Berry phase correction to electron density of states in solids

Di Xiao, Junren Shi, and Qian Niu
Department of Physics, The University of Texas, Austin, TX 78712-0264, USA
(Dated: February 14, 2005)

Liouville's theorem on the conservation of phase space volume is violated by Berry phase in the semiclassical dynamics of Bloch electrons. This leads to a modification of the phase space density of states, whose significance is discussed in a number of examples: field modification of the Fermi-sea volume, connection to the anomalous Hall effect, and a general formula for orbital magnetization. The effective quantum mechanics of Bloch electrons is also sketched, where the modified density of states plays an essential role.

PACS numbers: 73.43.-f, 72.15.-v, 75.20.-g

Semiclassical dynamics of Bloch electrons in external fields has provided a powerful theoretical framework to account for various properties of metals, semiconductors and insulators [1]. In recent years, it has been made increasingly clear that essential modification of the semiclassical dynamics is necessary for a proper understanding of a number of phenomena. It was known earlier that global geometric phase effects [2, 3] on Bloch states are very important for insulators in our understanding of the quantum Hall effect [4], quantized adiabatic pumps [5], and electric polarization [6, 7]. It was shown in 1996 [8] and more generally in 1999 [9] that geometric phase also modifies the local dynamics of Bloch electrons and thus affects the transport properties of metals and semiconductors. Recently these ideas have been applied to the anomalous Hall effect in ferromagnetic semiconductors and metals [10, 11, 12, 13], achieving quantitative comparisons with experiments for the first time over a long history of study. More recently, geometric phase has also been found to be important in spin transport [14, 15, 16].

In this Letter, we reveal a general property of the Berry-phase [2] modified semiclassical dynamics which has been overlooked so far: the violation of Liouville's theorem for the conservation of phase space volume. Liouville's theorem was originally established for standard classical Hamiltonian dynamics, and its importance cannot be over emphasized as it serves as a foundation for classical statistical physics. The Berry phase makes, in general, the equations of motion non-Hamiltonian, rendering the violation of Liouville's theorem. Nevertheless, we are able to remedy the situation by modifying the measure of density of states in the phase space.

This modified phase-space density of states enters naturally in the semiclassical expression for the expectation value of physical quantities, and has profound effects on equilibrium as well as transport properties. We demonstrate this with several examples. First, we consider a Fermi sea of electrons in a weak magnetic field, and show that the Fermi sea volume can be changed linearly by the field. Second, we show how the Berry phase formula for the intrinsic anomalous Hall conductivity may be derived from equilibrium thermodynamics using the Středa formula [17]. Third, we provide a general derivation of an orbital-magnetization formula which is convenient for first-principles calculations.

In addition, we present an effective quantum mechanics for Bloch electrons in solids by quantizing the semiclassical dynamics with the geometric phase. The density of states enters in a nontrivial manner into the commutators of the phase space coordinates, and relates directly to the minimal uncertainty volume in the phase space.

To begin with, we write down the semiclassical equations of motion for a Bloch electron in weak electric and magnetic fields [9]

$$\dot{\boldsymbol{r}} = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\boldsymbol{k})}{\partial \boldsymbol{k}} - \dot{\boldsymbol{k}} \times \boldsymbol{\Omega}_n(\boldsymbol{k}) \,, \tag{1a}$$

$$\hbar\dot{\boldsymbol{k}} = -e\boldsymbol{E}(\boldsymbol{r}) - e\dot{\boldsymbol{r}} \times \boldsymbol{B}(\boldsymbol{r}) \,, \tag{1b}$$

where $\boldsymbol{\Omega}_n(\boldsymbol{k})$ is the Berry curvature of electronic Bloch states defined by $\boldsymbol{\Omega}_n(\boldsymbol{k}) = \mathrm{i}\langle\boldsymbol{\nabla}_{\boldsymbol{k}} u_n(\boldsymbol{k})| \times |\boldsymbol{\nabla}_{\boldsymbol{k}} u_n(\boldsymbol{k})\rangle$ with $|u_n(\boldsymbol{k})\rangle$ being the periodic part of Bloch waves in the nth band. We use the convention that electron charge is $-e$. It is well known that, in the absence of the Berry curvature field, the above equations can be written into a Hamiltonian form using the Peierls substitution [1, 18]. On the other hand, if the magnetic field is zero, one can still turn these equations into a Hamiltonian form in a similar manner [28]. However, this cannot be done when both fields are present, leading to the violation of Liouville's theorem.

To account for the breakdown of Liouville's theorem, we consider the time evolution of a volume element $\Delta V = \Delta\boldsymbol{r}\Delta\boldsymbol{k}$ in the phase space. The equation of motion for ΔV is given by $(1/\Delta V)\mathrm{d}\Delta V/\mathrm{d}t = \boldsymbol{\nabla}_{\boldsymbol{r}} \cdot \dot{\boldsymbol{r}} + \boldsymbol{\nabla}_{\boldsymbol{k}} \cdot \dot{\boldsymbol{k}}$ [19]. A straightforward but somewhat tedious calculation shows that the right hand side is equal to $-\mathrm{d}\ln(1+e\boldsymbol{B}\cdot\boldsymbol{\Omega}/\hbar)/\mathrm{d}t$, which is a total time derivative. Therefore we can solve for the time evolution of the volume element and obtain

$$\Delta V = \Delta V_0/(1 + e\boldsymbol{B} \cdot \boldsymbol{\Omega}_n/\hbar) \,. \tag{2}$$

The fact that the Berry curvature is generally $\boldsymbol{k}$ dependent (and the magnetic field can also depend on $\boldsymbol{r}$) shows that the phase space volume element changes during time evolution of the state variables $(\boldsymbol{r}, \boldsymbol{k})$.

Nevertheless, we have a remedy to this breakdown of Liouville's theorem. Equation (2) shows that the volume element is a local function of the state variables (through the magnetic field and the Berry curvature) and has nothing to do with the history of time evolution. We can thus introduce a measure of density of states

$$D_n(\boldsymbol{r},\boldsymbol{k}) = (2\pi)^{-d}(1+e\boldsymbol{B}\cdot\boldsymbol{\Omega}_n/\hbar)\ , \tag{3}$$

such that the number of states in the volume element, $D_n(\boldsymbol{r},\boldsymbol{k})\Delta V$, remains constant in time, where d is the spatial dimensionality of the system. The prefactor $(2\pi)^{-d}$ is obtained by demanding that the density of states $D_n(\boldsymbol{r},\boldsymbol{k})$ reduces to the conventional form when the Berry curvature vanishes. As will be shown later, this density of states corresponds to the minimal quantum uncertainty volume of the state variables. Therefore, it does serve as the semiclassical measure for the number of quantum states per unit volume in the phase space. Based on this understanding, we write the classical phase-space probability density as

$$\rho_n(\boldsymbol{r},\boldsymbol{k},t) = D_n(\boldsymbol{r},\boldsymbol{k})f_n(\boldsymbol{r},\boldsymbol{k},t)\ , \tag{4}$$

with $f_n(\boldsymbol{r},\boldsymbol{k},t)$ being the occupation number of the state labeled by $(\boldsymbol{r},\boldsymbol{k})$. Probability conservation demands that $\rho_n(\boldsymbol{r},\boldsymbol{k},t)$ satisfies the continuity equation in phase space. On the other hand, our density of states satisfies $\mathrm{d}D_n/\mathrm{d}t = -(\boldsymbol{\nabla}_{\boldsymbol{r}}\cdot\dot{\boldsymbol{r}} + \boldsymbol{\nabla}_{\boldsymbol{k}}\cdot\dot{\boldsymbol{k}})D_n$. It then follows that the occupation number introduced above has the desired property of being invariant along the trajectory, i.e., $\mathrm{d}f_n/\mathrm{d}t = 0$ [29].

We can thus write the real space density of a physical observable $\hat{O}$ in the form [16]

$$\bar{O}(\boldsymbol{R}) = \sum_n \int \mathrm{d}\boldsymbol{k} D_n(\boldsymbol{r},\boldsymbol{k})f_n(\boldsymbol{r},\boldsymbol{k},t)\langle\hat{O}\delta(\hat{\boldsymbol{r}}-\boldsymbol{R})\rangle_{\boldsymbol{r}\boldsymbol{k}n} \tag{5}$$

where $\langle\cdots\rangle_{\boldsymbol{r}\boldsymbol{k}n}$ denotes the expectation value in the wavepacket state centered at $(\boldsymbol{r},\,\boldsymbol{k})$ with the band index n. In the spatially homogeneous case, it reduces to:

$$\bar{O} = \sum_n \int \mathrm{d}\boldsymbol{k} D_n(\boldsymbol{k})f_n(\boldsymbol{k})O_n(\boldsymbol{k})\ , \tag{6}$$

where $O_n(\boldsymbol{k})$ is the expectation value of $\hat{O}$ in a Bloch state. In the following, before more general considerations, we will present a number of applications of the above formula. For simpler notation, we will drop the band index n and assume that the integral over $\boldsymbol{k}$ includes the sum over n.

In our first example, we consider the quantity of electron density and show that the Fermi sea volume can be changed linearly by a magnetic field when the Berry curvature is non-zero. Assuming zero temperature and using Eq. (3), we have the electron density as

$$n_e = \int^{\mu} \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d}\left(1+\frac{e\boldsymbol{B}\cdot\boldsymbol{\Omega}}{\hbar}\right)\ , \tag{7}$$

where the upper limit means that the integral is over states with energies below the chemical potential μ. Noting that the electron density is fixed by the background charge density, we conclude that the chemical potential must change with the magnetic field. To first order, this change is given by

$$\delta\mu\,\rho(\mu_0) = -\int^{\mu_0} \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d}\frac{e\boldsymbol{B}\cdot\boldsymbol{\Omega}}{\hbar}\ . \tag{8}$$

where $\rho(\mu_0)$ is the density of states at the Fermi energy μ_0 at zero field. The left hand side of this equation also stands for the change in the Fermi sea volume (divided by $(2\pi)^d$, to be precise). We note that while Landau levels make the Fermi sea volume oscillate with the field, the effect described above gives an overall shift on average. Such a shift has important implications to those Fermi-surface related behaviors such as transport properties. For instance, in metals, it can induce a magnetoresistance linearly depending on the magnetic field. On the other hand, in band insulators, the $\boldsymbol{k}$ space is limited to the Brillouin zone. Electrons must populate a higher band if $(e/\hbar)\int_{\mathrm{BZ}}\mathrm{d}\boldsymbol{k}\,\boldsymbol{B}\cdot\boldsymbol{\Omega}$ is negative. When this quantity is positive, holes must appear at the top of the valence bands. Discontinuous behavior of physical properties in a magnetic field is therefore expected for band insulators with non-zero integral of the Berry curvatures (Chern numbers).

In our second example, we show a connection between our phase space density of states to the intrinsic anomalous Hall effect. In the context of the quantum Hall effect, Středa derived a formula relating the Hall conductivity to the field derivative of the electron density at a fixed chemical potential [17], $\sigma_{xy} = -e(\partial n_e/\partial B_z)_\mu$. There is a simple justification of this relation by a thermodynamic argument by considering the following adiabatic process in two dimensions. A time dependent magnetic flux generates an electric field with an emf around the boundary of some region; and the Hall current leads to a net flow of electrons across the boundary and thus a change of electron density inside. This argument can be straightforwardly applied to the case of anomalous Hall effect and to three dimensions. Using the identity, $(\partial n_e/\partial B_z)_\mu = -(\partial n_e/\partial\mu)_{B_z}(\partial\mu/\partial B_z)_{n_e}$, and making use of Eq. (8), we find that

$$\sigma_{xy} = -\frac{e^2}{\hbar}\int^{\mu}\frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d}\Omega_z \tag{9}$$

This is the Berry phase formula for the intrinsic anomalous Hall conductivity extensively discussed in recent years [10, 11, 12, 13].

As a third example of application, we now derive a semiclassical formula for orbital magnetization. In the presence of a weak magnetic field $\boldsymbol{B}$, the electron band structure energy $\varepsilon_0(\boldsymbol{k})$ acquires a correction term from the orbital magnetic moment [8, 9], $\varepsilon(\boldsymbol{k}) = \varepsilon_0(\boldsymbol{k}) - \boldsymbol{m}(\boldsymbol{k})\cdot$

$\boldsymbol{B}$, where $\boldsymbol{m}(\boldsymbol{k})$ is the orbital magnetic moment of a Bloch electron [30], $\boldsymbol{m}(\boldsymbol{k}) = -\mathrm{i}(e/2\hbar)\langle\boldsymbol{\nabla}_{\boldsymbol{k}}u| \times [\hat{H}_0(\boldsymbol{k}) - \varepsilon_0(\boldsymbol{k})]|\boldsymbol{\nabla}_{\boldsymbol{k}}u\rangle$ with $\hat{H}_0$ being the unperturbed Hamiltonian. Using Eq. (6), the total energy is

$$E = \int^{\mu} \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d}\Big(1 + \frac{e\boldsymbol{B}\cdot\boldsymbol{\Omega}}{\hbar}\Big)\Big(\varepsilon_0(\boldsymbol{k}) - \boldsymbol{m}(\boldsymbol{k})\cdot\boldsymbol{B}\Big) \ . \quad (10)$$

To first order in $\boldsymbol{B}$, there are three sources of corrections to the total energy: the change in the electron band energy $\varepsilon(\boldsymbol{k})$, the change of density of states in Eq. (3), and the change of Fermi surface in Eq. (8). Taking differential of E with respect to $\boldsymbol{B}$, we obtain the magnetization

$$\begin{aligned}\boldsymbol{M} &= \int^{\mu_0} \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d}\Big(\boldsymbol{m}(\boldsymbol{k}) + \frac{e\boldsymbol{\Omega}}{\hbar}\big[\mu_0 - \varepsilon_0(\boldsymbol{k})\big]\Big) \quad (11)\\ &= \frac{e}{2\hbar}\int^{\mu_0} \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^d}\mathrm{i}\Big\langle\frac{\partial u}{\partial\boldsymbol{k}}\Big| \times [2\mu_0 - \varepsilon_0(\boldsymbol{k}) - \hat{H}_0]\Big|\frac{\partial u}{\partial\boldsymbol{k}}\Big\rangle \ .\end{aligned}$$

Gat and Avron obtained a similar result for the special case of Hofstadter model [20]. Our derivation provides a more general formula that is applicable to other systems. Following the discussions on band insulators in our first example, there will be a discontinuity of the orbital magnetization if the integral of the Berry curvature over the Brillouin zone, or the anomalous Hall conductivity, is non-zero and quantized. Depending on the direction of the field, the chemical potential μ_0 in the above formula should be taken at the top of the valence bands or the bottom of the conduction bands. The size of the discontinuity is given by the quantized anomalous Hall conductivity times E_g/e, where E_g is the energy gap. For insulators with zero Chern numbers, the orbital magnetization can be directly evaluated from Wannier functions, with result consistent with our general formula [21]. Our general formula can also be derived from a full quantum mechanical linear response analysis [22].

The central result of this paper, equation (3), can be extended to the more general case when Berry curvature includes the components of $\overleftrightarrow{\Omega}^{\boldsymbol{kr}}$ as well as $\overleftrightarrow{\Omega}^{\boldsymbol{kk}}$ and $\overleftrightarrow{\Omega}^{\boldsymbol{rr}}$ [9]. In this case, we introduce the Berry curvature in phase space,

$$\overleftrightarrow{\boldsymbol{\Omega}} = \begin{pmatrix}\overleftrightarrow{\Omega}^{\boldsymbol{rr}} & \overleftrightarrow{\Omega}^{\boldsymbol{rk}}\\ \overleftrightarrow{\Omega}^{\boldsymbol{kr}} & \overleftrightarrow{\Omega}^{\boldsymbol{kk}}\end{pmatrix} \ , \quad (12)$$

where each block is a 3×3 matrix; $\overleftrightarrow{\Omega}^{\boldsymbol{rk}} = -(\overleftrightarrow{\Omega}^{\boldsymbol{kr}})^T$. The phase space density of states then reads,

$$D = (2\pi)^{-d}\sqrt{\det(\overleftrightarrow{\boldsymbol{\Omega}} - \overleftrightarrow{\mathbf{J}})} \ . \quad (13)$$

with $\overleftrightarrow{\mathbf{J}} = \left(\begin{smallmatrix} 0 & \overleftrightarrow{\mathrm{I}}\\ -\overleftrightarrow{\mathrm{I}} & 0\end{smallmatrix}\right)$. In the special case of electromagnetic perturbations with $\overleftrightarrow{\Omega}^{\boldsymbol{kk}}_{ab} = \epsilon_{abc}\Omega_c$, $\overleftrightarrow{\Omega}^{\boldsymbol{rr}}_{ab} = -(e/\hbar)\epsilon_{abc}B_c$ and $\overleftrightarrow{\Omega}^{\boldsymbol{kr}} = 0$, it reduces to (3). On the other hand, when either $\overleftrightarrow{\Omega}^{\boldsymbol{kk}}$ or $\overleftrightarrow{\Omega}^{\boldsymbol{rr}}$ vanishes, it has a simpler form

$$D = (2\pi)^{-d}\det(\overleftrightarrow{\mathrm{I}} - \overleftrightarrow{\Omega}^{\boldsymbol{rk}}) \ . \quad (14)$$

This result has found application in the study of spin-force induced charge-Hall effect [23].

Finally, we show how the density of states emerges naturally in the effective quantum mechanics of Bloch electrons. Although our system is not canonical, it can nevertheless be quantized following a standard procedure developed for non-holonomic systems with second class constraints [24, 25]. First, one redefines the Poisson bracket $\{f,g\}^* = (\partial f/\partial\xi^a)M_{ab}(\partial g/\partial\xi^b)$, where ξ^a are the components of phase space coordinates $\boldsymbol{\xi} \equiv (\boldsymbol{r},\ \boldsymbol{k})$ and $\overleftrightarrow{\mathbf{M}} = (\overleftrightarrow{\boldsymbol{\Omega}} - \overleftrightarrow{\mathbf{J}})^{-1}$. Our equations of motion (1) can then be written as $\dot{\xi}^a = \{\xi^a,\varepsilon\}^*$, where the energy $\varepsilon(\boldsymbol{\xi})$ plays the role as the Hamiltonian function. Then, one promotes the Poisson brackets into quantum commutators:

$$[\hat{\xi}^a,\hat{\xi}^b] = \mathrm{i}M_{ab} \ , \quad (15)$$

where $\hat{\xi}^a$ is the quantum operator corresponding to the phase space coordinates. It then follows that a phase space point acquires a minimal uncertainty volume given by [26]

$$\min\Big(\prod_a \Delta\xi^a\Big) = 2^{-d}\Big[\det(\overleftrightarrow{\boldsymbol{\Omega}} - \overleftrightarrow{\mathbf{J}})\Big]^{-1/2} \ . \quad (16)$$

This can be understood as the phase space volume occupied by a single quantum state, therefore Eq. (13), which is proportional to the reciprocal of this volume, can naturally be regarded as the semiclassical expression for the number of quantum states per unit volume in the phase space.

Equation (15) presents the effective quantum mechanics of Bloch electrons. As a demonstration for the validity of the quantization scheme as well as the quantum effect of the phase space density of states, we consider a simple toy model of two dimensional electron system with a constant Berry curvature, subjected to a uniform magnetic field. The commutators read,

$$\begin{aligned}&[\hat{x},\hat{y}] = \mathrm{i}\frac{\Omega}{1+(e/\hbar)B\Omega} \ , \quad [\hat{k}_x,\hat{k}_y] = -\mathrm{i}\frac{(e/\hbar)B}{1+(e/\hbar)B\Omega} \ ,\\ &[\hat{x},\hat{k}_x] = [\hat{y},\hat{k}_y] = \mathrm{i}\frac{1}{1+(e/\hbar)B\Omega} \ . \quad (17)\end{aligned}$$

In the absence of the Berry curvature, we reduce the problem to a known case with the familiar nontrivial commutator $[\hat{k}_x,\hat{k}_y] = -\mathrm{i}(e/\hbar)B$. In the absence of the B field, we have the nontrivial commutator $[\hat{x},\hat{y}] = \mathrm{i}\Omega$ discussed extensively in the literature on non-commutative geometry. It is interesting to see that in the presence of both fields, we do not just have a combination of these nontrivial commutators. Instead, we have a nontrivial density of states which enters into all of the commutators.

Assuming $\varepsilon(\boldsymbol{k}) = \hbar^2\boldsymbol{k}^2/2m$, the system can be solved algebraically to yield the energy spectrum and degeneracy. We found that the spectrum consists of a set of

Landau levels with the renormalized cyclotron frequency $\omega_c = \omega_c^0/[1 + (e/\hbar)B\Omega]$, where $\omega_c^0 = eB/m$ is the usual cyclotron frequency [27]. At the same time, it is more important to note that each Landau level still has the same degeneracy of eB/h as in the absence of the Berry curvature. It is known that this degeneracy is directly related to the quantized Hall conductance e^2/h for a filled Landau level [31]. Had the density of states not entered in the commutators, the Landau level degeneracy would be modified, violating the topological requirement that the Hall conductance for a filled Landau level is quantized.

Before closing, we note that the phase space density of states also enters naturally in the alternative quantization scheme with Feynman path integral. The S matrix is calculated by [24]

$$\langle \text{out}|S|\text{in}\rangle = \int \prod_t [D(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi}] \exp\Big[\frac{\mathrm{i}}{\hbar}\int L\mathrm{d}t\Big] \ . \qquad (18)$$

where L is the Lagrangian for our system [9],

$$L = \frac{1}{2}\dot{\xi}^a J_{ab} \xi^b - \varepsilon(\boldsymbol{\xi}) + \dot{\xi}^a \mathcal{A}_a(\boldsymbol{\xi}) \qquad (19)$$

with $\mathcal{A}_a(\boldsymbol{\xi}) \equiv \mathrm{i}\langle u(\boldsymbol{\xi})|\nabla_\alpha u(\boldsymbol{\xi})\rangle$ being the phase space gauge potentials associated with the Berry curvature field $\overleftrightarrow{\boldsymbol{\Omega}}$.

In summary, we have found a Berry phase correction to the phase space density of states for Bloch electrons. This correction emerges naturally in both semiclassical and quantum mechanics of Bloch electrons, and has profound effects on the equilibrium and transport properties. Because of the fundamental change introduced by this correction, it could have important implications on other aspects of condensed matter physics, such as the Fermi liquid theory. For instance, in the presence of a magnetic field, interaction between electrons can change the Fermi sea volume by modifying the Berry curvature and thus the phase space density of states.

We acknowledge useful discussions with M. C. Chang, R. Resta, G. Y. Guo, Y. G. Yao, and D. Vanderbilt. This work is supported by DOE grant DE-FG03-02ER45958.

[1] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Saunders, Philadelphia, 1976).

[2] M. V. Berry, Proc. Roy. Soc. London **A392**, 45 (1984).

[3] A. Bohm, A. Mostafazadeh, H. Koizumi, Q. Niu, and J. Zwanziger, *The Geometric Phase in Quantum Systems: Foundations, Mathematical Concepts, and Applications in Molecular and Condensed Matter Physics* (Springer-Verlag, Berlin, 2003).

[4] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. **49**, 405 (1982).

[5] D. J. Thouless, Phys. Rev. B **27**, 6083 (1983).

[6] R. D. King-Smith and D. Vanderbilt, Phys. Rev. B **47**, R1651 (1993).

[7] R. Resta, Rev. Mod. Phys. **66**, 899 (1994).

[8] M.-C. Chang and Q. Niu, Phys. Rev. B **53**, 7010 (1996).

[9] G. Sundaram and Q. Niu, Phys. Rev. B **59**, 14915 (1999).

[10] T. Jungwirth, Q. Niu, and A. H. MacDonald, Phys. Rev. Lett. **88**, 207208 (2002).

[11] Z. Fang, N. Nagaosa, K. S. Takahashi, A. Asamitsu, R. Mathieu, T. Ogasawara, H. Yamada, M. Kawasaki, Y. Tokura, and K. Terakura, Science **302**, 92 (2003).

[12] Y. Yao, L. Kleinman, A. H. MacDonald, J. Sinova, T. Jungwirth, D.-S. Wang, E. Wang, and Q. Niu, Phys. Rev. Lett. **92**, 37204 (2004).

[13] F. D. M. Haldane, Phys. Rev. Lett. **93**, 206602 (2004).

[14] S. Murakami, N. Nagaosa, and S.-C. Zhang, Science **361**, 1348 (2003).

[15] J. Sinova, D. Culcer, Q. Niu, N. A. Sinitsyn, T. Jungwirth, and A. H. MacDonald, Phys. Rev. Lett. **92**, 126603 (2004).

[16] D. Culcer, J. Sinova, N. A. Sinitsyn, T. Jungwirth, A. H. MacDonald, and Q. Niu, Phys. Rev. Lett. **93**, 46602 (2004).

[17] P. Středa, J. Phys. C: Solid State Phys. **15**, L717 (1982).

[18] R. Peierls, Z. Phys. **80**, 763 (1933).

[19] L. E. Reichl, *A Modern Course in Statistical Physics* (University of Texas Press, Austin, TX, 1980).

[20] O. Gat and J. E. Avron, Phys. Rev. Lett. **91**, 186801 (2003).

[21] Private communication with authors of the following paper, where some partial results are presented: R. Resta, D. Ceresoli, T. Thonhauser and D. Vanderbilt, *Orbital magnetization in extended systems*, submitted to Chem. Phys. Chem.

[22] J. Shi, D. Xiao, and Q. Niu, to be published.

[23] P. Zhang, J. Shi, D. Xiao, and Q. Niu, to be published.

[24] P. Senjanovic, Ann. Phys. **100**, 227 (1976).

[25] D. M. Gitman and I. V. Tyutin, *Quantization of Fields with Constraints* (Springer-Verlag, New York, 1990).

[26] H. P. Robertson, Phys. Rev. **46**, 794 (1934).

[27] P. A. Horvathy, L. Martina, and P. Stichel, hep-th/0412090.

[28] In the absence of the magnetic field, the equations of motion (1) can be written into a Hamiltonian form with $\boldsymbol{R} = \boldsymbol{r} + \boldsymbol{\mathcal{A}}$ and $\hbar\boldsymbol{k}$ being conjugate variables and $\varepsilon_n(\boldsymbol{k}) - \phi(\boldsymbol{R} - \boldsymbol{\mathcal{A}})$ as the Hamiltonian, where $\phi(\boldsymbol{r})$ is the scalar potential and $\boldsymbol{\mathcal{A}}(\boldsymbol{k}) = \mathrm{i}\langle u_n(\boldsymbol{k})|\boldsymbol{\nabla}_{\boldsymbol{k}} u(\boldsymbol{k})\rangle$ is the vector potential in $\boldsymbol{k}$-space.

[29] In the presence of collision, the function satisfies the usual Boltzmann equation:

$$\frac{\mathrm{d}f_n}{\mathrm{d}t} \equiv \Big(\frac{\partial}{\partial t} + \dot{\boldsymbol{r}}\cdot\nabla_{\boldsymbol{r}} + \dot{\boldsymbol{k}}\cdot\nabla_{\boldsymbol{k}}\Big) f_n(\boldsymbol{k},\boldsymbol{r},t) = \Big(\frac{\partial f_n}{\partial t}\Big)_{\text{coll}}$$

The right hand side denotes the collision contribution.

[30] There is a typo in Ref. [9]. The expression for orbital magnetic moment in Eq. (3.6) misses a factor of $-1/2$.

[31] The Hall conductance is given by $\sigma = ne/B$, where n is the electron density. The quantized value is obtained if we substitute the degeneracy density for n.