Berry phase correction to electron density in solids and “exotic”
dynamics

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Abstract

Recent results on the semiclassical dynamics of an electron in a solid are explained using
techniques developed for “exotic” Galilean dynamics. The system is indeed Hamiltonian and
Liouville’s theorem holds for the symplectic volume form. Suitably defined quantities satisfy
hydrodynamic equations.

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The effective semiclassical dynamics of a Bloch electron in a solid is modified by a Berry curvature term [1]. Putting $\hbar = 1$, the equations of motion in the $n^{th}$ band read indeed

$$\dot{r} = \frac{\partial \epsilon_n(k)}{\partial k} - \dot{k} \times \Omega(k), \quad (1)$$

$$\dot{k} = -eE - e\dot{r} \times B(r), \quad (2)$$

where $r = (x^i)$ and $k = (k_j)$ denote the electron’s intracell position and quasimomentum, respectively, $\epsilon_n(k)$ is the band energy. The purely momentum-dependent $\Omega$ is the Berry curvature of the electronic Bloch states, $\Omega_i(k) = \epsilon_{ijl} \frac{\partial}{\partial k_j} A_l(k)$, where $A$ is the Berry connection. The electronic charge is $-e$. The new Berry-curvature dependent term in eqn. (1) has been instrumental in explaining the anomalous Hall effect in ferromagnetic materials [2], and also the spin Hall effect [3].

Much of the transport phenomena rely on the Liouville’s theorem on the conservation of the phase-space volume element. Recently, Xiao et al. observed that, due to the Berry curvature term, the naive phase-space volume form $d\mathbf{r}d\mathbf{k}$ is no more conserved. They attribute this fact to the non-Hamiltonian character of the equations (1)-(2), and suggest to redefine the phase-space density by including a pre-factor,

$$\rho \rightarrow \rho_n = D_n f_n(r, k, t), \quad D = \frac{1}{(2\pi)^d} (1 + eB \cdot \Omega), \quad (3)$$

where $d$ is the spatial dimension and $f_n$ is the occupation number of the state labeled by $r, k$. If the latter is conserved along the motion, $df_n/dt = 0$, then $\rho_n$ satisfies the continuity equation on phase space. Eqn. (3) is the starting point of Xiao et al. to derive interesting applications.

Xiao et al. derive Eq. (3), their main result, by calculating the change of $d\mathbf{r}d\mathbf{k}$ using the equations of motion and then finding a compensating factor. This may appear somewhat mysterious at first sight. Our Note is to the end to point out that the equations (1)-(2) are indeed Hamiltonian in a by-now standard sense [9], and the validity of Liouville’s theorem is restored if the symplectic volume form, Eq. (7) below, is used. Then Eq. (3) follows at once. Our clue is the relation to “exotic” Galilean dynamics, introduced independently and equivalent to non-commutative mechanics in [5, 6, 7, 8].

Let us first summarize the general principles of Hamiltonian dynamics [9]. The first ingredient is the symplectic form on $2d$-dimensional phase space, i.e., a closed and regular 2-form $\omega = \frac{1}{2} \omega_{\alpha\beta} d\xi^\alpha \wedge d\xi^\beta$, where $\xi^\alpha$ denotes the phase space coordinates $r$ and $k$ collectively. Then the Poisson bracket of two functions $f$ and $g$ on phase space is

$$\{f, g\} = \omega^{\alpha\beta} \partial_\alpha f \partial_\beta g, \quad (4)$$

where $\omega^{\alpha\beta}$ is the inverse of the symplectic matrix, $\omega^{\alpha\gamma} \omega_{\gamma\beta} = \delta^{\alpha\beta}$. Since $\omega$ is closed, the Poisson bracket (4) satisfies the Jacobi identity. Then Hamilton’s equations read

$$\dot{\xi}^\alpha = \{h, \xi^\alpha\}, \quad (5)$$

where $h = h(\xi)$ is some given Hamiltonian, which is the second ingredient we need. Such a framework is obtained [10], in particular, starting with a first-order Lagrangian $L = a_\alpha(\xi) \dot{\xi}^\alpha - h(\xi)$ on phase-space, whose Euler-Lagrange equations read

$$\omega_{\alpha\beta} \dot{\xi}^\beta = \partial_\alpha h, \quad \text{where} \quad \omega_{\alpha\beta} = \partial_\alpha a_\beta - \partial_\beta a_\alpha, \quad (6)$$

and multiplying (6) by the inverse matrix $\omega^{\alpha\beta}$ yields Hamilton’s equations, (5).
Now the natural volume form on phase space is the \( d^d \) power of the symplectic form \[9\] which, in arbitrary coordinates \( \xi^\alpha \) on phase space, reads
\[
dV = \frac{1}{d!} \omega^d = \sqrt{\det(\omega_{\alpha\beta})} \prod_{\alpha=1}^d d\xi^\alpha. \tag{7}
\]

The intrinsic expression \[7\] is invariant w.r.t. coordinate transformations. The naive expression \( \prod d\xi^\alpha \), changes in fact as \( \prod d\xi^\alpha \rightarrow \prod d\zeta^\alpha = \det(\partial^\alpha \zeta / \partial \xi^\beta) \prod d\xi^\alpha \) under a transformation \( \xi \rightarrow \zeta \). This is, however, compensated by the change of the determinant. As a bonus, the validity of Liouville’s theorem is restored: the r.h.s. of \[5\] generates the classical flow of the phase space, w.r.t. which the symplectic volume form, \[7\], is invariant, since the classical flow is made of symplectic transformations \[9\].

Now Darboux’s theorem tells that one can always find canonical local coordinates \( p_i, q^j \) (say) such that the symplectic matrix has the canonical form \( \Omega = dp_i \wedge dq^j \). Then the general Hamilton equations, \[5\] take their familiar form \( \dot{q}^i = \partial p_i / \partial \dot{h}, \dot{p}_j = -\partial q^j / \partial \dot{h} \). The volume form is simply \( \prod dp_i \wedge dq^j \). Xiao et al. use the restricted terminology, referring to canonical coordinates. Non-canonical coordinates may be useful, though. The equations of motion \[1\]-\[2\] can indeed be put into the form \[6\] with symplectic and resp. Poisson matrix
\[
\omega_{\alpha\beta} = \begin{pmatrix}
-\varepsilon_{ijk} B^k & -\delta_{jk} \\
\delta_{jk} & \varepsilon_{ijk} \Omega^k
\end{pmatrix} \quad \implies \quad \omega^{\alpha\beta} = \frac{1}{1 + eB \cdot \Omega} \begin{pmatrix}
\varepsilon_{ijk} \Omega^k & \delta_{jk} + eB_j \Omega_k \\
-\delta_{jk} - e\Omega_j B_k & -\varepsilon_{ijk} B^k
\end{pmatrix} \tag{8}
\]
where \( i, j, k = 1, 2, 3 \). The Poisson bracket relations are therefore
\[
\{x^i, x^j\} = \frac{\varepsilon_{ijk} \Omega_k}{1 + eB \cdot \Omega}, \tag{9}
\]
\[
\{x^i, k_j\} = \frac{\delta^i_j + eB^i \Omega_j}{1 + eB \cdot \Omega}, \tag{10}
\]
\[
\{k_i, k_j\} = -\frac{\varepsilon_{ijk} eB^k}{1 + eB \cdot \Omega}. \tag{11}
\]
The Berry curvature is divergence-free, \( \partial_{k_j} \Omega^j = 0 \), because it is a curl. The Jacobi identity follows hence from \( \partial_{\delta} B^j = 0 \), cf. \[11\]. The Hamiltonian is \( h = \epsilon_n - eV \). Note, in particular, that the coordinates do not commute: the model is indeed equivalent to non-commutative mechanics \[5\] \[6\] \[11\].

When both the \( B \), and the Berry curvature, \( \Omega = \text{const.} \) are directed in the third direction, these relations reduce to those of the ”exotic” model in the plane, derived from first principles \[6\] \[8\]. The crucial anomalous velocity term in \[11\] arises, in particular, by minimal coupling of the ”exotic” model to a gauge field \[6\]. Eq. \[8\] is obtained, furthermore, by the Faddeev-Jackiw \[10\] construction mentioned above, if we start with the Lagrangian \[11\] \[6\] \[8\]
\[
L^{\text{Bloch}} = (k_i - eA_i(r, t)\dot{x}^i) \dot{x}^i - (\epsilon_n(k) - eV(r, t)) + A^i(k) \dot{k}_i, \tag{12}
\]
where \( V \) and \( A_i \) are the scalar resp. vector potential for the electromagnetic field and \( A \) is the potential for the Berry curvature. The conserved volume form is \[7\]
\[
\sqrt{\det(\omega_{\alpha\beta})} \prod dk_i \wedge dx^i = (1 + eB \cdot \Omega) \prod_i dk_i \wedge dx^i. \tag{13}
\]
Consistently with Darboux’s theorem, canonical coordinates can be found.
In the planar case, for example, if \( B \) is constant such that \( 1 + eB\Omega \neq 0 \),
\[
P_i = \sqrt{1 + eB\Omega} k_i + \frac{1}{2} eB\epsilon_{ij} Q^j
\]
\[
Q^i = x^i - \frac{1}{eB} \left( 1 - \sqrt{1 + eB\Omega} \right) \epsilon^{ij} k_j
\] (14)

are canonical \([7]\), so that the Poisson bracket reads simply \( \{ F, G \} = \sum \partial_{Q_i} F \partial_{P_j} G - \partial_{Q_i} G \partial_{P_j} F \). (The disadvantage is that the Hamiltonian becomes rather complicated). When expressed in terms of canonical coordinates, the four-dimensional volume form reads simply
\[
\omega = \sqrt{\det(g_{ij}^{-1})} \wedge \epsilon^{ijkl} \langle dx^i \rangle \wedge \langle dx^j \rangle \wedge \langle dx^\alpha \rangle \wedge \langle dk_1 \wedge dk_2 \wedge dk_3 \rangle
\]

\( \omega = dV = \omega^3/6 \) is invariant by the Liouville theorem, \( f dV \) is an integral invariant of the flow, provided \( df/dt = 0 \). Further, multiplied with the square root of the determinant removes the unwanted term, though:
\[
\rho = f \sqrt{\det(\omega_{\alpha\beta})}
\] (16)

do not satisfy the continuity equation \( \partial_t \rho + \nabla_\xi \cdot (\hat{\xi} \rho) = 0 \) on phase space (and time). In the coordinates \( (r, k) \), \( [10] \) reduces to the expression \( [5] \) of Xiao et al., which is hence simply the coefficient of \( \prod d\xi^a \) in \( [13] \), written in a local coordinate system. The (modified) Boltzmann transport equation for \( \rho \) is
\[
\frac{d\rho}{dt} = \{ \rho, h \} + \partial_t \rho = \frac{1}{1 + eB \cdot \Omega} \left[ (\nabla_k \epsilon_n + eE \times \Omega + eB(\Omega \cdot \nabla_k \epsilon_n)) \cdot \nabla_r \rho \right.
\]
\[
- e \left( E + \nabla_k \epsilon_n \times B - e\Omega (E \cdot B) \right) \cdot \nabla_k \rho \left. + \frac{\partial \rho}{\partial t} = \frac{e(B \cdot \Omega)}{1 + eB \cdot \Omega} \rho, \right]
\] (17)

where \( (B \cdot \Omega) = \partial_t (B \cdot \Omega) + \Omega^i \hat{r} \cdot \nabla_r B_i + B_i \hat{k} \cdot \nabla_k \Omega^i \) is the material derivative.

Using the equations of motion and Maxwell equations \( \nabla \cdot B = 0 \) and \( \partial_t B + \nabla_r \times E = 0 \), a tedious but straightforward calculation shows, furthermore, that
\[
\varphi = \int \rho dk \quad \text{and} \quad \mathbf{v} = \frac{1}{\varphi} \int \hat{r} \rho dk
\] (18)

[where the integration is over the first Brillouin zone] satisfy the continuity equation \( \partial_t \varphi + \nabla_r \cdot (\mathbf{v} \varphi) = 0 \) in ordinary space-time. Similarly, we also have the Euler equation
\[
\varphi (\partial_t + \mathbf{v} \cdot \nabla_r) \mathbf{v} = \mathbf{f} - \nabla \sigma,
\] (19)

where \( \mathbf{f} = \int \hat{r} \rho dk \) is the mean force and \( \sigma = (\sigma_{ij}) \) with \( \sigma_{ij} = \int (\hat{x}_i - v_i)(\hat{x}_j - v_j) \rho dk \) is the kinetic stress tensor \([7]\).
All these remarks hold when

$$\det(\omega_{\alpha\beta}) = (1 + eB \cdot \Omega)^2 \neq 0.$$  \hspace{1cm} (20)

In the singular planar case $eB\Omega = -1$ [which can only happen if $\Omega$ and $B$ are constants], the volume element degenerates and the phase space looses 2 dimensions. The symplectic matrix can not be inverted and one can not get from a Lagrangian to the Hamiltonian framework. The only allowed motion follow the Hall law [6, 7, 8]. Hamiltonian reduction yields, however, a well-behaved 2-dimensional phase space with symplectic form proportional to the surface form in the plane, $\omega_{\text{red}} = -eBdx \wedge dy$. The fluid moves collectively, governed by a generalized Hall law [7].

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