Dynamics of semiclassical Bloch wave - packets

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Abstract

The semiclassical approximation for electron wave-packets in crystals leads to equations which can be derived from a Lagrangian or, under suitable regularity conditions, in a Hamiltonian framework. In the plane, these issues are studied using the method of the coadjoint orbit applied to the “enlarged” Galilei group.

1 Introduction

The standard semiclassical dynamics of a Bloch electron in a solid [1] accounts for various properties of metals, semiconductor and insulators. More recently it was argued, however, that a correct wave packet dynamics requires taking into account also geometric (Berry) phase effects [2]. The latter modify the transport properties of metals and semiconductors, and provide us with a new insight into the Anomalous Hall Effect [3] [4].

From the theoretical point of view, two problems arose : i) the accuracy of the semi-classical approximation derived from a time dependent variational principle in Quantum Mechanics [5]; ii) the geometrical structure of the dynamical systems describing the evolution of the electron wave-packets. The Hamiltonian structure of these models takes into account the Berry Phase effects by non commuting coordinates and realizes, at least in the planar case, a two-fold central extension of the Galilean symmetry [6].
For uniform electromagnetic fields, the structure can further be extended: position-independent fields can be viewed as extra “coordinates” that can be added to the ordinary space-time variables. The symmetries of the combined structure form the “enlarged” or “Maxwell-Galilei” group [7, 8], which involves, besides the usual Galilean space-time symmetries, also field components, see (46).

Firstly, physical realizations of such a symmetry have been presented in [9, 10]. Particles of this type are related to “anyons”, and may be used in explaining the Fractional Quantum Hall Effect [11]. Difficulties arise when coupling to an external electromagnetic field, but this can be partially overcome by resorting to the methods of the coadjoint orbits on a larger symmetry group [7]. Similar symplectic structures may appear also in 3 space dimensions [12, 13].

In Sec. 2 we briefly review the main ideas involved in the semiclassical approximation of Bloch electron wave-packets. In Sec. 3 their Lagrangian and Hamiltonian formulations are considered. Then in Sec. 4, considering a simplified version (in the plane but interacting with constant external fields), we study their general geometric formulation, by resorting to the coadjoint orbit method [15].

2 Semiclassical Approximation

The Schrödinger equation can be derived from the action functional

$$S = \int_{t_1}^{t_2} L_S dt, \quad L_S = \frac{i}{2} \frac{\langle \Psi | \frac{d\Psi}{dt} \rangle - \langle \frac{d\Psi}{dt} | \Psi \rangle}{\langle \Psi | \Psi \rangle} - \frac{\langle \Psi | \hat{H} | \Psi \rangle}{\langle \Psi | \Psi \rangle},$$

requiring the action to be stationary at the “classical” wave function |\Psi⟩. The latter belongs to a suitable Hilbert space, acted upon by an hermitian Hamiltonian operator \(\hat{H}\). The usual Schrödinger equation is obtained after a suitable phase normalization [5].

The derivation of the semiclassical approximation from a variational principle requires restricting ourselves to a predetermined domain of the Hilbert space by a suitable parametrization of the wave-function |\Psi⟩, such that the variational principle singles out the best approximate time evolution. In particular, for a spinless point-like particle one can introduce the mean position and momentum values,

$$\bar{r}_c (t) = \frac{\langle \Psi | \hat{r} | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \quad \bar{p}_c (t) = \frac{\langle \Psi | \hat{p} | \Psi \rangle}{\langle \Psi | \Psi \rangle},$$

as main parameters. Neglecting all other details of the time evolution of the wave-packets, we replace |\Psi⟩ → |\Psi[\bar{r}_c (t), \bar{p}_c (t)]⟩ into the Lagrangian (1) and look for self-consistent equations for the parameters.
As usual, the dynamics of an electron in a crystal lattice is described by a first quantized Hamiltonian operator

\[ \hat{H} \left[ \hat{r}, \hat{p}, f \left( \hat{r}, t \right) \right], \]

where \( \hat{r} \) and \( \hat{p} \) are position and momentum operators, satisfying the Heisenberg algebra. The (possibly vectorial and/or time dependent) function \( f \) represents differentiable “slow” modulations in space with respect to a fixed lattice background potential, such that \( \hat{H}_c = \hat{H} \left[ \hat{r}, \hat{p}, c \right] \) is a periodic Hamiltonian operator for any constant parameter \( c \). To justify the previous parametrization, three phenomenological length scales have to be considered, namely the typical lattice constant length \( l_{\text{att}} \), the wave-packet dispersion length \( l_{\text{wp}} \) and the modulation wave-length \( l_{\text{mod}} \). They are related by \( l_{\text{att}} \ll l_{\text{wp}} \ll l_{\text{mod}} \). Assuming regular dependence of the Hamiltonian operator (2) on the modulations, one can truncate it at the first order around the instantaneous mean position \( \bar{r}_c \), yielding

\[ \hat{H} = \hat{H}(\bar{r}_c, t) + \frac{1}{2} \left[ \partial_f \hat{H} \nabla_{\bar{r}_c} f (\bar{r}_c, t) \cdot (\hat{r} - \bar{r}_c) \right] + h.c. \],

where \( \hat{H}(\bar{r}_c, t) \) belongs to the family of the \( \hat{H}_c \), with \( c = (\bar{r}_c, t) \). Thus, we postulate that the physical states does not only include a (approximate) solution of the Schrödinger equation for a special value of \( \bar{r}_c \), but for all possible \( \bar{r}_c \) belonging to some configuration space, which has to be determined self-consistently. Then, for any \( \bar{r}_c \), one can choose an orthonormal basis of eigenvectors of the Bloch parameter-dependent Hamiltonians \( \hat{H}(\bar{r}_c, t) \), that is

\[ \hat{H}(\bar{r}_c, t) \left| \psi_{n,\bar{q}}^{\bar{r}_c, t} \right\rangle = E_{n,\bar{q}}^{\bar{r}_c, t} \left| \psi_{n,\bar{q}}^{\bar{r}_c, t} \right\rangle, \quad \langle \psi_{n,\bar{q}}^{\bar{r}_c, t} | \psi_{n',\bar{q}'}^{\bar{r}_c, t} \rangle = \delta_{n,n'} \delta (\bar{q} - \bar{q}'), \]

where the energy eigenvalues \( E_{n,\bar{q}}^{\bar{r}_c, t} \) are labelled by a band index \( n \) and by the quasi-momentum \( \bar{q} \), which can be limited to belong to the first Brillouin zone (IBZ). In the position representation the Bloch eigenfunctions take the form

\[ \langle \bar{r} | \psi_{n,\bar{q}}^{\bar{r}_c, t} \rangle = e^{i \bar{q} \cdot \bar{r}} u_{n,\bar{q}}^{\bar{r}_c, t} (\bar{r}) , \quad u_{n,\bar{q}}^{\bar{r}_c, t} (\bar{r} + \bar{a}) = u_{n,\bar{q}}^{\bar{r}_c, t} (\bar{r}), \]

\( u_{n,\bar{q}}^{\bar{r}_c, t} (\bar{r}) \) being the periodic part of the wave-function, assumed to be analytic in \( (\bar{r}_c, t) \). In the eigenvalue problem (3) time dependence is assumed adiabatic, so that the eigenvalues \( E_{n,\bar{q}}^{\bar{r}_c, t} \) form well separated bands. This is not always the case, but one can assume that the degeneracy occurs in isolated points of the IBZ not considered in the present discussion. However, there are effects which could depend on the detailed behavior of (quasi)-degenerate bands, if the Fermi level is close to these values [4]. Moreover, we assume that the modulations are so weak that band jumping is forbidden.

Now, it is a classical result by Karplus and Luttinger [2] that the matrix element of the position operator between two Bloch wave-functions is given by

\[ \langle \psi_{n,\bar{q}}^{\bar{r}_c, t} | \hat{r} | \psi_{n',\bar{q}'}^{\bar{r}_c, t} \rangle = \left[ i \nabla_\bar{q} + \langle u_{n,\bar{q}}^{\bar{r}_c, t} | i \nabla_\bar{q} u_{n,\bar{q}}^{\bar{r}_c, t} \rangle_{\text{cell}} \right] \delta (\bar{q} - \bar{q}') \delta_{n,n'}. \]

That is, in the space generated by the Bloch waves, \( \hat{r} \) acts as

\[ \hat{r} = i \nabla_\bar{q} + \hat{Q}^n(\bar{r}_c, \bar{q}, t), \quad \text{with} \quad \hat{Q}^n(\bar{r}_c, \bar{q}, t) = \langle u_{n,\bar{q}}^{\bar{r}_c, t} | i \nabla_\bar{q} u_{n,\bar{q}}^{\bar{r}_c, t} \rangle_{\text{cell}}, \]
where $\langle \cdot | \cdot \rangle_{cell}$ is the restriction of the scalar product for $L^2_{cell}$ to the unite cell with periodic boundary conditions. $(2\pi)^3 / V_{cell}$ is a normalization factor. The quantity $\mathbf{Q}^n(\mathbf{r}_c, \mathbf{q}, t)$ here can be interpreted as a $U(1)$ gauge connection and is identified with Berry’s connection.

The components of the position operator no longer commute in general,

$$[\hat{r}_j, \hat{r}_l] = i \left( \partial_{q_l} Q^n(\mathbf{r}_c, \mathbf{q}, t) - \partial_{q_j} Q^n(\mathbf{r}_c, \mathbf{q}, t) \right) \equiv i \Theta^n_{j,l}(\mathbf{r}_c, \mathbf{q}, t),$$

where the antisymmetric tensor

$$\Theta^n(\mathbf{r}_c, \mathbf{q}, t) = \Theta^n_{j,l} = i \langle \nabla_{\mathbf{q}} \mathbf{u}(\mathbf{r}_c, \mathbf{q}, t) | \times | \nabla_{\mathbf{q}} \mathbf{u}(\mathbf{r}_c, \mathbf{q}, t) \rangle_{cell},$$

is the gauge invariant Berry curvature.

Thus, the Berry phase converts the dynamics of an ordinary particle, in a periodic background potential, into a quantum mechanical system living in a non-commutative configuration space [14].

Now we want to build wave-packets from the Bloch wave-functions (4-5) chosen from a single energy band (say $n$; we drop the index in what follows) of the form

$$|\tilde{\Psi}[\mathbf{r}_c(t), \mathbf{q}_c(t)]\rangle = \int_{IBZ} \Phi(\mathbf{q}, t) |\psi(\mathbf{r}_c, \mathbf{q}, t)\rangle d\mathbf{q},$$

where the quasi-momentum normalized amplitude $\Phi(\mathbf{q}, t)$ (taking $\int_{IBZ} |\Phi(\mathbf{q}, t)|^2 d\mathbf{q} = 1$) is chosen in such a way that its dispersion $\Delta_q$ in momentum space is small compared to the first typical Brillouin size $\sim 2\pi / l_{latt}$. Moreover, we describe the semiclassical approximate wave function by the mean quasi-momentum

$$\mathbf{q}_c(t) = \int_{IBZ} \mathbf{q} |\Phi(\mathbf{q}, t)|^2 d\mathbf{q},$$

completed with the mean position

$$\mathbf{r}_c(t) = \langle \tilde{\Psi}[\mathbf{r}_c(t), \mathbf{q}_c(t)] | \hat{r} | \tilde{\Psi}[\mathbf{r}_c(t), \mathbf{q}_c(t)] \rangle$$

$$= \int_{IBZ} |\Phi(\mathbf{q}, t)|^2 \left[ -\nabla_q \arg[\Phi(\mathbf{q}, t)] + \mathbf{Q}(\mathbf{r}_c, \mathbf{q}, t) \right] d\mathbf{q}$$

$$\approx -\nabla_{\mathbf{q}_c} \arg[\Phi(\mathbf{q}_c, t)] + \mathbf{Q}(\mathbf{r}_c, \mathbf{q}_c, t),$$

were the relation (5) has been used. In the last approximate equality only contributions of zero order in the wave-packet space and momentum dispersion lengths, $l_{wp}$ and $\Delta_q$ respectively, were retained. This is the meaning of the semiclassical approximation, which we use to evaluate the Lagrangian (1) after inserting the wave-function (10). Thus, one finds the following approximate relations:

$$\langle \tilde{\Psi} | i \frac{d}{dt} | \tilde{\Psi} \rangle \approx -\partial_t \arg[\Phi(\mathbf{q}_c, t)] + \langle u_{\mathbf{q}_c} \mathbf{u}(\mathbf{r}_c, \mathbf{q}_c, t) \rangle_{cell} + \hat{\mathbf{r}}_c \cdot \langle u_{\mathbf{q}_c} \mathbf{u}(\mathbf{r}_c, \mathbf{q}_c, t) \rangle_{cell}$$

$$= -\partial_t \arg[\Phi(\mathbf{q}_c, t)] + \mathbf{T}(\mathbf{r}_c, \mathbf{q}_c, t) + \hat{\mathbf{r}}_c \cdot \mathbf{R}(\mathbf{r}_c, \mathbf{q}_c, t),$$

(14)
where we have introduced the connection components $\mathcal{T}$ and $\vec R$ in analogy with $\bar Q$ in (11). The first term in (14) involving the partial time derivative of the phase in the quasi-momentum distribution can be rearranged in terms of the total time derivative

$$\partial_t \arg [\Phi(\vec q_c, t)] = \frac{d}{dt} \arg [\Phi(\vec q_c, t)] - \vec q_c \cdot \nabla \arg [\Phi(\vec q_c, t)]$$

$$= \frac{d}{dt} \arg [\Phi(\vec q_c, t)] + \vec q_c \cdot \left[ \vec R(\vec r_c, \vec q_c, t) \right], \quad (15)$$

where eq. (13) has been used. Thus, taking account the third term in (14), the final expression of the approximate Lagrangian will contain only linearly first derivatives of the “generalized coordinates” $(\vec r_c, \vec q_c).$ In fact, dropping total time derivatives, allows us to write down a Lagrangian for a point - like classical particle

$$L_{app} = \dot{\vec q}_c \cdot \left( \vec q_c + \vec R(\vec r_c, \vec q_c, t) \right) + \dot{\vec q}_c \cdot \bar Q(\vec r_c, \vec q_c, t) + \mathcal{T}(\vec r_c, \vec q_c, t)$$

$$- E(\vec r_c, \vec q_c, t) - \Delta E(\vec r_c, \vec q_c, t), \quad (16)$$

where

$$\mathcal{E} = \langle \tilde \Psi | \hat H_{(\vec r_c, t)} | \tilde \Psi \rangle \quad \text{and} \quad \Delta \mathcal{E} = \frac{i}{2} \langle \tilde \Psi | \left[ \partial_f \hat H \cdot \nabla_{\vec r_c} \hat f(\vec r_c, t) \cdot \left( \hat r - \vec r_c \right) \right] + h.c. | \tilde \Psi \rangle. \quad (17)$$

In general, the last expression is quite involved [2], but it is easy to check its elegant form when applying an external electromagnetic field represented by the potentials $(\vec A(\vec r, t), V_{el}(\vec r, t)).$ In fact, for slowly changing vector potentials, the solution of the approximate Bloch eigenvalue problem

$$\left[ \frac{1}{2m} \left( \vec p + e \vec A(\vec r_c, t) \right)^2 + V_{latt}(\vec r, t) - e V_{el}(\vec r_c, t) \right] \psi = E\psi \quad (18)$$

can be written in terms of the function

$$\psi^{(\vec r_c, t)}_c \approx \exp \left[ i \left( \vec q - e \vec A(\vec r_c, t) \right) \cdot \vec r_c \right] u^{(\vec r_c, t)}_c, \quad (19)$$

where $u^{(\vec r_c, t)}_c$ is the periodic part of the Bloch solution for the same crystal in the absence of a magnetic field. Because of its definition in (7), a space - time dependent change of phase does not have any influence on the Berry connection. Moreover, $\bar Q(\vec r_c, \vec q_c, t) = \bar Q(\vec k_c),$ where

$$\vec k_c = \vec q_c + e \vec A(\vec r_c, t) \quad (20)$$

is the gauge invariant quasi-momentum. On the other hand, from (14) one has $\vec R(\vec r_c, \vec k_c, t) \simeq e \nabla_{\vec r_c} \left( \vec A(\vec r_c, t) \cdot \vec r_c \right) - e \vec A(\vec r_c, t)$ and $\mathcal{T}(\vec r_c, \vec k_c, t) \simeq e \partial_t \vec A(\vec r_c, t) \cdot \vec r_c.$ Furthermore, the expressions for the semiclassical approximate energy band and its first order correction take the form

$$\mathcal{E} = \mathcal{E}_0(\vec k_c) + e V_{el}(\vec r_c, t) \quad \Delta \mathcal{E} = -\vec M(\vec r_c, \vec k_c, t) \cdot \vec B(\vec r_c, t), \quad (21)$$

where $\vec M(\vec r_c, \vec k_c, t) = \frac{e}{2m_e} \langle \tilde \Psi | \hat L | \tilde \Psi \rangle$ is the local mean magnetic moment of the wave-packet and $\vec B(\vec r_c, t) = \nabla_{\vec r_c} \times \vec A(\vec r_c, t)$ is the usual expression of the mean magnetic field acting
on the wave-packet. This is subject also the mean electric field \( \vec{E}(\vec{r}, t) = \partial_t \vec{A}(\vec{r}, t) - \nabla_{\vec{r}} V_{el}(\vec{r}, t) \).

Finally, let us observe that the discrete symmetry properties of the crystals induce restrictions in the expressions of the above Berry’s connections. In particular, the time reversal invariance implies the transformation \( \vec{k} \to -\vec{k} \) and \( \vec{\Theta}(\vec{r}, -\vec{k}) = -\vec{\Theta}(\vec{r}, \vec{k}) \). So always \( \vec{\Theta} \) vanishes at \( \vec{k} = 0 \). Moreover, the spatial inversion implies that \( \vec{\Theta}(\vec{r}, \vec{k}) = \vec{\Theta}(\vec{r}, \vec{k}) \).

The simultaneous space-time inversion symmetry implies \( \vec{\Theta}(\vec{r}, -\vec{k}) \equiv 0 \). In conclusion, crystals admitting time and space inversions cannot carry any dual magnetic structure. On the contrary, there exist concrete examples of crystals for which one, or both, inversion invariances are broken, so the geometric phase effects are significant [2, 4].

3 Hamiltonian Structure

From the semiclassical Lagrangian (16) we can derive the equations of motion of the wave-packet

\[
(1 + \Xi) \dot{\vec{r}} + \Theta \dot{\vec{q}} = \nabla_{\vec{q}} [\mathcal{E} + \Delta \mathcal{E} - \mathcal{T}] + \partial_t \vec{Q},
\]

\[
X \dot{\vec{r}} + (1 + \Xi) \dot{\vec{q}} = -\nabla_{\vec{r}} [\mathcal{E} + \Delta \mathcal{E} - \mathcal{T}] - \partial_t \vec{R},
\]

(dropping the index “c” for simplicity) where the antisymmetric matrices \( \Xi \) and \( X \) have elements

\[
\Xi_{ij}(\vec{r}, \vec{q}, t) = \partial_{r_i} Q_j - \partial_{q_j} R_i = i \left( \frac{\langle \nabla_{\vec{q}} u_{(\vec{r},t)}^{\vec{q}} \times |\nabla_{\vec{r}} u_{(\vec{r},t)}^{\vec{q}} \rangle_{cell} \rangle_{ij} }{2} \right),
\]

\[
X_{ij}(\vec{r}, \vec{q}, t) = \partial_{r_i} R_j - \partial_{r_j} R_i = i \left( \frac{\langle \nabla_{\vec{r}} u_{(\vec{r},t)}^{\vec{q}} \times |\nabla_{\vec{r}} u_{(\vec{r},t)}^{\vec{q}} \rangle_{cell} \rangle_{ij} }{2} \right). \tag{23}
\]

We also have

\[
\partial_t \vec{Q} - \nabla_{\vec{q}} \mathcal{T} = 2\text{Im}(\nabla_{\vec{q}} u_{(\vec{r},t)}^{\vec{q}} |\partial_t u_{(\vec{r},t)}^{\vec{q}} \rangle_{cell}), \quad \nabla_{\vec{r}} \mathcal{T} - \partial_t \vec{R} = -2\text{Im}(\nabla_{\vec{r}} u_{(\vec{r},t)}^{\vec{q}} |\partial_t u_{(\vec{r},t)}^{\vec{q}} \rangle_{cell}). \tag{24}
\]

This dynamical system is defined on the tangent manifold \( TM \) of the configuration space, parametrized by the generalized coordinates \( \vec{\xi} = (\vec{r}, \vec{q}) \).

The system (22) can be written (at least when \( \partial_t \vec{Q} = \partial_t \vec{R} = 0 \)) in terms of the symplectic 2-form

\[
\omega = (\delta_{i,j} + \Xi_{ij}) \, dr_i \wedge dq_j + \frac{1}{2} [X_{ij} \, dq_i \wedge dq_j - \Theta_{ij} \, dr_i \wedge dr_j] \tag{25}
\]

and the Hamiltonian function

\[
\mathcal{H} = \mathcal{E} + \Delta \mathcal{E} - \mathcal{T} \tag{26}
\]

6
in the form \( i_{\Delta} \omega = dH \) where \( \Delta = \dot{r} \frac{\partial}{\partial r} + \dot{\theta} \frac{\partial}{\partial \theta} \) [15][16]. The motions can be viewed therefore, as the integral curves of the vector field \( \Delta \).

Furthermore, we assume that the 2-form \( \omega \) closed, (i.e. \( d\omega = 0 \)). The closure condition on \( \omega \) is equivalent to the set of differential constraints

\[
\varepsilon_{i,j,k} \partial_{q_i} \Theta_{j,k} = 0, \quad \varepsilon_{i,j,k} \partial_{r_i} X_{j,k} = 0, \quad \partial_{q_j} \Xi_{i,j} = -\partial_{r_j} \Theta_{i,j}, \quad \partial_{r_j} \Xi_{i,j} = \partial_{q_j} X_{i,j}, \quad (1 - \delta_{h,k}) \varepsilon_{k,i,j} \partial_{q_k} \Xi_{i,j} = \varepsilon_{h,i,j} \partial_{r_h} \Theta_{i,j}, \quad (1 - \delta_{h,k}) \varepsilon_{k,i,j} \partial_{r_k} \Xi_{i,j} = -\varepsilon_{h,i,j} \partial_{q_h} X_{i,j}.
\]

Because of the antisymmetry and the differentiability properties of the tensors \( \Theta, \Xi \) and \( X \) as defined in (9) and (24), the equations above are automatically satisfied for a variational system. In particular, let us observe that the first pair of equations in (28) are the divergenceless conditions for the two vector-fields \( \varepsilon_{i,j,k} \Theta_{j,k} \) and \( \varepsilon_{i,j,k} \partial_{r_i} X_{j,k} \) in the \( \vec{q} \)- and \( \vec{r} \)-space, respectively. This will take a precise physical meaning in the case of Bloch electrons interacting with external electromagnetic fields.

If \( \omega \) is non degenerate, it can be inverted and the system takes a Hamiltonian form [15][16]. A non-degenerate and closed 2-form \( \omega = \omega_{\alpha,\beta} \, d\xi_\alpha \wedge d\xi_\beta \) defines indeed a Poisson bracket. For any pair of functions \( f(\vec{r}, \vec{q}) \) and \( g(\vec{r}, \vec{q}) \) is associated \( \{ f, g \} = \omega^\alpha_\gamma \partial_\alpha f \partial_\beta g \), where \( \omega^\alpha_\gamma \omega_\gamma^\beta = \delta^\alpha_\beta \) is the inverse of the symplectic matrix. Then Hamilton’s equations read

\[
\dot{\xi}_\alpha = \{ \xi_\alpha, \mathcal{H} \}.
\]

In the degenerate case one has to resort to symplectic reduction [15][17].

In the present case here one has a \( 6 \times 6 \) block matrix

\[
(\omega_{\alpha,\beta}) = \frac{1}{2} \begin{pmatrix} X & 1 + \Xi \\ -1 + \Xi & -\Theta \end{pmatrix}
\]

which is non degenerate when \( 1 - \frac{1}{2} \text{Tr} (\Xi^2 + X (1 + 2 \Xi) \Theta) \neq 0 \). Then the inverse of the symplectic matrix is

\[
(\omega^\alpha_\beta) = -2 \left( 1 - \frac{1}{2} \text{Tr} (\Xi^2 + X (1 + 2 \Xi) \Theta) \right)^{-1}
\]

\[
\begin{pmatrix} \Theta + [\Theta, \Xi] & [1 - \frac{1}{2} \text{Tr} (\Xi^2 + X \Theta) ] 1 + (\Xi^2 + X \Theta)^T \\ -[1 - \frac{1}{2} \text{Tr} (\Xi^2 + X \Theta) ] 1 - (\Xi^2 + X \Theta) - X + [\Xi, X] \end{pmatrix}
\]

Consistently with the Darboux’s theorem on non degenerate symplectic forms, canonical coordinates i.e. such that \( \omega_{\alpha,\beta} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \) can be found. Then the equation (28) takes the usual canonical form; the disadvantage is that the Hamiltonian may become rather complicated.
It should be noticed that our description is formulated on the tangent space $T\mathcal{M}$, instead of the cotangent bundle $T^*\mathcal{M}$, usually used in the theory a Hamiltonian system.

A general consequence of the geometrical formulation is that the Liouville theorem remains true for the Bloch electron wave-packets and the invariant volume is modified with respect to standard semiclassical approximation form \[1\] as follows

\[
\sqrt{\det (\omega_{\alpha\beta})} \prod dr_i \wedge dq_i = \frac{1}{8} \left( 1 - \frac{1}{2} \Tr (\Xi^2 + X (1 + 2 \Xi) \Theta) \right) \prod_i dr_i \wedge dq_i. \tag{31}
\]

Before proceeding, let us notice that, in presence of an external electromagnetic field, eq.s (22) take the form

\[
\dot{\vec{r}} = \nabla \vec{q} \left[ \mathcal{E}_0 (\vec{k}) - \vec{M} (\vec{r}, \vec{k}, t) \cdot \vec{B} (\vec{r}, t) \right] - \vec{k} \times \Theta (\vec{k}), \\
\dot{\vec{k}} = -e (\vec{k} \times \vec{B} (\vec{r}, t) + \vec{E} (\vec{r}, t)) + \nabla \vec{r} \left[ \vec{M} (\vec{r}, \vec{k}, t) \cdot \vec{B} (\vec{r}, t) \right], \tag{32}
\]

where the so-called “dual”, or “reciprocal magnetic field” $\Theta_i (\vec{k}) = \frac{1}{2} \epsilon_{ijk} \Theta_{j,k} (\vec{k})$ has been introduced.

The electron mean velocity $\vec{v} = \langle \Psi | \nabla_{\vec{k}} \hat{H} | \Psi \rangle \approx \langle \tilde{\Psi} | \nabla_{\vec{k}} \hat{H} | \tilde{\Psi} \rangle$ can be estimated from the eq.s (32). In particular, this can explain the Anomalous Hall Effect predicted by Karplus and Luttinger half a century ago \[3\]. In fact, for vanishing external magnetic field and choosing the electric field $\vec{E} = E \hat{x}$, one obtains the

\[
\begin{align*}
\dot{\vec{r}} &= \vec{v} (\vec{k}) = \nabla_{\vec{k}} \mathcal{E}_0 (\vec{k}) + e E \Theta_z (\vec{k}) \vec{y}, \\
\dot{\vec{k}} &= \vec{k}_0 - e E t \vec{x}.
\end{align*} \tag{33}
\]

At the macroscopic level, for static uniform electric and temperature fields, the electric current will be given by the mean value

\[
\vec{j} = -e \int_{IBZ} \frac{d^3\vec{k}}{4\pi^3} \vec{v} (\vec{k}) g (\vec{r}, \vec{k}) \
\]

with respect to the appropriate non equilibrium distribution function $g (\vec{r}, \vec{k})$. A good approximation \[1\] of such a distribution is $g (\vec{r}, \vec{k}) = f_{FD} (\mathcal{E}) + e \tau (\mathcal{E}) \frac{\partial f_{FD}}{\partial \mathcal{E}} \vec{E} \cdot \vec{v}$, where $f_{FD} (\mathcal{E} (\vec{k}))$ denotes the Fermi - Dirac distribution and $\tau$ is the relaxation time, that is the inverse of the probability for unit time that an electron of momentum $\vec{k}$ be scattered. In the simplest situation of a filled band, i.e. for $f_{FD} \equiv 1$, the current expression (34) will contain only the Hall contribution, which takes the form

\[
\begin{align*}
j_y &= -e^2 E \int_{IBZ} \frac{d^3\vec{k}}{(2\pi)^3} \Theta_z (\vec{k}) \
j_y &= -e^2 E \int_{IBZ} \frac{d^3\vec{k}}{(2\pi)^3} \Theta_z (\vec{k}). \tag{35}
\end{align*}
\]
Thus, this “anomalous” Hall effect is entirely due to the existence of the reciprocal magnetic field $\hat{\Theta}$. Moreover, for a prismatic fundamental cell in the reciprocal lattice, the expression (35) is proportional to the $k_z$-integrated flux of $\Theta_z$ through the surface, obtained by the intersection of the IBZ with the $(k_x, k_y)$ plane. In fact, from the curvature nature of the integrand (see eq. (9)), such a flux is interpreted as the first Chern number (that is a topological invariant taking integer values) of the principal bundle generated by attaching to each point of the IBZ an $U(1)$-fiber, to which the Berry connection belongs [18, 19].

4 Symmetry Group and Symplectic Structure

Now, equations of motion of the type (32) in (2+1)-dimensions were studied by several authors from the point of view of symmetries, in particular, starting from the planar Galilei group [6]. This admits a two-fold central extension, labeled by the mass $m$ and the “exotic” parameter $\kappa$. The latter can be viewed as a particular case of Berry’s phase, as it is involved in the model considered in [10] and [8], where the coupling to an external electromagnetic field was also considered.

In the 2-dim gauge-invariant momentum space we consider the linear Berry’s connection $\mathbf{Q}_i (\mathbf{k}) = -\frac{\theta}{2} \varepsilon_{i,j} k_j$, modulo further gauge transformations in $\mathbf{k}$. This leads to the constant Berry’s curvature $\Theta_3 = -\theta$, which will be related to the “exotic” charge $\kappa$ of the symmetry Galilei group. Then, the first-order Lagrangian (16) is simplified to

$$L = \mathbf{k} \cdot \dot{\mathbf{r}} - \frac{\mathbf{k}^2}{2m} + e(\mathbf{A} \cdot \dot{\mathbf{r}} + V_{el}) + \frac{\theta}{2} \mathbf{k} \times \dot{\mathbf{k}},$$

where the electromagnetic field depends only on $(r_1, r_2, t)$. The corresponding Euler-Lagrange equations, specializing (32), are

$$m^* \dot{\mathbf{r}} = \mathbf{k} - e m \theta \dot{\mathbf{E}}, \quad \dot{\mathbf{k}} = eB \dot{\mathbf{r}} + e \mathbf{E},$$

where the effective mass $m^* = m(1 - e\theta B)$ appears and $\dot{\mathbf{E}}$ denotes the operator which rotates vectors of the plane counterclockwise by $\pi/2$. In the Hamiltonian framework the modified Poisson-brackets (29) and (32) become

$$\{r_i, r_j\} = \frac{m}{m^*} \theta \delta_{ij}, \quad \{r_i, k_j\} = \frac{m}{m^*} \delta_{ij}, \quad \{k_i, k_j\} = \frac{m}{m^*} e B \delta_{ij}. \quad (38)$$

The first important remark is that the Jacobi identity for (38) is identically satisfied for arbitrary space-time dependent magnetic fields. This can be directly checked restricting the equations (28) in 2 dimensions.

The second feature of the model is that when $m^* = 0$, i.e. when the magnetic field takes the critical value

$$B = B'_{crit} = \frac{1}{e\theta},$$

(39)
the system becomes singular, and the only allowed motions follow the Hall law \[10\]. This is an example of degeneracy of the symplectic 2-form \(\omega\) in \[31\]. Application of a uniform and constant magnetic field \(B = B'_{\text{crit}}\) amounts to restrict the motion to the lowest Landau level, and quantization allows to recover the “Laughlin” wave functions \[10\]. Furthermore, the vanishing of \(m^*\) signals a sort of “phase transition”, in the sense that the spectrum of the angular momentum can take only strictly positive integer values for \(m^* \leq 0\) \[20\].

Now, aiming to describe the system by a larger symmetry group, following \[7\] and \[8\], let us consider a homogeneous time dependent electric field \(\vec{E}(t)\) and its canonical conjugate momentum \(\vec{\pi}\) as further dynamical variables. Thinking to the components \(\pi_i\) as Lagrange multipliers, we define the new Lagrangian

\[
L^{\text{enl}} = L + \vec{\pi} \cdot \dot{\vec{E}},
\]

providing the supplementary equations of motion

\[
\dot{\vec{E}} = 0, \quad \dot{\vec{\pi}} = e\vec{r},
\]

i.e. the electric field is actually a constant. The Hamiltonian structure is “enlarged” appending \(\{E_i, \pi_j\} = \delta_{ij}\) to the fundamental Poisson brackets \(\{38\}\). The Hamiltonian is \(H_0 = \vec{k}^2/2m - e\vec{E} \cdot \vec{r}\), for a suitable choice of gauge for \(V_{el}\), and provides the equations of motion \(37\) and \(41\).

The enlarged Lagrangian \(10\) is (quasi-)invariant w. r. t. the infinitesimal variations

\[
\begin{aligned}
\text{translations} & \quad \delta\vec{r} = \vec{a}, \quad \delta\vec{k} = 0, \quad \delta\vec{E} = 0, \quad \delta\vec{\pi} = e\vec{a}t, \\
\text{rotations} & \quad \delta\vec{r} = -\phi \dot{\vec{r}}, \quad \delta\vec{k} = -\phi \dot{\vec{k}}, \quad \delta\vec{E} = -\phi \dot{\vec{E}}, \quad \delta\vec{\pi} = -\phi \dot{\vec{\pi}}, \\
\text{boosts} & \quad \delta\vec{r} = \vec{b}t, \quad \delta\vec{k} = m\vec{b}, \quad \delta\vec{E} = -B\dot{\vec{b}}, \quad \delta\vec{\pi} = \frac{e}{2} \dot{\vec{b}} t^2, \\
\text{electric} & \quad \delta\vec{r} = 0, \quad \delta\vec{k} = 0, \quad \delta\vec{E} = \vec{d}, \quad \delta\vec{\pi} = 0, \\
\text{superposition} &
\end{aligned}
\]

where the 2-components vectors \(\vec{a}, \vec{b}, \vec{d}\) are parameters related to the space translations, boosts and linear changes of the electric field, respectively. The scalar \(\phi\) is the rotational parameter.

Conserved quantities are readily constructed by Noether theorem. Actually, direct integration of the second equation in \(37\) yields the constant of the motion

\[
\vec{P} = \vec{k} - eB\dot{\vec{r}} - e\vec{E} t,
\]

describing uniform motions of the guiding center of the charged particle. Using the commutation relations

\[
\{r_i, P_j\} = \delta_{ij}, \quad \{k_i, P_j\} = 0, \quad \{E_i, P_j\} = 0 \quad \{\pi_i, P_j\} = et \delta_{ij},
\]

10
one recognizes that (43) generates the enlarged translations in (42). Similarly,

$$\mathcal{J} = r \times k + \frac{eB}{2} r^2 + \frac{\theta}{2} k^2 + \vec{E} \times \vec{\pi} + s_0, \quad \vec{K} = m \vec{r} - \left( \vec{P} + \frac{e \vec{E} t}{2} \right) t + m \theta \vec{k} - B \vec{\pi}. \quad (45)$$

are conserved quantities and generate rotations and boosts, respectively, accordingly with (42). In (43) the “anyonic” spin $s_0$ has been added by hand to the angular momentum $\mathcal{J}$, which contains also the magnetic flux and new “exotic” (or “dual”) flux, proportional to the “area” swept in momentum space. Of course also the electric field $\vec{E}$ is considered as a further conserved quantity. Together with the Hamiltonian $H_0$, they span a 11-dimensional symmetry Lie algebra, whose non vanishing Lie-Poisson commutation relations are

$$\{P_i, H_0\} = eE_i, \quad \{K_i, H_0\} = P_i, \quad \{P_i, J\} = -\epsilon_{ij} P_j,$$

$$\{P_i, P_j\} = -eB \epsilon_{ij}, \quad \{K_i, J\} = -\epsilon_{ij} K_j, \quad \{P_i, K_j\} = -m \delta_{ij}, \quad (46)$$

$$\{K_i, K_j\} = -\theta m^2 \epsilon_{ij}, \quad \{E_i, J\} = -\epsilon_{ij} E_j, \quad \{E_i, K_j\} = B \epsilon_{ij},$$

with $m$ and $B$ as central charges. But the key observation is that the boosts generators $K_i$ do not commute among them-selves as usual. In fact, their commutator yields the “exotic” central charge $\kappa = -\theta m^2$ and, then, providing us with an explicit realization of the second central extension of the Galilei group.

The action of the symmetry group on these functions, formally belonging to the dual space of the symmetry algebra, is given by

$$H'_0 = H_0 - \vec{b} \cdot R_{\phi} \vec{P} + \frac{1}{2} m \vec{b}^2 - e \vec{a} \cdot \vec{E}', \quad \vec{P}' = R_{\phi} \vec{P} + e \tau \vec{E}' - eB \vec{a} - m \vec{b},$$

$$\mathcal{J}' = \mathcal{J} + \frac{1}{2} eB \vec{a}^2 - m \vec{a} \times \vec{b} + \frac{1}{2} m^2 \theta \vec{b}^2 + \vec{a} \times R_{\phi} \vec{P} + \vec{b} \times R_{\phi} \vec{K} + \left( R_{\phi} \vec{d} + e \tau \vec{a} \right) \times \vec{E}',$$

$$\vec{K}' = R_{\phi} \vec{K} + m \vec{a} + \tau m \vec{b} - m^2 \theta \vec{e} \vec{b} + \frac{1}{2} e \tau^2 \vec{E}' - \tau R_{\phi} \vec{P}, \quad \vec{E}' = R_{\phi} \vec{E} + B \vec{e} \vec{b}, \quad (47)$$

where $R_{\phi}$ represents the plane rotation by an angle $\phi$ and the parameter $\tau$ is the time translation. Besides $m, \kappa = -m^2 \theta$ and $B$, the enlarged Galilei group has the independent Casimir functions

$$C = e\theta \left( BH_0 - \vec{P} \times \vec{E} + \frac{m}{2B} \vec{E}' \right) = \frac{e\theta B}{2m} \left( k_i - \frac{m}{B} \epsilon_{ij} E_j \right)^2, \quad \quad (48)$$

$$C' = \frac{\vec{P}^2}{2m} - H_0 - \frac{e}{m} \left( \vec{K} \cdot \vec{E} + \mathcal{J} B \right) - \frac{me\theta}{2B} \vec{E}'^2 = -C - \frac{es_0 B}{m}, \quad (49)$$

where $C'$ is interpreted as the internal energy of the system and $C + C'$ is the spin, expressed in an energy scale. These are non trivial convex Casimir functions, so they restrict the group orbits in the dual of the symmetry algebra to 6-dimensional manifolds, except at the critical point defined by $C = 0$, where they define a 4-dimensional manifold. All these submanifolds can be endowed with suitable Poisson structures. The 6-dim orbits labeled by the $(m, \kappa, B, C (\neq 0), s_0)$ are endowed by local coordinates $(\vec{P}, \vec{K}, \vec{E})$. The restricted
Hamiltonian $H_0$ to such an orbit becomes linear in the momenta $P_i$, i.e.

$$H_1 = \frac{\vec{P} \times \vec{E}}{B} - \frac{m}{2B^2} \vec{E}^2 + \frac{C}{e \theta B}. \quad (50)$$

The relevant Poisson brackets are extracted from (46), yielding the non singular symplectic form on the orbit

$$\omega_1 = \frac{1}{B} dP_1 \wedge dP_2 + \frac{m}{B^2 e} dP_i \wedge dE_i - \frac{\epsilon_{ij}}{B} dK_i \wedge dE_j + \frac{mm^*}{B^3 e} dE_1 \wedge dE_2. \quad (51)$$

On such an orbit, the equations of motion can be read off directly from the first to relation in (46). Their immediate solution

$$\vec{P} = e\vec{E}_0 t + \vec{P}_0, \quad \vec{K} = \frac{1}{2} \vec{E}_0 t^2 + \vec{P}_0 t + \vec{K}_0, \quad \vec{E} = \vec{E}_0, \quad (52)$$

describes the solutions of the original equations of motion (37) in terms of the new variables. Thus one obtains the usual cycloidal motions, with guiding center, radius and frequency, given in terms of integrals of motion by

$$\vec{r}_0 = \frac{1}{B^2 e} \left( m \vec{E}_0 + B \vec{P}_0 \right) + \vec{E}_0 t, \quad \rho = \frac{m}{e B} \sqrt{\frac{C}{e m \theta B}}, \quad \Omega = \frac{e B}{m^*}. \quad (53)$$

The singular 4 dimensional orbits can be expressed equivalently by

$$\vec{P} = \frac{m}{B} \hat{\epsilon} \vec{E} + \alpha \vec{E}, \quad (\alpha \in \mathbb{R}). \quad (54)$$

In terms of the original variables, from the second equality in (50) one has constrained both components of the momentum $\vec{k}$. Consequently, the equations of motion (37) become

$$\dot{\vec{r}} = \hat{\epsilon} \frac{\vec{E}}{B}, \quad \vec{k} = \frac{m}{B} \hat{\epsilon} \vec{E}, \quad (55)$$

as predicted by (39) at $m^* = 0 \iff B = B_{\text{crit}}$. Notice also that the above formulae give vanishing cycloid radius and diverging frequency $\Omega$. In other words, all motions reduce to uniform translations, driven at the Hall velocity. On the orbits $(m, \kappa, B, C = 0, s_0)$ naturally the set of coordinates $(\vec{K}, \vec{E})$ is introduced, and defined the non degenerate symplectic 2-form

$$\omega_2 = \epsilon_{ij} dK_i \wedge dE_j + em^2 \theta^2 dE_1 \wedge dE_2. \quad (56)$$

The Hamiltonian becomes $H_2 = \frac{m}{2B_{\text{crit}}^2} \vec{E}^2$ and yields the equations $\dot{\vec{E}} = 0, \quad \dot{\vec{K}} = \frac{m}{B} \hat{\epsilon} \vec{E}$, showing again that the particle motion is reduced to the uniform translations of the guiding center.

Following a procedure introduced by Bacry [21], a direct generalization of the system (37)-(41), endowed with the enlarged Galilei symmetry, can be derived from the unique polynomial Hamiltonian

$$H_{\text{anom}} = H_0 + \frac{g}{2} C' = -\frac{\vec{k}^2}{2m} \left( 1 - \frac{g}{2} e\theta B \right) - e\vec{E} \cdot \vec{r} - \mu B + \frac{g e \theta}{2} \vec{k} \times \vec{E} - \frac{m g e \theta}{4B} \vec{E}^2. \quad (57)$$
Here $\mu = g e s_0/2m$ with $g$ a real parameter, interpreted as the anomalous gyromagnetic factor. The kinetic energy term gets a field-dependent factor, which can be seen also as wave-packet magnetic dipole interaction, with $M = \frac{g e B}{4 m} \vec{k}^2$, accordingly to (21) and (32). The Hamiltonian (57) contains, together with the standard magnetic moment term $\mu B$, also contributions similar to the Hamiltonian (50), proportional to $g$. However, we have to consider that we are using now “natural” coordinates. The corresponding equations of motion are

$$m^* \ddot{\vec{r}} = (1 - \frac{g}{2} e \theta B) \vec{k} - \left(1 - \frac{g}{2}\right) e m \theta \vec{E}, \quad \ddot{\vec{k}} = e B \dot{\vec{r}} + e \vec{E}. \quad (58)$$

This is a special case of (32) and reminiscent of Eq. (5.3) in [22]. In particular, for $g = 2$ and $e \theta B \neq 1$ one obtains $m \vec{r} = \vec{k}$, so that our equations describe an ordinary charged particle in an electromagnetic field. For $g = 2$ and $e \theta B = 1$, Eq. (58) is identically satisfied. Of course, since the symmetry structure of this new anomalous system is the same as for the standard case $g = 0$, the analysis of the motions follows essentially the same considerations as above. The only change is that the frequency of the rotational motion is $\Omega = \frac{e B}{2m^*}(1 - \frac{g}{2} e \theta B)$, which for $g = 2$ reduces to the usual Larmor frequency $e B/m$. But, now $\Omega$ vanishes at the new critical point $B = B_{crit}^{''} = \frac{2}{egg}$. At this value $m^* = m(1 - 2/g)$ and the equation (58) becomes an identity at $g = 2$. On the other hand, for $g \neq 2$ it reduces to $\vec{r} = \frac{g}{2} e \theta \vec{E}$, which again defines motions following the Hall law (55), except that now $\vec{k} = 0$, that is the momentum is an arbitrary constant.

A different kind of generalization can be obtained by a deformation of the symmetry algebra, although the symmetry generators remain essentially the same. In particular, we would change only the Hamiltonian, combining $H_0$ with the other generators. Although a systematic study lies beyond the scope of the present work, let us consider the Hamiltonian with the magnetic interaction

$$H_{mag} = H_0 + \mu B \mathcal{J}. \quad (59)$$

This model has not to be confused with that introduced at the beginning in the context of the solid state physics, since $\mathcal{J}$ has a physical different meaning with respect to $\vec{M}$. However, it could be useful in some limit. The Poisson brackets in (46) are modified only when commuting with $H_{mag}$. Specifically,

$$\{H_{mag}, \vec{P}\} = -e \vec{E} + \mu B \vec{e}, \quad \{H_{mag}, \vec{K}\} = -\vec{P} + \mu B \vec{e}, \quad \{H_{mag}, \vec{E}\} = \mu B \vec{e}. \quad (60)$$

Notice that the presence of the $\vec{P}$ in $\mathcal{J}$ induces the non constancy of the electric field. Moreover, one can find only one Casimir operator, namely

$$C_{mag} = \frac{1}{2} \vec{\mathcal{P}}^2 - e B \mathcal{J} + \frac{mm^*}{B^2} \vec{E}^2 - e \vec{K} \cdot \vec{E}^2 - \frac{m}{B} \vec{P} \times \vec{E} = \frac{m^*}{m} B^2 \left(\vec{k} - \frac{m}{B} e \vec{E}\right)^2 - 2 e B^2 s_0. \quad (61)$$

This invariant is a convex function, and therefore we expect dimensional reduction of the group orbit as in (54). The equations of motion, in term of the natural coordinates $\vec{r}$ and
$\vec{k}$, take the form

$$m^* \vec{r} = \vec{k} - e m \theta \vec{E}, \quad \dot{\vec{k}} = e (1 + B m \theta \mu) \vec{E} + B (e + m^* \mu) \left( \dot{\vec{r}} - B \mu \vec{r} \right),$$

$$\dot{\vec{E}} = -B \mu \dot{\vec{E}}, \quad \dot{\vec{\pi}} = B \mu \vec{\pi} + e \vec{r}. \quad (62)$$

5 Discussion

In conclusion, the semiclassical Bloch electron provides a physical motivation for the “exotic” particle models in the plane, and the “enlarged Galilean symmetry” provides us with further hints. Generalizations of the “exotic” models are built by adding a Casimir to the Hamiltonian, accommodating in certain limits anomalous moment coupling and orbital magnetic dipole interactions. An algebraic characterization of the Hall motions in terms of criticality conditions for the symmetry Casimir operators was shown.

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