol{y}\cdot\boldsymbol{B}) - 2y_i(\boldsymbol{B}\cdot\sigma)). \quad (56)$$

Hence, the force linear in velocity becomes

$$m\ddot{r}_i = -\frac{\partial}{\partial r_i}(V + \mu_B\sigma\cdot\boldsymbol{B}) + \frac{\hbar}{2mc^2}\epsilon_{ijk}\sigma^j v_l\frac{\partial^2 V}{\partial r_l\partial r_k} + \frac{e}{c}\epsilon_{ijk}v_j B_k$$
$$+ \frac{\mu_B}{2mc^2}\left(3\sigma_i B_l\frac{\partial V}{\partial r_l} + B_i\sigma_l\frac{\partial V}{\partial r_l} - 4\frac{\partial V}{\partial r_i}(B_l\sigma_l)\right) + \frac{\hbar}{8m^2c^4}\epsilon_{ijk}\sigma_l\frac{\partial V}{\partial r_l}v_j\frac{\partial V}{\partial r_k}. \quad (57)$$

The last term which is the transverse spin force on the spin current results to be the same[2]. However, the terms which depend on both the electric and magnetic fields are in dispute with (49). This discrepancy between the two nonrelativistic approximation schemes can be settled by experiments.

4.4. The spin Hall effect

Electrons constrained to move on a plane in the presence of a uniform external magnetic field perpendicular to the plane deviate and produce an electric field which is perpendicular to both the initial direction of the current and the magnetic field. This is the Hall effect which manifests itself as the Hall conductivity. We would like to present a derivation of the Hall conductivity which will inspire a simple formulation of the intrinsic spin Hall effect utilizing our semiclassical approach. To this aim let us deal with the Hamiltonian

$$H_0 = \frac{1}{2m}\boldsymbol{y}^2 + V(r_1, r_2), \quad (58)$$

where the scalar potential is given in terms of the uniform electric field components E_i as

$$V(r_1, r_2) = -eE_1 r_1 - eE_2 r_2. \quad (59)$$

In order to constrain the electron to move on the r_1r_2-plane we set $y_3 = 0$. We consider the vanishing Berry gauge fields $\mathcal{A} = 0, \mathcal{B} = 0$ and let there be a uniform magnetic field in the r_3 direction:

$$f_{12} = B. \quad (60)$$

[2] In [32] it was claimed that this method leads to a transverse force in conflict with [15].

The related coupling constant is $\eta = e/c$. The equations of motion following from (32) and (33) are

$$\dot{r}_i = \frac{y_i}{m}, \tag{61}$$

$$\dot{y}_1 = eE_1 + \frac{eB}{mc} y_2, \tag{62}$$

$$\dot{y}_2 = eE_2 - \frac{eB}{mc} y_1. \tag{63}$$

The force acting on an electron can be read from (61) to (63), in terms of the velocity $\boldsymbol{v} \equiv \dot{\boldsymbol{r}}$, as

$$\mathcal{F}_1 = m\ddot{r}_1 = \dot{y}_1 = eE_1 + \frac{eB}{c} v_2, \tag{64}$$

$$\mathcal{F}_2 = m\ddot{r}_2 = \dot{y}_2 = eE_2 - \frac{eB}{c} v_1. \tag{65}$$

Till now we have considered a single particle dynamics. To connect it to a system of electrons let us introduce the density of electrons κ. Thus, the electric current is defined by

$$\boldsymbol{j} = e\kappa \boldsymbol{v}. \tag{66}$$

We demand that the net force acting on electrons vanish $\mathcal{F}_i = 0$, so that the electrons move without deflection (see, e.g. [33]). We can solve this condition for the velocity and plug it into (66), which yields the electric current

$$\begin{pmatrix} j_1 \\ j_2 \end{pmatrix} = \begin{pmatrix} 0 & -\sigma_H \\ \sigma_H & 0 \end{pmatrix} \begin{pmatrix} E_1 \\ E_2 \end{pmatrix}, \tag{67}$$

where

$$\sigma_H = -\frac{ec\kappa}{B}$$

is the Hall conductivity.

The intrinsic spin Hall effect is envisaged in [21] in terms of the Rashba spin–orbit coupling [22]. By generalizing the Hall effect formulation we can introduce a simple method of acquiring the spin Hall conductivity employing the Rashba spin–orbit coupling. The Hamiltonian is still given by (58) with $y_3 = 0$. However, there is no magnetic field: $a_i = 0$. To consider the linear Rashba spin–orbit coupling we set $\mathcal{B} = 0$ and define

$$\mathcal{A}_i = \epsilon_{ijk} \sigma_j e^z_k. \tag{68}$$

Here, $\boldsymbol{e}^z$ is the unit vector in the third direction $e^z_k = \delta_{k3}$ and σ_i are the Pauli matrices. Moreover, in the original formulation (11) we should take $\rho = -\alpha m/\hbar$, where α is the Rashba coupling constant [22].

The related field strength can be calculated as

$$F_{ij} = -\frac{\mathrm{i}\rho}{\hbar} [\mathcal{A}_i, \mathcal{A}_j] = \frac{2\rho}{\hbar} \sigma_3 \epsilon_{ijk} e^z_k. \tag{69}$$

The equations of motion of the canonical variables are

$$\dot{r}_i = \frac{y_i}{m}, \tag{70}$$

$$\dot{y}_i = -\frac{\partial V}{\partial r_i} + \frac{\rho}{m} F_{ij} y_j. \tag{71}$$

Hence, the force acting on the particle is

$$\mathcal{F}_i = m\ddot{r}_i = eE_i + \frac{2\rho^2}{\hbar}\sigma_3\epsilon_{ijk}e^z_k v_j. \tag{72}$$

Imitating the formulation of the Hall effect we set $\mathcal{F}_i = 0$, in order to have a motion without deflection. This condition is solved for the velocity as

$$v_1^\uparrow = \frac{e\hbar}{2\rho^2}E_2, \qquad v_1^\downarrow = -\frac{e\hbar}{2\rho^2}E_2, \tag{73}$$

$$v_2^\uparrow = -\frac{e\hbar}{2\rho^2}E_1, \qquad v_2^\downarrow = \frac{e\hbar}{2\rho^2}E_1. \tag{74}$$

The arrows $\uparrow$ and $\downarrow$ correspond, respectively, to the positive and negative eigenvalues of σ_3. It is natural to define the spin current as

$$\boldsymbol{j}^z = \frac{\hbar}{2}(n^\uparrow \boldsymbol{v}^\uparrow - n^\downarrow \boldsymbol{v}^\downarrow), \tag{75}$$

where $n^\uparrow$ and $n^\downarrow$ denote the concentrations of states with spins along the e^z and $-e^z$ directions. Employing (73), (74) in (75) yields

$$\boldsymbol{j}^z = \sigma_{\mathrm{SH}}\boldsymbol{e}^z \times \boldsymbol{E}, \tag{76}$$

where

$$\sigma_{\mathrm{SH}} = \frac{-e\hbar^2}{4\rho^2}(n^\uparrow + n^\downarrow) \equiv \frac{-e\hbar^4}{4\alpha^2m^2}n \tag{77}$$

is the spin Hall conductivity. In this simplistic approach, the total concentration of states $n = (n^\uparrow + n^\downarrow)$ is an input which should be given by other means. Although its calculation is beyond the scope of this work, for having an insight let

$$n = sn^*_{2D}, \tag{78}$$

where s is a constant and n^*_{2D} is the concentration of states occupying the lower energy state of the Rashba Hamiltonian [22]:

$$n^*_{2D} = \frac{\alpha^2m^2}{\pi\hbar^4}.$$

Using (78) in (77) leads to the spin Hall conductivity

$$\sigma_{\mathrm{SH}} = -\frac{es}{4\pi}. \tag{79}$$

This agrees with the universal behavior obtained in [21] for $s = 1/2$. However, when the vertex corrections are taken into account it is known that this universal behavior does not survive [23], as far as the linear Rashba coupling is considered. The vertex corrections were calculated employing Green functions within the Born approximation. Hence, it is not clear how one can incorporate the vertex corrections into our semiclassical scheme. To cure the defects of the linear theory, it would be useful to study the Rashba couplings which are higher orders in momenta (see [24] and references therein). Although we will not discuss it here, our semiclassical approach can be used to investigate higher order generalizations of the Rashba spin–orbit coupling.

5. Discussions

Semiclassical limit designated as the bracket (8) can be utilized to study diverse dynamical problems where spin degrees of freedom are not ignored. Hence, instead of dealing with wave packets one can consider the single particle interpretation of the semiclassical dynamics of spin-dependent systems.

It can be shown that the constrained Hamiltonian system which we presented here is suitable to investigate properties of some topological quantum phases. Moreover, as we will present in a future work it constitutes a new gauge-invariant method of studying dynamical systems in noncommutative spaces.

Any model concerning spin dynamics utilizing Berry gauge fields which give rise to noncommutativity of coordinates and/or momenta can be studied in terms of the semiclassical approach presented here. We focused on some recent formalisms where some of persisting discussions can be clarified. The results which we derived are valid up to the first order in $\hbar$. However, in this formulation keeping the track of the higher orders is possible. When higher order $\hbar$ corrections are considered there may be some different sources: gauge fields which we consider may depend on higher $\hbar$, the limit of the Moyal bracket will have another term and the inversion of the matrix $C_{\alpha\beta}^{zz'}$ may lead to some higher $\hbar$ terms.

Obviously, the formalism of the spin Hall conductivity which we reported here should be elaborated. Nevertheless, due to its resemblance with the Hall effect and simplicity, it may be profitable to predict some basic properties of the spin Hall effect.

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