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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. We show that both the position and momentum operators acquire a Berry-phase dependence, leading to a non-canonical Hamiltonian dynamics. The equations of motion turn out to be identical to the ones previously derived in the context of electron wave-packets dynamics.

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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. 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 fields [2], as well as in semiconductors [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 have been the focus of several other works [1, 4, 5], and have 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 $\mathcal{E}(\mathbf{k}) = \mathcal{E}_0(\mathbf{k}) - \mathbf{m}(\mathbf{k}).\mathbf{B}$ is the energy of the nth 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 nth 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]. Eqs.1 were 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 Eqs.1 led the authors of [12] to conclude that the naive phase space volume is not conserved in the presence of a Berry phase, thus violating Liouville's theorem. To remedy this situation these authors introduced a modified density of state in the phase space $D(\mathbf{r}, \mathbf{k}) = (2\pi)^{-d}(1 + e\mathbf{B}.\Theta/\hbar)$ 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 in the solid-state physicists community. Additionally, 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 corresponds 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. We show that both dynamical variables $(\mathbf{r},\mathbf{k})$ in Eqs. 1 are not the usual Galilean operators, but new covariant operators defined in a particular nth Bloch band, and including Berry gauge potentials. These potentials induce noncanonical commutation relations between the covariant variables. In our context, the equations of motion are given by the tandard dynamical laws $\hbar d\mathbf{r}/dt = i\left[\mathbf{r},H\right]$ and $d\mathbf{k}/dt = i[\mathbf{k},H]$ leading to Eqs.1 in a semiclassical approximation. Our approach thus reveals the Hamiltonian nature of Eqs.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 $(\mathbf{r},\mathbf{k})$, as already found in the context of the Dirac equation in [15].

It should be noted that focusing on a 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 Eqs.1 for electrons in magnetic Bloch waves, as they missed the Berry phase dependence of the intraband momentum operator. A similar Hamiltonian approach has also been 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 crystal lattice perturbated by the presence of an external electromagnetic field. As 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

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

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 $\mathbf{T}(\mathbf{R}_i) = \exp(i\mathbf{K}.\mathbf{R}_i)$, with $\mathbf{K}$ the generator of translation, are commuting quantities allowing to exactly diagonalize the Hamiltonian and to treat $\delta A(\mathbf{R})$ as a small perturbation. The state space of the Bloch electron is spanned by the basis vector $|n,\mathbf{k}>=|\mathbf{k}>\otimes|n>$ with n corresponding to a band indice. In this representation $\mathbf{K}|n,\mathbf{k}>=\mathbf{k}|n,\mathbf{k}>$ 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 $UHU^+ = \mathcal{E}(\mathbf{K}) - e\phi(U\mathbf{R}U^+)$, 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., $\mathbf{k} = U\mathbf{K}U^+ = \mathbf{K}$, the position operator becomes:

$$\mathbf{r} = U\mathbf{R}U^+ = \mathbf{R} + iU\partial_{\mathbf{k}}U^+ \qquad (3)$$

in the new representation owing to the fact that $[R_i,K_j] = i\delta_{i,j}$. In the adiabatic or one-band approximation, which consists of 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 nth intraband position operator $\mathbf{r}_n = \mathcal{P}_n(\mathbf{r})$ reads $\mathbf{r}_n = \mathbf{R} + \mathcal{A}_n$. The quantity $\mathcal{A}_n = i\mathcal{P}_n(U\partial_{\mathbf{k}}U^+)$ is a Berry connection, as it can be readily shown that its matrix elements are given by $\mathcal{A}_n(\mathbf{k}) = i < u_n(\mathbf{k})|\partial_{\mathbf{k}}|u_n(\mathbf{k})>$, where we used $U^+(\mathbf{k})|n>=|u_n(\mathbf{k})>$ with $|u_n(\mathbf{k})>$ 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)

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

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

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

Due to the Berry connection in the definition of the position operator, the equations of motion should be changed. But to compute commutators like $\left[r^k,\phi(\mathbf{r})\right]$, one resorts to the semiclassical approximation $\left[r^k,\phi(\mathbf{r})\right] = i\partial_l\phi(\mathbf{r})\Theta^{kl} + O(\hbar)$ leading to the following semiclassical equations of motion

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

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 those derived first in [8, 9] (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 an 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

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

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 in Eq.2 is diagonalized by the matrix $U(\delta\mathbf{A}) = U(\mathbf{K} + e\delta\mathbf{A}/\hbar)$, as we have just shifted the momentum $\mathbf{K}$. To diagonalize Eq. 2 in the general case, we now consider 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. $< n|\delta\mathbf{A}|m >= 0$ for $m \neq n$. Before implementing effectively the canonical transformation on the Hamiltonian, it appears 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 nth 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 as we obtain

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

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

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

which at the order $\hbar$ can also be written

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

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 an electron in a magnetic Bloch band.

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

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

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

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

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

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

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 Hamiltonians in the presence of electromagnetic fields [17]. In the present case, the approximate diagonalization $\tilde{U}H\tilde{U}^+$ is performed by formally expanding $\tilde{U}$ and H in a 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 $\mathbf{R}$. In doing so, we arrive at the following expression

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

which after projection on the nth band can be written:

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

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

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

We mention that this magnetization (the orbital magnetic moment of Bloch electrons), has been obtained previously in the context of electron wave packets dynamics [8, 9].

Notice that because a semiclassical computation was considered here, we kept only terms of order $\hbar$. As $\delta\mathbf{A}$ is small, we chose 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. 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 the 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 semiclassical equations of motion. Dropping now the index n we have:

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

These equations differ from the ones derived in [16], but are exactly the same equations of motion as in [8, 9] apart from the magnetization contribution (which should also be present in [9]). It is also clear that the correct volume form in the phase space $(\mathbf{r}, \tilde{\mathbf{k}})$ has to include the Jacobian $D(\mathbf{r}, \tilde{\mathbf{k}}) = (1 + e\delta\mathbf{B}.\Theta/\hbar)$ of the transformation from $(\mathbf{R}, \tilde{\mathbf{K}})$ to $(\mathbf{r}, \tilde{\mathbf{k}})$. This Jacobian is precisely the density of state introduced in [12], in order to ensure the validity of the Liouville theorem. As a consequence, and by comparing Eqs.1 and 16 we can conclude that the operators $(\mathbf{r}, \tilde{\mathbf{k}})$ correspond to the dynamical variables in Eqs. 1, denoted $\mathbf{x_c}$ and $\mathbf{q_c}$ in Ref. [9]. The variable $\mathbf{x_c}$ is the wave-packet center, and $\mathbf{q_c}$ the mean wave vector. The equations of motion for $\mathbf{x_c}$ and $\mathbf{q_c}$ were obtained, using a time-dependent variational principle in a Lagrangian formulation [9] . It was then found that the derivation of a semiclassical Hamiltonian presents some difficulties in the presence of Berry-phase terms. Actually, as explained in [9], this derivation requires the knowledge of the commutation relations between $\mathbf{x_c}$ and $\mathbf{q_c}$ (a re-quantization procedure), but these relations cannot be found from the Lagrangian formulation. One of the advantages of our approach is to show that these commutation relations are in fact a direct consequence of the semiclassical diagonalization of the quantum Hamiltonian.

In summary, our semiclassical diagonalization of the electromagnetic Bloch Hamiltonian leads to a well defined semiclassical Hamiltonian with Berry-phase corrections. The resulting semiclassical equations turn out to be the ones obtained previously from a semiclassical Lagrangian formalism [9]. When the correct dynamical variables are used the Liouville theorem is restored. Moreover, the present approach also confirms 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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[1] A. Bérard, H. Mohrbach, Phys. Rev. D **69** (2004) 127701; Phys. lett. A **352** (2006) 190.
[2] K. Y. Bliokh, Eur. Lett. **72** (2005) 7.
[3] S. Murakami, N. Nagaosa, S. C. Zhang, Science **301** (2003) 1348.
[4] K. Y. Bliokh, Y. P. Bliokh, Phys. Lett A **333** (2004), 181; Phys. Rev. E **70** (2004) 026605.
[5] M. Onoda, S. Murakami, N. Nagasoa, Phys. Rev. Lett. **93** (2004) 083901.
[6] C. Duval, Z. Horváth, P. A. Horváthy, Phys. Rev. D **74** (2006) 021701; and math-ph/0509031.
[7] N. W. Ashcroft and N. D. Mermin, Solid State Physics (Saunders, Philadelphia, 1976).
[8] M. C. Chang, Q. Niu, Phys. Rev. Lett **75** (1995) 1348; Phys. Rev. B **53** (1996) 7010;
[9] G. Sundaram, Q. Niu, Phys. Rev. B **59** (1999) 14915.
[10] R. Shindou, K. I. Imura, Nucl. Phys. B, **720** (2005) 399.
[11] R. Karplus and J. M. Luttinger, Phys. Rev. **95** (1954) 1154; W. Kohn and J. M. Luttinger, Phys. Rev. **108** (1957) 590.
[12] D. Xiao, J. Shi and Q. Niu, Phys. Rev. Lett **95** (2005) 137204.
[13] P. A. Horváthy, L. Martina, P. Stichel, Phys. Lett. B **615** (2005) 87.
[14] C. Duval, et al., Phys.Rev.Lett. **96** (2006) 099701; Mod. Phys. Lett. B **20**, 373 (2006)
[15] K. Y. Bliokh, Phys. Lett. A **351** (2006) 123.
[16] E. N. Adams and E. I. Blount, J. Phys. Chem. Solids **10** (1959) 286.
[17] P. Gosselin, A. Bérard, H. Mohrbach, hep-th/0603192.
[18] E. M. Lifshitz and L. P. Pitaevskii, Statistical Physics, vol 9, Pergamon Press, 1981.