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Semiclassical Dynamics of Electrons in Magnetic Bloch Bands: an Hamiltonian Approach

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By formally diagonalizing with accuracy \hbar the Hamiltonian of electrons in a crystal subject to electromagnetic perturbations, we resolve the debate on the Hamiltonian nature of semiclassical equations of motion with Berry phase corrections, and therefore confirm the validity of the Liouville theorem. Contrary to previous treatment based on the study of electron wave-packets dynamics, it is found that both the position and momentum are Berry-phase dependent. This allows us to find a well defined semi-classical Hamiltonian in the presence of Berry-phase terms. The resulting equations of motion turn out to be only formally equivalent to previous ones derived from wave-packets dynamics. Besides, our method is more general as we are not limited to the uniform magnetic field case.

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The notion of Berry phase has found many applications in several branches of quantum physics such as atomic and molecular physics, optic and gauge theories and more recently in spintronics to cite just a few of them. Most studies focused on the geometric phase a wave function acquires when a quantum mechanical system has an adiabatic evolution. It is only recently that a possible influence of the berry phase on semiclassical dynamics of several physical systems has been investigated. It was then shown that Berry phases modify semiclassical dynamics of spinning particles in electric [1] and magnetic field [2] as well as in semiconductor [3]. In the above cited examples, a noncommutative geometry, originating from the presence of a Berry phase which turns out to be a spin-orbit coupling, underlies the semiclassical dynamics. Also, spin-orbit contributions to the propagation of light has been the focus of several other works [1, 4, 5] and has led to a generalization of geometric optics called geometric spinoptics [6].

Semiclassical methods in solid state physics have also played an important role in studying the dynamics of electrons to account for the various properties of metals, semiconductors and insulators [7]. In a series of papers [8][9] (see also [10]), the following new set of semiclassical equations with a Berry phase correction was proposed to account for the semiclassical dynamic of electrons in magnetic Bloch bands (in the usual one band approximation)

$$\begin{aligned}\dot{\mathbf{r}} &= \partial \mathcal{E}(\mathbf{k}) / \hbar \partial \mathbf{k} - \dot{\mathbf{k}} \times \Theta(\mathbf{k}) \\ \hbar \dot{\mathbf{k}} &= -e \mathbf{E} - e \dot{\mathbf{r}} \times \mathbf{B}(\mathbf{r})\end{aligned}\quad (1)$$

where \mathbf{E} and \mathbf{B} are the electric and magnetic fields respectively and $\mathcal{E}(\mathbf{k}) = \mathcal{E}_0(\mathbf{k}) - \mathbf{m}(\mathbf{k}) \cdot \mathbf{B}$ is the energy of the n th band with a correction due to the orbital magnetic

moment [9]. The correction term to the velocity $-\dot{\mathbf{k}} \times \Theta$ with $\Theta(\mathbf{k})$ the Berry curvature of electronic Bloch state in the n th band is known as the anomalous velocity predicted to give rise to a spontaneous Hall conductivity in ferromagnets [11]. For crystals with broken time-reversal symmetry or spatial inversion symmetry, the Berry curvature is nonzero [9]. Eq.1 was derived by considering a wave packet in a band and using a time-dependent variational principle in a Lagrangian formulation. The derivation of a semiclassical Hamiltonian was shown to lead to difficulties in the presence of Berry phase terms [9]. The apparent non-Hamiltonian character of Eq.1 led the authors of [12] to conclude that the naive phase space volume is not conserved in the presence of a Berry phase, violating thus Liouville's theorem. To remedy this situation these authors introduced a modified density of state in the phase space $D(\mathbf{r}, \mathbf{k}) = (2\pi)^{-d} (1 + e \mathbf{B} \cdot \Theta / \hbar)$ such that $D(\mathbf{r}, \mathbf{k}) d\mathbf{r} d\mathbf{k}$ remains constant in time.

This point of view was immediately criticized by several authors. In particular, by relating the semiclassical dynamics of Bloch electron to "exotic" Galilean dynamics introduced independently in the context of noncommutative quantum mechanics [13], C. Duval et al. [14] found that Eqs.1 are indeed Hamiltonian in a standard sense, restoring the validity of Liouville's theorem when the correct symplectic volume form is used. This approach, relying on a symplectic structure on a classical Hamiltonian formulation, though very elegant, does not stem from the quantum Hamiltonian for electrons in a solid and is consequently not widely known from the solid state physicists community. Besides the role of the Berry phase is hidden in this approach. In a different but related work [15] the Hamiltonian nature of semiclassical equations of motion of Dirac electrons in electromagnetic field with Berry phase corrections (in this case it corre-

sponds to a spin-orbit coupling) was established.

This letter presents an alternative approach for the derivation of the equations of motion of an electron in magnetic Bloch bands based on a direct semiclassical diagonalization of the full quantum Hamiltonian. It is important to stress that our result is only formally identical to Eq.1 since the momentum obtained in the diagonal representation, denoted $\tilde{\mathbf{k}}$, turns out to be different from \mathbf{k} in Eq.1. Actually both dynamical variables $(\mathbf{r}, \tilde{\mathbf{k}})$ are not the usual Galilean operators, but are defined in a particular n th Bloch band which takes into account Berry phase contributions rendering the commutation relations non-trivial. In this approach the equations of motion are given by the standard dynamical laws $\hbar d\mathbf{r}/dt = i[\mathbf{r}, H]$ and $d\tilde{\mathbf{k}}/dt = i[\tilde{\mathbf{k}}, H]$ formally leading to Eq.1 in a semiclassical approximation. Our approach thus reveals the Hamiltonian nature of Eq.1 and confirms the importance of the Berry phase on the semiclassical dynamics of Bloch electrons. The origin of the density of state $D(\mathbf{r}, \mathbf{k})$ is then obvious; it is simply equal to the Jacobian of the transformation between the canonical variables (\mathbf{R}, \mathbf{K}) and the covariant ones $(\mathbf{r}, \tilde{\mathbf{k}})$ as already found in the context of the Dirac equation in [15].

One should mention that focusing on an Hamiltonian formalism for electrons in solids in order to account for the anomalous velocity was first initiated by Adams and Blount [16] who showed that this term arises from the noncommutability between the components of the intraband position operator which acquires a Berry phase contribution. But their approach does not lead to the correct equations Eq.1 for electrons in magnetic Bloch waves as they missed the Berry phase dependence of the intraband momentum operator. A similar Hamiltonian approach has been also realized for arbitrary spinning (massive and massless) particles in an electric field [1] and extended to the case of Dirac electron in an arbitrary electromagnetic field [2, 15]. The common feature of these Hamiltonian formulations is that a noncommutative geometry underlies the algebraic structure of both coordinates and momenta. Actually, a Berry phase contribution to the coordinate operators stems from the representation where the kinetic energy is diagonal (Foldy-Wouthuysen or Bloch representation). The components of the coordinate become noncommutative when interband transitions are neglected (adiabatic motion).

Consider an electron in an cristal lattice perturbed by the presence of an external electromagnetic field. As it is usual, we express the total magnetic field as the sum of a constant field \mathbf{B} and small nonuniform part $\delta\mathbf{B}(\mathbf{R})$. The Hamiltonian can be written $H = H_0 - e\phi(\mathbf{R})$, with H_0 the magnetic contribution (ϕ being the electric potential) which reads

$$H_0 = \left(\frac{\mathbf{P}}{2m} + e\mathbf{A}(\mathbf{R}) + e\delta\mathbf{A}(\mathbf{R}) \right)^2 + V(\mathbf{R}) \quad (2)$$

where $\mathbf{A}(\mathbf{R})$ and $\delta\mathbf{A}(\mathbf{R})$ are the vectors potential of

the homogeneous and inhomogeneous magnetic field respectively and $V(\mathbf{R})$ the periodic potential. The large constant part \mathbf{B} is chosen such that the magnetic flux through a unit cell is a rational fraction of the flux quantum h/e . The advantage of such a decomposition is that for $\delta\mathbf{A}(\mathbf{R}) = 0$ the magnetic translation operators $\mathbf{T}(\mathbf{R}_i) = \exp(i\mathbf{K} \cdot \mathbf{R}_i)$ with \mathbf{K} the generator of translation are commuting quantities allowing to diagonalize exactly the Hamiltonian and to treat $\delta\mathbf{A}(\mathbf{R})$ as a small perturbation. The state space of the Bloch electron is spanned by the basis vector $|n, \mathbf{k}\rangle = |\mathbf{k}\rangle \otimes |n\rangle$ with n corresponding to a band indice. In this representation $\mathbf{K}|n, \mathbf{k}\rangle = \mathbf{k}|n, \mathbf{k}\rangle$ and the position operator is $\mathbf{R} = i\partial/\partial\mathbf{K}$, which implies the canonical commutation relation $[R_i, K_j] = i\delta_{ij}$.

We first perform the diagonalization of the Hamiltonian in Eq.2 for $\delta\mathbf{A} = 0$ by an unitary matrix $U(\mathbf{K})$ (whose precise expression is not necessary for the derivation of the equations of motion) such that $UHU^\dagger = \mathcal{E}(\mathbf{K}) - e\phi(U\mathbf{R}U^\dagger)$, where $\mathcal{E}(\mathbf{K})$ is the diagonal energy matrix made of elements $\mathcal{E}_n(\mathbf{K})$ with n the band indice. Whereas the quasi-momentum is invariant through the action of U , e.g., $\mathbf{k} = U\mathbf{K}U^\dagger = \mathbf{K}$, the position operator becomes:

$$\mathbf{r} = U\mathbf{R}U^\dagger = \mathbf{R} + iU\partial_{\mathbf{K}}U^\dagger \quad (3)$$

in the new representation owing to the fact that $[R_i, K_j] = i\delta_{ij}$. In the adiabatic or one band approximation which consists in neglecting interband transitions, one has to project the position coordinate (the momenta operator is diagonal and so invariant by construction) on a certain band such that the n th intraband position operator $\mathbf{r}_n = \mathcal{P}_n(\mathbf{r})$ reads $\mathbf{r}_n = \mathbf{R} + \mathcal{A}_n$. The quantity $\mathcal{A}_n = i\mathcal{P}_n(U\partial_{\mathbf{K}}U^\dagger)$ is a Berry connection since it can be readily shown that its matrix elements are given by $\mathcal{A}_n(\mathbf{k}) = i \langle u_n(\mathbf{k}) | \partial_{\mathbf{K}} | u_n(\mathbf{k}) \rangle$, where we used $U^\dagger(\mathbf{k})|n\rangle = |u_n(\mathbf{k})\rangle$ with $|u_n(\mathbf{k})\rangle$ the periodic part of the magnetic Bloch waves. The price to pay when considering the one-band approximation, is that the algebra of the coordinates becomes noncommutative (as we consider only one band we drop the index n)

$$[r^i, r^j] = i\Theta^{ij}(\mathbf{k}) \quad (4)$$

with $\Theta^{ij}(\mathbf{k}) = \partial^i \mathcal{A}^j(\mathbf{k}) - \partial^j \mathcal{A}^i(\mathbf{k})$ the Berry curvature. Observe that the replacement of \mathbf{k} by \mathbf{p}/\hbar shows that $\Theta^{ij}(\mathbf{p})$ is actually of order \hbar^2 . In the one-band approximation the full Hamiltonian including the electric potential is now given by

$$\mathcal{P}_n(UHU^\dagger) = \mathcal{E}(\mathbf{k}) - e\phi(\mathbf{r}). \quad (5)$$

Due to the Berry connection in the definition of the position operator the equations of motion should be changed. But to compute commutators like $[r^k, \phi(\mathbf{r})]$, one resorts to the semiclassical approximation $[r^k, \phi(\mathbf{r})] =$

$i\partial_l\phi(\mathbf{r})\Theta^{kl} + O(\hbar)$ leading to the following semiclassical equations of motion

$$\dot{\mathbf{r}} = \partial\mathcal{E}(\mathbf{k})/\hbar\partial\mathbf{k} - \dot{\mathbf{k}} \times \Theta(\mathbf{k}), \quad \hbar\dot{\mathbf{k}} = -e\mathbf{E} \quad (6)$$

where \mathbf{E} is the external electric field. Whereas the momentum equation of motion is the usual one, the velocity operator acquires an anomalous contribution due to presence of the Berry curvature. Notice that the contribution of the magnetic field stems only from the presence of the Berry curvature through the Band structure. This equation was first derived by Adams and Blount [16] using a similar approach, and later rederived by Niu and coworkers [8][9] by looking at the dynamics of wave packets from a Lagrangian formalism. In the following we will extend our approach to carry out a semiclassical diagonalization of the full electromagnetic Hamiltonian (with $\delta\mathbf{A}(\mathbf{R}) \neq 0$). Contrary to the work of [16], we show that the momentum also acquires a Berry phase contribution leading to different semiclassical equations of motion. These last ones turn out to be formally those derived first in [9] (and also Duval et al. [14] in another context). Our rigorous approach has the merit to show without ambiguities that the equations of motion are indeed Hamiltonian in the standard sense.

The diagonalization of the Hamiltonian in the presence of an arbitrary magnetic field is now the focus of the rest of the paper. Consider first the Hamiltonian Eq.2 in the absence of electric field and set $\tilde{\mathbf{K}} = \mathbf{K} + e\delta\mathbf{A}(\mathbf{R})/\hbar$. As the flux $\delta\mathbf{B}$ on a plaquette is not a rational multiple of the flux quantum we cannot diagonalize simultaneously its components \tilde{K}_i since they do not commute anymore. Actually

$$\hbar[\tilde{K}^i, \tilde{K}^j] = -e\varepsilon^{ijk}\delta B_k(\mathbf{R}) \quad (7)$$

As a consequence of this non-commutativity, we just aim at "quasi-diagonalizing" our Hamiltonian at the semiclassical order (with accuracy \hbar). To perform this approximate diagonalization $\tilde{U}H\tilde{U}^+$ with accuracy \hbar we first consider the limiting case of a constant potential $\delta\mathbf{A}(\mathbf{R}) = \delta\mathbf{A}_0$ (this is obviously a formal consideration). Clearly the Hamiltonian Eq.2 is diagonalized by the matrix $U(\delta\mathbf{A}) = U(\mathbf{K} + e\delta\mathbf{A}/\hbar)$, since we have just shifted the momentum \mathbf{K} . To diagonalize Eq. 2 in the general case we consider now a unitary matrix $\tilde{U}(\mathbf{K} + e\delta\mathbf{A}(\mathbf{R})/\hbar)$ which has the same series expansion as $U(\delta\mathbf{A}(\mathbf{R}))$ when \mathbf{R} is considered as a parameter commuting with \mathbf{K} . Of course this matrix is not unique, due to the noncommutativity of \mathbf{K} and \mathbf{R} , but it can be shown that the various choices lead to the same projected Hamiltonian. Note that in the sequel, a small $\delta\mathbf{A}$ perturbation, which preserves the band structure determined previously is assumed, i.e. $\langle n|\delta\mathbf{A}|m \rangle = 0$ for $m \neq n$. Before implementing effectively the canonical transformation on the Hamiltonian it will appear more convenient to implement first the canonical transformation on the dynamical operators. Therefore, in

the new representation the position operator is again given by $\mathbf{r} = \mathbf{R} + i\tilde{U}\partial_{\tilde{\mathbf{K}}}\tilde{U}^+$. As before the projection on a band defined the n th intraband position operator $\mathbf{r}_n = \mathbf{R} + \mathcal{A}_n(\tilde{\mathbf{K}})$, with $\mathcal{A}_n(\tilde{\mathbf{K}}) = \mathcal{P}_n(\tilde{U}\partial_{\tilde{\mathbf{K}}}\tilde{U}^+)$ a new Berry connection.

The pseudo-momentum $\tilde{\mathbf{K}}$ is no more invariant since we obtain

$$\begin{aligned} \tilde{\mathbf{k}} &= \tilde{U}\tilde{\mathbf{K}}\tilde{U}^+ = \tilde{\mathbf{K}} + \tilde{U}\partial_{\tilde{\mathbf{K}}^j}\tilde{U}^+ [\tilde{\mathbf{K}}, \tilde{K}^j] \\ &= \tilde{\mathbf{K}} - ie\tilde{U}\partial_{\tilde{\mathbf{K}}}\tilde{U}^+ \times \delta\mathbf{B}(\mathbf{R})/\hbar \end{aligned} \quad (8)$$

The n th intraband momentum operator $\tilde{\mathbf{k}}_n = \mathcal{P}_n(\tilde{\mathbf{k}})$ is then

$$\hbar\tilde{\mathbf{k}}_n = \hbar\tilde{\mathbf{K}} - e\mathcal{A}_n(\tilde{\mathbf{K}}) \times \delta\mathbf{B}(\mathbf{R}) \quad (9)$$

which at the order \hbar can also be written

$$\hbar\tilde{\mathbf{k}}_n \simeq \hbar\tilde{\mathbf{K}} - e\mathcal{A}(\tilde{\mathbf{k}}_n) \times \delta\mathbf{B}(\mathbf{r}_n) + O(\hbar^2) \quad (10)$$

This new contribution to the momentum has been overlooked before in the work of Adams and Blount [16] but is crucial for the correct determination of the semiclassical equations of motion of electron in a magnetic Bloch band. Note that this additional term in the momentum is also absent in [9] and this may leads to the trouble in defining a semi-classical Hamiltonian (see discussion below).

The commutation relations between the components of the intraband momenta are therefore given by (at leading order)

$$\hbar[\tilde{k}_n^i, \tilde{k}_n^j] = -ie\varepsilon^{ijk}\delta B_k(\mathbf{r}_n) + ie^2\varepsilon^{ipk}\delta B_k\varepsilon^{jqk}\delta B_l\Theta^{pq}/\hbar \quad (11)$$

with $\Theta^{ij}(\tilde{\mathbf{k}}_n) = \partial^i\mathcal{A}^j(\tilde{\mathbf{k}}_n) - \partial^j\mathcal{A}^i(\tilde{\mathbf{k}}_n)$ the Berry curvature. The commutation relation between position and momentum can be computed leading to

$$[r_n^i, \hbar\tilde{k}_n^j] = i\hbar\delta^{ij} + ie\varepsilon^{jlk}\delta B_k(\mathbf{r}_n)\Theta^{il}(\tilde{\mathbf{k}}_n) \quad (12)$$

The third useful commutator is as in Eq.4 given by

$$[r_n^i, r_n^j] = i\Theta(\tilde{\mathbf{k}}_n)^{ij} \quad (13)$$

at leading order. The set of nontrivial commutations relations given by Eqs.11, 12, 13 is the same as the one deduced in [15] in the context of the Dirac electron using an approximate explicit Foldy Wouthuysen transformation. This shows that a common structure underlies the quasi-diagonalization of general quantum Hamiltonian in the presence of electromagnetic field [17]. In the present case, the approximate diagonalization $\tilde{U}H\tilde{U}^+$ is performed by formally expanding \tilde{U} and H in series of \mathbf{K} and $\delta\mathbf{A}(\mathbf{R})$. The recombination of the series includes corrections of order \hbar due to the noncommutativity of \mathbf{K} and \mathbf{R} . Doing so we arrive at the following expression

$$\begin{aligned} \tilde{U}H\tilde{U}^+ &= \mathcal{E}(\tilde{\mathbf{k}}) - \frac{ie}{4\hbar} [\mathcal{E}(\tilde{\mathbf{K}}), \mathcal{A}_i(\tilde{\mathbf{K}})] \varepsilon^{ijk}\delta B^k(\mathbf{R})\mathcal{A}_j(\tilde{\mathbf{K}}) \\ &\quad - \frac{ie}{4\hbar} \mathcal{A}_j(\tilde{\mathbf{K}}) [\mathcal{E}(\tilde{\mathbf{K}}), \mathcal{A}_i(\tilde{\mathbf{K}})] \varepsilon^{ijk}\delta B^k(\mathbf{R}) \end{aligned}$$

which after projection on the n th band can be written:

$$\mathcal{P}_n(\tilde{U}H\tilde{U}^+) = \mathcal{E}_n(\tilde{\mathbf{k}}_n) - \mathcal{M}(\tilde{\mathbf{K}})\delta\mathbf{B}(\mathbf{r}_n) + O(\hbar^2) \quad (14)$$

with $\mathcal{M}(\tilde{\mathbf{K}}) = \mathcal{P}_n(\frac{ie}{2\hbar} [\mathcal{E}(\tilde{\mathbf{K}}), \mathcal{A}(\tilde{\mathbf{K}})] \times \mathcal{A}(\tilde{\mathbf{K}}))$ the magnetization. This term can also be written under the usual form in the (\mathbf{K}, n) representation [18]:

$$\mathcal{M}_{nn}^i = \frac{ie}{2\hbar} \varepsilon^{ijk} \sum_{n' \neq n} (\mathcal{E}_n - \mathcal{E}_{n'}) (\mathcal{A}_j)_{nn'} (\mathcal{A}_k)_{n'n} \quad (15)$$

At this point, a comment might be necessary. Since a semiclassical computation was considered here, we kept only terms of order \hbar , and as $\delta\mathbf{A}$ is small, we are perfectly allowed to neglect terms of order $\hbar\delta\mathbf{A}^2$. But, as we do not consider a perturbation expansion, our method keeps all contributions of order $\delta\mathbf{A}^n$. In a perturbation expansion, instead of evaluating $\tilde{U}H\tilde{U}^+$, one would compute $U(\mathbf{K})HU(\mathbf{K})^+ = \mathcal{E}(\mathbf{K}) + U\delta HU^+$ (and neglect all terms of order higher than $\delta\mathbf{A}$). In this representation the position operator is still given by Eq.3 but \mathbf{K} is invariant as in [8]. But doing so would lead us to neglect contributions of order \hbar that are fundamental for the correct determination of the equations of motion. A perturbation expansion is then not allowed here.

The commutation relations Eqs.11, 12, 13, together with the semiclassical Hamiltonian of Bloch electron in the full electromagnetic field $E_n(\tilde{\mathbf{k}}_n) - \phi(\mathbf{r}_n)$ with $E_n(\tilde{\mathbf{k}}_n) = \mathcal{E}_n(\tilde{\mathbf{k}}_n) - \mathcal{M}(\tilde{\mathbf{K}}_n)\delta\mathbf{B}(\mathbf{r}_n)$, allow us to deduce the semi-classical equations of motion. Dropping now the index n we have:

$$\begin{aligned} \dot{\mathbf{r}} &= \partial E(\tilde{\mathbf{k}})/\hbar \partial \tilde{\mathbf{k}} - \tilde{\mathbf{k}} \times \Theta(\tilde{\mathbf{k}}) \\ \hbar \dot{\tilde{\mathbf{k}}} &= -e\mathbf{E} - e\dot{\mathbf{r}} \times \delta\mathbf{B}(\mathbf{r}) - \mathcal{M}\partial\delta\mathbf{B}/\partial\mathbf{r} \end{aligned} \quad (16)$$

which are formally the same equations of motion than in [9] but important differences have to be mentioned. First, our equations are more general since $\delta\mathbf{B}$ is non-zero, leading to the additional contribution $\mathcal{M}\partial\mathbf{r}\delta\mathbf{B}$. More importantly, whereas the coordinate \mathbf{r} is the same in both approach, our momentum $\tilde{\mathbf{k}}$ is different. Therefore both functions $E(\tilde{\mathbf{k}})$ and $\Theta(\tilde{\mathbf{k}})$ are different from the ones in [9]. The apparent trouble with semi-classical Hamiltonian formalism in [9] may be due to an incorrect choice of the dynamical variables which in [9] are \mathbf{r} and $\tilde{\mathbf{K}}$. But $\tilde{\mathbf{K}}$ is not invariant through the canonical transformation, and one should better consider \mathbf{r} and $\tilde{\mathbf{k}}$ as conjugate dynamical variables. Doing so there is no problem to deduce a semi-classical Hamiltonian in the presence of Berry-phase terms. Clearly, the correct volume form in the phase space $(\mathbf{r}, \tilde{\mathbf{k}})$ has to include the Jacobian

$D = (1 + e\delta\mathbf{B}\cdot\Theta/\hbar)$ of the transformation from $(\mathbf{R}, \tilde{\mathbf{K}})$ to $(\mathbf{r}, \tilde{\mathbf{k}})$, which in turn assures the validity of the Liouville theorem.

In summary our semiclassical diagonalization of the electromagnetic Bloch Hamiltonian leads to semiclassical equations which are only formally equivalent to those obtained previously [9]. The principal difference stems from the definition of the momentum which in our computation acquires also a Berry Phase contribution. When the correct dynamical variables are chosen the semi-classical Hamiltonian is well defined and the Liouville's theorem is restored. The present approach confirms also the result of Duval et al. [6] and Bliokh [15] about the Hamiltonian nature of these semiclassical equations of motion with Berry phase corrections, which is a hotly debated subject.

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