

# Coherent wave-packet evolution in coupled bands

Dimitrie Culcer, Yugui Yao, and Qian Niu

*Department of Physics, The University of Texas at Austin, Austin TX 78712-1081 and  
International Center for Quantum Structures, Chinese Academy of Sciences, Beijing 100080, China*

(Dated: November 12, 2004)

We develop a formalism for treating *coherent* wave-packet dynamics of charge and spin carriers in degenerate and nearly degenerate bands. We consider the two-band case carefully in view of spintronics applications, where transitions between spin-split bands often occur even for relatively weak electromagnetic fields. We demonstrate that much of the semiclassical formalism developed for the single-band case can be generalized to multiple bands, and examine the nontrivial non-Abelian corrections arising from the additional degree of freedom. Along with the center of mass motion in crystal momentum and real space, one must also include a pseudo-spin to characterize the dynamics between the bands. We derive the wave packet energy up to the first order gradient correction and obtain the equations of motion for the real- and  $k$ -space center of the wave-packet, as well as for the pseudo-spin. These equations include the non-Abelian Berry curvature terms and a non-Abelian correction to the group velocity. As an example, we apply our formalism to describe coherent wave-packet evolution under the action of an electric field, demonstrating that it leads to electrical separation of up and down spins. A sizable separation will be observed, with a large degree of tunability, making this mechanism a practical method of generating a spin polarization. We then turn our attention to a magnetic field, where we recover Larmor precession, which cannot be obtained from a single-band point of view. In this case, the gradient energy correction can be regarded as due to a magnetic moment from the self-rotation of the wave-packet, and we calculate its value for the light holes in the spherical four-band Luttinger model.

PACS numbers: 72.10.Bg, 72.20.My, 72.25.Dc, 73.23.-b

## I. INTRODUCTION

It often happens, in transport phenomena, that one has to consider carrier dynamics in bands which are coupled together. This coupling arises either through strong interband scattering or as a result of the bands being degenerate, or both. The nearly degenerate case is particularly relevant in transport theory as transitions often occur between bands even at relatively weak electromagnetic fields. Such situations include two-dimensional systems described by the Rashba Hamiltonian<sup>1</sup> with strong scattering, the doubly degenerate heavy and light hole bands in the Luttinger model<sup>2</sup>, which is frequently used to model the valence bands of bulk zincblende semiconductors, and the conduction bands of wurtzite structures<sup>3</sup>. The case of nearly degenerate bands has not, to date, received the attention it deserves<sup>4</sup>, despite the important role played by such bands in semiconductor spintronics systems<sup>5,6</sup>, whether in dealing with spin currents<sup>7</sup>, spin generation<sup>8</sup> and relaxation<sup>9</sup>, or spin injection across a semiconductor interface<sup>10</sup>.

Spintronics systems lend themselves to a semiclassical treatment, as the external electromagnetic fields vary on scales that are considerably larger than atomic size. The semiclassical formalism has had much success in describing carrier dynamics and transport phenomena in condensed matter physics. In the non-degenerate case, the carrier dynamics can be obtained semiclassically then combined with the Boltzmann equation to produce accurate descriptions of the transport properties of many materials. This approximation is used in the descriptions of cyclotron orbits, conduction in solids, the Hall effect

and magnetoresistance<sup>11</sup>. An essential application of the semiclassical model, which is specifically relevant to our discussion, is in treating external fields that are not represented by bounded operators, so that a perturbative expansion will not converge<sup>12</sup>. The most common example is provided by uniform electric and magnetic fields, where the potential is linear in position.

We therefore develop, in this paper, a semiclassical description of transport in degenerate and nearly degenerate bands. One of our main purposes is to extend the semiclassical approach, as developed by Sundaram and Niu<sup>13</sup>, to the case of coupled Bloch bands, in order to take into account the spin degree of freedom. We illustrate the underlying physics by treating two bands, without loss of generality. Two-band models are frequently an adequate description of the conduction bands of many semiconductors<sup>14</sup>. In experiments on spin transport in semiconductors the carriers have traditionally been electrons<sup>15</sup>, as the strong spin-orbit coupling in the valence band causes holes to lose spin information much faster<sup>6</sup>. However, in recent years research has also focused on spin currents in the valence bands of semiconductors<sup>7</sup>, with a degeneracy which is usually greater than two, and the formalism we outline is straightforwardly extended to multiple bands.

To formulate a description of coherent transport in coupled bands we may no longer work with each band individually but must instead treat the coupled-band manifold as a whole. The condition for our theory to be valid, which in the one-band case states that there must be no transitions out of that band<sup>11</sup>, translates into the requirement that there be no transitions out of the manifold un-

der consideration. We will consider a wave packet made up of two bands, which is a suitable description of *coherent* transport, when the density matrix has off-diagonal terms and the relative phase of the two wave functions plays a crucial role. This approach allows us to retain the notion of the real-space center of the wave-packet,  $\mathbf{r}_c$ , which remains well defined. Moreover, in extending the formalism to two bands we are able, in the presence of a magnetic field, to recover Larmor precession, which is not possible from a one band picture. The additional degree of freedom of the two-band system can be taken into account by defining a wave function with the Bloch periodicity in such a way as to incorporate both bands, which allows us to derive the dynamics from a single-band point of view. The coefficients of the bands can then be grouped into a vector which we shall call the pseudo-spin, the structure and dynamics of which makes clear the gauge structure of the problem. An interesting fact which will emerge from our analysis is that the effect of the external perturbations can be incorporated entirely into the Berry curvatures<sup>13</sup>, which in turn are generated by a set of connections in real and reciprocal space as well as in time. The Berry curvatures acquire additional terms needed to ensure gauge covariance, and in the framework we present they take the form of field strength tensors associated with the connections.

The organization of this paper is as follows. In Section II we develop the semiclassical formalism for coherent transport in the presence of electromagnetic fields, deriving the Lagrangian, based on a time-dependent variational principle, and the equations of motion. In Section III we use our formalism to show how coherent wave-packet evolution under the action of an electric field leads to the separation of up and down spins. This idea is similar in principle to the spin transistor proposed by Datta and Das<sup>16</sup>. We demonstrate that a large degree of tunability can be achieved by varying the gate field and number density. Finally, in section IV we examine the case of a magnetic field. We show that the gradient correction to the energy can be interpreted as an intrinsic magnetic moment of the wave-packet<sup>13,17,18</sup>, and we calculate this magnetic moment correction for the light holes in the spherical four-band model of the Luttinger Hamiltonian.

## II. DEVELOPMENT OF THE FORMALISM

The semiclassical model describes the dynamics of wave-packets. The wave-packet we consider is well localized in reciprocal space, and it is assumed it sees only a small part of the lattice at any one time. It is chosen in such a way that its spread in wave vector is much smaller than the size of the Brillouin zone, so that its motion at any moment is dependent only on the local properties of the band structure. In order for this to happen, the uncertainty principle dictates that the spread in real space must be greater than the size of the lattice constant

We consider systems whose Hamiltonians are functions of slowly varying parameters, such as the potentials of weak external electromagnetic fields, which vary on larger length scales than that of the wave-packet, and are treated classically. The periodic potential of the ions on the other hand, changing over dimensions small compared to the wave-packet spread, must be treated quantum mechanically<sup>11</sup>. When these conditions are fulfilled, the Hamiltonian can be expanded<sup>13</sup> about the center of the wave-packet, which we denote by  $\mathbf{r}_c$ :

$$\begin{aligned} \hat{H} &= \hat{H}_c + \Delta\hat{H} = \\ &= \hat{H}_c + \frac{1}{2}[(\hat{\mathbf{r}} - \mathbf{r}_c) \cdot \frac{\partial \hat{H}_c}{\partial \mathbf{r}_c} + c.c.] \end{aligned} \quad (1)$$

The term  $\hat{H}_c$  represents the Hamiltonian  $\hat{H}$  evaluated at  $\mathbf{r}_c$ , while the gradient term gives rise to a correction to the energy, which will play an important role in our discussion below. Since the wave-packet senses only a small part of the lattice and the Hamiltonian varies on a larger scale than the wave-packet, we can truncate the expansion to first order.

We take the Hamiltonian to have the following general form:

$$\hat{H} = \hat{H}_0 + \hat{H}_{so} + H_Z, \quad (2)$$

where the term  $H_0$  contains the kinetic energy and the lattice periodic potential, while  $H_{so}$  represents the spin-orbit coupling and  $H_Z$  is the Zeeman term, representing the interaction between the spin and a magnetic or exchange field. The energy spectrum of the Hamiltonian consists, as usual, of a series of bands, of which several are close together in energy and are separated from the others by larger gaps. It is these bands that constitute the focus of our attention. When the external fields are smoothly varying the states move within this subset, which henceforth, for simplicity and without loss of generality, we take to be two-dimensional. In order to have a well defined velocity it is necessary for the energy to be well defined, therefore the model does not allow transitions outside the subspace. We regard the fields in this problem as small enough that Zener tunneling to the remote bands is negligible, but they may induce transitions within the subset.

The subset is spanned by two basis functions, which are eigenstates of  $\hat{H}_c$ , the local Hamiltonian, evaluated at  $\mathbf{r}_c$ , which has the periodicity of the unperturbed crystal:

$$\hat{H}_c|\Psi_i\rangle = \varepsilon_c^i|\Psi_i\rangle. \quad (3)$$

For a given  $\mathbf{r}_c$ , therefore, these eigenstates have the Bloch form, with the functions  $|u_i\rangle$  representing the lattice periodic parts of the wave functions:

$$\begin{aligned} |\Psi_1(\mathbf{r}_c, \mathbf{q}, t)\rangle &= e^{i\mathbf{q}\cdot\hat{\mathbf{r}}}|u_1(\mathbf{r}_c, \mathbf{q}, t)\rangle \\ |\Psi_2(\mathbf{r}_c, \mathbf{q}, t)\rangle &= e^{i\mathbf{q}\cdot\hat{\mathbf{r}}}|u_2(\mathbf{r}_c, \mathbf{q}, t)\rangle \end{aligned} \quad (4)$$

The wave functions  $|u_i(\mathbf{r}_c, \mathbf{q}, t)\rangle$  are spinors with the full periodicity of the lattice. Despite the fact that the two

bands are spin split, it cannot be assumed that their local spin quantization axes are antiparallel, as the interactions with neighboring bands may affect the direction of quantization. Therefore, in principle, a finite overlap exists between the spinors corresponding to the two bands and it is not revealing to make a further decomposition of the eigenfunctions into an orbital and a spin part. Additionally, the Hamiltonian contains terms describing the spin-orbit interaction, which may depend on wave vector and position.

Employing the crystal momentum representation, the wave-packet is therefore expanded in the basis of Bloch eigenstates:

$$|w\rangle = \int d^3q \{a(\mathbf{q}, t)[\eta_1(t)|\Psi_1\rangle + \eta_2(t)|\Psi_2\rangle\}. \quad (6)$$

As the wave-packet depends only on the local properties of the band structure, the basis functions  $|\Psi_1\rangle, |\Psi_2\rangle$  are functions of the position of the wave packet center,  $\mathbf{r}_c$ , wave vector and time, although implicit in the ket notation is dependence on position. The function  $a(\mathbf{q}, t) = |a(\mathbf{q}, t)|e^{-i\Gamma(\mathbf{q}, t)/2}$ , which incorporates the overall phase term, is a narrow distribution function describing the extent of the wave-packet in reciprocal space and is sharply peaked at the center of the wave packet, denoted by  $\mathbf{q}_c$ , as discussed by Sundaram and Niu<sup>13</sup>. The functions  $\eta_1$  and  $\eta_2$  describe the composition of the wave-packet in terms of the two bands. They are functions of time only, not of wave vector, since defining the  $\eta_i$  as functions of wave vector is tantamount to redefining the Bloch wave functions, in other words a rotation in the coupled-band manifold. In addition, since the distribution function  $a(\mathbf{q}, t)$  is narrow, it effectively singles out one wave-vector, so the wave-vector dependence of the  $\eta_i$  can be ignored. The wave-packet satisfies the normalization conditions:

$$\begin{aligned} \int d^3q |a|^2 &= 1 \\ |\eta_1|^2 + |\eta_2|^2 &= 1. \end{aligned} \quad (7)$$

The wave-packet can be rewritten by grouping together the coefficients in an overall wave function  $|u\rangle$ , which retains the Bloch periodicity:

$$|w\rangle = \int d^3q |a| e^{-i\Gamma/2} e^{i\mathbf{q}\cdot\hat{\mathbf{r}}} |u\rangle \quad (8)$$

Note that  $|u\rangle$  is not an eigenstate of the Hamiltonian, but an expansion in eigenstates, a crucial difference from the one-band situation. In addition, the time dependence of  $|u\rangle$  comes both from the time dependence of the Bloch states and that of the coefficients.

We require the real-space center of the wave-packet to be given by:

$$\mathbf{r}_c = \langle w | \hat{\mathbf{r}} | w \rangle = \frac{\partial \Gamma_c}{\partial \mathbf{r}_c} + \mathbf{R}_c \quad (9)$$

The subscript  $c$  signifies that the quantity is evaluated at the center of the wave-packet in reciprocal space, that is  $\mathbf{q} = \mathbf{q}_c$ . The vector  $\mathbf{R}$ , representing a connection in reciprocal space, is defined as follows:

$$\mathbf{R} = \langle u | i \frac{\partial}{\partial \mathbf{q}} | u \rangle. \quad (10)$$

The energy of the wave-packet is given by the expectation value

$$\langle w | \hat{H} | w \rangle = \langle w | \hat{H}_c | w \rangle + \langle w | \Delta \hat{H} | w \rangle \equiv \varepsilon + \Delta. \quad (11)$$

Both  $\varepsilon$  and  $\Delta$  are expressible entirely in terms of the Bloch wave function  $|u\rangle$ :

$$\varepsilon = \langle u | \hat{H}_c | u \rangle \quad (12)$$

$$\Delta = \frac{i}{2} (\langle u | \frac{\partial \hat{H}_c}{\partial \mathbf{r}_c} \cdot | \frac{\partial u}{\partial \mathbf{q}} \rangle - c.c.) - \mathbf{R} \cdot \langle u | \frac{\partial \hat{H}_c}{\partial \mathbf{r}_c} | u \rangle$$

This energy correction takes on an additional significance when a magnetic field is present, as will be seen in the last section.

The Lagrangian  $\mathcal{L}$  is obtained semiclassically by means of a variational principle:

$$\mathcal{L} = \langle w | (i\hbar \frac{d}{dt} - \hat{H}) | w \rangle \quad (13)$$

Its use is justified by the fact that the Euler-Lagrange equation of motion for  $|w\rangle$  derived from it is the time-dependent Schrodinger equation. Following the method used by Sundaram and Niu<sup>13</sup>, the following expression is found for the Lagrangian:

$$\begin{aligned} \mathcal{L} &= \langle u | i\hbar \frac{\partial u}{\partial t} \rangle + \hbar \dot{\mathbf{r}}_c \cdot (\mathbf{q}_c + \mathbf{Q}_c) + \hbar \dot{\mathbf{q}}_c \cdot \mathbf{R} - \langle w | \hat{H} | w \rangle = \\ &= \hbar T + \hbar \mathbf{q}_c \cdot \dot{\mathbf{r}}_c - \varepsilon - \Delta \end{aligned} \quad (14)$$

The time and real space connections,  $T$  and  $\mathbf{Q}$ , are defined in analogy with  $\mathbf{R}$  by

$$\begin{aligned} T &= \langle u | i \frac{d}{dt} | u \rangle \\ \mathbf{Q} &= \langle u | i \frac{\partial}{\partial \mathbf{r}} | u \rangle \end{aligned} \quad (15)$$

In the above,  $\frac{d}{dt}$  represents the total time derivative, including both the explicit time dependence and the implicit, which is due to the dependence on  $\mathbf{r}_c$  and  $\mathbf{q}_c$ . In this picture we regard  $|u\rangle$  itself as a dynamical variable (due to the presence of  $\eta_1, \eta_2$ ), which allows us to keep the same Lagrangian as in the one-band case. Since  $|u\rangle$  is a dynamical variable, it will give rise to additional equations of motion:

$$\hbar \dot{\mathbf{q}}_c = - \frac{\partial}{\partial \mathbf{r}_c} \langle u | \hat{H} | u \rangle + (\boldsymbol{\Omega}_{\mathbf{r}\mathbf{r}} \dot{\mathbf{r}}_c + \boldsymbol{\Omega}_{\mathbf{r}\mathbf{q}} \dot{\mathbf{q}}_c) - \boldsymbol{\Omega}_{\mathbf{t}\mathbf{r}} \quad (16)$$

$$\hbar \dot{\mathbf{r}}_c = \frac{\partial}{\partial \mathbf{q}_c} \langle u | \hat{H} | u \rangle - (\boldsymbol{\Omega}_{\mathbf{q}\mathbf{r}} \dot{\mathbf{r}}_c + \boldsymbol{\Omega}_{\mathbf{q}\mathbf{q}} \dot{\mathbf{q}}_c) + \boldsymbol{\Omega}_{\mathbf{t}\mathbf{q}}$$

$$i\hbar \langle u_1 | \frac{\partial u}{\partial t} \rangle = \langle u_1 | (\hat{H} - \hbar \dot{\mathbf{r}}_c \cdot \frac{\partial}{\partial \mathbf{r}_c} - \hbar \dot{\mathbf{q}}_c \cdot \frac{\partial}{\partial \mathbf{q}_c}) | u \rangle$$

$$i\hbar \langle u_2 | \frac{\partial u}{\partial t} \rangle = \langle u_2 | (\hat{H} - \hbar \dot{\mathbf{r}}_c \cdot \frac{\partial}{\partial \mathbf{r}_c} - \hbar \dot{\mathbf{q}}_c \cdot \frac{\partial}{\partial \mathbf{q}_c}) | u \rangle$$

The curvature tensor  $\Omega_{\mathbf{r}\mathbf{r}}^{\alpha\beta}$  is defined by:

$$\Omega_{\mathbf{r}\mathbf{r}}^{\alpha\beta} = i(\langle \frac{\partial u}{\partial r_\alpha} | \frac{\partial u}{\partial r_\beta} \rangle - \langle \frac{\partial u}{\partial r_\beta} | \frac{\partial u}{\partial r_\alpha} \rangle) \quad (17)$$

and the vector  $\Omega_{t\mathbf{q}}$  by:

$$\Omega_{t\mathbf{q}}^\alpha = i(\langle \frac{\partial u}{\partial t} | \frac{\partial u}{\partial q_\alpha} \rangle - \langle \frac{\partial u}{\partial q_\alpha} | \frac{\partial u}{\partial t} \rangle) \quad (18)$$

The others can be deduced analogously. These quantities have exactly the same form as the curvatures defined in the paper by Sundaram and Niu<sup>13</sup>.

We specialize in the case of an external electromagnetic field. The effect of such an external field is discussed thoroughly by Sundaram and Niu<sup>13</sup>. The wave vector  $\mathbf{q}$  must be replaced by  $\mathbf{k} = \mathbf{q} + \frac{e}{\hbar}\mathbf{A}(\mathbf{r}, t)$ , which is the gauge invariant crystal momentum (for electrons with charge  $-e$ ), and therefore the Hamiltonian will have the form  $\hat{H}(\mathbf{k}) + eV(\mathbf{r}, t)$ . Provided the magnetic or exchange field is constant and uniform, so that the Zeeman term has no time or space dependence, the basis states  $\{|u_i\rangle\}$  will depend only on  $\mathbf{k}$ . The reason for this is that all the spatial and time dependence of the wave functions will only come from the spatial and time dependence of the vector potential  $\mathbf{A}(\mathbf{r}, t)$ . We will therefore restrict our attention to constant uniform magnetic fields, while the electric fields may be space- and time-dependent. As the electromagnetic fields vary on a spatial scale which is large compared to that of the wave-packet, the local Hamiltonian will have the form  $\hat{H}[\mathbf{q} + \frac{e}{\hbar}\mathbf{A}(\mathbf{r}_c, t)] + eV(\mathbf{r}_c, t)$ . The band eigenstates  $\{|\Psi_{n\mathbf{k}}\rangle\}$  take the form  $|\psi_{n\mathbf{k}}\rangle = e^{i\mathbf{q}\cdot\mathbf{r}}|u_{n\mathbf{k}}\rangle = e^{i(\mathbf{k} - \frac{e\mathbf{A}}{\hbar})\cdot\mathbf{r}}|u_{n\mathbf{k}}\rangle$ . The time dependence of  $|u\rangle$  comes both from the Bloch wave functions  $\{|u_i\rangle\}$ , which depend only on  $\mathbf{k}$ , and from the coefficients, which depend only on time. Therefore, the Lagrangian in the presence of electromagnetic fields can be written as:

$$\mathcal{L} = \langle u | i\hbar \frac{d}{dt} | u \rangle + [\hbar\mathbf{k}_c - e\mathbf{A}(\mathbf{r}_c, t)] \cdot \dot{\mathbf{r}}_c - \varepsilon - \Delta - eV(\mathbf{r}_c, t), \quad (19)$$

and the equations of motion now take the following form:

$$\begin{aligned} \hbar\dot{\mathbf{k}}_c &= -e(\mathbf{E} + \dot{\mathbf{r}}_c \times \mathbf{B}) \quad (20) \\ \hbar\dot{\mathbf{r}}_c &= \frac{\partial}{\partial \mathbf{k}_c} \langle u | \hat{H} | u \rangle - \hbar\dot{\mathbf{k}}_c \times \boldsymbol{\Omega} + \boldsymbol{\Omega}_{t\mathbf{k}} \\ i\hbar\langle u_1 | \frac{du}{dt} \rangle &= \langle u_1 | \hat{H} | u \rangle \\ i\hbar\langle u_2 | \frac{du}{dt} \rangle &= \langle u_2 | \hat{H} | u \rangle \end{aligned}$$

where  $\boldsymbol{\Omega} = i\langle \frac{\partial u}{\partial \mathbf{k}} | \times | \frac{\partial u}{\partial \mathbf{k}} \rangle$ . Note that the position-vector equation of motion is very similar to the one band case<sup>13</sup>, excepting the presence of the vector  $\boldsymbol{\Omega}_{t\mathbf{k}}$ , which is nonzero due to the time dependence of  $|u\rangle$  through the coefficients. The equation of motion for  $|u\rangle$ , if a magnetic field is present, leads to the formula for Larmor precession. The equations may be solved to any desired order in the external fields and are not limited to the linear response regime (the fields are weak enough that they do not induce transitions to remote bands).

### III. THE PSEUDO-SPIN

The treatment we have presented so far is an exact analogy with the single-band dynamics. The equations of motion (20) are complete. However, the form of the equations hides the fact that the last two of them are in fact equations of motion for the coefficients  $\eta_i$ . The equations of motion can be made more explicit in terms of these coefficients, and the non-Abelian quantities emerging in the process illustrate the gauge structure of the Hilbert space.

The coefficients  $\eta_1, \eta_2$  give the composition of the wave-packet in terms of the two bands, and it is natural to think of them as a vector,  $(\frac{\eta_1}{\eta_2})$ , which will be referred to as the pseudo-spin. The connections  $\mathbf{R}, \mathbf{Q}$  and  $T$  can be expanded in terms of  $\eta$ :

$$\begin{aligned} R^\alpha &= \eta^\dagger \mathcal{R}^\alpha \eta, \quad \mathcal{R}_{ij}^\alpha = \langle u_i | i \frac{\partial u_j}{\partial q_\alpha} \rangle; \quad (21) \\ Q^\alpha &= \eta^\dagger \mathcal{Q}^\alpha \eta, \quad \mathcal{Q}_{ij}^\alpha = \langle u_i | i \frac{\partial u_j}{\partial r_\alpha} \rangle; \\ T &= \eta^\dagger \mathcal{T} \eta + i\eta^\dagger \frac{d\eta}{dt}, \quad \mathcal{T}_{ij} = \langle u_i | i \frac{du_j}{dt} \rangle. \end{aligned}$$

The Lagrangian in this picture takes the form:

$$\mathcal{L} = i\hbar\eta^\dagger \frac{D\eta}{Dt} + \hbar\mathbf{q}_c \cdot \dot{\mathbf{r}}_c - \eta^\dagger \mathcal{H} \eta. \quad (22)$$

where  $\mathcal{H}_{ij} = \langle u_i | \hat{H} | u_j \rangle$  and the covariant derivative with respect to time, defined as  $\frac{D}{Dt} = \frac{d}{dt} - i\mathcal{T}$ , has been introduced. Specializing in electromagnetic fields, we end up with the following Lagrangian:

$$\mathcal{L} = \eta^\dagger (i\hbar \frac{D}{Dt}) \eta + [\hbar\mathbf{k}_c - e\mathbf{A}(\mathbf{r}_c, t)] \cdot \dot{\mathbf{r}}_c - \eta^\dagger \mathcal{H} \eta \quad (23)$$

The equations of motion derived from this electromagnetic Lagrangian are as follows:

$$\begin{aligned} \hbar\dot{\mathbf{k}}_c &= -e(\mathbf{E} + \dot{\mathbf{r}}_c \times \mathbf{B}) \quad (24) \\ \hbar\dot{\mathbf{r}}_c &= \eta^\dagger [\frac{D}{D\mathbf{k}}, \mathcal{H}] \eta - \hbar\dot{\mathbf{k}}_c \times \eta^\dagger \mathcal{F} \eta \\ i\hbar \frac{D\eta}{Dt} &= \mathcal{H} \eta \end{aligned}$$

The covariant derivative with respect to the wave vector, which has the form  $\frac{D}{Dk_\alpha} = \frac{\partial}{\partial k_\alpha} - i\mathcal{R}^\alpha$ , has been introduced. The non-Abelian Berry curvature matrix,  $\mathcal{F}_{ij}^\gamma$ , is expressed in terms of the field strength tensor corresponding to the covariant wave vector derivatives:

$$\mathcal{F}_{ij}^\gamma = \frac{1}{2} \epsilon^{\alpha\beta\gamma} \mathcal{F}_{ij}^{\alpha\beta} \quad (25)$$

where

$$\begin{aligned} \mathcal{F}_{ij}^{\alpha\beta} &= i[\frac{D}{Dk_\alpha}, \frac{D}{Dk_\beta}]_{ij} = \quad (26) \\ &= \frac{\partial \mathcal{R}_{ij}^\beta}{\partial k_\alpha} - \frac{\partial \mathcal{R}_{ij}^\alpha}{\partial k_\beta} - i[\mathcal{R}^\alpha, \mathcal{R}^\beta]_{ij} \end{aligned}$$

This form, which includes the non-Abelian correction from the commutator of the connection matrices, makes evident its gauge covariance with respect to unitary transformations of the pseudo-spin. The curvature tensor is antisymmetric under interchange of  $\alpha$  and  $\beta$ , while the indices  $i$  and  $j$  satisfy  $\mathcal{F}_{ij}^{\alpha\beta} = (\mathcal{F}_{ji}^{\alpha\beta})^*$ .

It is seen from the equations of motion that working in the coupled-band manifold entails the presence of non-Abelian quantities such as the modified Berry curvature and gauge covariant group velocity  $\frac{1}{\hbar}[\frac{D}{D\mathbf{k}}, \mathcal{H}]$ , which are corrections to the one band equations of motion needed to ensure gauge covariance. The matrix  $\mathcal{H}$  is not necessarily diagonal, as it includes the energy gradient correction  $\Delta$ .

#### IV. CONSTANT ELECTRIC FIELD

We will examine first the case of a constant uniform electric field acting on two degenerate bands. We choose a gauge such that the scalar electric potential need not be included in the Hamiltonian, and the electric field is represented purely by the vector potential  $\mathbf{A}$ . With experiment in mind, we take  $\mathbf{E} = (0, 0, E)$ , modelling a gate field, and study its effect on transport in the  $xy$ -plane.

We choose as an example the light hole bands of the spherical four-band model. The wave functions are eigenstates of  $\mathbf{k} \cdot \hat{\mathbf{J}}$ , where  $\hat{\mathbf{J}}$  is the total angular momentum operator. In this system, the equation of motion for  $\eta$  takes the form

$$i\hbar \frac{d\eta}{dt} = (\mathcal{H} - eER^z)\eta, \quad (27)$$

where the connection matrix  $\mathcal{R}^z = -\frac{k_x}{k^2}\sigma^y$  has off-diagonal elements only, with  $\mathbf{k}_\perp = (k_x, k_y)$  and  $\sigma^y$  a Pauli spin matrix. The equations of motion for the position and wave vector are:

$$\begin{aligned} \hbar \dot{\mathbf{k}} &= e\mathbf{E} \\ \hbar \dot{\mathbf{r}}_c &= \frac{\partial \varepsilon_l}{\partial \mathbf{k}} - e\mathbf{E} \times \eta^\dagger \mathcal{F} \eta, \end{aligned} \quad (28)$$

in which  $\mathbf{k}_0$  is the initial value of  $\mathbf{k}$ ,  $\varepsilon_l = \frac{\hbar^2 k^2}{2m_l}$  is the light hole energy,  $m_l$  is the light hole effective mass, and the curvature  $\mathcal{F} = \frac{3}{2} \frac{\mathbf{k}}{k^3} \sigma^z$ . The wave vector equation of motion is readily integrated to give  $\mathbf{k} = \mathbf{k}_0 + \frac{e\mathbf{E}t}{\hbar}$ . Since the Berry curvature is parallel to  $\mathbf{k}$ , there are two limiting cases to consider: the case  $\mathbf{k}_0 // \mathbf{E}$  is trivial because the curvature correction vanishes and the bands decouple, so we will focus on the more interesting case  $\mathbf{k}_0 \perp \mathbf{E}$ .

The equations of motion can be solved exactly. The pseudo-spin is given by:

$$\eta = \begin{pmatrix} \eta_1^{(0)} \cos \alpha + \eta_2^{(0)} \sin \alpha \\ \eta_2^{(0)} \cos \alpha - \eta_1^{(0)} \sin \alpha \end{pmatrix}, \quad (29)$$

with the angle  $\alpha(\tau) = \arctan\left(\frac{\tau + \cos \theta_0}{\sin \theta_0}\right) - \left(\frac{\pi}{2} - \theta_0\right)$ , where we have introduced the dimensionless time  $\tau = \frac{eEt}{\hbar}$  and

$\theta_0$  is the polar angle of  $\mathbf{k}_0$ , and where  $\eta_i^{(0)}$  are the values of the pseudospin at  $\tau = 0$ .

In this system, the contraction  $\eta^\dagger \hat{\sigma}^i \eta$  (with  $i = 1, 2, 3$ ) is the expectation value of the pseudo-spin. Its components evolve in time as:

$$\begin{aligned} \langle \hat{\sigma}^1 \rangle &= \langle \hat{\sigma}^1 \rangle_{\tau=0} \cos 2\alpha - \langle \hat{\sigma}^3 \rangle_{\tau=0} \sin 2\alpha \\ \langle \hat{\sigma}^2 \rangle &= \langle \hat{\sigma}^2 \rangle_{\tau=0} \\ \langle \hat{\sigma}^3 \rangle &= \langle \hat{\sigma}^3 \rangle_{\tau=0} \cos 2\alpha + \langle \hat{\sigma}^1 \rangle_{\tau=0} \sin 2\alpha \end{aligned} \quad (30)$$

The electric field therefore only rotates the 1 and 3 components of the pseudo-spin into combinations of each other, while the 2 component remains unaffected. To understand the significance of these results we will examine a concrete example, taking initially a positive helicity eigenstate so that  $\eta_1^{(0)} = 1, \eta_2^{(0)} = 0$ , and fixing the initial wave vector along the  $x$ -axis such that  $\mathbf{k}_0 = k_0 \hat{\mathbf{x}}$ , which means that  $\theta_0 = \frac{\pi}{2}$ . As  $t \rightarrow \infty$ ,  $\alpha$  reaches the limiting value of  $\frac{\pi}{2}$  and the components of the pseudo-spin become:

$$\begin{aligned} \langle \hat{\sigma}^1 \rangle &= -\langle \hat{\sigma}^1 \rangle_{\tau=0} \\ \langle \hat{\sigma}^2 \rangle &= \langle \hat{\sigma}^2 \rangle_{\tau=0} \\ \langle \hat{\sigma}^3 \rangle &= -\langle \hat{\sigma}^3 \rangle_{\tau=0}. \end{aligned} \quad (31)$$

Thus the 1 and 3 components of the pseudo-spin are reversed while the 2 component is conserved.

The  $\mathbf{r}_c$  equation of motion can be integrated to give the trajectory of the carriers:

$$\mathbf{r}_c = \frac{\hbar^2 k_0^2}{eEm_l} (\tau \hat{\mathbf{x}} + \frac{\tau^2}{2} \hat{\mathbf{z}}) - \frac{\tau(3 + \tau^2)(|\eta_1^{(0)}|^2 - |\eta_2^{(0)}|^2)}{2k_0(1 + \tau^2)^{3/2}} \hat{\mathbf{y}}. \quad (32)$$

We have omitted a term proportional to  $\eta_1^{(0)} \eta_2^{(0)}$  since in our setup either one of them will be zero (we assume the carriers have been polarized, either optically or by a ferromagnet, so that their initial pseudo-spin is either up or down). From the above and Fig. 1 it can be seen that the maximum separation in the  $y$ -direction occurs at  $\tau = 1$ . Taking  $k_0 = 10^8 \text{m}^{-1}$  and  $E = 1000 \text{Vm}^{-1}$  as typical values of the Fermi wave vector and the electric field, this yields a separation of 14nm after a waiting time of 60ps. This effect is certainly measurable provided one uses a clean sample with a long scattering time, and is broadly tunable by adjusting the Fermi wave vector (and thus the number density) and the electric field. In addition, although the present example treats only convective transport, this formalism explains the principle behind effects such as the spin Hall effect, since it can be seen directly that the carriers with different helicities are separated in the  $xy$ -plane by the electric field normal to the plane.

#### V. CONSTANT MAGNETIC FIELD

When a constant uniform magnetic field is present, the gradient correction to the energy takes the form:

$$\Lambda = -\mathbf{M} \cdot \mathbf{B} \quad (33)$$

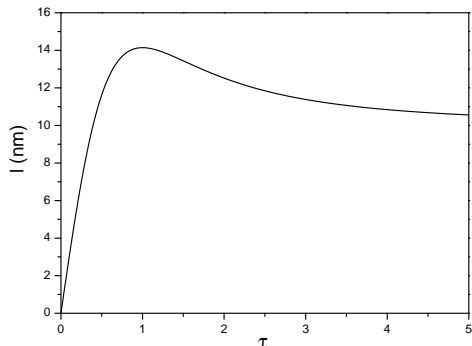


FIG. 1: Separation  $l$  in the  $y$ -direction between light holes of opposite helicities as a function of  $\tau$ , the dimensionless time. The maximum separation occurs for  $\tau = 1$ .

$\mathbf{M}$ , which is identified with the intrinsic magnetic moment of the wave packet<sup>13,17,18</sup>, is given by the expression:

$$\begin{aligned} \mathbf{M} &= \mp e R e \langle u | \hat{\mathbf{v}} \times (i \frac{\partial}{\partial \mathbf{k}} - \mathbf{R}) | u \rangle = \\ &= \mp e R e (\eta_i^* \langle u_i | \hat{\mathbf{v}} \times (i \frac{\partial}{\partial \mathbf{k}} - \mathbf{R}) | u \rangle \eta_j), \end{aligned} \quad (34)$$

where the sign is negative for electrons and positive for holes. The form of  $\Delta$  shows that it can be regarded as a correction to the Zeeman term. Written explicitly in component form, the magnetic moment is:

$$M^\alpha = \mp \frac{e}{2} \epsilon^{\alpha\beta\gamma} \eta_i^* \langle u_i | \{ \hat{v}_\beta, (i \frac{\partial}{\partial k_\gamma} - R^\gamma) \} | u_j \rangle \eta_j. \quad (35)$$

$\epsilon^{\alpha\beta\gamma}$  represents the antisymmetric tensor. We can expand the expression for  $M^\alpha$  in terms of the pseudo-spin, whereupon it becomes:

$$\begin{aligned} M^\alpha &= \mp e \left[ \frac{1}{2} \epsilon^{\alpha\beta\gamma} \sum_{i,j}^{in} \sum_l^{all} \eta_i^* (v_{il}^\beta \mathcal{R}_{lj}^\gamma + \mathcal{R}_{il}^\gamma v_{ij}^\beta) \eta_j - \right. \\ &\quad \left. - \epsilon^{\alpha\beta\gamma} \left( \sum_{i,j}^{in} \eta_i^* v_{ij}^\beta \eta_j \right) \left( \sum_{k,l}^{in} \eta_k^* \mathcal{R}_{kl}^\gamma \eta_l \right) \right]. \end{aligned} \quad (36)$$

The abbreviation  $v_{ij}^\beta$  stands for the matrix elements of the velocity operator between Bloch eigenfunctions,  $\langle u_i | \hat{v}^\beta | u_j \rangle$ , *in* indicates that the index runs only over the bands in the degenerate subspace and *all* over all bands. Thus the magnetic moment consists of a term which is first order in the pseudo-spin and summed over all bands as well as a term which is second order in the pseudo-spin and summed only over the degenerate subspace.

We take as an example once again the light-hole manifold of the four-band Luttinger model in the spherical approximation in the presence of a constant uniform magnetic field. The Hamiltonian in this case is:

$$\hat{H} = \frac{\hbar^2}{2m} \left[ \left( \gamma_1 + \frac{5}{2} \gamma_2 \right) k^2 - 2\gamma_2 (\mathbf{k} \cdot \hat{\mathbf{J}})^2 \right] - \frac{g e}{2} \hat{\mathbf{S}} \cdot \mathbf{B}, \quad (37)$$

where  $g$  is the Lande  $g$ -factor. The Zeeman interaction between the spin and the magnetic field does not contribute to the velocity operator and therefore it does not contribute to the magnetic moment.

The velocity operator takes the form:

$$\hat{\mathbf{v}} = \left( \gamma_1 + \frac{5}{2} \gamma_2 \right) \frac{\hbar \mathbf{k}}{2m} - \frac{\hbar \gamma_2}{m} (\{ \mathbf{k} \cdot \hat{\mathbf{J}}, \hat{\mathbf{J}} \}) = \hat{\mathbf{v}}_I + \hat{\mathbf{v}}_{II} \quad (38)$$

Since  $\hat{\mathbf{v}}_I$  is proportional to the identity matrix, the contribution it makes to the magnetic moment is zero, due to the fact that  $\langle u | i \frac{\partial}{\partial \mathbf{k}} - \mathbf{R} | u \rangle = 0$ . In addition, as shown in the Appendix,  $\hat{\mathbf{v}}_{II}$  can be separated into two contributions: one that spans the LH and HH subspaces and one inter-subspace contribution. The former, when restricted to the LH subspace, is again proportional to the identity matrix and thus the second term in (37) is actually second order in  $\eta$  and cancels the intra-subspace part of the first term in (37). Therefore, for the light holes  $\mathbf{M}$  can be expressed as:

$$M^\alpha = \frac{e}{2} \epsilon^{\alpha\beta\gamma} \sum_{i,j}^{in} \sum_l^{out} \eta_i^* [(v_{II}^\beta)_{il} \mathcal{R}_{lj}^\gamma + \mathcal{R}_{il}^\gamma (v_{II}^\beta)_{lj}] \eta_j, \quad (39)$$

where *out* signifies that  $l$  runs over all bands outside the degenerate subspace, that is  $l \neq i, j$ . In our approximation, we take  $l$  to run over the heavy-hole manifold. Using the expressions for  $v_{II}^\beta$  and  $\mathcal{R}$  given in the appendix, the light-hole intrinsic magnetic moment in the spherical four-band model is given by the following expression:

$$\mathbf{M} = - \frac{3e \hbar \gamma_2 \hat{\mathbf{k}}}{m} \eta^\dagger \sigma^z \eta. \quad (40)$$

Thus, depending on the weight of each band in the wavepacket the intrinsic magnetic moment can be positive or negative and if the bands are equally represented it will be zero.

Note added - After completion of this work, we became aware of a related effort by R. Shindou and K. Imura<sup>19</sup>.

This work was supported by the DOE under grant number DE-FG03-02ER45958.

## VI. APPENDIX

The reciprocal-space connection matrix  $\mathcal{R}$  is given by the following expression:

$$\mathcal{R} = \frac{\partial \theta}{\partial \mathbf{k}} J^y + \frac{\partial \phi}{\partial \mathbf{k}} (J^z \cos \theta - J^x \sin \theta). \quad (41)$$

Restricting to the light-hole manifold, we have that the angular momentum matrices  $J^x$ ,  $J^y$  and  $J^z$  become:

$$\begin{aligned} J^x &= \sigma^x \\ J^y &= \sigma^y \\ J^z &= \frac{1}{2} \sigma^z, \end{aligned} \quad (42)$$

so the connection is:

$$\mathcal{R} = \frac{\partial \theta}{\partial \mathbf{k}} \sigma^y + \frac{\partial \phi}{\partial \mathbf{k}} \left( \frac{1}{2} \sigma^z \cos \theta - \sigma^x \sin \theta \right). \quad (43)$$

As explained in the text, the velocity operator consists of two parts, the first of which is parallel to  $\mathbf{k}$  and proportional to the identity matrix. The second part,

$\hat{\mathbf{v}}_{II}$ , in the  $\mathbf{k} \cdot \hat{\mathbf{J}}$  basis has a contribution that is non-zero in either the light- or the heavy-hole subspace, and an inter-subspace contribution. The former is given by  $-\frac{2\hbar\gamma_2}{m} J_z^2 \mathbf{k}$ , which restricted to the light-hole manifold is proportional to the identity matrix. The components of the latter contribution are shown on the following page.

$$\hat{v}_{II}^x|_{inter} = -\frac{\sqrt{3}\hbar\gamma_2 k}{m} \left[ \cos \theta \cos \phi \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix} + i \sin \phi \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \right]$$

$$\hat{v}_{II}^y|_{inter} = -\frac{\sqrt{3}\hbar\gamma_2 k}{m} \left[ \cos \theta \sin \phi \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & -1 & 0 \end{pmatrix} + i \cos \phi \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix} \right] \quad (44)$$

$$\hat{v}_{II}^z|_{inter} = -\frac{\sqrt{3}\hbar\gamma_2 k}{m} \sin \theta \begin{pmatrix} 0 & -1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (45)$$

- 
- <sup>1</sup> Yu. A. Bychkov and E. I. Rashba, JETP Lett. (Engl. transl.) **39**, 66 (1984).
- <sup>2</sup> See, for example, Chapter 5 of *Semiconductor Laser Fundamentals: Physics of the Gain Materials* by W. W. Chow and S. W. Koch (Springer, Berlin, 1999).
- <sup>3</sup> L. C. Lew Yan Voon *et al.*, Phys. Rev. B **53** (16), 10703 (1996).
- <sup>4</sup> Y. Qi and S. Zhang, Phys. Rev. B **65**, 214407 (2002); *ibid.* **67**, 052407 (2003).
- <sup>5</sup> For a review of spin injection in metals and semiconductors, see M. Johnson, Semicond. Sci. Technol. **17**, 298 (2002).
- <sup>6</sup> For a review of spin injection into semiconductors, see G. Schmidt and L. W. Molenkamp, Semicond. Sci. Technol. **17**, 310 (2002).
- <sup>7</sup> There is already a vast theoretical literature on spin currents from the past few years. The following is a selection: D. Culcer *et al.*, Phys. Rev. Lett. **93**, 046602 (2004); S. Murakami *et al.*, Science **301**, 1348 (2003); S. Murakami *et al.*, Phys. Rev. B **69**, 235206 (2004); S. Zhang and Z. Yang, cond-mat/0407704 (2004); T. Damker, H. Bottger, V. V. Bryksin, Phys. Rev. B **69**, 205327 (2004); L.Hu *et al.* cond-mat/0401231 (2004); E.G.Mishchenko, A.V.Shytov, and B. I. Halperin, cond-mat/0406730; A.G.Aronov, Yu.B.Lyanda-Geller, and G.E.Pikus, Sov.Phys. JETP **73**, 537 (1991); J Inoue, G.W.Bauer, L. W. Molenkamp, Phys. Rev. B **67**, 033104 (2003).
- <sup>8</sup> Recent experiments on spin generation include: Y. Kato *et al.* cond-mat/0403407; Y. Kato *et al.* Nature **427**, 50 (2004); J. Stephens *et al.*, cond-mat/0401197 (2004). Theoretical efforts include: D. Culcer *et al.*, cond-mat/0408020 (2004); L. I. Magarill *et al.*, Semiconductors **35** (9), 1081 (2001); V.M.Edelstein, Solid State Comm. **73**, 233 (1990); O.Bleibaum, Phys. Rev. B **69**, 205202, (2004); M.Q.Weng, M.W.Wu and L. Jiang, Phys. Rev. B **69**, 245320 (2004); S.Saikin, J.Phys. Cond.Matt. **16**, 5071 (2004); Y.Pershin, Physica E **23**, 226 (2004); see S.Saikin *et al.*, J. Appl. Phys. **94**, 1769 (2003) for a general treatment of spin transport based on the drift-diffusion model.
- <sup>9</sup> I. Malajovich *et al.*, Phys. Rev. Lett. **84**, 1015 (2000); R. Fiederling *et al.*, Appl. Phys. Lett. **82**, 2160 (2003).
- <sup>10</sup> N. W. Ashcroft and N. D. Mermin, *Solid State Physics*, 2<sup>nd</sup> edition (Saunders College Publishing, New York, 1976).
- <sup>11</sup> J. Callaway, *Quantum Theory of the Solid State* (Academic Press, New York, 1976).
- <sup>12</sup> G. Sundaram and Q. Niu, Phys. Rev. B **59**, 14915 (1999).
- <sup>13</sup> E. G. Mishchenko and B. I. Halperin, Phys. Rev. B **68**, 045317 (2003); D. Culcer *et al.*, Phys. Rev. B **68**, 045327 (2003); Y. S. Gui *et al.*, Europhys. Lett. **65** (3), 393 (2004); see also Ref. [2] and [3].
- <sup>14</sup> Y. Ohno *et al.*, Phys. Rev. Lett. **83**, 4196 (1999); Y. Ohno *et al.*, Nature **402**, 790 (1999); V. Daumer *et al.*, Appl. Phys. Lett. **83**, 1376 (2003).
- <sup>15</sup> S. Datta and B. Das, Appl. Phys. Lett. **56**(7), 665 (1990).
- <sup>16</sup> R. B. Diener *et al.*, cond-mat/0306184.
- <sup>17</sup> M.-C. Chang and Q. Niu, Phys. Rev. B **53**, 7010 (1996).
- <sup>18</sup> R. Shindou and K. Imura, cond-mat/0411105 (2004).