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Wave-packet dynamics of Bloch electrons—Role of Berry phase

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Abstract

Motivated by a recent proposal on the possibility of observing a monopole in the band structure, and by an increasing interest in the role of Berry phase in spintronics, we reconsidered the problem of adiabatic motion of a wave packet of Bloch functions, under a perturbation varying slowly and incommensurately to the lattice structure. We showed, using only the fundamental principles of quantum mechanics, that the effective wave-packet dynamics of Bloch electrons is conveniently described by a set of equations of motion (EOM) in which a *non-Abelian* Berry phase associated with the internal degree of freedom appears.

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1. Introduction

A quantized magnetic monopole was found recently [1] in the band structure. In crystal momentum space, monopoles of the reciprocal magnetic field do appear, in the study of geometric Berry phase of Bloch electrons [2,3]. The Berry phase has also attracted much attention on the technological side, in particular, in the context of *spintronics* [4].

In the following, we sketch our recent study [5] on the Berry phase in the wave-packet dynamics of a Bloch electron under perturbations $\beta(\mathbf{x}, t)$ slowly varying in space and in time. We derived and analyzed a set of equations of motion (EOM) which describes the center-of-mass motion of such a wave packet together with its internal motion associated with its (pseudo) spin. A reciprocal gauge field of geometric origin (Berry connection) appears naturally in such EOM. Combining our formalism with the Boltzmann transport theory, we addressed such phenomena as spin and orbital transport.

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Our EOM can be viewed as a generalization of the standard Ehrenfest's theorem, in the sense that we derived them, based only on the fundamental principles of quantum mechanics. We developed the concept of *local* Bloch bands for describing the adiabatic motion of a wave packet. One of the advantages of our approach is that the various types of gauge fields were classified into two categories by their different physical origin. Using those gauge fields, we wrote our EOM in a covariant form, whereas the gauge-invariant field strength stemmed from the *noncommutativity* of covariant derivatives along different axes of the reciprocal parameter space. On the other hand, the degeneracy of Bloch bands made the gauge field *non-Abelian*.

2. Non-Abelian gauge field, encoding information on the band structure

Let us focus on the adiabatic motion of a wave packet localized in the phase space in the vicinity of $(\bar{\mathbf{k}}, \bar{\mathbf{x}})$. $\bar{\mathbf{k}}$ is a crystal momentum characterizing the Bloch function. In the case of nondegenerate band, the reciprocal magnetic field $\tilde{B}(\bar{\mathbf{k}})$ appears in our EOM for $\bar{\mathbf{x}}$ as $\mathrm{d}\bar{\mathbf{k}}/\mathrm{d}t \times \tilde{B}(\bar{\mathbf{k}})$ exactly in parallel with the Lorentz force in the EOM for $\bar{\mathbf{k}}$ [3]. $\tilde{B}(\bar{\mathbf{k}})$ encodes information on the topological nature of band structure, in particular, that of band crossings. The Berry curvature $\tilde{B}(\bar{\mathbf{k}})$ associated with such a crossing of two levels takes the form of a *magnetic monopole* in the space spanned by an appropriate set of adiabatic parameters, [6] which are basically $\bar{\mathbf{k}}$ for Bloch electrons.

Let us now consider a more general case of N-fold degenerate bands. In this case, we may introduce a reciprocal vector potential (Berry connection) in the form of a $N \times N$ matrix, whose (m, n)-component is given by

$$(\tilde{A}_q)_{mn} = \mathrm{i}\left\langle u_m(\bar{\mathbf{k}}, \bar{\mathbf{x}}, t) \middle| \frac{\partial u_n(\bar{\mathbf{k}}, \bar{\mathbf{x}}, t)}{\partial q} \right\rangle, \tag{1}$$

where q should be understood as a general coordinate $q = \bar{k}_\mu, \bar{x}_\nu, t$ and $\mu, \nu = 1, \ldots, D$. $|u_n(\bar{\mathbf{k}}, \bar{\mathbf{x}}, t)\rangle = \exp(-\mathrm{i}\bar{\mathbf{k}} \cdot \mathbf{x})|\phi_n(\bar{\mathbf{k}}, \bar{\mathbf{x}}, t)\rangle$ is the periodic part of a *local* Bloch state, i.e., $\langle \mathbf{x} + \mathbf{a}|u_n(\bar{\mathbf{k}}, \bar{\mathbf{x}})\rangle = \langle \mathbf{x}|u_n(\bar{\mathbf{k}}, \bar{\mathbf{x}})\rangle$ with $\mathbf{a}$ being a primitive vector of the Bravais lattice. Inner products involving the periodic part $|u_n(\bar{\mathbf{k}}, \bar{\mathbf{x}}, t)\rangle$, mean an integration over the unit-cell, with a normalization $\langle u_n(\bar{\mathbf{k}}, \bar{\mathbf{x}}, t)|u_n(\bar{\mathbf{k}}, \bar{\mathbf{x}}, t)\rangle = 1$. In the Abelian case $N = 1$, this vector potential is related simply to the reciprocal magnetic field $\tilde{B}(\bar{\mathbf{k}})$ as $\tilde{B}(\bar{\mathbf{k}}) = \partial/\partial\bar{\mathbf{k}} \times \tilde{A}_{\bar{\mathbf{k}}}$. In the non-Abelian case, the gauge-invariant reciprocal field strength is defined as

$$\tilde{F}_{q_1 q_2} = \partial_{q_1}\tilde{A}_{q_2} - \partial_{q_2}\tilde{A}_{q_1} + \mathrm{i}[\tilde{A}_{q_1}, \tilde{A}_{q_2}], \tag{2}$$

where $q_1, q_2 = \bar{k}_\mu, \bar{x}_\mu, t$. The matrix elements of Eq. (2) contain Berry curvatures of two different physical origins:

(i) Projection onto a subspace spanned by N Bloch bands,
(ii) *local* Bloch basis which evolves in time.

In order to clarify the above points, let us now formulate our problem together with the assumptions which we will make later.

3. Local Hamiltonian and its local Bloch eigenstates

We considered the wave-packet dynamics in the phase space in the presence of space and time-dependent external perturbation $\beta(\mathbf{x}, t)$, which varies *adiabatically* but *incommensurately* to the lattice structure. In order to define a crystal momentum under such circumstances, we replace the spatial coordinate $\mathbf{x}$ in $\beta(\mathbf{x}, t)$ by the center-of-mass coordinate $\bar{\mathbf{x}}$ of a wave packet under consideration. This recovers the lattice periodicity $\mathbf{a}$ of the Hamiltonian, leading us to the concept of *local* Hamiltonian,

$$H_{\mathrm{loc}} = H(\mathbf{p}, \mathbf{x}; \beta(\bar{\mathbf{x}}, t)),$$

and its *local* Bloch eigenstates,

$$H_{\mathrm{loc}}|\phi_n(\mathbf{k}, \bar{\mathbf{x}}, t)\rangle = \varepsilon_n(\mathbf{k}, \bar{\mathbf{x}}, t)|\phi_n(\mathbf{k}, \bar{\mathbf{x}}, t)\rangle.$$

A *local* Bloch eigenstate, $|\phi_n(\mathbf{k}, \bar{\mathbf{x}}(t), t)\rangle$, evolves as a function of time (cf. (ii) above and below), both explicitly (through t) and implicitly (through $\bar{\mathbf{x}}(t)$). Thus $\bar{\mathbf{x}}(t)$ plays, together with $\bar{\mathbf{k}}(t)$, the role of adiabatic parameters in the standard