Spin Transverse Force on Spin Current in an Electric Field

Shun-Qing Shen

Department of Physics, and Center for Theoretical and Computational Physics, The University of Hong Kong, Pokfulam Road, Hong Kong, China

(Received 27 June 2005; published 25 October 2005)

As a relativistic quantum mechanical effect, it is shown that the electron field exerts a transverse force on an electron spin 1/2 only if the electron is moving. The spin force, analogue to the Lorentz force on an electron charge in a magnetic field, is perpendicular to the electric field and the spin current whose spin polarization is projected along the electric field. This spin-dependent force can be used to understand the Zitterbewegung of the electron wave packet with spin-orbit coupling and is relevant to the generation of the charge Hall effect driven by the spin current in semiconductors.

DOI: 10.1103/PhysRevLett.95.187203

PACS numbers: 85.75.—d, 71.10.Ca, 72.20.My

In recent years, spintronics has become an emerging field because of its potential application to the semiconductor industry, and more and more attention is focused on the effect of spin-orbit coupling in metals and semiconductors [1]. The spin-orbit coupling is a relativistic effect describing the interaction of the electron spin, momentum, and electric field, and provides a route to manipulate and to control the quantum spin states via external fields [2,3]. It is desirable to understand the motion of electron spin with spin-orbit coupling in an electromagnetic field. In electrodynamics it is known that a magnetic field would exert a Lorentz force on an electric charge if it were moving. This Lorentz force can generate a lot of fundamental phenomena such as the Hall effect in solids [4]. The interaction of the spin in the electromagnetic field behaves as if the spin is a gauge charge and the interaction is due to the spin-orbit coupling in metals and semiconductors [1]. In the last step we neglect the higher order terms of expansion. Thus the Dirac equation is reduced to the ordinary wave function satisfies the following equation, $i\hbar \frac{\partial}{\partial t} \Psi = \left[ \begin{array}{c} c\alpha \cdot \left( p + eA \right) + mc^2\gamma + V \end{array} \right] \Psi,$ (1)

where $\alpha$ and $\gamma$ are the $4 \times 4$ Dirac matrices, $m$ and $e$ are the electron mass and charge, respectively, and $c$ is the speed of light. We let $\Psi = \left( \begin{array}{c} \psi_L \psi_R \end{array} \right)$ such that the rest mass energy of electron is removed from the energy eigenvalue of the electron. In the nonrelativistic limit, $\chi$ is a very small component, $\chi = \frac{1}{m^2c^2} \varepsilon \sigma \cdot \left( p + \frac{e}{c} A \right) \varphi$ where $\sigma$ are the Pauli matrices. Thus the component $\varphi$ of the wave function satisfies the following equation, $i\hbar \frac{\partial}{\partial t} \varphi = i\hbar \frac{\partial}{\partial t} \varphi = H \varphi,$ where

$$H = \frac{\left( p + \frac{e}{c} A \right)^2}{2m} + \frac{V_{\text{eff}}}{m} + \frac{\mu_B}{2} \sigma \cdot B + \frac{\hbar( p + \frac{e}{c} A)}{4m^2c^2} \cdot (\sigma \times \nabla V),$$

(2)

where $\mu_B = e\hbar/2mc$ and $V_{\text{eff}} = V + \frac{\hbar^2}{8mc^2} \nabla^2 V$. In the last step we neglect the higher order terms of expansion. Thus the Dirac equation is reduced to the Schrödinger equation with the spin-orbit coupling. The same form of effective spin-orbit coupling and Zeeman splitting can be also derived from the $8 \times 8$ Kane model that takes into account only the $k \cdot p$ coupling between the $\Gamma_6$ conduction band and the $\Gamma_5$ and $\Gamma_7$ valence bands, although the effective mass, the effective Lande $g$ factor, and the effective coupling coefficients have to be introduced as material-specific parameters such as $m \rightarrow m^*$, $\mu_B \rightarrow g \mu_B/2$, and $h^2/(4m^2c^2) \rightarrow r_{6 \rightarrow 6}^\text{He} \epsilon$. [6]

In the Heisenberg picture the kinetic velocity is

$$\mathbf{v} = \frac{1}{i\hbar} \left[ \mathbf{r}, H \right] = \frac{1}{m} \left[ \mathbf{p} + \frac{e}{c} \left( \mathbf{A} + \mathbf{A} \right) \right]$$

(3)

where $\mathbf{A} = \frac{\hbar}{2mc^2} \sigma \times \nabla V$ and comes from the spin-orbit coupling. It indicates clearly that $\mathbf{A}$ plays a role of a SU(2) gauge vector potential. The spin dependence of the gauge field can separate the charged carriers with different spins in cyclotron motion experimentally [7]. Even though we have $[p_\alpha, p_\beta] = 0$ for canonical momentum,
the analogous commutators do not vanish for the kinetic velocity
\[ [v_\alpha, v_\beta] = -i \frac{\hbar e}{m c^2} \epsilon_{\alpha\beta\gamma} B_\gamma + \frac{e^2}{m c^2} [A_\alpha, A_\beta] \tag{4} \]
where the total magnetic field \( B = B + \nabla \times A \), and \( \nabla \times A = \hbar [\sigma \cdot (\nabla^2 \psi) - (\sigma \cdot \nabla) \nabla \psi] / (4mc^2) \). Notice that
\[ [A_\alpha, A_\beta] = 2i\hbar (\sigma \cdot \nabla) e_{\alpha\beta\gamma} \partial_\gamma \psi / (4mc^2)^2. \]
We can derive the quantum mechanical version of the force,
\[ m \frac{dv}{dt} = F_h + F_g + F_f \tag{5} \]
with
\[ F_h = -\frac{e}{c} (\mathbf{v} \times \mathbf{B} - \mathbf{B} \times \mathbf{v}) / 2 - \nabla (V_{\text{eff}} + \mu_B \sigma \cdot \mathbf{B}), \tag{6a} \]
\[ F_g = \frac{\mu_B}{2mc^2} \left[ \sigma (\mathbf{B} \cdot \nabla \psi) - \mathbf{B} (\sigma \cdot \nabla \psi) \right], \tag{6b} \]
\[ F_f = \frac{\hbar}{8m^2c^4} (\sigma \cdot \nabla \psi) (\mathbf{v} \times \nabla \psi). \tag{6c} \]

This is the quantum mechanical analogue of Newton’s second law. Of course we should notice that this is just an operator equation. The uncertainty relationship tells us that the position and momentum cannot be measured simultaneously, and there is no concept of force in quantum mechanics. To see the physical meaning of the equation, we take the expectation values of both sides with respect to a Heisenberg state \( |\Phi \rangle \) which does not vary with time. The expectation values of the observable describe the motion of the center of the wave packet of electrons. In this sense we have an equation of the force experienced by the moving electron. Actually the first term \( F_h \) in Eq. (5) is the Lorentz force for a charged particle in a magnetic field \( \langle \mathbf{B} \rangle \) which contains the contribution from the SU(2) gauge field \( A \), as well as the conventional electromagnetic field. We have recovered the Ehrenfest theorem as one of the examples of the corresponding principle in quantum mechanics. The term, \( \nabla (\mu_B \sigma \cdot \mathbf{B}) \), results from the nonuniform magnetic field. Its role was first realized in the Stern-Gerlach experiment, where a shaped magnet is used to generate a nonuniform magnetic field to split the beam of silver atoms. In the classical limit it is written as the interaction between the magnetic momentum \( \mu = -\langle \mu_B \sigma \rangle \) and magnetic field. This spin force depends on the spin. Recently it is proposed that the force can generate a pure spin current if we assume \( \nabla \mathbf{B} \) is a constant [8]. In the term \( F_g \) we can also use \( \mu \) to replace the spin. It is nonzero only when the electric and magnetic fields coexist, as suggested by Anandan and others [5]. This term will play an essential role in generating spin Hall current in two-dimensional Rashba systems, which we will discuss it later. The last term, \( F_f \), comes from the SU(2) gauge potential or spin-orbital coupling. As the force is related to the Planck constant it has no counterpart in classical mechanics and is purely quantum mechanic effect. The force is irrelevant of the magnetic field. In the classical limit we cannot simply use the magnetic momentum \( \mu \) to replace the spin \( \sigma \) in the potential \( A \). Otherwise the force vanishes. To see the physical meaning of the force, we write the spin force for a single electron on a quantum state in a compact form,
\[ \langle F_f \rangle = \frac{e^2 |\mathcal{E}|^2}{4mc^2} \mathbf{j}^\perp \times \mathcal{E}, \tag{7} \]
where the spin current is defined conventionally, \( \mathbf{j}^\perp = \frac{1}{2} \langle (\mathbf{v} \cdot \sigma \cdot \mathcal{E}) / |\mathcal{E}| \rangle \), and in the last step the relation \( \{A, \sigma \cdot \mathcal{E}\} = 0 \) has been used. This is the main result in this Letter. The force is proportional to the square of electric field \( \mathcal{E} \) and the spin current whose polarization is projected along the field. It is important to note that an electron in a spin state perpendicular to the electric field \( \mathcal{E} \) and the spin current whose polarization is projected along the field. It is important to note that an electron in a spin state perpendicular to the electric field will not experience any force. Comparing with a charged particle in a magnetic field, \( \mathbf{j} \times \mathbf{B} \), where \( \mathbf{j} \) is a charge current density, the spin force is nonlinear to the electric field and depends on the spin state of electron.

We discuss several examples relevant to the spin force. Though the gauge field \( A \) provides a spin-dependent magnetic field \( \nabla \times A \), the Lorentz force caused by the field on the charge will vanish in a uniform electric field \( \nabla \mathbf{V} = e \mathcal{E} \). The spin dependent force \( F_g \) also vanishes in the absence of magnetic field. Here we consider the motion of an electron confined in a two-dimensional plane subjected to a perpendicular electric field,
\[ H = \frac{\mathbf{p}^2}{2m} + \lambda (\mathbf{p}_x \sigma_y - \mathbf{p}_y \sigma_x), \tag{8} \]
where \( \lambda = \hbar e \mathcal{E} / (4mc^2) \) from Eq. (2). This can be regarded as counterpart of a charged particle in a magnetic field. On the other hand it has the same form of the Rashba coupling in a semiconductor heterojunction with the structural inversion asymmetry [9], where the spin-orbit coupling is induced by the offsets of valence bands at the interfaces and the structure inversion asymmetry [6]. A typical value of this coefficient \( \lambda \) is of order \( 10^{-5}c \) (the speed of light), and can be adjusted by an external field [10]. Because of the spin-orbit coupling the electron spin will precess with time,
\[ \frac{d\sigma(t)}{dt} = \frac{2\lambda}{\hbar} \sigma(t) \times (\mathbf{p} \times \mathbf{z}). \tag{9} \]
Since the momentum \( \mathbf{p} \) is a good quantum number, without loss of generality, we take \( p = p_x \), just along the \( x \) direction. Correspondingly the wave function in the position space \( \langle r | \Psi \rangle = \exp(ip_x x) \chi_s / \sqrt{L} \) where \( \chi_s \) is the initial spin state. Equivalently the spin-orbit coupling provides an effective magnetic field along the \( y \) direction, \( B_{eff} = \lambda \mathbf{p}_y \mathbf{z} \). This problem can be solved analytically, and the electron spin precesses in the spin \( x-z \) plane [11], \( \sigma_z(t) = \sigma_z \cos \omega t - \sigma_x \sin \omega t, \sigma_y(t) = \sigma_y \cos \omega t + \sigma_z \sin \omega t, \) and \( \sigma_z(t) = \sigma_z \) where the Larmor frequency...
\( \omega_c = 2p_e \lambda / h \). The spin \( \sigma_z(t) \) varies with time and the spin current is always along the \( x \) direction, \( \langle j_x \rangle = \frac{2}{m} \left( \langle \sigma_x \rangle \times \cos \omega_c t + \langle \sigma_y \rangle \sin \omega_c t \right) \hat{x} \) where \( \langle \ldots \rangle \) means the expectation value over an initial state \( \langle \tau | \Phi \rangle \). As a result the spin transverse force on the spin is always perpendicular to the \( x \) direction. Correspondingly the kinetic velocity \( v_x \) and \( v_y \) at a time \( t \) are

\[
\langle v_x \rangle_t = \frac{p_x}{m} + \lambda \langle \sigma_z \rangle, \tag{10a}
\]

\[
\langle v_y \rangle_t = - \lambda (\langle \sigma_x \rangle \cos \omega_c t - \langle \sigma_y \rangle \sin \omega_c t), \tag{10b}
\]

respectively. Though \( p_y = 0 \) the kinetic velocity \( \langle v_y \rangle_t \) oscillates with the frequency \( \omega_c \) while \( \langle v_x \rangle_t \) remains constant. The \( y \) component of the position is

\[
\langle y \rangle_t = \langle y \rangle_{t=0} - \frac{\hbar}{p_x} \sin \omega_c t \left( \langle \sigma_x \rangle \cos \frac{\omega_c t}{2} - \langle \sigma_y \rangle \sin \frac{\omega_c t}{2} \right), \tag{11}
\]

If the initial state is polarized along the \( y \) direction the electron spin does not vary with time as it is an energy eigenstate of the system, as discussed by Datta and Das [2]. In this case the spin current \( \langle j_y \rangle \) carried by the electron is always zero and the spin transverse force is zero. Thus \( \langle v_y \rangle_t = 0 \). If the initial state is along the spin \( z \) direction at \( t = 0 \), i.e., \( \langle \sigma_z \rangle = s = \pm 1 \), it is found that \( \langle v_y \rangle_{t=0} = -2s \lambda \sin \omega_c t \). Different spins will move in opposite directions. It can be understood that the spin precession makes the spin current whose polarization is projected along the electric field changes with time such that the spin force along the \( y \) direction also oscillates with the frequency \( \omega_c \). This force will generate a nonzero velocity of electron oscillating along the \( y \) direction. Though \( \langle v_y \rangle_{t=0} = 2s \lambda \), the velocity does not contribute to the spin current along the \( y \) direction, \( \langle v_y \rangle_t = 0 \). The trajectory oscillates with time. The amplitude of the oscillation is \( \hbar / p_x \) and the frequency is \( \omega_c = 2p_e \lambda / h \). For a typical two-dimensional electron gas the electron density is \( n_e = 10^{11} \sim 10^{12}/\text{cm}^2 \) and the wavelength near the Fermi surface \( \hbar / p_x \sim 3-10 \) nm. For a typical Rashba coupling \( \lambda = 10^{-4} c, \omega_c = 0.3 \sim 1.0 \times 10^{-14} \text{ s} \). The rapid oscillation of the electron wave packet is known in the literature as the Zitterbewegung of an electron as a relativistic effect, which is usually regarded as a result of admixture of the positron state in an electron wave packet as a relativistic effect [12]. In semiconductors the Rashba coupling reflects the admixture of the particle and hole states in the conduction and valence bands. Recently Schliemann et al. obtained the solution of the trajectory and proposed that this effect can be observed in III-V zinc-blend semiconductor quantum wells [13]. In the p-doped semiconductors described by the Luttinger model there also exists a spin force, and will generate the Zitterbewegung as calculated by Jiang et al. [14]. Though the spin transverse force on a moving spin is very analogous to the Lorentz force on a moving charge, because of spin precession, its effect is completely different with the motion of a charged particle in a magnetic field, where the amplitude of the Lorentz force is constant and the charged particle moves in a circle. The Zitterbewegung of the electronic wave package near the boundary will cause some edge effect as shown in recent numerical calculations [15]. The edge effect is determined by the electron momentum. The smaller the momentum, the larger the edge effect. The amplitude and frequency of the Zitterbewegung satisfy a relation that \( (\hbar/2p_e)(2p_e \lambda / h) = \lambda \), which is the amplitude of oscillation of the velocity \( v_y \). In Fig. 1 it is illustrated that two electrons with different spins experience opposite forces in an electric field.

Furthermore we consider a two-dimensional electron gas lacking both the bulk and structural inversion symmetries. A Dresselhaus term \( \beta (p_x \sigma_x - p_y \sigma_y) \) will be included in the total Hamiltonian in Eq. (8) [16]. In this model the spin force formula gives [17]

\[
\langle F_j \rangle = \frac{4m^2}{\hbar^2} (\lambda^2 - \beta^2) \langle j_z \times \hat{z} \rangle, \tag{12}
\]

for each moving electron. First of all, the force disappears at the symmetric point of \( \lambda = \pm \beta \). At this point the operator \( \sigma_x \pm \sigma_y \) is a good quantum number and there is no spin flip in the system. For \( \lambda \neq \pm \beta \), the moving electron will experience a spin-dependent force and the force will change its sign near \( \lambda = \beta \). A heuristic picture from this formula is that when a nonzero spin current \( j_z \) goes through this system the spin-orbit coupling exerts the spin transverse force on the spin current, and drives electrons to form a charge Hall current perpendicular to the spin current. The injected spin current can be generated in various ways, such as by the spin force \( \nabla (\mu \cdot B) \) [8] and circularly or linearly polarized light injection [18,19]. For instance we assume the spin current \( j_z \) is generated by the linear polarized light injection which is proportional to the transition rate from the valence band to the conduction band with finite momentum and the life time of electrons at the excited states. In the relaxation time \( \tau \) approximation in a steady state the drift velocity orthogonal to the spin current is \( \langle v_x \rangle = \frac{4m}{h} (\lambda^2 - \beta^2) j_z \tau \) if \( \tau \) is not so long, i.e., \( 2p_e \sqrt{\lambda^2 + \beta^2} \tau \ll h \). This nonzero

\[\text{FIG. 1 (color online). The electric field exerts opposite forces on electrons with different spins polarized along the field.}\]
drift velocity will form a Hall current orthogonal to the spin current. This is the charge Hall effect driven by the spin current. In ferromagnetic metal or diluted magnetic semiconductors the charge current is spin polarized; it can generate the spin polarized Hall current via the spin transverse force. Thus the spin transverse force can also be regarded a driven force of an anomalous Hall effect [20] and the spin-resolved Hall effect [17,21]. A detailed calculation for this Hall conductance is given by the Kubo formula as a linear response to the field $B = \Delta B \hat{z}$. This field will generate a spin force, $-\nabla(g \mu_B B \sigma) = -g \mu_B \Delta B \sigma \hat{x}$, which will circulate a spin current along the $x$ direction, and, furthermore, the spin-orbit coupling provides a driving force to generate a transverse charge current, $j_{cx}$. In the clear limit the Hall conductance $\sigma_{xy} = j_{xy}/(g \mu_B \Delta B) = 0$ for $\lambda = \pm \beta$ and $(e/4\pi \hbar) \times (\lambda^2 - \beta^2)/|\lambda^2 - \beta^2|$. However, following Inoue et al. and Mishchenko et al. [22] the inclusion of impurities scattering will suppress the Hall conductance completely just like the spin Hall effect. On the other hand numerical calculation in mesoscopic systems shows the existence of the effect [19]. Another example is the two-dimensional $p$-doped system with the cubic Rashba coupling [23],

$$H = \frac{p_x^2}{2m} + i \alpha (p_+^3 \sigma_+ - p_-^3 \sigma_-)$$

where $\sigma_{\pm}$ are spin increasing and decreasing operators, and $p_\pm = p_x \pm ip_y$. The spin force on the moving electron in this system is $F_f = (2m \alpha \sqrt{\hbar})^2 (j_\parallel \times \hat{z})$. The linear response theory gives the Hall conductance $-9e/(2\pi \hbar)$ which is robust against the vertex correction from impurities scattering. Calculations by means of the Green-Keldysh function technique and linear response theory [8,19] show the existence of charge Hall effect driven by the spin current, and the Onsager relation between the charge Hall effect and its reciprocal. The key features of the numerical results are in good agreement with the picture of spin force qualitatively.

In conclusion, an electric field exerts a transverse force on a moving spin just like a magnetic field exerts a Lorentz force on a moving charge. This force is proportional to the square of electric field and the spin current with spin projected along the field. This is a purely relativistic quantum mechanical effect. As the origin of the force the spin current should be also observable physically. From the solution of the motion of a single electron in an electric field, the Zitterbewegung of electronic wave packet in the spin-orbit coupling can be regarded as an explicit consequence of this force. Because of the similarity of this spin transverse force and the Lorentz force, the spin transverse force plays a similar role in the formation of the charge Hall effect driven by the spin current and the spin Hall effect driven by the charge current as the Lorentz force does in the Hall effect in a magnetic field.

The author thanks F.C. Zhang for helpful discussions. This work was supported by the Research Grant Council of Hong Kong (No. HKU 7039/05P), and a CRCG grant of The University of Hong Kong.

Resonant spin Hall conductance in quantum Hall systems lacking bulk and structural inversion symmetry

Shun-Qing Shen,1 Yun-Juan Bao,1 Michael Ma,2 X. C. Xie,3,4 and Fu Chun Zhang1,2,5

1Department of Physics, The University of Hong Kong, Pokfulam Road, Hong Kong, China
2Department of Physics, University of Cincinnati, Cincinnati, Ohio 45221, USA
3Department of Physics, Oklahoma State University, Stillwater, Oklahoma 74078, USA
4ICQS, Institute of Physics, Chinese Academy of Sciences, Beijing, China
5Department of Physics, Zhejiang University, Hangzhou, Zhejiang, China

(Received 7 October 2004; revised manuscript received 26 January 2005; published 19 April 2005)

A previous work [Shen, Ma, Xie, and Zhang, Phys. Rev. Lett. 92, 256603 (2004)] on two-dimensional quantum wells with Rashba type spin-orbit interaction under a strong perpendicular magnetic field is generalized to include the Dresselhaus coupling. The Rashba coupling and the Dresselhaus coupling interplay with the Zeeman effect in opposing ways. The former tends to produce a resonant spin Hall effect at certain magnetic fields while the latter suppresses it. Due to the resonant spin Hall effect, the spin Hall current is highly nonohmic at low temperatures. The condition for the resonant spin Hall conductance in the presence of both Rashba and Dresselhaus couplings is derived using a perturbation method. In the presence of disorder, we argue that the resonant spin Hall conductance occurs when the two Zeeman split extended states near the Fermi level become degenerate due to the Rashba coupling, and that the quantized charge Hall conductance changes by $2e^2/h$ instead of $e^2/h$ as the magnetic field changes through the resonant field.

DOI: 10.1103/PhysRevB.71.155316 PACS number(s): 75.47.—m

I. INTRODUCTION

Spintronics, which exploits electron spin rather than charge to develop a new generation of electronic devices, has emerged as an active field in condensed matters because of both the underlying fundamental physics and its potential impact on the information industry.1–3 One key issue in spintronics is the generation and efficient control of spin current. Spin-orbit interaction of electrons exists extensively in metals and semiconductors and mix spin states. It provides an efficient way to control the coherent motion of electron spins. Recently, it has been proposed theoretically that an electric field may generate a spin current in hole-doped semiconductors and in two-dimensional electron gases (2DEG) in heterostructures with spin-orbit coupling due to the spin helicity and the noncollinearity of the velocity of the single particle wave function.4–6 Studies of this intrinsic spin Hall effect have evolved into a subject of intense research.7–13 The spin Hall effect in a paramagnetic metal with magnetic impurities has also been discussed, in which a transverse spin imbalance will be generated when a charge current circulates.14–17 We also note that the spin chirality in systems with strong spin-orbit interaction may induce a pure spin current.18

Over the past two decades, remarkable phenomena have been observed in the 2DEG, most notably, the discovery of integer and fractional quantum Hall effect.19–21 Research in spin transports provides a good opportunity to explore spin physics in the 2DEG with spin-orbit couplings. The spin-orbit coupling leads to a zero-field spin splitting, and it competes with the Zeeman spin splitting when a perpendicular magnetic field is applied. The result can be detected as beating in Shubnikov-de Haas oscillations.22,23

Very recently we have studied the spin Hall effect in the 2DEG with Rashba type spin-orbit coupling in a strong perpendicular magnetic field and predicted a resonant spin Hall effect caused by the Landau level crossing near the Fermi energy.6 In this paper we present detailed calculations of the problem. The resonance shows up below a characteristic temperature of the order of the Zeeman energy $E_Z$. The peak of the resonance diverges as $1/|B−B_0|$, its weight diverges as $−\ln T$ at low $T$ as $E→0$. Near the resonant magnetic field $B_0$, $G_s \propto 1/|B−B_0|$. The resonance arises from the Fermi level degeneracy of the Zeeman-split Landau levels in the presence of the Rashba coupling. More generally, the spin-orbit interaction present in the 2DEG may be of the Dresselhaus type rather than the Rashba type, or a combination of both. It is thus of interest to extend the analysis of Ref. 6 to beyond the pure Rashba coupling. To do so, it is useful to analyze certain symmetries in systems with the Rashba and/or Dresselhaus couplings. We will show that in contrast to the zero magnetic field case, where two physical systems differing only in a pure Rashba vs a pure Dresselhaus coupling exhibit identical essential physical behavior, this is not the case when a magnetic field is present. The difference arises from the way the Rashba coupling vs the Dresselhaus coupling interplays with the Zeeman effect. In particular, the Rashba coupling opposes the Zeeman splitting and causes resonance while the Dresselhaus coupling enhances Zeeman splitting and thereby suppresses the resonance. By using linear response theory, we calculate the spin Hall conductance $G_s$ including its magnetic field and temperature dependences for realistic parameters of InGaAs/InGaAlG. For systems possessing both Rashba and Dresselhaus couplings, the resonant condition is derived within a perturbation theory which is accurate for the small ratio of the Zeeman energy to the cyclotron frequency.

The paper is organized as follows. In Sec. II we introduce the Hamiltonian of the system under consideration and ana-
lyze its symmetries. In Sec. III we study the spin Hall current for systems with only Rashba or only Dresselhaus coupling. In Sec. IV we consider systems with both Rashba and Dresselhaus couplings. By treating the couplings as small parameters, we develop a perturbation method to derive the resonance condition. The paper is concluded with a summary and a brief discussion on the effects of disorder in Sec. V.

II. MODEL HAMILTONIAN AND SYMMETRY

A. Spin-orbit coupling and model Hamiltonian

For the introduction, we start with the three-dimensional (3D) spin-orbit interaction known for III-V compounds such as GaAs and InAs, which is of the form

\[ V_{SO}^{3D} = \alpha_0 \mathbf{K}(\mathbf{p}) \cdot \sigma + \beta_0 \mathbf{E} \cdot (\mathbf{p} \times \sigma), \]

where \( \sigma \) (\( \mu = x, y, z \)) are the Pauli matrices for spin of electrons, \( \mathbf{p} \) is the momentum of the charge carrier, and

\[ K_\mu(p) = \sum_{\nu, \delta} p_\nu \sigma_\nu \epsilon_{\mu \nu \delta}. \]

In Eq. (1), the first term is the Dresselhaus coupling which originates from the lack of bulk inversion symmetry,\(^{24, 25}\) while the second term is the Rashba coupling which arises from the lack of structure inversion symmetry.\(^{25}\) The effective field \( \mathbf{E} \) is induced by the asymmetry of the external voltage to the system. In quantum wells, by neglecting the weak interband mixing and retaining the linear contribution of \( \mathbf{p} \) parallel to the \( x \)-y plane, the spin-orbit interaction in 3D is reduced to an effective one in 2D,

\[ V_{SO}^{2D} = H_{SO}^D + H_{SO}^R, \]

\[ H_{SO}^D(\alpha) = \frac{\alpha}{\hbar} (\sigma_x p_x - \sigma_y p_y), \]

\[ H_{SO}^R(\beta) = \frac{\beta}{\hbar} (\sigma_x p_x - \sigma_y p_y), \]

where \( \alpha = -\alpha_0 \hbar \langle p_x^2 \rangle \) and \( \beta = \beta_0 \hbar \langle \mathbf{E} \cdot \sigma \rangle \), with the average taken over the energy band of the quasi-2D quantum well. The Rashba coupling can be modulated up to 50% by a gate voltage perpendicular to the plane.\(^{22, 26}\) In some quantum wells such as GaAs the two terms are usually of the same order of magnitude, while in narrow gap compounds like InAs the Rashba coupling dominates.\(^{27-29}\) Experimentally the relative strength of the Rashba and Dresselhaus couplings can be extracted from photocurrent measurements.\(^{30}\)

In this paper we consider a spin-1/2 particle of charge \( -e \) and effective mass \( m \) confined by a semiconductor quantum well to a 2D \( x \)-\( y \) plane of length \( L_x \) and width \( L_y \).\(^{31}\) The particle is subjected to a spin-orbit interaction \( V_{SO}^{2D} \). A perpendicular magnetic field \( \mathbf{B} = -\mathbf{B}_Z = \mathbf{V} \times \mathbf{A} \) and an electric field \( \mathbf{E} = \mathbf{E}_y \) along the \( y \) axis are applied (see Fig. 1 in Ref. 6). Both electron-electron interaction and impurities will be neglected in our study. The Hamiltonian reads

\[ H = H_0 + e\mathbf{E}_y, \]

where \( g_x \) is the Lande \( g \) factor, and \( \mu_B \) is the Bohr magneton. In \( V_{SO}^{2D}(\mathbf{A}) \) the momentum \( \mathbf{p} \) is replaced by the canonical momentum, \( \mathbf{P} = \mathbf{p} + e/\mathbf{c} \mathbf{A} \). We choose the Landau gauge \( \mathbf{A} = y\mathbf{B} \) and consider a periodic boundary condition in the \( x \) direction, hence \( p_x = k \) is a good quantum number.

Below we rewrite the Hamiltonian in terms of lowering and raising operators. For each \( k \), we introduce the lowering operator

\[ a_k = \frac{1}{\sqrt{2l_B}} \left[ y + \frac{c}{e\mathbf{B}} (k + ip_x) \right], \]

and the corresponding raising operator \( a_k^\dagger = (a_k)^\dagger \), with the magnetic length \( l_B = \sqrt{\hbar c/e\mathbf{B}} \). \( a \) and \( a^\dagger \) satisfy the commutations \( [a_k, a_{k'}^\dagger] = \delta_{kk'} \), and \( [a_k, a_{k'}] = 0 \). In terms of \( a_k \) and \( a_k^\dagger \), we have

\[ H_0 / \hbar \omega = a_k^\dagger a_k + \frac{1}{2} (1 - g_x \sigma_z) i/\hbar (\tau = x, y), \]

from which we obtain

\[ v_x = \frac{\hbar}{\sqrt{2ml_B}} [a_k^\dagger + a_k + \sqrt{2} \eta_\theta \sigma_x + \sqrt{2} \eta_\theta \sigma_y], \]

\[ v_y = \frac{i\hbar}{\sqrt{2ml_B}} [a_k^\dagger + a_k + i\sqrt{2} \eta_\theta \sigma_x + i\sqrt{2} \eta_\theta \sigma_y]. \]

Comparing this with the standard expression of velocity for a charged particle in a magnetic field, \( \mathbf{v} = (\mathbf{p} + e/\mathbf{c} \mathbf{A}) / m \), the spin-orbit coupling effectively induces a spin-dependent vector potential.

B. Symmetries

We analyze three symmetries of the Hamiltonian in this section, which we will use in our calculations. 

Interchange symmetry of the two couplings. Under the unitary transformation, \( \sigma_x \rightarrow \sigma_y, \sigma_y \rightarrow -\sigma_x, \sigma_z \rightarrow -\sigma_z \), the Rashba and Dresselhaus couplings are interchanged,\(^7\)

\[ \alpha(\Pi_x \sigma_x - \Pi_y \sigma_y) \rightarrow \alpha(\Pi_y \sigma_y - \Pi_x \sigma_x); \]

\[ \beta(\Pi_x \sigma_x - \Pi_y \sigma_y) \rightarrow \beta(\Pi_y \sigma_y - \Pi_x \sigma_x); \]

\[ H_0 = \frac{1}{2m} \left( \frac{e}{c} + \mathbf{A} \right)^2 - \frac{g_x}{2} \mu_B \mathbf{B} \sigma_z + V_{SO}^{2D}(\mathbf{A}), \]
\( g_s \rightarrow -g_s. \) (7c)

Therefore a system with Rashba coupling \( \beta \), Dresselhaus coupling \( \alpha \), and Lande \( g \)-factor \( g_s \) is mapped onto a system with Rashba coupling \( \beta \), Dresselhaus coupling \( \alpha \), and Lande \( g \)-factor \(-g_s\). In particular, a system with only Dresselhaus coupling can be mapped onto a system with only Rashba coupling and an opposite sign in \( g_s \). This symmetry will be used in Sec. III. At the symmetric point \( \alpha = \beta, V_{SO}^D \) is invariant under the transformation. \( \alpha = -\beta \) is another symmetric point under the transformation, \( \alpha_s \rightarrow -\alpha_s, \sigma_s \rightarrow -\sigma_s, \sigma_s \rightarrow \sigma_s \). For physical parameters, we will always consider \( g_s \geq 0 \).

**Signs of the couplings.** Under the transformation, \( \alpha_s \rightarrow -\alpha_s, \sigma_s \rightarrow -\sigma_s, \sigma_s \rightarrow \sigma_s \), we have \( \alpha \rightarrow -\alpha \) and \( \beta \rightarrow -\beta \). The eigenenergy spectrum is invariant under the simultaneous sign changes of the two couplings. The eigenenergy spectrum is even in \( \eta_R \) if \( \theta_R = 0 \) and is even in \( \eta_D \) if \( \eta_R = 0 \).

**Charge conjugation.** Under the charge conjugation transformation, \( -e \rightarrow e \), the magnetic moment of the carrier also changes its sign, or effectively \( g_s \rightarrow -g_s \) in Eq. (4). This transformation is equivalent to the flip of the external magnetic field \( B \rightarrow -B \). Therefore a system of hole carriers has the same physical properties as the corresponding electron system except for possible directional changes in the observables. 31

\( H_0 \) can be solved analytically in the systems with only Rashba or only Dresselhaus coupling. An analytical solution is currently not available for \( H_0 \) with both couplings. 32–34 In the next section, we shall discuss the charge and spin Hall conductance of the electron system with a pure Rashba coupling. The results can be mapped easily onto the system with a pure Dresselhaus coupling and to the hole system in semiconductors by using the symmetries discussed above.

**III. SYSTEMS WITH PURE RASHBA OR PURE DRESSELHAUS COUPLING**

In this section we focus on systems with either Rashba coupling or Dresselhaus only. We will present the calculation with respect to the Rashba case. The Dresselhaus case can then be addressed using the interchange symmetry discussed above. After a brief review of the single particle solution in the absence of an electric field, we will discuss the spin Hall conductance by using linear response theory in Sec. III B, and its nonlinear effect and scaling behavior near the resonance in Sec. III C. Some of the analysis here has been previously reported. 9 For readability purposes we reproduce the highlights here for the linear response section. For the nonlinear effect, we expand the discussion from the previous work to emphasize that the spin Hall effect is not an artifact of perturbation theory.

**A. Single particle solution**

The single particle problem of \( H_0 \) with \( \eta_D = 0 \) can be solved. 25 The Rashba coupling hybridizes a spin down state in the \( n_0 \) Landau level with a spin-up state in the \((n_0 + 1)\)th Landau level, and the eigenenergies are given by

\[
\epsilon_{ns}^R = \hbar \omega \left( n + \frac{s}{2} \sqrt{(1-g)^2 + 8n\eta_R^2} \right),
\]

with \( s = \pm 1 \) for positive integer \( n \), and \( \epsilon_{0s}^R = \hbar \omega (1-g)/2 \). There is a large degeneracy \( N_{gs} = L_x L_y/(2\pi R^2) \) to each eigenenergy. The corresponding eigenstates are given by

\[
|n, k, s\rangle = \begin{pmatrix} \cos \theta_{ns} \phi_{nk} \\ i \sin \theta_{ns} \phi_{nk} \end{pmatrix}
\]

where \( \phi_{nk} \) is the eigenstate of the \( n^\text{th} \) Landau level with \( p_{nk} = k \) in the absence of the spin-orbit coupling, \( \theta_{nk} = 0 \), and \( \tan \theta_{ns} = -u_n s \sqrt{1 + u_n^2} \) for \( n \geq 1 \), with \( u_n = (1-g)/2nR\eta_R \).

The eigenenergies for the system with Dresselhaus coupling only can be obtained by replacing \( \eta_R \) by \( \eta_D \) and \( g \) by \(-g\).

\[
\epsilon_{ns}^D = \hbar \omega \left( n + \frac{s}{2} \sqrt{(1+g)^2 + 8n\eta_D^2} \right).
\]

The energy spectra versus \( \eta_R \) or \( \eta_D \) are plotted in Fig. 1. In the absence of the spin-orbit coupling, the Zeeman energy splits the two degenerate \( n_0 \)th Landau levels of spin-up and spin-down electron states into two nearby ones with the lower level for spin-up and the higher level for spin-down. As \( \eta_R \) increases from zero, the energy of the \( n_0 \)th Landau level state of spin-down is lowered because of its hybridization with the spin-up state at the \((n_0 + 1)\)th Landau level due to the Rashba coupling. The Rashba interaction competes with the Zeeman energy and there is an energy crossing at certain values of \( \eta_R \) or the magnetic fields as we can see in Fig. 1(a). The spin Hall resonance we examine is closely related to this level crossing. The energy level diagram in Fig. 1(b) for the Dresselhaus coupling has different features. In that case, a spin-up state, which is at the lower level due to the Zeeman splitting, mixes with a spin-down state at a higher Landau level, which separates further the Zeeman splitting, thus there is no resonance in the spin Hall current.

**B. Linear response theory: Spin Hall conductance**

We consider the charge and spin Hall currents along the \( x \) axis induced by an electric field along the \( y \) axis. In terms of the velocity operator, the charge and spin-\( z \) component current operators are defined by

\[
j_c = -e v_x,
\]

\[
j_s = \frac{\hbar}{4} (\sigma_z v_x + v_x \sigma_z),
\]

respectively. We refer readers to Ref. 6 for the discussions on the other spin components. The symmeterized form of the spin current operator guarantees that it is Hermitian. Each single particle state \(|\phi_{nk}\rangle\) carries a current \(|\phi_{nk}||c|\phi_{nk}\rangle\). The charge and spin Hall conductance are then given by

\[
G_{c,s} = \frac{1}{L_x L_y} \sum f_{nks} \langle \phi_{nk}|c|\phi_{nk}\rangle / E,
\]

where \( f_{nks} \) is the Fermi-Dirac distribution function. Note that since spin is not a conserved quantity in the presence of
spin-orbit couplings, the spin current defined above and the spin density do not satisfy a continuity equation. Nevertheless, the expectation values of the spin density and the spin current are well-defined. Unlike a free electron in a uniform magnetic field, the single particle problem with the spin-orbit coupling in the presence of an electric field $E\hat{y}$ is not analytically solvable, since the Landau levels mixing no longer truncate. After a replacement of $y \rightarrow y + eE/m\omega^2$ in the operator $a_k$ by $\bar{a}_k = a_k + eEh/\sqrt{2}\hbar\omega$, the Hamiltonian of the system in the presence of the electric field reads, apart from a constant, $H = H_0(E) + H'$, where $H_0(E)$ is the one in Eq. (5) by replacing $a_k$ with $\bar{a}_k$ and $H' = -eEh\eta R\sigma_y$. We now consider $H'$ as a perturbative Hamiltonian to study the charge and spin Hall currents. Up to the first order in $E$, we obtain

$$G_{c,d} = G_{c,d}^{(0)} + G_{c,d}^{(1)}$$

where the superscript refers to the zeroth order and first order in the perturbation in $H'$. The charge Hall conductance is found to be independent of the spin-orbit coupling, $G_c = n\hbar^2/2$, with $n = N_e/N_p$ being the filling factor. Within the perturbation theory, the spin Hall conductance $G_s$ can be divided into two parts. The part arising from the zeroth order in $H'$ is found to be the product of the spin polarization $\langle S^z \rangle$ per electron and the Hall conductance $G_e$, divided by the electron charge $(-e)$,

$$G_s^{(0)} = -\langle S^z \rangle G_e/e.$$  

The expectation value of the spin polarization per electron is

$$\langle S^z \rangle = \frac{1}{N_e} \sum_{n,k,s} \langle n,k,s | \sigma_z | n,k,s \rangle f_{nks} = \frac{1}{N_e} \sum_{n,k,s} \cos 2\theta_{ns} f_{nks}.$$  

The second part in $G_s$ arises from the first order in $H'$,

$$G_s^{(1)} = \frac{\epsilon \eta R}{8\pi\sqrt{2}} \sum_{n,k,s} \frac{f_{ns} - f_{ns'}}{E_{ns} - E_{ns'}} \times (\sqrt{n} \sin 2\theta_{ns} \sin^2 \theta_{ns'} - \sqrt{n'} \cos^2 \theta_{ns} \sin 2\theta_{ns'}).$$  

(17)

At $T=0$, if the two degenerate energy levels are partially occupied, $G_s^{(1)}$ may become divergent. Mathematically, the resonance is given by the condition $2n < \nu < 2n+1$ for the electron filling factor $\nu$, with $n$ an integer satisfying the equation

$$\sqrt{(1 - g)^2 + 8n\eta R} + \sqrt{(1 + g)^2 + 8(n + 1)\eta R} = 2.$$  

(18)

From the above condition, for a system with any $\eta R \neq 0$, $\eta D = 0$, and $g_s > 0$, there is a unique resonant magnetic field $B_0$ such that the resonant condition is satisfied. By symmetry, we obtain the resonance condition for the system with a pure Dresselhaus coupling, which is given by the solution for $n$ of the equation,

$$\sqrt{(1 + g)^2 + 8n\eta D} + \sqrt{(1 - g)^2 + 8(n + 1)\eta D} = 2.$$  

(19)

Unlike the pure Rashba coupling case, there is no solution for any $g_s > 0$ in the pure Dresselhaus coupling system. This is because the energy levels $E_{ns}$ and $E'_{ns'}$ with $n' = n \pm 1$ do not cross over, so the pairs of the crossing levels in the Dresselhaus coupling system correspond to $n' \neq n \pm 1$ and do not contribute to the spin Hall conductance.

We have calculated the spin Hall conductance numerically. $G_s$ at $T=0$ is shown in Fig. 2(b). In addition to the oscillation in $1/B$ similar to that of $\sigma_z$, there is a pronounced resonant peak at the filling $\nu = 12.6$. No such resonant peak occurs for the Dresselhaus case, as is shown in Fig. 2(d). In Fig. 3, we show $G_s$ at several temperatures for the Rashba

\[ FIG. 1. (a) Energy levels in units of $\hbar\omega$ as a function of the dimensionless Rashba coupling $\eta R$. The parameters are $\beta = 0.9 \times 10^{-11}$ eV m, $n_e = 1.9 \times 10^{16}/m^2$, $m_e = 0.05m_e$, and $g_s = 4$, taken from Ref. 22 for the inversion heterostructures In_{0.53}Ga_{0.47}As/In_{0.52}Al_{0.48}As. (b) Same as in (a), but for the Dresselhaus coupling $\eta D$ (with the same strength of the Rashba coupling). \]
The height of the resonance peak increases drastically as the temperature decreases below a few kelvin. In the inset of Fig. 3, we show the $T$-dependence of the height of the resonant peak and the two nearby side peaks. The characteristic temperature for the occurrence of the peak can be estimated to be the Zeeman energy $E_Z$, which is about 10 K at the resonant field for the parameters in the caption. More explicit derivation of this will be given in the next section.

C. Nonohmic spin Hall current and scaling behavior

In this section we study the nonlinear effect of the electric field to the resonant spin Hall current and the scaling behavior. Since the resonance originates from the interference of two degenerate levels near the Fermi energy, we will focus on those two levels to examine the problem. As an example, we shall consider In$_{0.53}$Ga$_{0.47}$As/In$_{0.52}$Ga$_{0.48}$As with the parameters given in Fig. 1, in which case the resonance occurs at the filling factor $n=12.6$ [see Fig. 1(b)] and the relevant two levels are $|1|=|n=6,k,s=+1\rangle$ and $|2|=|n+1=7,k,s=-1\rangle$. The energy levels below the two levels are assumed to be fully filled, and all levels above the two to be empty. This is valid if $\hbar \omega \gg k_B T$. The Hamiltonian is then, up to a constant, reduced to a $2 \times 2$ matrix,

$$H_{\text{reduced}} = \begin{pmatrix} \Delta \epsilon & \nu_0 \\ \nu_0 & -\Delta \epsilon \end{pmatrix},$$

where $\Delta \epsilon = (\epsilon_{6,+1}^R - \epsilon_{7,-1}^R)/2$, and
we obtain the singular part of the spin Hall conductance to be
\[ G_s = \frac{\delta_\ell e}{4\pi} \frac{E_Z}{v_0^2} \frac{f_-(1-f_+)}{f_++f_-} \left[ 1 - e^{-2\sqrt{(\Delta e)^2 + v_0^2}/k_B T} \right] \] (23)
where the factor \( f_-(1-f_+)/f_++f_- \) is a slowly varying function of \( T \) ranging from 1 at low temperatures to \( (1-\delta_\ell/2)/2 \) at high temperatures. At low temperatures \( G_s \) is given by
\[ G_s = -\frac{e}{4\pi |h|} \] (24)

It is only a function of the reduced magnetic field and the excess part of the filling factor from 2n. At the resonant magnetic field, i.e., \( b=0 \), the spin Hall current approaches with lowering temperature to a constant,
\[ f_- = -\varepsilon E_Z/(e\ell b \eta_R \cos \theta_{0,\pm} \sin \theta_{1,\pm}) \] as can be seen in Fig. 5. Using the resonance condition in Eq. (18), \( B_0 = 4nm^2c^2\beta^2/h^3 \) \((n=6)\) and using the fact that for large \( n \), \( n \) is proportional to \( 1/B_0 \) the resonant magnetic field \( B_0 \) \( \propto \beta \sqrt{|g|} \) approximately. Thus the resonant spin current is proportional to
\[ I_s = -\frac{\delta_\ell e^2}{8\pi m^2 c^2} \frac{g B_0^2}{\beta} \propto \delta_\ell \beta. \] (25)

Therefore for a given filling factor, the larger the spin-orbit coupling \( \beta \) is, the stronger the spin Hall resonance. The resulted spin Hall conductance diverges at \( T=0 \) as
\[ G_s = -\frac{\delta_\ell e}{4\pi |v_0|} \frac{E_Z}{8\pi m^2 c^2} \frac{g B_0^2}{\beta} E. \] (26)

At temperatures \( k_B T > \sqrt{(\Delta e)^2 + v_0^2} \),
\[ G_s = -\frac{\delta_\ell (1-\delta_\ell/2)e}{4\pi} \frac{2E_Z}{k_B T} \] (27)
and the integral
\[ \int G_x db = \frac{\delta_\ell e}{2\pi} \left[ \ln \frac{2E_Z}{k_B T} \right]. \]

This integral reflects the weight of the resonant peak of the spin Hall conductance.

Since the method used in this section is beyond perturbation theory, we conclude that the resonance spin Hall conductance we predict is not an artifact of the perturbation method. Instead, the resonance is caused by the interference between the two degenerate energy levels at the Fermi energy.

**IV. SYSTEMS WITH BOTH RASHBA AND DRESSELHAUS COUPLINGS**

In this section we briefly discuss the resonance in the spin Hall conductance in systems with both Rashba and Dresselhaus couplings. The Hamiltonian including the electric potential reads

\[ \Delta E_{\text{gap}} \]

**FIG. 4.** Schematic illustration of the energy shift due to the electric field in the two degenerate levels near the resonant point.

\[ \nu_0 = (2|H'|1) = -eE l_b \eta_R \cos \theta_{0,\pm} \sin \theta_{1,\pm}. \]

As we can see from the reduced Hamiltonian and from Fig. 4, the electric field breaks the level degeneracy and opens an energy gap \( \Delta E_{\text{gap}} = 2|\nu_0| \). Denoting the two eigenstates of the reduced Hamiltonian by \( |\Phi_\pm\rangle \), the spin Hall current density is given by
\[ I_s = \frac{1}{2\pi l_B^2} (i_{f_-} + i_{f_+}), \] (21)
where the Fermi-Dirac distribution \( f_\pm = (\exp[(\pm\sqrt{(\Delta e)^2 + v_0^2} - \mu)/k_B T])^{-1} \), with \( f_+ + f_- = \delta_\ell = \nu - 2n \), \( \mu \) the chemical potential, and \( i_s = \langle \Phi_\pm | j_x | \Phi_\pm \rangle \). The electric field and temperature dependences of the spin current \( I_s \) near the resonance point is plotted in Fig. 5. At low temperatures the resonant spin current approaches to a constant in a weak electric field.

Now we analyze the scaling behavior of the spin conductance near the resonance point. For simplicity we limit our discussion to the case of \( \delta_\ell < 1 \) and \( g \ll 1 \). Near the resonant point, \( \Delta e \approx -E_Z b \) where \( E_Z = g\hbar \omega_0/2 \) is the Zeeman energy and \( b = (B-B_0)/B_0 \) is the reduced dimensionless magnetic field. Using the identity
\[ f_- - f_+ = f_-(1 - f_+) [1 - e^{-2\sqrt{(\Delta e)^2 + v_0^2}/k_B T}], \] (22)
we obtain the singular part of the spin Hall conductance to be
The large number \( n \) with \( h \) generate if the following equation is satisfied: the perturbation to the second order. The two levels become degenerate if \( \eta_N = 0 \) is coupled to \( |n_0+1, \uparrow \rangle \) via the Rashba coupling, which is further coupled to \( |n_0+2, \downarrow \rangle \) due to the Dresselhaus coupling. In this way, a Landau level is coupled to an infinite number of other Landau levels, and the analytic solution is not available. The problem, however, may be approximately solved by using perturbation theory to treat \( \eta_R \) and \( \eta_D \) as small parameters. This is equivalent to the limit \( B \to \infty \), since \( \eta_{N,B} \to 1/\sqrt{B} \). For parameter values given in Fig. 1, \( \eta_N = 0.004 \ll 1 \) at the resonant field \( B = 6.1 \) T. In the absence of the electric field, the single particle energy, up to the second order in \( \eta_R \) and \( \eta_D \), is given by

\[
\frac{\epsilon_{n_0}}{\hbar \omega} = n_0 + \frac{1 - g}{2} + \frac{2n_0 \eta_R^2}{1 - g} - \frac{2(n_0 + 1) \eta_D^2}{1 + g}, \tag{29a}
\]

\[
\frac{\epsilon_{n_0}}{\hbar \omega} = n_0 + \frac{1 + g}{2} + \frac{2n_0 \eta_D^2}{1 + g} - \frac{2(n_0 + 1) \eta_R^2}{1 - g}. \tag{29b}
\]

Note that the mixed term of \( \eta_R \eta_D \) does not appear in the perturbation to the second order. The two levels become degenerate if the following equation is satisfied:

\[
\frac{g}{2(2n_0 + 1)} = \frac{\eta_R^2}{1 - g} - \frac{\eta_D^2}{1 + g}. \tag{30}
\]

It follows that a necessary condition for the resonant spin Hall current is \( \eta_R^2/\eta_D^2 > (1 - g)/(1 + g) \approx 1 \), for \( g \ll 1 \). At \( \eta_D = 0 \) and in the limit \( \eta_R \ll 1 \), Eq. (30) is consistent with Eq. (18) for the resonant condition we derived for the pure Rashba system. Alternatively the resonant magnetic field is

\[
B_0 = \frac{2(2n_0 + 1) mc^2}{g} \frac{B_0}{e h^2} (\beta^2 - \alpha^2). \tag{31}
\]

The large number \( n_0 \) increases with \( 1/B_0 \) for a specific density of particles. Thus for a certain Rashba coupling the increasing of Dresselhaus coupling will decrease the resonant magnetic field \( B_0 \). The singular part of the spin Hall conductance can be studied by examining the two level system in the presence of an electric field as we described in Sec. III C. At the resonant point and at low temperature,

\[
G_s = -\delta e^2 \hbar^2 \frac{g B_0^2}{8 \pi m^2 e^2 c^2 \sqrt{\alpha^2 + \beta^2}} \frac{1}{E}. \tag{32}
\]

As the Dresselhaus coupling increases from zero, the resonance is shifted to lower magnetic fields and occurs at higher Landau levels with a weaker resonant strength.

V. SUMMARY AND DISCUSSIONS

In summary, we have studied the spin Hall effect in a two-dimensional electron system with spin-orbit couplings in a strong perpendicular magnetic field. In systems with the Rashba coupling dominating over the Dresselhaus coupling, there is a resonant magnetic field at which the spin Hall conductance diverges at low temperature and low electric field. The physics for this resonance is the energy level crossing of the two Landau levels due to the competition of the Zeeman splitting and the Rashba coupling. For a given system, there is a unique resonant magnetic field, at which the two Landau levels become degenerate at the Fermi energy. In this case, some physical properties may show singularity. As studied earlier, the spin polarization will change its sign as the magnetic field is varied passing through the resonant field. Namely the magnetic susceptibility is divergent. The spin Hall conductance is another singular response due to this level crossing. When an infinitesimally weak dc electric field is applied in the plane, the two degenerate Landau levels are split accordingly and a finite spin Hall current is induced. The resonance is macroscopic in the sense that a huge number of the states in the same Landau level are involved in the process. We have calculated the temperature and electric field dependences of the resonance. The characteristic temperature for the resonant spin Hall current is of order of the Zeeman energy. As the temperature decreases, the height of the resonance peak diverges like \( \sim 1/T \) and the weight diverges like \( \sim \ln T \). While the spin orbit coupling has a dramatic effect on the spin Hall conductance, the charge Hall conductance is not affected and remains quantized. The spin Hall current is nonlinear with the electric field at the resonant field. At low temperatures, the spin Hall current rapidly rises linearly with the electric field and saturates at higher electric fields. At \( T = 0 \), the spin Hall conductance diverges as \( 1/E \) at resonance. Near the resonant magnetic field \( B_0 \), it is \( \sim 1/B_0 \). Contrary to the Rashba coupling, the Dresselhaus coupling further increases the Zeeman energy splitting to suppress the effect of the Rashba coupling. The strength of the Rashba coupling necessary to surpass the Dresselhaus coupling, in order to have the resonant spin Hall current, was estimated by using a perturbation method treating the couplings as small parameters. This is accurate as long as the Zeeman energy is much smaller than the cyclotron frequency.

We have assumed no potential disorder in our theory. The effects of disorder in 2DEG with Rashba coupling, especially in a strong magnetic field, is not well understood at this point. Nevertheless, it seems reasonable to assume that the spin-orbit coupling does not change the effects of disorder qualitatively. This is likely to be the case in the presence of a strong magnetic field, which ensures extended states in the Landau levels when the disorder is not sufficiently strong as evidenced by the experimentally observed quantization of the Hall conductance. We then assume that the disorder gives rise to broadening of the Landau level and localization so that the extended states in a Landau levels are separate in energy from those in the next one by localized states. Inspection of the spin-orbit coupling shows that Laughlin’s gauge argument still holds, and each Landau level with its extended states completely filled contribute \( e^2/h \) to the charge Hall conductance. Thus we conclude that the quantum Hall conductance remains intact with the spin-orbit interaction, except at the special degeneracy point. As the Fermi energy
varies across this degenerate extended state, the charge Hall conductance $G_c$ is expected to change by $2e^2/h$, instead of $e^2/h$ for the other extended levels. This fact can be used experimentally to determine the Rashba interaction induced degeneracy discussed in this paper.

This work was in part supported by the Research Grant Council in Hong Kong (S.Q.S. and F.C.Z.), NSF ITR Grant No. 0223574 (F.C.Z.), and DOE/DE-FG02-04ER46124 (X.C.X.).

ACKNOWLEDGMENTS

31A hole in semiconductor carries a positive charge $e$.
Edge spin current and spin polarization in quantum Hall regime

Yun-Juan Bao, Huai-Bing Zhuang, Shun-Qing Shen, and Fu-Chun Zhang*
Department of Physics, and Center for Theoretical and Computational Physics, The University of Hong Kong, Pokfulam Road, Hong Kong, China

(Received 29 September 2005; published 16 December 2005)

We study the edge spin current and spin polarization, and their responses to an external electric field in a two-dimensional electron gas with a Rashba spin-orbit coupling in the quantum Hall regime. The edge state carries a large spin current, which drops sharply away from the boundary. The spin Hall current of the edge states has a resonance at a critical magnetic field, accompanied by a spin rotation in the bulk. The spin Hall current is shown to be proportional to the spin polarization, which provides an explicit way to extract the spin current in experiment.

DOI: 10.1103/PhysRevB.72.245323 PACS number(s): 72.20.My, 71.10.Ca, 75.47.

I. INTRODUCTION

The edge state and edge charge current in two-dimensional electron gas (2DEG) in a magnetic field have been well studied in the past two decades and have played an important role in understanding the quantum Hall effect. Recent progress on spintronics stimulate extensive study of spin generation and transport in semiconductors. The relati-vistic quantum effect of moving electrons in a confining potential in 2DEG induces a spin-orbit coupling to split the energy spectra of electrons and provides an efficient way to control the electron’s spin. Driven by an external electric field, moving electrons may generate a pure spin Hall current via the magnetic impurity or spin-orbit coupling. Very recently the spin accumulation has been observed in both n-type semiconductors and p-type heterojunctions in experiments, which provides substantial evidence of pure spin current. In the presence of a strong magnetic field, the competition between the Rashba spin-orbit coupling and the Zeeman splitting in 2DEG introduces an additional degeneracy and gives rise to some interesting effects, such as the resonant spin Hall conductance and the anisotropic spin transport. In this paper we study the edge spin current and spin polarization, and their responses to an external electric field in 2DEG with a Rashba coupling in a magnetic field. The edge effect will cause the anticrossing of Landau levels. The spin Hall conductance is calculated using the edge state approach, and the result can be used to complement the bulk theory for the resonant spin Hall effect. The spin current is shown to be proportional to the spin polarization along the y direction in a finite magnetic field, which provides an explicit way to extract the spin current in experiments.

II. MODEL AND METHOD

We consider a 2DEG with the Rashba coupling in the x-y plane of area $L \times L$ subject to a perpendicular magnetic field $B = B \hat{z}$. The electrons are confined between $-L/2$ and $L/2$ in the y direction by an infinite potential wall, and its wave function is periodic along the x direction. We choose the Landau gauge $A = B y \hat{x}$. The Hamiltonian for a single electron with a Rashba coupling is given by:

$$H = \frac{\hat{p}^2}{2m} - g_S \mu_B B \sigma_z + \frac{\hbar}{2} (\sigma_y - \sigma_x),$$

where the confining potential is implied. $m$, $-e$, and $g_S$ are the electron’s effective mass, charge, and Landé-g factor, respectively. $\sigma_y = \hat{p} + eA/\hbar$ is the kinetic operator, $\mu_B$ is the Bohr magneton, and $\sigma$ are the Pauli matrices. The edge state and the edge charge current in the absence of the Rashba coupling have been studied previously. In that case, the eigenstate is given by

$$\Phi_{n,y_0} = e^{y_0 \sigma_y} \varphi_{n,y_0}(y) \chi_n,$$

with $n$ the Landau level index, $\varphi_{n,y_0}(y)$ the $x$-component momentum quantum number or the guiding center of the wave function $\phi_{n,y_0}(y)$, and the magnetic length $l_B = \sqrt{\hbar/c e B}$. $\chi_n$ is the eigenstate of spin $S_z = \pm 1/2$. Since the magnetic length is usually much smaller than the size of the sample, it can be regarded as the position of electron. The wave function $\phi_{n,y_0}(y)$ is the confluent hypergeometric function determined by the eigenvalue equation

$$a_0^{y_0} a_{y_0} \phi_{n,y_0} = \nu_{n,y_0} \phi_{n,y_0},$$

satisfying the boundary condition $\phi_{n,y_0}(\pm L/2) = 0$, where $a_0 = \sqrt{y_0 + i (c/\epsilon e B) p_y} / \sqrt{2} l_B$ and $[a_0, a_0^\dagger] = \delta_{y_0,y_0'}$. The energy eigenvalues are

$$E_{n,y_0}^{(0)}(y_0) = \nu_{n,y_0} + \frac{1}{2} (1 - g_S) \hbar \omega,$$

where $\omega = eB/mc$ is the cyclotron frequency. For $|y_0| \ll L/2$ far away from the edges, the problem is reduced to a simple harmonic oscillator and the eigenvalue $\nu_{n,y_0} = n$, a nonnegative integer. $\nu_{n,y_0}$ increases monotonically to $\nu_{n,y_0} = 2n + 1$ when $y_0$ approaches the two edges, $y_0 = \pm L/2$.

In the presence of the Rashba spin-orbit coupling, $p_x$ remains to be a good quantum number. In the Hilbert subspace of $y_0$, the Hamiltonian can be written as

1098-0121/2005/72(24)/245323(5)/$23.00 245323-1 ©2005 The American Physical Society
BAO et al. in the same Landau level, namely, the level anticrossing may be understood as follows. The general magnetic lengths as shown in Fig. 1. The edge effect on the Landau level splitting introduces an additional degeneracy, there is a competition between the Rashba coupling and the Zeeman splitting mixes only two states \( \Phi_{n,0} \) and \( \Phi_{n+1,0} \) so that an analytical solution can be obtained.\(^8\)\(^9\)\(^11\) Near the boundary, exact analytical solutions seem unlikely. We use \( \{\Phi_{n,0} \, | \, n \geq 0\} \), the eigenstates of \( H(y_0) \) at \( \lambda = 0 \), as the base functions. The lower energy spectra \( \{E_n(y_0)\} \) and the corresponding eigenvectors can be obtained numerically by truncating sufficiently higher Landau level states. In Fig. 1, we show a typical energy spectrum of the lowest 20 Landau levels at \( y_0 = L/2 - 4l_b \) as a function of the effective Rashba coupling \( \eta \), for a set of realistic parameters suitable for In\(_{0.53}\)Ga\(_{0.47}\)As/In\(_{0.52}\)Al\(_{0.48}\)As.\(^12\) Although the quantitative results depend on the precise parameters, the basic physics we address is quite general. Different from the bulk state, where the competition between the Rashba coupling and the Zeeman splitting introduces an additional degeneracy,\(^8\) there is a level anticrossing\(^13\) near the boundary of a distance of several magnetic lengths as shown in Fig. 1. The edge effect on the level anticrossing may be understood as follows. The Rashba coupling mixes the two edge states of opposite spins in the same Landau level, namely, \( \Phi_{n,1/0} = 1 \) and \( \Phi_{n,3/0,1} \), while this mixing vanishes for the bulk states.

III. EDGE SPIN CURRENT AND POLARIZATION

We now turn to the discussion of the charge and spin currents and the spin polarization near the boundary. The charge current operator of a single electron, in the Hilbert subspace of \( y_0 \), is given by

\[ j_c = -e \mathbf{v} \cdot \mathbf{s} \],

and \( \mathbf{v} = [x, H]/i \hbar \). The spin-\( \alpha \) component current operator is

\[ j^\alpha_x = \frac{\hbar}{4} (\sigma_y v_y + v_x \sigma_x) \].

Let \( (j^c)_x \) be the charge \( (c) \) or spin \( (s) \) current carried by an electron in the eigenstate of \( H \) in Eq. (1) with a collective index \( \tau = (n, y_0, s) \) and \( (S^\tau)_x = \langle \tau | \sigma_x | \tau \rangle \hbar/2 \) the average \( \alpha \) component spin polarization in that state. Note that the state represented by \( y_0 \) is extended in the \( x \) direction but localized around \( y = y_0 \) in the \( y \) direction. The calculated expectation values are plotted in Fig. 2 as functions of the position of the edge state described by \( y_0 = L/2 - \xi l_b (\xi > 0) \), where \( \xi \) is the distance to the edge in the unit of \( l_b \). In comparison with their bulk values, both \( (j^c)_x \) and \( (j^s)_x \) are markedly larger. As for the spin polarization, \( (S^c)_x = 0 \), while \( (S^s)_x \), and \( (S^s)_y \), display interesting features: the spin is mostly polarized along the \( z \)-axis in the bulk, while mostly polarized along the \( y \)-axis at the edges. It is interesting to note from Fig. 2 that the large polarization of \( S_y \) coincides with the large charge current at the edge. From a mean-field point of view, the Rashba coupling

\[ V_R(y_0) = \frac{\lambda m}{\hbar^2} (v_x \sigma_y - v_y \sigma_x) - \frac{2m \lambda}{\hbar^2} \]

introduces an effective magnetic field, which is proportional and normal to the charge current along the \( x \) direction. It is most interesting to note that the average of \( S_x \) is identical to the spin current \( j^s_x \) except for an overall proportionality.

\[ (j^c)_x = -0.831 \left( \frac{\hbar}{m l_b} \right) (S^c)_x \]

for the specific parameters in Fig. 2. In fact, there is an exact relation between the two quantities in the present case,
for the equation, we consider a commutator,\textsuperscript{14}

\[ [H, \sigma_z] = -i \left( \frac{4m \lambda^2}{\hbar^2} \right) \hat{j}_z - i g_s \mu_B B \sigma_y. \]  

To derive the above relation and to see the required condition for the equation, we consider a commutator,\textsuperscript{14}

\[ \lambda(\hat{j})_\tau = -\left( \frac{g_s \mu_B}{2m} \right) B(S^\tau)_\tau. \]  

In the present case, \( p_x \) is a good quantum number and the energy eigenstate \( |\tau\rangle \) is localized in the \( y \) direction around \( -y_0 \) and vanishes at the two edges. Because of these properties, the expectation value of this commutator

\[ \langle [H, \sigma_z] \rangle_\tau = \langle \tau | H \sigma_z - \sigma_z H | \tau \rangle = 0 \]

and, hence, Eq. (10) is approved. We note that the relation holds in the presence of an electric field \( E = E_y \). Because the relation applies to each eigenstate of \( H \) in the absence or in the presence of an electric field, the thermodynamic averages of the spin polarization and the spin current are also proportional. However, one has to be cautious to apply the relation to the case with \( B=0 \) and \( E \neq 0 \). At \( B=0 \), the states are extended in both the \( x \) and \( y \) directions, and the above derivation for the vanishing integral may not apply. We note that the spin Hall current at \( B=0 \) cannot be obtained by taking \( B \rightarrow 0 \). Inclusion of the Dresselhaus coupling\textsuperscript{15} will also give a relevant relation. In the presence of disorder and electron-electron interactions, the spin current and spin polarization vary in space, but such a relation between the spin current and the spin polarization can be shown to hold at any spatial point in the quantum Hall regime. The detailed discussion will be presented elsewhere.

IV. RESONANT SPIN HALL EFFECT: EDGE-STATE PICTURE

Now we come to discuss the effect of an electric field along the \( y \) direction, \( V_y = -eE_y \). We use the truncation approximation to solve the problem and evaluate the energy eigenvalues and eigenstates numerically. We find that the edge charge current responses linearly to the electric field. Here we focus on the nonlinear behaviors of the spin currents and spin polarization at or near the resonant magnetic field \( B_0 \) where the two levels in the bulk are degenerate.\textsuperscript{8} In Fig. 3, we plot \( \langle j_y \rangle_\tau \), \( (S^y)_\tau \), and \( (S^z)_\tau \) in a weak electric field \( E = 0.01 \text{ V/m} \). Our data show that \( \langle j_y \rangle_\tau \) is still proportional to \( (S^y)_\tau \) in the presence of the electric field; therefore, we plot \( \langle j_y \rangle_\tau \) and \( (S^y)_\tau \) in the same figure. At the resonant point we note that the electric field generates a finite spin current in the bulk, which is almost equal to the edge spin current at the edge of \( y_0 = -L/2 \). At the edge of \( y_0 = +L/2 \), the current has the same value, but different direction. \( (S^z)_\tau \) decreases quickly to zero, but the \( (S^y)_\tau \) increases to \( 1 \) approximately in a unit of \( h/2 \). Thus, the spin rotates from the \( z \) to \( y \) direction. Near the resonant magnetic field where the energy gap \( E_G \) of the two levels at the bulk is larger than but comparable with the electric field energy, \( E_G = eE_l \), both the spin current and spin polarization vary nonlinearly with the electric field. When the energy gap \( E_G \) is much larger than the electric field energy, \( E_G \gg eE_l \), the response becomes linear to the field. The rotation of the spins of the two levels in a weak field can be understood in the theory of resonant spin Hall effect.\textsuperscript{8} A weak field removes the degeneracy of the two levels of the bulk along the spin \( z \) direction, and as a result, the mixed two levels give the spin along the \( y \) direction. The rotation of spin from the spin \( z \) direction to the spin \( y \) direction should be observed near the resonant point experimentally.

With the periodic boundary condition along the \( x \) direction, the velocity operator in the Hilbert subspace of \( y_0 \) can
Following the works by Halperin and MacDonald and Streda, the total spin Hall current in the filled Landau level \((n,s)\) can be expressed as

\[
(j^z)_{n,s} = \frac{e}{2\pi} \int_{-L/2}^{+L/2} \frac{dy_0}{\gamma_0} \left[ E_{n,s}(y_0) - E_{n',s'}(y_0) \right] \times \langle \tau | \partial_{y_0} \tau' \rangle \langle \sigma_z | \tau' \rangle - \langle \tau' | \sigma_z | \tau \rangle \langle \tau' | \partial_{y_0} | \tau \rangle.
\]

where \(\tau' = (n',y_0,s')\). Without the spin-orbit coupling the energy eigenstate satisfies \(\langle \tau | \sigma_z | \tau' \rangle = s \delta_{n,n'} \delta_{s,s'}\), so that

\[
(j^z)_{n,s} = -\frac{seV}{4\pi},
\]

which is only determined by the voltage difference at the two edges,

\[
E_{n,s}(L/2) - E_{n,s}(-L/2) = -eV,
\]

and the inclusion of impurities and Coulomb interactions in the Hamiltonian does not affect this result as for the charge Hall current. The spin Hall conductance displays a series of plateaus in the quantum Hall regime, corresponding to the quantum Hall conductance, \(G_c = ne^2/h\). In the presence of spin-orbit coupling, the states with different spins will be mixed together, and the spin gradually deviates from the \(z\) to \(y\) direction and the spin Hall conductance varies with the effective Rashba coupling or magnetic field through tuning the energy gap between the two states especially near the Fermi level. We calculate the total spin Hall conductance numerically as a function of \(1/B\) for a fixed chemical potential assuming that the voltage drops only near the edges and the bulk state does not contribute to the total conductance numerically as a function of \(1/B\) for a fixed chemical potential assuming that the voltage drops only near the edges and the bulk state does not contribute to the total conductance numerically as a function of \(1/B\) for a fixed chemical potential assuming that the voltage drops only near the edges and the bulk state does not contribute to the total conductance.

\[
G_s = \frac{e}{8\pi} \left[ 1 - (-1)^n \right]
\]

FIG. 3. (Color online) The spin polarization and spin current of the two levels that are almost degenerated subjected to an fixed external electric field, \(E_0 = 0.01 \text{ V/m}\). The left is for \(y_0 = L/2 - \delta y\) and the right is for \(y_0 = -L/2 + \delta y\). (a) The solid line is for the two levels with an energy gap \(\Delta E\) in the bulk less than the electric field energy \(eE_0\); (b) the dashed line for the two levels with \(\Delta E = eE_0\); (c) the dashed-dotted line for the two levels of \(\Delta E \gg eE_0\). (The energy gap \(\Delta E\) is controllable by the magnetic field near the resonant point.)

![Figure 3](image1)

FIG. 4. (Color online) The spin Hall conductance (pillars shape) and charge Hall conductance (staircase shape) as a function of \(1/B\) for a fixed chemical potential, \(\mu = 14.539 \text{ meV}\). The inset is spin Hall conductance for a fixed density of charge carriers, \(n_e = 1.9 \times 10^{12} \text{ cm}^{-2}\).
spin Hall current. Both charge and spin Hall conductances are plotted in Fig. 4. As expected the Hall conductance is quantized: the spin Hall conductance has the order of $e/4\pi$ if an odd number of Landau levels are occupied, and is of order \(10^{-3} - 10^{-4}e/4\pi\) if an even number of Landau levels are occupied. The spin Hall conductance is a function of the effective spin-orbit coupling, which varies with the magnetic field. The resonant peak appears only when the two degenerate bulk Landau levels cross over a special value of chemical potential with decreasing the magnetic field. In the inset of Fig. 4, we extract the spin Hall conductance for a fixed density of charge carriers from the results for a fixed chemical potential if \(L \gg l_s\). The values of the spin Hall conductance are consistent with the bulk theory for the fully filled Landau levels.\(^8\)

V. CONCLUSION AND DISCUSSION

The spin and charge edge currents will become dominant when the bulk states are localized due to the impurities and the charge Hall conductance is quantized. In a realistic sample of a finite size, both charge and spin bulk Hall current densities will not be suppressed completely, but decay with the size of the sample if the impurities are taken into account. The total charge and spin Hall currents consist of both the edge and bulk currents. The ratio of the edge and bulk Hall currents or the distribution of the electric field are determined by the disorder, Coulomb interaction, and the rigidity of the confining potential wall as studied by several authors.\(^16\) The quantum Hall effect can be understood from both the bulk and edge-state point of view. In this paper, we have presented a picture of edge states for spin Hall conductance for a 2DEG with a Rashba coupling. The theory is consistent with and complementary to the bulk theory for resonant spin Hall conductance, especially in the quantum Hall regime. In this system the motion of electrons will induce an effective magnetic field via the Rashba coupling and generate spin polarization. Since the spin current is proportional to the spin polarization along the \(y\) direction, this relation will provide an explicit way to extract spin current from the distribution of spin polarization.

ACKNOWLEDGMENTS

The authors would like to thank Kun Yang and Qian Niu for helpful discussions. This work was supported by the Research Grant Council of Hong Kong (No. HKU7039/05P).

---

\(^8\) On leave from Department of Physics, University of Cincinnati, Ohio


\(^10\) The Dresselhaus coupling appears in narrowband semiconductors without bulk inversion symmetry. Its competition with the Rashba coupling will change the electron spectra and shift the resonant points of the Landau levels. Inclusion of the Dresselhaus coupling will not change the main results in this paper qualitatively.


\(^13\) A. Reynoso, G. Usaj, M. J. Sanchez, and C. A. Balseiro, Phys. Rev. B 70, 235344 (2004); A similar commutator was considered by O. V. Dimitrova, condmat/0407612 (unpublished), and by E. I. Rashba, Phys. Rev. B 70, 201309(R) (2004). In the absence of an external magnetic field, they observed that \(j_y^s = -(\hbar^2/2m^*)[V_{\perp}, \sigma_y]\).


Contractor renormalization group theory of SU(N) chains and ladders

Peng Li and Shun-Qing Shen

Department of Physics, The University of Hong Kong, Pokfulam Road, Hong Kong, China

(Received 8 December 2004; revised manuscript received 7 March 2005; published 1 June 2005)

The contractor renormalization group (CORE) method is applied to the SU(N) chain and ladders in this paper. In our designed schemes, we show that two classes of systems can return to their original form of Hamiltonian after CORE transformation. Successive iteration of the transformation leads to a fixed point so that the ground state energy and the energy gap to the ground state can be deduced. The result of SU(N) chain is compared with the one by Bethe ansatz method. The transformation on spin-1/2 ladders gives a finite gap in the excited energy spectra to the ground state in an intuitive way. The application to SU(3) ladders is also discussed.

DOI: 10.1103/PhysRevB.71.212401 PACS number(s): 75.10.Pq, 64.60.Ak, 05.50.+q

The contractor renormalization (CORE) group method combines the contraction and cluster expansion techniques with the real space renormalization group approach to solve the electron and spin lattice problems. It was first applied to spin-1/2 Heisenberg chain and (1+1)-dimensional Ising model, and later to the frustrated antiferromagnets and the Haldane conjecture. The results are satisfactory and encouraging. Since then the method has been applied to investigate low energy physics in many strongly correlated systems. In this paper, we are concerned with a class of models showing that CORE is at its critical point, which means that the symmetry of the system is restored or the same form of Hamiltonian is recovered iteratively and a quite satisfactory result can be obtained. The recovery of the form of the Hamiltonian owes highly to the SU(2) symmetry and an adequate designed CORE scheme. As a generalization, we found that their CORE scheme on SU(2) chain is a specimen picked out from a general CORE scheme on the SU(N) chain. Though the SU(N) chain had been exactly solved by Bethe ansatz method long time ago, it is still instructive to see how CORE works in the system.

Let us start with a one-dimensional SU(N) chain in terms of the exchange operator, \( H = \sum_{j=1}^{N} P_{j} \). Here we limit our discussion to the antiferromagnetic case by setting \( J = 1 > 0 \). For a SU(N) system each site \( j \) has \( N \) quantum states \( | j, \alpha \rangle \) with \( (\alpha = 1, 2, \ldots, N) \). The exchange operator \( P_{j} \) swaps two states on sites \( j \) and \( j+1 \), i.e., \( P_{j;j+1} | j, \alpha; j+1, \beta \rangle = | j, \beta; j+1, \alpha \rangle \). Usually \( P_{j;j+1} \) can be expressed in terms of the SU(N) generators as \( P_{j;j+1} = \sum_{\alpha \beta} a_{\alpha \beta}^{\mu} a^{\dagger}_{\beta \alpha} \), where the operators \( J_{\mu}^{\beta}(j) \) satisfy the SU(N) algebra \( [J_{\mu}^{\alpha}(j), J_{\nu}^{\beta}(j')] = \delta_{\mu\nu}[\delta_{\alpha\beta}(j)-\delta_{\beta\alpha}(j')] \). Alternatively, \( P_{j;j+1} \) can also be expressed by spin operators. Many spin systems as well as spin-orbit systems concerning SU(N) symmetry have been studied extensively.

In the CORE scheme, the first step is to divide the original chain into a chain of blocks and retain adequate number of energy levels in each block. We found two obvious schemes to be readily applied to this system: one is \( (N-1) \)-site block partition with \( N \)-state truncation (scheme A), and the other is \( (N+1) \)-site block partition with \( N \)-state truncation (scheme B). The treatment on SU(2) case in Ref. 1 obviously falls into scheme B with \( P_{j;j+1} = 2S_{j}S_{j+1} + 1/2 \) when \( N = 2 \). We will see the scheme B gives better results than scheme A. The existence of the two schemes can be understood from the single column Young tableaux with \( (N-1) \) or \( (N+1) \) boxes. In fact the SU(N) model on both \( (N-1) \)-site block and \( (N+1) \)-site block have one unique \( N \)-dimensional ground state space. We denote the truncated space for a single block by \( \Phi_{l} = \{| \phi_{j,1}, | \phi_{j,2}, \ldots, | \phi_{j,N} \} \). Then in the range-2 CORE calculation, we should retain appropriate \( N^{2} \) low levels from the exact diagonalization of two blocks. All the retained low levels should have nonzero projection to the product space \( \Phi_{l} \otimes \Phi_{j+1} \), so the eligible levels are not always the lowest ones. Fortunately this job is easy to be done due to the SU(N) symmetry. The range-2 CORE calculation leads to the effective Hamiltonian.
The range-4 result for scheme B of CORE gives better results and the numerical errors are about $-0.0106$, $-0.0006$, and $0.0021$ for $N=2, 3, 4$, respectively, compared to the results by Bethe ansatz method (see Ref. 9).

\[ H^{(2)} = \frac{1}{N+1} \sum_j (-C_+ + K_+ \tilde{P}_{j,j+1}), \]

where the sign $\tilde{\pm}$ corresponds to the two schemes A ($-$) and B ($+\cdot$), $\tilde{P}_{j,j+2}$ is a renormalized exchange operator connecting blocks $j$ and $j+1$ after each block “contracts” to a single site. The coefficients $C_+$ and $K_+$ are listed in Table I. It can be confirmed that the effective interaction between the two blocks along the rung can also recover the Heisenberg interaction.

Successive application of CORE in Eq. (1) will lead the running coupling approaching a gapless fixed point. And no phase transition is observed. The ground energy is read out as

\[ E_0 = -\frac{C_+}{(N+1)} - K_+ , \]

where the sign $\tilde{\pm}$ corresponds to the two schemes. Figure 1 shows that the result of the range-2 CORE of scheme B agrees quite well with the one by Bethe ansatz method. The numerical error can be reduced by higher range calculation. The range-4 result for $N=2$ by Weinstein shows the error is reduced to $-0.0025$.2

In fact the traditional RG gives an effective Hamiltonian having the same form of Eq. (1). It can produce results consistent with CORE though not so good. The two schemes above are still applicable and the corresponding coefficients can be found in Table I. The advantages of CORE are obvious. In many cases one can design more flexible schemes in CORE while selecting basic blocks and truncating at low levels. A more careful analysis shows that RG based on $(N-1)$-site block partition scheme (scheme A) can give an effective Hamiltonian for general $N$.

![FIG. 1. (Color online) The ground energy of SU(N) chain. Scheme B of CORE gives better results and the numerical errors are about $-0.0106$, $-0.0006$, and $0.0021$ for $N=2, 3, 4$, respectively, compared to the results by Bethe ansatz method (see Ref. 9).](1)

\[ H^{RG} = \frac{1}{N-1} \sum_j \left[ -\frac{NN-2}{(N-1)^2} + \frac{1}{(N-1)^2} \tilde{P}_{j,j+1} \right], \]

which exhibits a ground energy coinciding with the one by Bethe ansatz method at large $N$, $E_0=\frac{-N(N-2)}{(N^2-N+1)}-1$.

The two-leg spin-1/2 ladders aroused a lot of attention when a finite spin gap was observed.11 A simple picture says that the ground state is a product state with the spins on each rung forming a spin singlet. Then the lowest energy excitation is a $S=1$ magnon. Here we show that our scheme of CORE produces exactly the same picture and refined results can be achieved following the CORE algorithm. We start from the Hamiltonian

\[ H = \sum_j \left[ (S_j^A \cdot S_{j+1}^A + S_j^B \cdot S_{j+1}^B) + \alpha S_j^A \cdot S_j^B \right], \]

where the indices $A$ and $B$ refer to the two rails of the ladders, $\alpha=J_{\text{rung}}/J_{\text{rail}}$ is the ratio between the rung and rails couplings, and we have set $J_{\text{rail}}=1$.

Our first step is to divide the ladder into triads along the rail direction [Fig. 2(a)]. The problem on the rail direction is just the SU(2) chain that had been solved. Detailed calculation shows that the effective interaction between the two blocks along the rung can also recover the Heisenberg interaction. Thus ladders with renormalized couplings can be obtained. The second step is to parse out the effective block-
Table II. An example of the range-2 CORE iteration procedure at \( \alpha = 1 \).

<table>
<thead>
<tr>
<th>( n )</th>
<th>( E_0 )</th>
<th>( \delta_0 )</th>
<th>( \Lambda_0(\alpha) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>1.0</td>
<td>1.0</td>
</tr>
<tr>
<td>1</td>
<td>-0.460796</td>
<td>0.491582</td>
<td>0.81919</td>
</tr>
<tr>
<td>2</td>
<td>-0.558041</td>
<td>0.241653</td>
<td>0.64499</td>
</tr>
<tr>
<td>5</td>
<td>-0.587214</td>
<td>0.028706</td>
<td>0.420144</td>
</tr>
<tr>
<td>10</td>
<td>-0.587867</td>
<td>0.000824</td>
<td>0.382715</td>
</tr>
<tr>
<td>15</td>
<td>-0.587869</td>
<td>0.000024</td>
<td>0.381603</td>
</tr>
<tr>
<td>20</td>
<td>-0.587869</td>
<td>6.7907 \times 10^{-2}</td>
<td>0.381571</td>
</tr>
<tr>
<td>21</td>
<td>-0.587869</td>
<td>3.3382 \times 10^{-2}</td>
<td>0.38157</td>
</tr>
<tr>
<td>22</td>
<td>-0.587869</td>
<td>1.641 \times 10^{-2}</td>
<td>0.381576</td>
</tr>
</tbody>
</table>

block interactions from all possible configurations of connected blocks. As defined by Morningstar and Weinstein, \( r \) connected blocks contain range-\( r' \) interactions with \( r' = 0, 1, \ldots, r \) \([r'=0 \text{ corresponds to the constant term as in Eq. (5)}]\). To parse out all range interactions the exact diagonalization is employed on the connected blocks. We present range-2 and range-3 results here. It is notable that the range-3 blocks should include a configuration in Fig. 2(b). This unsymmetric configuration may cause higher problems. The range-2 CORE result simply regains the original form of Hamiltonian except for a constant term

\[
H^{(2)} = \frac{1}{3} \sum_j \left[ -C(\alpha) + \delta(\overline{S}_j^A \cdot \overline{S}_{j+1}^A + \overline{S}_j^B \cdot \overline{S}_{j+1}^B) + \Lambda(\alpha)S_j^A \cdot \overline{S}_{j+1}^B \right],
\]

where \( \delta = 0.491582, C(\alpha) \) and \( \Lambda(\alpha) \) vary with \( \alpha \). The iteration on the range-2 effective Hamiltonian is always applicable because the retained four low levels are always one spin singlet and three spin triplets just like the SU(2) chain case. After \( n \) steps of iteration on Eq. (5) we will get running coupling terms as

\[
h_i = \delta_i(\overline{S}_j^A \cdot \overline{S}_{j+1}^A + \overline{S}_j^B \cdot \overline{S}_{j+1}^B) + \Lambda_i(\alpha)S_j^A \cdot \overline{S}_{j+1}^B,
\]

where the coefficients are determined recursively, \( \delta_i = \delta_i', \Lambda_i(\alpha) = \Lambda_i(\alpha)'/\delta_i' \cdots, \Lambda_1(\alpha) = \Lambda(\alpha)/\delta, \Lambda_1(\alpha) = \Lambda(\alpha) = \alpha \). So the coupling approaches zero \( \delta_i' \to 0 \) as \( n \to \infty \). While the coupling goes to a fixed value \( \Lambda_n(\alpha) \neq 0 \) for \( \alpha > 0 \) (we observed that \( \Lambda_n(\alpha) \to 0 \) only when \( \alpha = 0 \), which is in agreement with the conclusion drawn by DMRG \([10,20]\) and exact diagonalization). \([21]\) So the system flows to a fixed point exhibiting dimer covering on each rung of the ladder. The spin gap is read out as \( \Delta_1(\alpha) = \Lambda_{n(\alpha)}(\alpha) \). The ground energy \( E_0 \) is obtained by cumulating the constant term. Table II gives an example of iterations procedure for \( \alpha = 1 \).

The range-3 CORE result at the first run of iteration contains the next-nearest-neighbor interactions

\[
H^{(3)} = \frac{1}{3} \sum_j \left[ -C(\alpha) + \delta(\overline{S}_j^A \cdot \overline{S}_{j+1}^A + \overline{S}_j^B \cdot \overline{S}_{j+1}^B) + \Lambda(\alpha)S_j^A \cdot \overline{S}_{j+1}^B + \Omega(\alpha)(\overline{S}_j^A \cdot \overline{S}_{j+1}^A + \overline{S}_j^B \cdot \overline{S}_{j+1}^B) + \gamma(\overline{S}_j^A \cdot \overline{S}_{j+2}^A + \overline{S}_j^B \cdot \overline{S}_{j+2}^B) \right],
\]

The ground energy \( E_0 \) and the gap for the spin-1/2 two-leg ladder. The log-log plot shows that CORE and RG give correct gap in strong coupling limit \( \alpha \to \infty \). Data by other methods are adapted from Refs. 11 and 23–25.

where \( C(\alpha), \delta(\alpha), \) and \( \Lambda(\alpha) \) are different from the ones in Eq. (5). \( \gamma = 0.333795 \). \( \gamma \) will vary with \( \alpha \) in the successive iterations, \( \gamma_0 = \gamma_1(\alpha), \cdots, \gamma_n = \gamma \). After \( n \)-step iterations, we find that the only nonvanishing coupling is still the interaction along the rung \( \Lambda_{n(\alpha)}(\alpha) \neq 0 \), so the physical picture obtained by the range-2 CORE does not change, i.e., the ground energy and the spin gap are produced in the same way.

As we noted above, the unsymmetric configuration of blocks in Fig. 2(b) brings some troubles to the range-3 CORE iteration. Unlike the SU(2) chain, the desired low levels may not always stay at the lowest positions during the iterations. And sometimes it is hard to select out the eligible set of levels from several possible candidates since each of them will lead to a recovered SU(2) symmetry. So different iteration procedures with different results are inevitable. When these situations take place, we resort to the principle: retaining the iteration procedure that gives the lowest energy, \([22]\) although in our observations the values of the results only have small difference. The range-2 and range-3 CORE results for the ground state energy and the spin gap are illustrated in Fig. 3. For a comparison, data by other methods \([11,23–25]\) are presented together. The ground energy agrees well with those by other methods in the whole range of interchain coupling \( \alpha \). This means that CORE algorithm can successively capture the low energy physics of the system. The gap has relatively larger deviation at intermediate values of \( \alpha \). Nevertheless the discrepancy can be remedied through higher range CORE calculation. The range-3 gap is a little zigzag. This may be due to the unsymmetric configuration of range-3 blocks in Fig. 2(b). It is noteworthy that RG gives a gap simply as \( \Delta_R = \alpha \), which captures the correct behaviour of the gap at strong coupling limit \( \alpha \to \infty \).\([11]\)

We also applied CORE to the two-leg SU(3) ladders, \( H = \sum_j [P_j a_{j+1, A} + \gamma P_j a_{j+1, B} + \alpha P_j a_{j, B} - \alpha P_j a_{j, B}] \). The applicable schemes are presented in Figs. 4(a)–4(c). Notice that all
blocks are equivalent and a three-state truncation is made in each scheme. Scheme (a) should be valid when the rung interaction $\alpha$ is large enough. While for small $\alpha$, the schemes (a) ($\alpha<1.0$) and (b) ($\alpha<1.58$) are appropriate and scheme (b) is better than (a). All three schemes lead to the fixed point with zero gap. We see that scheme (a) will be mapped to a SU(3) chain, which had been solved previously and gives a zero gap. And after the first mapping we applied four-site block partition scheme on the chain in the successive iteration steps to produce the ground energy in Fig. 4.

In conclusion, we have studied the SU(N) chain and ladders by the CORE schemes. We have shown that the effective Hamiltonian in the appropriate CORE schemes can regain its original form such that it approaches a fixed point by iteration of the CORE schemes. The ground state energy and the lowest excitations can be deduced from the fixed point. The results show that the SU(N) chain and the two-leg SU(3) ladders are gapless, while the two-leg spin-1/2 ladder exhibits gapped phase originated from the rung dimmerization.

This work was supported by the Research Grant Council of Hong Kong under the Project No. HKU7038/04P.
Spin and orbital valence bond solids in a one-dimensional spin-orbital system: Schwenker boson mean-field theory

Peng Li and Shun-Qing Shen

Department of Physics and Center for Theoretical and Computational Physics, The University of Hong Kong, Pokfulam Road, Hong Kong, China

(Received 2 August 2005; revised manuscript received 24 October 2005; published 30 December 2005)

A generalized one-dimensional SU(2) × SU(2) spin-orbital model is studied by means of Schwinger boson mean-field theory (SBMFT). We focus on exploring the dimer phases and clarify how to capture properly the low-temperature properties of the system. The phase diagrams for the cases of $S=T=1/2$ and of $S=1$ and $T=1/2$ are presented. Three dimer phases, the orbital valence bond state, spin valence bond state and spin-orbital valence bond state, are found to arise in proper parameter regions. The results indicate that the SU(2) × SU(2) type of spin-orbit coupling can serve as both the spin-Peierls and orbital-Peierls mechanisms which are responsible for the formations of spin singlet and orbital singlet, respectively. We have also calculated the static spin and pseudospin susceptibilities in the SBMFT scheme to characterize and distinguish the three types of dimer phases.

DOI: 10.1103/PhysRevB.72.214439

PACS number(s): 75.10.Jm, 71.27.+a, 75.40.Cx

I. INTRODUCTION

Spin-orbital models arose from the consideration of orbital degeneracy in addition to the spin degeneracy of $d$ or $f$ electrons of metal ions in transition metal oxides.\textsuperscript{1-3} The interplay between the spin and orbital degrees of freedom in electrons may generate the complexity of the magnetic structures in a lot of materials. For simplicity, a spin-orbital model with SU(2) × SU(2) symmetry was recurrently proposed and studied in connection with real materials. Motivated by the structure of tetrahedral(dimethylamino)ethylene- (TDAE-) $\text{C}_6\text{O}$, an effective multicomponent superexchange coupling was proposed and several special points with SU(2) × SU(2) symmetry were realized as limits of a hopping model.\textsuperscript{4} The spin-gap materials Na$_2$Ti$_2$Sb$_2$O and NaV$_2$O$_5$ were also thought to be related to the one-dimensional spin-orbital model with spin $S=1/2$ and double orbital degeneracy.\textsuperscript{5,6} Recently a spin-orbital model with spatial anisotropy and higher spin $S=1$ was deduced by Khaliullin et al. to describe the cubic vanadates LaVO$_3$ and YVO$_3$, which also take on the SU(2) × SU(2) symmetry in the limit where the Hund’s coupling vanishes.\textsuperscript{7,8}

The phase diagrams of spin-orbital systems have been investigated extensively. Various methods have been applied to these spin-orbital models, such as exact diagonalization, density matrix renormalization group, non-Abelian bosonization, and series expansion.\textsuperscript{5,9-11} Because of the strong correlation of electrons in these systems, except for the conventional ferromagnetic and antiferromagnetic phases, the spin-orbital coupling may also break the translational invariance of the system, and form the nonuniform valence bond states consisting of spin spinlets or orbital singlets. For the system of $S=1/2$ the strong spin-orbital coupling drives the system to form a spin-orbital valence bond (SOVB) state based on numerical calculation and symmetric analysis.\textsuperscript{5,10-12} For a system with higher spin, it was found that an orbital valence bond (OVB) state arises at low temperatures.\textsuperscript{9} A magnetic neutron scattering experiment of YVO$_3$ was identified as tentative evidence of the OVB state or an orbital Peierls state.\textsuperscript{13,14}

In this paper, we apply the Schwinger boson mean-field theory (SBMFT) to study the phase diagram of the generalized one-dimensional (1D) SU(2) × SU(2) spin-orbital model at low temperatures. We shall focus on exploring the dimer phase which consists of either spin or orbital singlets. There are three kinds of valence bond (VB) phases: the orbital valence bond solid state, the spin valence bond solid (SVB) state, and the spin-orbital valence bond solid state. The SOVB state is a spin and orbital singlet while the OVB and SVB states exhibit only one channel singlet, i.e., the orbital singlet and spin singlet, respectively. All of the three states are gapped, but they can be well characterized by the spin and orbital susceptibilities, and thus are distinguishable experimentally. Generally speaking, the SU(2) × SU(2) type of spin-orbit coupling is responsible for both the spin-Peierls and orbital-Peierls phenomena occurring in this 1D model.

The paper is organized as follows. In Sec. II, we present a detailed Schwinger boson mean-field scheme of the spin-orbital model. Then in Sec. III, we study the phase diagrams for two cases: (i) $S=1$ and $T=1/2$; (ii) $S=1/2$ and $T=1/2$. The OVB and SVB phases appear in the parameter space. In Sec. IV, we derive the spin and pseudospin susceptibilities for various phases. Finally, a brief conclusion is given in Sec. V.

II. MODEL HAMILTONIAN AND SCHWINGER BOSON MEAN-FIELD THEORY

The one-dimensional spin-orbital Hamiltonian with SU(2) × SU(2) symmetry reads

$$H = \sum_m (S_m \cdot S_{m+1} + x)(T_m \cdot T_{m+1} + y),$$

where $S$ and $T$ are spin and pseudospin operators with eigenvalues $S$ and $T$, respectively, and both satisfy the SU(2) al-
gebra. The pseudospin $T$ describes the orbital degree of freedom. The two parameters $x$ and $y$ adjust the strength of spin coupling, orbital coupling, and spin-orbital coupling.11 These two material-specific parameters are given by the interaction of electrons of transition metal ions and the band structure. The pseudospin interaction is considered to be rotationally invariant here for simplicity.5 The model can also be viewed as a spin ladder system with four-operator interactions. There exist two special points which can be solved exactly in this model. The first point is the dimer point $D: (x, y) = (S(S + 1), T(T + 1))$, whose ground state is perfectly dimerized and can be recognized as a twofold degenerate dimerized valence bond solid.15 The other point is the ferromagnetic (FM) point $F$, which is, we will see in the phase diagrams later, the critical point of three uniform phases. For $x < -S^2$ and $y < -T^2$, the ground state is fully polarized and possesses the maximal values for both $S_{\text{total}} = \sum_{m} S_{m}$ and $T_{\text{total}} = \sum_{m} T_{m}$. The model for $S = 1/2$ and $T = 1/2$, which further exhibits a solvable SU(4) point $S, (x, y) = (1/4, 1/4)$,15 has been extensively studied by both analytical and numerical methods. Its phase diagram was proposed by several authors.5,10,11 Except for the phases with ferromagnetic and antiferromagnetic (AFM) orders for spins and pseudospins, the phase characterized by the mixed spin-orbital valence bond state, which exhibits no long-range correlation and no energy gap between the ground state and excited states, inhabits a considerable region in the phase diagram near the SU(4) point $S,T$.10 The model for $S = 1$ and $T = 1/2$ has not yet been fully understood very well. Around the point $O, (x, y) = (1, 1/4)$, it was revealed to exhibit the OVB state.5,13,14

We now develop a SBMFT to study the phase diagram and focus on exploring the dimer phases. The SBMFT was introduced to the field of strongly correlated systems, and shows its merit in describing spin systems at low temperatures. It can describe the spin liquid phase and spin gap close to the ground state as well as the phases with long-range correlation, though it predicted wrongly a gap for the half-integer spin chain.16–19 In the Schwinger boson representation, one can introduce two boson operators $a$ and $b$ to represent a spin operator $S_{m}$:

$$S_{m}^{\uparrow} = a_{m}^{\dagger}b_{m}, \quad S_{m}^{\downarrow} = a_{m}^{\dagger}b_{m}, \quad S_{m} = \frac{1}{2}(a_{m}^{\dagger}a_{m} - b_{m}^{\dagger}b_{m})$$

with the local constraint

$$a_{m}^{\dagger}a_{m} + b_{m}^{\dagger}b_{m} = 2S.$$

For the Heisenberg system one can introduce two types of bond operators,

$$F_{mn} = \frac{1}{2}(a_{m}^{\dagger}a_{n} + b_{m}^{\dagger}b_{n}),$$

$$A_{mn} = \frac{1}{2}(a_{m}b_{n} - b_{m}a_{n}),$$

(2)

(3)

(4a)

(4b)

to mimic the ferromagnetic and antiferromagnetic channels of the spin-$S$ Heisenberg interactions. The low-energy physics can be well captured by the mean fields, $\Delta_{F} = \langle F_{mn} \rangle$ or $\Delta_{A} = \langle A_{mn} \rangle$, where $\langle \cdots \rangle$ stands for the thermodynamic average. Likewise, the mean fields for the pseudospin $T$ are denoted by $\Theta_{F}$ and $\Theta_{A}$ for the FM and AFM channels, respectively.

As revealed by Ceccatto et al.,20 the exchange coupling can be expressed in terms of $F_{mn}$ and $A_{mn}$,

$$S_{m} \cdot S_{n} = :F_{mn}^{\dagger}F_{mn}: - A_{mn}^{\dagger}A_{mn}$$

(5)

where $: :$ denotes normal order. In the mean-field scheme, the bond operators are decomposed as

$$F_{mn}^{\dagger}F_{mn} \rightarrow \Delta_{F}(F_{mn} + F_{mn}^{\dagger}) - \Delta_{F}^{2},$$

$$A_{mn}^{\dagger}A_{mn} \rightarrow \Delta_{A}(A_{mn} + A_{mn}^{\dagger}) - \Delta_{A}^{2},$$

(6)

(7)

where the higher-order terms $(F_{mn} - \Delta_{F})(F_{mn} - \Delta_{F})$ and $(A_{mn}^{\dagger} - \Delta_{A})(A_{mn} - \Delta_{A})$ are ignored. The identity

$$F_{mn}^{\dagger}F_{mn} + A_{mn}^{\dagger}A_{mn} = S^2$$

is equivalent to the constraint of Eq. (3) and implies

$$S_{m} \cdot S_{n} = \begin{cases} 2:F_{mn}F_{mn}: - S^2 & \text{for FM,} \\ - 2A_{mn}^{\dagger}A_{mn} + S^2 & \text{for AFM.} \end{cases}$$

(8)

The identity Eq. (7) may be largely violated when the constraint is imposed only on average and even when the Gaussian-fluctuation corrections are considered.21

To show the advantage of Eq. (5), we present a two-site example $H = JS_{1}^{\dagger}S_{2}$, which can be solved analytically. After solving it by SBMFT, one can find, in the FM ($J < 0$) case, that Eq. (5) gives the ground energy $f_{0} = JS^{2}$ with $\Delta_{F} = S$ and $\Delta_{A} = 0$, and Eq. (8) gives the same ground energy with $\Delta_{F} = S$. They both are in agreement with the exact solution. In the AFM ($J > 0$) case, Eq. (5) gives $f_{0} = JS(S + 1)$ with $\Delta_{A} = \sqrt{S(S + 1)}$ and $\Delta_{F} = 0$, while Eq. (8) gives $f_{0} = -JS(S + 2)$ with $\Delta_{A} = \sqrt{S(S + 1)}$. The former is just the exact energy, and the latter approaches the exact value only in the limit of $S \rightarrow \infty$. Thus Eq. (8) overestimates the ground energy in AFM channel. We have also found that Eq. (5), instead of Eq. (8), can produce the exact energy of the dimer point in the spin-orbital model of Eq. (1). Thus for a small $S$, the mean-field scheme of Eq. (5) is better than that of Eq. (8). In practice, we found that only one of the FM and AFM channels can survive on a bond for 1D and 2D unfrustrated systems.

To perform the mean-field approach, we decompose Eq. (1) into the spin $S$ and the pseudospin $T$ chains,

$$H = \sum_{m} [J_{S}(m)S_{m} \cdot S_{m+1} + J_{T}(m)T_{m} \cdot T_{m+1}] + \sum_{m} [yJ_{F}(m) + xJ_{S}(m) + J_{S}(m)J_{T}(m)],$$

(9)

where the effective couplings

$$J_{F}(m) = \langle S_{m} \cdot S_{m+1} \rangle,$$

$$J_{S}(m) = \langle T_{m} \cdot T_{m+1} \rangle.$$

(10a)

(10b)

The two chains are coupled by the effective couplings, which will be determined self-consistently. And Eq. (5) ensures a reasonable estimation of the strength of the effective couplings Eq. (10) for both of the FM and AFM channels. One
FIG. 1. Two schemes to approach the dimer phases. The single and double arrow lines represent T and S, respectively. Two parallel arrows represent the FM channel, and two antiparallel arrows represent the AFM channel.

should notice that, for $S=1/2$, the mixed channel of $S$ and $T$ must be considered around the SU(4) point $(x, y) = (1/4, 1/4)^{5,10,12,22}$ which is not the focus of this paper. In the following we apply the bond operators in Eq. (5) for both spin $S$ and pseudospin $T$ in Eq. (9).

There are four combinations of uniform FM and AFM phases: (1) S-FM ($J_s = y + \Theta^2_0 < 0$), T-FM ($J_T = x + \Delta^2_0 < 0$); (2) S-FM ($J_s = y - \Theta^2_0 < 0$), T-AFM ($J_T = x + \Delta^2_0 > 0$); (3) S-AFM ($J_T = y + \Theta^2_0 > 0$), T-FM ($J_T = x - \Delta^2_0 < 0$); (4) S-AFM ($J_T = y - \Theta^2_0 > 0$), T-AFM ($J_s = x - \Delta^2_0 > 0$). The inequalities in the parentheses should be satisfied when the mean fields are solved. The four phases correspond to four separate regions in the $(x, y)$ plane. We omit details for these uniform phases. Let us focus on more interesting cases. It was pointed out by Shen et al. that the OVB state should be a preferred ground state around the point $O$, $(x, y) = (1, 1/4)$, for $S=1$ and $T=1/2$, and the possibility of a segment with more than two sites has been ruled out by exact numerical diagonalization and linear spin-wave analysis. This dimerization effect is also confirmed by the finite-temperature density-matrix renormalization group (TDMRG) calculation of the orbital-orbital correlation function, and is also thought to be responsible for the observation on the neutron scattering experiment of YVO$_3$. In fact, the generalized model of Eq. (1) provides two other valence bond states, SVB and SOVB states. The three kinds of dimer phases have not yet been studied and distinguished within a unified framework in previous works. To approach the dimer phases, we have two schemes as depicted in Figs. 1(a) and 1(b). They complement each other in the whole dimer phase region. It turns out that the scheme (b) is only appropriate for exploring the SOVB phase and does not produce the OVB and SVB phases. So, in the following, we present detailed treatment of the scheme (a).

One can find, for the scheme (a), that the spin $S$ chain and the pseudospin $T$ chain are the same object mathematically: a dimerized chain with alternating FM and AFM bonds. For the spin $S$ part, we can divide it into two sublattices $A$ and $B$ by assuming that the translational invariance is broken simultaneously. In fact, the period length of the chain is doubled due to the spin-Peierls phenomenon. We use two sets of Schwinger bosons $(a, b)$ and $(c, d)$ to represent spins on the sublattices $A$ and $B$, respectively, and choose the unit cell to be composed of two lattice sites with one for sublattice $A$ and the other for sublattice $B$. Then the Fourier transformations read

$$\begin{align*}
\left( \begin{array}{c} d_A \\ b_A \\ d_B \\ b_B \\ d_A \\ b_A \\ d_B \\ b_B \\ \vdots \\
\end{array} \right) &= \frac{1}{\sqrt{N}} \sum_k e^{i(k R_j - \delta)} \left( \begin{array}{c} d_k \\ c_k \\ c_k \\ d_k \\ c_k \\ c_k \\ c_k \\ c_k \\ \vdots \\
\end{array} \right),
\end{align*}$$

(11a)

The supposed nonzero real mean fields are

$$\begin{align*}
\Delta_A &= \left( \frac{1}{2} (a^+_j a^+_j - b^+_j b^+_j) \right), \\
\Delta_F &= \left( \frac{1}{2} (a^+_j a^+_j + b^+_j b^+_j) \right).
\end{align*}$$

(12a, 12b)

The Lagrangian multipliers $\lambda^{(A)}_{l,S}$ and $\lambda^{(B)}_{l,S}$ are imposed to realize the constraints on the spin $S$ by adding the term to the total Hamiltonian,

$$\sum_j \lambda^{(A)}_{l,S} (a^+_j a_j + b^+_j b_j - 2S) + \sum_j \lambda^{(B)}_{l,S} (c^+_j c_j + d^+_j d_j - 2S).$$

(13)

For the mean-field approach we take $\lambda^{(A)}_{l,S} = \lambda^{(B)}_{l,S} = \lambda$. After the Fourier transform, we introduce the Nambu spinor in the momentum space, $\phi = (a^+_1, b^+_1, c^+_1, d^+_1, a^+_2, b^+_2, c^+_2, d^+_2)$. One can arrive at the mean-field Hamiltonian for the spin $S$ chain in a compact form,

$$H^S = \frac{1}{2} \sum_k \phi^0_k M^S \phi_k + e^S_0,$$

(14)

where

$$e^S_0 = M[(\Theta^2_F + y) \Delta^2_F + (\Theta^2_F - y) \Delta^2_F] - 2N \lambda (2S + 1).$$

(15)

and the matrix $M^S$ is constructed by the Kronecker products of the Pauli matrices,

$$M^S = \lambda \sigma_0 \otimes \sigma_0 \otimes \sigma_0 + j_{A,S} \cos \frac{k}{2} \sigma_0 \otimes \sigma_y \otimes \sigma_y + j_{F,S} \sin \frac{k}{2} \sigma_0 \otimes \sigma_x \otimes \sigma_z - j_{F,S} \cos \frac{k}{2} \sigma_0 \otimes \sigma_\sigma \otimes \sigma_z + j_{F,S} \sin \frac{k}{2} \sigma_0 \otimes \sigma_y \otimes \sigma_z + j_{A,S} \sin \frac{k}{2} \sigma_0 \otimes \sigma_x \otimes \sigma_z + j_{A,S} \cos \frac{k}{2} \sigma_0 \otimes \sigma_y \otimes \sigma_z + j_{F,S} \sin \frac{k}{2} \sigma_0 \otimes \sigma_x \otimes \sigma_z + j_{F,S} \cos \frac{k}{2} \sigma_0 \otimes \sigma_y \otimes \sigma_z$$

(16)

with $j_{A,S} = (\Theta^2_F + y) \Delta^2_F / 2$, $j_{F,S} = (\Theta^2_F - y) \Delta^2_F / 2$, $j_{A,T} = (\Delta^2_T + x) \Theta^2_A / 2$, and $j_{F,T} = (\Delta^2_T - x) \Theta^2_A / 2$. Then we can read out the spectra from the poles of the bosonic Matsubara Green’s function $(8 \times 8$ matrix),

$$G^S(k, i\omega_n) = (i\omega_n \sigma_\sigma \otimes \sigma_0 \otimes \sigma_\sigma - M^S)^{-1}$$

(17)

where $\omega_n = n \pi / \beta$ (n is an integer and $\beta$ is the inverse temperature). Similarly, we repeat the mean-field calculation on the pseudospin $T$ chain. Both the spin and the pseudospin chains have two spectra, which read

$$\omega_{\alpha,\nu}(k) = \sqrt{\lambda^2_{\alpha} - j_{A,\alpha}^2 + 2v_{\nu,F}^e \Omega_{\nu}(k)},$$

(18)

where $\alpha = (S, T)$, $\nu = \mp$, and $\Omega_{\nu}(k) = \sqrt{\lambda^2_{\alpha} - j_{A,\alpha}^2 + j_{F,\alpha}^2 \cos^2 k}$. The lower quasiparticle spectrum $\omega_{\alpha,\nu}(k)$ is found to be gapped at
By optimizing the total free energy

\[ F = \varepsilon_0 - \frac{1}{2} \sum_{\alpha, \sigma} \ln(n_B(\omega_{\alpha,\sigma}(k))[n_B(\omega_{\alpha,\sigma}(k)) + 1]), \]

(19)

where \( n_B(\omega) \) is the Bose-Einstein distribution, and

\[ \varepsilon_0 = N[\alpha_3(\Delta_0^2 + \Delta_F^2) + 2\alpha_x(\Delta_0^2 - \Delta_F^2)y + (\Theta_0^2 - \Theta_F^2)x - 2\lambda_F(2S + 1) - 2\lambda_T(2T + 1)], \]

(20)

a set of mean-field equations are established,

\[ W(\tilde{J}_{A,S}, \tilde{J}_{F,S}) = 2S + 1, \]

(21a)

\[ W(\tilde{J}_{A,T}, \tilde{J}_{F,T}) = 2T + 1, \]

(21b)

\[ X(\tilde{J}_{A,S}, \tilde{J}_{F,S}) = \Delta_A, \]

(21c)

\[ X(\tilde{J}_{A,T}, \tilde{J}_{F,T}) = \Theta_A, \]

(21d)

\[ Y(\tilde{J}_{A,S}, \tilde{J}_{F,S}) = \Delta_F, \]

(21e)

\[ Y(\tilde{J}_{A,T}, \tilde{J}_{F,T}) = \Theta_F, \]

(21f)

\[ \frac{(\Theta_0^2 + y)\Delta_0}{\tilde{J}_{A,S}} = \frac{(\Theta_0^2 - y)\Delta_F}{\tilde{J}_{F,S}} = 2\lambda_S, \]

(21g)

\[ \frac{(\Delta_0^2 + x)\Theta_0}{\tilde{J}_{A,T}} = \frac{(\Delta_0^2 - x)\Theta_F}{\tilde{J}_{F,T}} = 2\lambda_T, \]

(21h)

where we have defined integrals (the symbols tildes mean dimensionless quantities, \( \tilde{J}_{A,\sigma} = J_{A,\sigma}/\lambda_{A,\sigma}, \tilde{J}_{F,\sigma} = J_{F,\sigma}/\lambda_{F,\sigma}, \tilde{\Omega}_\alpha = \Omega_\alpha/\lambda_{A,\sigma} \), and we have substituted the sum by an integral: \((1/N)\sum_k \rightarrow \int dk/2\pi \) in the thermodynamic limit)

\[ W(\tilde{J}_{A,\alpha}, \tilde{J}_{F,\alpha}) = \int \frac{dk}{2\pi} \sum_{\alpha, \sigma} \left( 1 + \frac{\tilde{J}_{F,\alpha}}{\tilde{\Omega}_\alpha} \right) \coth(\beta\omega_{\alpha,\sigma}/2), \]

(22a)

\[ X(\tilde{J}_{A,\alpha}, \tilde{J}_{F,\alpha}) = \int \frac{dk}{2\pi} \sum_{\alpha, \sigma} \left( 1 + \frac{\tilde{J}_{F,\alpha}}{\tilde{\Omega}_\alpha} \right) \coth(\beta\omega_{\alpha,\sigma}/2), \]

(22b)

\[ Y(\tilde{J}_{A,\alpha}, \tilde{J}_{F,\alpha}) = -\int \frac{dk}{2\pi} \sum_{\alpha, \sigma} \left( \tilde{J}_{F,\alpha} + \nu\tilde{\Omega}_\alpha \right) \coth(\beta\omega_{\alpha,\sigma}/2), \]

(22c)

### III. Phase Diagram

For the transition metal oxides, the pseudospin for the orbital is usually one-half, i.e., \( T = 1/2 \), reflecting almost double degeneracy of unfrozen \( e_g \) or \( t_{2g} \) orbitals. The spin-gaps materials Na2Ti2Sb2O and NaV2O5 are related to the S =1/2 case in the model of Eq. (1), while the cubic vanadates LaVO3 and YVO3 are related to the \( S = 1 \) case due to the large Hund’s coupling.

The phase diagrams are obtained by solving the mean-field equations numerically at zero temperature. Figure 2(a) shows the case of \( S = 1 \) and \( T = 1/2 \). We obtained three dimer phases: (1) the OVB phase with \( \Theta_A = \sqrt{3}/2, \Theta_F = 0, \Delta_A \neq 0 \); and \( \Delta_F \neq 0 \); (2) the SBV phase with \( \Theta_A = 0, \Theta_F \neq 0, \Delta_A = \sqrt{2} \), and \( \Delta_F = 0 \); (3) the SOVB phase with \( \Theta_A = \sqrt{3}/2, \Theta_F = 0, \Delta_A = \sqrt{2} \), and \( \Delta_F = 0 \). As expected, the point \( O, (x, y) = (1, 1/4) \), lies in the OVB phase region. At the mean-field level, the dimer phases are captured by the staggered nonzero AFM mean fields \( \Theta_A \) and/or \( \Delta_A \), which provide a perfect dimer picture of spin and/or pseudospin in the whole phase region. The reason for this may lie in two effects: the mean-field treatment omits part of the quantum fluctuations; and the dimerization effect is very strong in such a system at least at low temperatures. In fact, TDMRG has confirmed the orbital dimerization at the point \( O, (x, y) = (1, 1/4) \), since the correlation function \( \langle T_{\alpha} T_{\alpha'} \rangle \) extrapolates to \(-3/8 \) per bond at zero temperature, although this point is not exactly soluble. And the OVB phase is quite robust even when the anisotropy, Hund’s coupling, and atomic spin-orbit interaction are taken into account for cubic vanadates and other relevant systems. We also anticipate that these dimer phases may survive in two dimensions, although no rigorous soluble point can be referred to. A dimerized OVB configu-
SPIN AND ORBITAL VALENCE BOND SOLIDS IN A...

...tion in two dimensions has been proposed and checked by the spin-wave theory in Ref. 9, which indeed exhibits lower energy than the uniform phases. However, it is still an interesting problem whether SOVB can survive in two dimensions.

Figure 2(b) shows the case for $S=1/2$ and $T=1/2$. In Fig. 2(b), the SU(4) gapless region is quoted from Ref. 10. We found that the SVB and OVB phases still occupy two blocks that are sandwiched between the SOVB and the SU(4) gapless region. The three dimer phases with corresponding mean fields are (1) the OVB phase with $\Theta_A = \sqrt{3}/2$, $\Theta_B = 0$, $\Delta_4 \neq 0$, and $\Delta_6 \neq 0$; (2) the SVB phase with $\Theta_A \neq 0$, $\Theta_B \neq 0$, $\Delta_4 = \sqrt{3}/2$, and $\Delta_6 = 0$; (3) the SOVB phase with $\Theta_A = \sqrt{3}/2$, $\Theta_B = 0$, $\Delta_4 = \sqrt{3}/2$, and $\Delta_6 = 0$. Previous work ignored the SVB and OVB phases.\(^5\,\!^10\) And there is an $S$-AFM and $T$-AFM phase region from the point of view of SBMFT.

The results here in fact suggest that the spin-orbit coupling of SU(2) $\times$ SU(2) type plays the role of the intrinsic spin-Peierls and orbital-Peierls mechanisms. The SVB formation in this 1D model is an example that expresses the concept of an orbitally driven Peierls state.\(^26\) Here we did not consider the lattice distortion. For a larger spin $S$, the SVB phase is harder to realize since the region shrinks.

**IV. SUSCEPTIBILITY**

The spin structures of the dimer phases are detectable by their spin susceptibility. Let us consider the spin susceptibility (the pseudospin case is handled in the same way). We can define spin-density waves on sublattices $A$ and $B$ (due to the rotational symmetry, we only consider the $z$ component of the spin),

$$S_A^z(q) = \frac{1}{\sqrt{N}} \sum_j e^{-i q R_j} S_{A,j}^z,$$

(23a)

$$S_B^z(q) = \frac{1}{\sqrt{N}} \sum_j e^{-i q (R_j + \delta)} S_{B,j + \delta}^z.$$

(23b)

The spin susceptibility contains contributions from both the intrasublattice and intersublattice fluctuations,

$$\chi(q) = \frac{1}{N_{m,n,A,B}} \langle S_{n,A}^z S_{m,\delta B}^z \rangle e^{i q (R_n - R_m)} = \chi_{AA}(q) + \chi_{AB}(q) + \chi_{BB}(q).$$

(24)

In Matsubara formalism, the intrasublattice and intersublattice contributions read

$$\chi_{AA}(q, \tau) = \langle S_{A}^z(q, \tau) S_{A}^z(-q, 0) \rangle$$

$$= \frac{1}{4} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left[ G_{11}^S(-k, \tau) G_{11}^S(k + q, \tau) - G_{66}^S(-k, \tau) \times G_{11}^S(k + q, \tau) - G_{22}^S(-k, \tau) G_{66}^S(k + q, \tau) \right],$$

(25a)

FIG. 3. Static spin susceptibilities for $S=1$ and $T=1/2$ at the OVB point $O$, $(x, y) = (1, 1/4)$ (solid line), and the dimer point $D$, $(2, 3/4)$ (dashed line).

$$\chi_{AB}(q, \tau) = \langle S_{A}^z(q, \tau) S_{A}^z(-q, 0) \rangle$$

$$= \frac{1}{4} \int_{-\pi}^{\pi} \frac{dk}{2\pi} \left[ G_{11}^S(-k, \tau) G_{11}^S(k + q, \tau) - G_{66}^S(-k, \tau) \times G_{11}^S(k + q, \tau) - G_{22}^S(-k, \tau) G_{66}^S(k + q, \tau) \right].$$

(25b)

The numerical solutions of the static spin susceptibilities $\chi_{AA}(q, \tau=0^+)$ and $\chi_{AB}(q, \tau=0^+)$ for $S=1$ and $T=1/2$ at the OVB point $O$, $(x, y) = (1, 1/4)$, and the dimer point $D$, $(2, 3/4)$, are shown in Fig. 3. At the OVB point $O$, the static spin susceptibilities exhibit finite sharp peaks at $q=\pi$ for $\chi_{AA}(q, \tau)$ and $q=0$ for $\chi_{AB}(q, \tau)$ reflecting the strong AFM fluctuation among sites in sublattice $A$ (or $B$) and FM fluctuation between sites in sublattice $A$ and sites in sublattice $B$. The finite peaks also indicate that no long-range order exists at zero temperature. While there is no sharp peak at the dimer point $D$, since the formation of spin singlets leads to dispersionless spin spectra, $\omega_{\pm}(k) = \omega_{\mp}(k) = \sqrt{J_{A,\pm}^2 + J_{A,\pm}^2}$. The spin susceptibilities at the OVB point $O$ and the dimer point $D$ characterize the whole OVB region and SOVB region, respectively. As we go from OVB phase to SBV phase, the spin and pseudospin change their roles. In the SOVB phase, the sharp peaks will disappear for both spin and pseudospin. Thus the three dimer phases are well characterized by the spin and pseudospin susceptibilities and distinguishable experimentally.

**V. CONCLUSION**

In conclusion, we have employed SBMFT to study various nonuniform valence bond states as well as uniform FM and AFM states in the 1D SU(2) $\times$ SU(2) spin-orbital model. The phase diagrams are constructed by comparing the ground-state energies of proposed possible states. In the valence bond states the translational invariance is broken in space; FM and AFM order parameters compete with each
other and are determined self-consistently. Specifically, two sublattices were introduced to approach the three dimerized SVB, OVB, and SOVB phases by SBMFT. We clarified how to capture properly the low-temperature properties of such a system by SBMFT. The main result of the paper is that the SVB and OVB states have lower energy than the SOVB state in some regions. And the SU(2) × SU(2) type of spin-orbit coupling provides both spin-Peierls and orbital-Peierls mechanisms. For \( S = 1 \), the well studied point \( (x, y) = (1, 1/4) \), lies properly in the OVB region. This intrinsic tendency to orbital dimerization may be relevant to the experimental observation of the splitting of magnon branches in the cubic vanadate YVO\(_3\), which is well described by this phase.\(^{13}\) For \( S = 1/2 \), our result suggests that the dimer phase also splits into three types. Careful experimental analyses on the related spin-gap materials, such as Na\(_2\)Ti\(_2\)Sb\(_2\)O and NaV\(_2\)O\(_5\), are expected to identify which dimer phase they belong to. The results still should be compared with other phases including those with translational invariance. Static spin and pseudospin susceptibilities have been calculated in the present theory and are available to distinguish spin-singlet and orbital-singlet formations in real materials.

ACKNOWLEDGMENTS

This work was supported by the Research Grant Council of Hong Kong under Grants No. HKU7109/02P and No. HKU7038/04P.
Spin-resolved Hall effect driven by spin-orbit coupling

Jian Li, Liangbin Hu, and Shun-Qing Shen

1Department of Physics, The University of Hong Kong, Pokfulam Road, Hong Kong, China
2Department of Physics, South China Normal University, Guangzhou 510631, China

(Received 4 February 2005; revised manuscript received 15 April 2005; published 14 June 2005)

Spin and electric Hall currents are calculated numerically in a two-dimensional mesoscopic system with Rashba and Dresselhaus spin-orbit coupling by means of the Landauer-Büttiker formalism. It is found that both electric and spin Hall currents circulate when two spin-orbit couplings coexist, while the electric Hall conductance vanishes if either one is absent. The electric and spin Hall conductances are suppressed in strong disorder, but survive in weak disorder. Physically it can be understood that the spin transverse “force” generated by spin-orbit coupling is responsible for the formation of the spin Hall current and the lack of transverse reflection symmetry is the origin of the electric Hall current.

DOI: 10.1103/PhysRevB.71.241305 PACS number(s): 72.25.−b, 75.47.−m

When a metallic sample is subjected to a perpendicular external magnetic field, the Lorentz force acting on the charge carriers gives rise to a transverse voltage between two edges of the sample; this is well known as the ordinary Hall effect. Actually, the Hall effect family has a number of important members. The anomalous Hall effect may occur even in the absence of an external magnetic field in a ferromagnetic metal with spin-orbit coupling.1–8 In the past few years it has been recognized that the spin-orbit coupling may provide an efficient way to manipulate a spin-resolved current in metals and semiconductors.9–15 In a two-dimensional electronic metal with spin-orbit coupling,1–8 the charge carriers gives rise to a transverse voltage between two edges of the sample.16

The Hamiltonian is given by

\[ H = \frac{p^2}{2m} + \lambda (\sigma^x p_x - \sigma^y p_y) + \beta (\sigma^z p_x - \sigma^y p_y), \]

where the second term is the Rashba spin-orbit coupling and the third one is the Dresselhaus spin-orbit coupling. \( \sigma^\mu (\mu = x, y, z) \) are the Pauli matrices, and the coupling parameters \( \lambda \) and \( \beta \) have the dimension of velocity. Using the Heisenberg equation of motion the second derivative of the position operator \( r \)

\[ m^* \frac{\partial^2}{\partial t^2} r = \frac{2m^* (\lambda^2 - \beta^2) \sigma^\mu}{\hbar} p \times \hat{z}. \]  

Compared with the Lorentz force brought by the magnetic field upon a charged particle, the spin-orbit coupling produces a spin transverse “force” on a moving electron. It has no classical counterpart as the coefficient is divided by \( \hbar \), but it reflects the tendency of spin asymmetric scattering of a moving electron subject to the spin-orbit coupling. When charge carriers are driven by an external electric field, this force tends to form a transverse spin current.

In this paper we calculate the spin and electric Hall conductances in a 2DEG mesoscopic system with Rashba and Dresselhaus coupling by using the Landauer-Büttiker formula and the Green’s function technique. It is found that both electric and spin Hall currents circulate while these two types of spin-orbit coupling coexist, but the electric Hall current disappears when either one is absent. The spin and electric Hall conductances are suppressed in strong disorder, but survive in weak disorder. The numerical results are in good agreement with the symmetry analysis of the system.

We consider a cross-shape device with four semi-infinite metallic leads as shown in Fig. 1. The scattering region (the shadowed part in Fig. 1) is described by the effective Hamiltonian in Eq. (1), and when it is treated as an \( L \times L \) lattice with the tight-binding approximation, the model Hamiltonian reads

\[ H = -t \sum_{ij, \sigma} c_{i, \sigma}^\dagger c_{j, \sigma} + t_{so}^R \sum_l (J_{1, l} - J_{1, l}^s) + t_{so}^D \sum_l (J_{1, l} - J_{1, l}), \]

where \( t_{so}^R \) and \( t_{so}^D \) are the dimensionless parameters for Rashba and Dresselhaus coupling strength in the unit of \( t \), respectively, and the local spin current operator \( J_{1, \alpha}^\mu \) is defined as

\[ J_{1, \alpha}^\mu = -it \sum_{\sigma, \sigma'} (c_{i, \sigma}^\dagger \sigma^\mu_{\sigma, \sigma'} c_{i+\alpha, \sigma'} - H.c.), \]

where \( \alpha \) stands for the unit vector along the axes of the lattice and \( \mu \) stands for the direction of spin polarization.17

FIG. 1. Cross-shape device with four semi-infinite metallic leads. The spin-orbit coupling is supposed to exist in the shadowed area only, and the effect of the semi-infinite leads is treated exactly through self-energy terms.
The transmission probability coefficients can be calculated from the Landauer–Büttiker formalism.18,19 Assume $T_{q,p}^{\mu}$ to be the spin-resolved transmission probability of electrons transmitted from spin channel $\mu$ of lead $p$ to spin channel $\nu$ of lead $q$, and $V_p$ to be the electric voltage in lead $p$, then, respectively, the outgoing electric current and spin current polarized along $\mu$ direction in lead $p$ are

$$I_p^\mu = \frac{e}{h} \sum_{q,\mu,\nu} (T_{q,p}^{\mu,\nu} V_q - T_{q,p}^{\mu,\nu} V_p),$$

$$I_p^\mu = -\frac{e}{4\pi} \sum_{q,\nu} \{ [T_{q,p}^{\mu,\nu} - T_{p,q}^{\mu,\nu}] V_q - (T_{q,p}^{\mu,\nu} - T_{q,p}^{\mu,\nu}) V_p \}. \quad (6)$$

The transmission probability coefficients can be calculated by using the Green’s function technique, $T_{q,p}^{\mu,\nu} = \text{Tr}[\Gamma_q \Gamma_p G^{\mu,\nu} G]$. And the retarded and advanced Green functions are given by $G^{R,A}(E) = 1/(E-H_e - \Sigma_\nu G^{\nu,\nu} A)$, where $E$ is the electron energy and $H_e$ is the model Hamiltonian in the shadowed region in Fig. 1. The retarded and advanced self-energy terms introduced by the semi-infinite lead $p$, $(\Pi^R)^p_{\sigma \rho,\sigma' \rho'} = -\Sigma_\nu \chi_\nu(p) e^{\pm i k m a \nu} \chi_\nu(p) \delta_{\sigma \sigma'}$ and $(\Pi^A)^p_{\sigma \rho,\sigma' \rho'} = -\Sigma_\nu \chi_\nu(p)$, where $\chi_\nu(p)$ is the transverse mode wave function at site $p$ in lead $p$ connected to the scattering region. It should be noted that in Eq. (6) $\mu$ may stand for an arbitrary direction of spin polarization, and this is done by incorporating a transformation in the definition of $\Gamma_p^\mu$, that is, $\Gamma_p^\mu(p, \sigma, \rho, \sigma') = 2\pi R_{\sigma \sigma'} \rho_{\sigma \rho} \Sigma_\nu \chi_\nu(p) \sin(k_m a) \chi_\nu(p)$ and $R$ is the rotation matrix to transform the eigenstates of $\sigma^z$ to those of $\mathbf{r} \cdot \mathbf{a}$ ($\mathbf{r}$ is a unit vector).20

In this paper we consider an initial electric current driven through leads 1 and 2. $I_1 = -I_2$, by setting the bias voltage $V_1 = -V_2 = V_0/2$ and $V_1 = V_2 = 0$. The currents in leads 3 and 4 are perpendicular to the current through leads 1 and 2. Thus the electric and spin Hall conductances are defined as

$$G_{eH} = I_1^o/(V_1 - V_2);$$

$$G_{sH}^\mu = I_1^o/(V_1 - V_2), \quad (8)$$

respectively, where the spin current has three components, $\mu = x, y, z$. Electric and spin Hall conductances are evaluated as functions of the Fermi energy for different ratios of Rashba and Dresselhaus coupling strength in Fig. 2. Generally speaking, the electric Hall conductance is symmetric about the Fermi energy $E_F$ while the spin Hall conductance is antisymmetric such that the spin Hall conductance vanishes at the band center, $E_F = 0$. This is consistent with the symmetry analysis for the tight-binding Hamiltonian.23 In the case of the pure Rashba or Dresselhaus coupling, the electric Hall conductance disappears, but the spin Hall conductance still exists. In the two cases of $R^0_{SO} = 1$ and $D^0_{SO} = 1$, the electric Hall conductances are equal. However the spin Hall conductances $G_{sH}^x$ differ by a minus sign, with $G_{sH}^x$ and $G_{sH}^y$ swapped, and the former is consistent with the work of Shen23 and Sinitsyn et al.26 for free 2DEG systems. A special case is at the symmetric point of $D^0_{SO}$.

![Fig. 2.](image.png)

**FIG. 2.** (Color online) Electric and spin Hall conductances as functions of the electron Fermi energy for different ratios of the Rashba and Dresselhaus coupling strengths. $L = 40$ for all the results in this figure.

$= t_{SO}^D$. The spin Hall conductance $G_{sH}^z = 0$, while $G_{sH}^x$ and $G_{sH}^y$ are equal and nonzero, which means the current is polarized within the $x$-$y$ plane. In this case the operator $\sigma^x + \sigma^y$ commutes with the total Hamiltonian, and actually there is no spin flip in the scattering region.22 On the other hand the longitudinal electric and spin conductances are also nonzero. The longitudinal conductances are about one order larger than the Hall conductances in magnitude, i.e., $I_1^o/I_2^o = 10$. And the electric conductance is also symmetric with respect to the Fermi energy, just like the electric Hall conductance, while the longitudinal spin current is antisymmetric. According to the symmetry properties of such a system,23 under the transformation: $\sigma^x \rightarrow \sigma^x$, $\sigma^y \rightarrow -\sigma^y$, and $\sigma^z \rightarrow -\sigma^z$, $D^0 \rightarrow D^0$, and $t_{SO}^D \rightarrow t_{SO}^D$, correspondingly $G_{sH}^x \rightarrow G_{sH}^x$, $G_{sH}^y \rightarrow G_{sH}^y$, and $G_{sH}^z \rightarrow -G_{sH}^z$ while the electric Hall conductance remains unchanged. At the symmetric point, $t_{SO}^D = t_{SO}^D$, it yields that $G_{sH}^x = G_{sH}^x$ and $G_{sH}^z = 0$. Our numerical results obviously agree with this symmetry analysis.

The Hall conductances as functions of the Rashba coupling strength are also evaluated, with the specific Dresselhaus coupling strength $t_{SO}^D = 1.0$ and electron Fermi energy $E_F = 2.0 t$ as shown in Fig. 3. It indicates clearly that the electric Hall conductance increases with increasing the Rashba couple strength, and reaches its maximal value at $t_{SO}^D = 2.0 t$. Then it turns to decrease when $t_{SO}^D > 2.0 t$, and approaches to zero for a large Rashba coupling strength. The figure shows that $G_{sH}^z = 0$ and $G_{sH}^x = G_{sH}^y$ at $t_{SO}^D = t_{SO}^D$ as expected by the symmetry analysis. For a large spin-orbit coupling both electric and spin Hall conductance approaches to zero because the spin-orbit coupling in the scattering region forms a large potential barrier and the incident electrons will be completely reflected. Unlike bulk systems,25,26 where the spin Hall conductance in the clean limit has a universal value $\pm e/8\pi$ and the sign is given by the relative ratio of two coupling strength in Eq. (1), Fig. 3 shows that the value of spin Hall conductance varies with the relative ratio as well as the sign, but the change of sign is compatible with the bulk systems case. And this result is also compatible with the previous numerical work in the case of pure Rashba coupling.23,24
Spin Hall conductances for $L_G/\sigma_H$ consistent with symmetry analyses. Coupling strength with a fixed Rashba coupling strength, which are obtained for the Hall conductances as functions of the Dresselhaus coupling strength with a fixed Rashba coupling strength, which are consistent with symmetry analyses.

To see the finite-size effect we calculate the electric and spin Hall conductances for $L=20, 30, 40,$ and $50$. $G_{cH}/L$ and $G_{sH}/L$ as functions of $E_f$ are plotted in Fig. 4. We notice that these curves for different sizes fit a single one very well. Thus we conclude that both electric and spin Hall conductance are proportional to the size $L$ of the sample. In other words, in our calculation the electric and spin Hall currents are determined by both the number of the incident channels and that of the outgoing channels. Thus the Hall currents induced by a specified longitudinal electric field are not proportional to the size $L$ linearly, but to $L \times L$.

The disorder effect is an interesting issue in the spin Hall effect in 2DEG. It is still greatly controversial whether the spin Hall effect may survive when the impurity scattering is taken into account. We consider the disorder effect by including the disorder potential term $V_{\text{disorder}} = \sum_{i} \epsilon_i c_i^\dagger c_i$ in Eq. (3), where $\epsilon_i$ are randomly distributed between $[-W/2, +W/2]$. Selectively the electric and spin Hall conductances, $G_{cH}$ and $G_{sH}$, for two couplings with equal strength are plotted in Fig. 5. $G_{cH}$ is exactly equal to zero according to the symmetry. It shows that both electric and spin Hall conductances can survive in weak disorder, but be suppressed in strong disord. We also did calculation for several other cases, and obtained similar results. The case of pure Dresselhaus coupling is in agreement with the work of Sheng et al. for pure Rashba coupling.

Physically the spin Hall conductance can be well understood from the spin transverse force caused by the spin-orbit coupling in Eq. (2). The electric field drives electrons moving along the field such that the electrons with spin-up or spin-down experience opposite the transverse force and thus a nonzero spin current is induced perpendicular to the field. The relative ratio of the two coupling strength determines the direction of the spin Hall current as the spinomotive force changes its sign around $\lambda = \beta$ and vanishes at the point. All calculated results are consistent with this. However, the spinomotive force is not a direct origin of the nonzero $G_{sH}$, since $G_{sH}$ arises only when two couplings are present simultaneously. From the symmetry properties of the system we notice that the Hamiltonian with pure Rashba coupling is invariant under the transformation: $k_x \rightarrow -k_x$, $k_y \rightarrow -k_y$, and $\sigma^x \rightarrow -\sigma^x$, $\sigma^y \rightarrow \sigma^y$, $\sigma^z \rightarrow -\sigma^z$. Similarly the Hamiltonian with pure Dresselhaus coupling is invariant under the transformation: $k_x \rightarrow k_x$, $k_y \rightarrow -k_y$, and $\sigma^x \rightarrow \sigma^x$, $\sigma^y \rightarrow -\sigma^y$, $\sigma^z \rightarrow -\sigma^z$. This is why the electric Hall current vanishes in these two cases, while the spin Hall current circulates because there is no symmetry constraint on it as both $k_z$ and $\sigma^z$ change their signs under such transformation. On the other hand, the Hamiltonian with both Rashba and Dresselhaus couplings does not possess the reflection symmetry of $k_x \rightarrow -k_x$, $k_y \rightarrow -k_y$. Therefore the coexistence of both couplings breaks the reflection symmetry of the system, which makes the electric current not parallel to the electric field such that it gives rise to a nonvanishing Hall conductance $G_{cH}$. This unconven-

![FIG. 3. (Color online) Electric and spin Hall conductances as functions of the Rashba coupling strength with a fixed Dresselhaus coupling strength $t_{so}^D=1.0$ at $E_f=-2.0t$ and $L=40$. Similar results are obtained for the Hall conductances as functions of the Dresselhaus coupling strength with a fixed Rashba coupling strength, which are consistent with symmetry analyses.](image)

![FIG. 4. (Color online) Electric and spin Hall conductances divided by sample size $L$ as functions of the electron Fermi energy. Here the Rashba and Dresselhaus coupling strengths are equal and the results for $L=20, 30, 40,$ and $50$ are shown simultaneously. It implies a size effect that both Hall conductances are proportional to $L$ in this calculation.](image)

![FIG. 5. (Color online) Electric and spin Hall conductances as functions of the logarithm of the disorder strength $W/t$. Results are obtained with equal Rashba and Dresselhaus coupling strengths at $E_f=-2.0t$ and $L=30$. Standard deviations in the calculation are shown through the error bars.](image)
tional Hall conductance may be related to some discussions in terms of the anomalous Hall effect due to parity anomaly and additional band crossing.\textsuperscript{5} Moreover, since the diagonal spin conductance is nonzero in this case,\textsuperscript{26} the diagonal spin current along leads 1 and 2 might generate a charge Hall current via the reciprocal spin Hall effect.\textsuperscript{32}

In conclusion, we studied the electric Hall conductance as well as the spin Hall conductance for a finite-size system with four leads. Both electric and spin Hall conductances are nonzero when both Rashba and Dresselhaus couplings are present, thus the current is actually spin polarized. Unlike the anomalous Hall effect, the present electric Hall current is driven by the spin-orbit coupling, not by the exchange coupling with the magnetic impurities.\textsuperscript{33} This effect also differs from the one resulted from a spin polarized current via the Rashba coupling.\textsuperscript{34} Though the incident current is not spin polarized, the Hall current is polarized in our case.

The authors would like to thank L. Sheng and D. N. Sheng for helpful discussions. This work was supported by the Research Grant Council of Hong Kong (S.Q.S.), and by the National Science Foundation of China under Grant No. 10474022 (L.B.H.).

\textsuperscript{1} The Hall Effect and its Applications, edited by C. L. Chien and C. R. Westgate (Plenum, New York, 1980).
\textsuperscript{3} J. Smit, Physica (Amsterdam) 21, 887 (1955).
\textsuperscript{9} M. I. D’yakonov and V. I. Perel, JETP Lett. 13, 467 (1971).
\textsuperscript{17} The unit of the spin current operator is at (a is the lattice space), and here we take $\alpha = 1$.

We take $+\mu$ as up (\(\uparrow\)) and $-\mu$ as down (\(\downarrow\)) as the indices of the rotation matrix $R$.
\textsuperscript{24} S. Q. Shen, Phys. Rev. B 70, 081311(R) (2004).
Non-exponential relaxation and the distribution of the second-order transverse anisotropic parameters in Mn$_{12}$

Z.-D. Chen$^{1,2,*}$ and S.-Q. Shen$^1$

$^1$ Department of Physics, The University of Hong Kong, Hong Kong, P.R. China
$^2$ Department of Physics, Jinan University, Guangzhou 510632, P.R. China

Received 22 July 2005
Published online 23 December 2005 – © EDP Sciences, Società Italiana di Fisica, Springer-Verlag 2005

Abstract. The Landau-Zener multi-crossing relaxation in Mn$_{12}$ molecule is studied based on the tunnel splitting obtained from the spin-coherent-state path integral including the local stray field. It is found that the spins with larger second-order transverse anisotropic parameters will finish the relaxation before the higher resonance is reached. Such a pre-relaxation seriously modifies the relaxation behavior at higher resonance and makes the distributions of the second-order transverse anisotropic parameters extracted from different resonances un-scaled. Our analysis shows that scaled distributions can be found from the relaxation curves of $k = 6$ and $k = 7$ resonance by including the effect of pre-relaxation.

PACS. 75.45.+j Macroscopic quantum phenomena in magnetic systems – 75.50.Xx Molecular magnets

Since the first signature of quantum effect (i.e., the so-called quantum steps) was observed in the hysteresis loop of single-molecule magnet(SMM) Mn$_{12}$ acetate [1,2], such a SMM has raised intense interesting in the field of molecular magnetism. However, the origin of the tunnel splitting in Mn$_{12}$ acetate is still far from being absolutely clear. The main controversy comes from the origin of the second-order transverse anisotropy which plays an important role in quantum tunnelling in Mn$_{12}$ acetate. Chudnovsky and Garanin have suggested a distribution of the second-order transverse anisotropy due to the crystal dislocations [3], and gained experimental support from the electronic paramagnetic resonance (EPR) and other experimental measurements [9–11]. Recently, Cornia et al. suggested that the disorder of solvent molecules in Mn$_{12}$ acetate is the origin of the second-order transverse anisotropy [4] and del Barco et al. shown there is not strict tetragonal symmetry in Mn$_{12}$ acetate [7]. The solvent-disorder theory was confirmed by some recent experiments using the higher quality of the deuterated crystal [5,6,8] and also some further theoretical works were done [12]. The first evidence of the distribution of the second-order transverse anisotropic parameters in magnetic relaxation is the non-exponential behavior which comes from a distribution of tunnel splitting. As a matter of fact, it has been shown that the random local stray field raising from the environmental spins can lead to a distribution of tunnel splitting and non-exponential relaxation in Fe$_{6}$ [15], but in Mn$_{12}$ acetate, the distribution of tunnel splitting is much broader [6,9] and hence should come mainly from the distribution of second-order transverse anisotropic parameters, but the random local stray field as well. In a recent experimental analysis [6], the distribution of the second-order transverse anisotropic parameters $P(E)$ is extracted from the relaxation curve based on the tunnel splitting obtained from the perturbation theory [3]. However, the extracted distributions $P(E)$ for different resonances (say, $k = 6$ and $k = 8$) do not overlap (scale). The result looks physically unreasonable since the distribution $P(E)$ should be independent of the resonance index. This is the motivation of the present paper. We present a detail analysis on the way of extracting $P(E)$ from the relaxation curve basing on the result obtained from the spin-coherent-state path integral with the random local stray field. It is shown that the spins with larger second-order transverse anisotropic parameters will finish relaxation before the higher order resonance is reached. This pre-relaxation makes both the distribution center and width of $P(E)$ become smaller for higher order resonance. By including the effect of pre-relaxation, the extracted distributions of the second-order transverse anisotropic parameters for $k = 6$ and $k = 7$ do overlap (scale) very well.

Up to the second-order anisotropy, the Hamiltonian of the Mn$_{12}$ acetate molecule is given by

$$H = -DS^2 + E(S_+^2 - S_-^2) - g\mu_B S \cdot (B + h),$$

(1)

where $D = 0.5483$ K [6,8,9], $B$ is the applied magnetic field, and $h$ is the local stray field which may originate from the interactions between the giant spin and the environmental spins (including other giant spins or nuclear spins) [17] and also the misalignment (or the tilt) of the easy axis in Mn$_{12}$ acetate molecule as the longitudinal field.

*a* e-mail: zhidechen@21cn.com
is applied [6,8,9]. Due to the crystal dislocation or the solvent disorder, the second-order transverse anisotropic parameter \( E \) has a random distribution \( P(E) \) which can be chosen as a Gaussian [6,8]

\[
P(E) = (2\pi w^2)^{-1/2} e^{-(E-E_0)^2/2w^2}.
\]

Our main interest is the Landau-Zener multi-crossing relaxation which is done by sweeping the longitudinal field at a constant rate \( \alpha = dB_z/dt \) over a resonance for many times [8,9], a method firstly developed to measure the ground state tunnel splitting in Fe\(_8\) [13,14]. For a given \( E \), the relaxation equation is

\[
dM/dn = -MP_{LZ},
\]
where \( n \) is the time crossing the resonance, \( P_{LZ} \) is the Landau-Zener transition rate and in low transition rate limit is given by

\[
P_{LZ} = 1 - e^{-a_k\Delta^2(E,h)/\alpha} \approx a_k\Delta^2(E,h)/\alpha,
\]

where \( a_k = \pi/\sqrt{2\hbar g\mu_B(2S-k)} \), \( k \) is the index of the resonance (i.e., \( |S_z = -S \leftrightarrow |S_z = S - k \) ), and \( \Delta^2(E,h) \) is the tunnel splitting including the local transverse stray field

\[
\Delta^2(E,h) = \Delta^2_{E_0}(E,h)\gamma_k(E,h),
\]

\( \Delta^2_{E_0}(E,h) \) can be found by the spin-coherent-state path integral with the instanton method [16,17] and the renormalization factor \( \gamma_k(E,h) = \{ \cosh[2q(E)h_y] + (-1)^{2\pi-k} \times \cos[2dk(E,h)] \}/2 \) with \( \lambda = (D-E)/(D+E) \),

\[
q(E) = g\mu_B \pi \sqrt{X}/[2(D-E)(1-\lambda)^{1/2}],
\]

\[
dk(E) = \frac{g\mu_B}{2(D+E)} \int_0^\pi \frac{d\phi}{1-\lambda \sin^2 \phi - k\frac{\partial}{\partial (2\pi \phi)} \cos \phi},
\]

By setting \( M(n \rightarrow \infty) = M_{eq} \) and \( M(n = 0) = M_0 \), the solution of equation (3) is

\[
R_k = \frac{M_n - M_{eq}}{M_0 - M_{eq}} = \int P(E)dE \times \int W(h)dh \exp\{-a_k(n/\alpha)\Delta^2_{E_0}(E)\gamma_k(E,h)\},
\]

where \( W(h) = W(h_x)W(h_y) \) represents the distribution of the transverse local stray field. In the present case, since the amplitude of the sweeping field is much larger than the strength of the local stray field and \( n \) is much larger than 1 [8,14], we can approximately ignore the variation of the distribution center and width with the magnetization and \( W(h_i)(i = x,y) \) will be chosen as a Gaussian with a fixed distribution center \( h_0 \) and width \( \sigma \) [15,18–21].

Using equation (8), the experimental relaxation curves for \( k = 6 \) and \( k = 7 \) resonance can be fitted by choosing appropriate distribution center and width of \( P(E) \) and \( W(h) \). It is found that, for \( k = 6 \) resonance, the relaxation curve can be best fitted by taking \( E_0 = 0.0225 \) K,

\[ w = 0.0025 \text{ K}, \sigma = 0.08 \text{ T and } h_0 = 0 \] [22], while for \( k = 7 \), the corresponding parameters are: \( E_0 = 0.0172 \) K, \( w = 0.0011 \text{ K}, \sigma = 0.08 \text{ T and } h_0 = 0 \). The fitted relaxation curves and the extracted \( P(E) \) are shown in Figures 1 and 2. Here we get the same problem as that of the experimental analysis [6] based on the result from the perturbation theory, that is, the \( P(E) \) extracted from \( k = 6 \) and \( k = 7 \) relaxation curve do not overlap (scale). It is seen that both the distribution center \( E_0 \) and width \( w \) decrease as \( k \) increases. del Barco et al. attributed this problem to “the origin of the tunnel splitting cannot only be due to a second-order transverse anisotropy” [6]. We have checked this point by comparing the tunnel splitting obtained from numerical diagonalization with the distribution center of tunnel splitting extracted from the experimental relaxation curves for \( k = 6 \) and \( k = 8 \) resonance (see Fig. 2b in Ref. [6]). It is found that the inclusion of the higher order term like \( C(S^z_1 + S^z_2) \) does not help to solve the problem, for example, by omitting the local stray field, numerical diagonalization of the Hamiltonian.

![Fig. 1. Illustration of fitting the experimental relaxation curves for \( k = 6 \) and \( k = 7 \). The solid line is the experimental relaxation curves for \( k = 6 \) and \( w = 0.0025 \).](image1)

![Fig. 2. The unscaled distribution of the second-order transverse anisotropic parameters extracted from the relaxation curves using a complete Gaussian distribution.](image2)
\[ H + C(S^4 + S^4) \] with \( D = 0.5483 \text{ K}, \ E = 0.0045 \text{ K} \) and \( C = 2.2 \times 10^{-5} \text{ K} \) [23] tells that \( \Delta_k \approx 4.654 \times 10^{-8} \text{ K} \) which is very close to the experimentally extracted distribution center of \( k = 6 \) (i.e., \( 4.571 \times 10^{-8} \text{ K} \)), while the corresponding \( \Delta_k \approx 4.632 \times 10^{-5} \text{ K} \) is nearly 2 orders larger than the extracted distribution center of \( k = 8 \) (i.e., \( 8.511 \times 10^{-7} \text{ K} \)). On the other hand, recent experiment suggested that the second-order transverse anisotropy should be the main contribution to quantum tunnelling in Mn_{12} acetate molecule [7]. Consequently some important elements must have been ignored in extracting \( P(E) \) from the relaxation curve for \( k > 6 \) resonance.

The physical origin is that the initial state of the \( k = 7 \) resonance is different from that of \( k = 6 \) resonance. Let us scrutinize the experiment process [6,8], starting from the negative saturated magnetization, the system is brought to the resonance by sweeping the field to the positive resonant field and relaxation under a sweeping field is measured. Experimental data shows there is not observable magnetization relaxation before \( k = 6 \) resonance is reached [6,8], approximately the relaxation due to quantum tunnelling is reached [6,8], approximately the relaxation due to the quantum tunnelling of \( k < 6 \) resonances can be omitted, hence the relaxation of \( k = 6 \) resonance can be considered as contributed as by the complete \( P(E) \). For \( k = 7 \) resonance, however, the relaxation due to quantum tunnelling as the field swept over the \( k = 6 \) resonance leads to an obvious magnetization step (see Fig. 16 in Ref. [8]) which has important sequence. It is known that the spins with larger \( E \) have larger tunnel splitting and thus higher Landau-Zener transition rate. This implies that some spins with larger \( E \) have finished quantum tunnelling before the measurement of relaxation for \( k = 7 \) resonance begins. In other words, the measured relaxation curve of \( k = 7 \) resonance is not contributed by the complete \( P(E) \), but by an incomplete \( P(E) \) with some larger \( E \) being cut. Accordingly, the \( P(E) \) contributed to the relaxation of \( k = 7 \) resonance can be expressed as

\[
P(E) = \begin{cases} C(2\pi \sigma^2)^{-1/2} e^{-(E-E_c)^2/2\sigma^2}, & E \leq E_{c2} \\ 0, & E > E_{c1} \end{cases} \quad (9)
\]

where \( C \) is the re-normalization factor to assure that \( \int_{E \leq E_{c1}} P(E)dE = 1 \), \( E_0 \) and \( \sigma \) are the same as extracted from relaxation curve of \( k = 6 \) resonance. In this way, it is found that the relaxation curve of \( k = 7 \) resonance can be best fitted by taking \( E_0 = 0.0225 \text{ K}, \ w = 0.0025 \text{ K}, \ E_c = 0.018 \text{ K}, \sigma = 0.09 \text{ T} \) and \( b_0 = 0 \). The result of fitting for \( k = 7 \) relaxation curve is shown in Figure 1 and the extracted \( P(E) \) is shown in Figure 3. The increase of the distribution width of \( W(h) \) is easy to understand since \( h \) includes contribution from the misalignment of the easy axis, which will increase as the applied longitudinal field increases.

By considering the pre-relaxation happened before the \( k = 7 \) resonance is reached, the extracted \( P(E) \) from \( k = 6 \) and \( k = 7 \) resonance do overlap (scale) very well. However, as one can see form Figure 3, the value of \( E_c \) seems to be smaller than the expected one. Physically \( E_c \) can be determined from the pre-relaxation happened in \( k = 6 \) resonance. Suggest that the pre-relaxation can be effectively represented as sweeping over the \( k = 6 \) resonance for \( n_1 \) times, then \( E_c \) can be found approximately by [15]

\[
P_{LZ}(E_c, k = 6, \alpha) \simeq \frac{a_0}{\alpha} \int W(h)dh \Delta h^2(E_c, h) = 1/n_1.
\]

Now we show the way to find out \( n_1 \). According to equation (3), one can safely set \( M_{\theta} = 0 \) [24] and we know that \( M_{\theta} = 1 \) for \( k = 6 \), this implies that \( R_0 = M_{\theta}(k = 6) \), namely \( R_0 \) just represents the magnetization. Since the magnetization is continuous for crossing from \( k = 6 \) to \( k = 7 \), we have

\[
M_{\theta}(k = 7) = M(n_1, k = 6),
\]

alternatively speaking, \( n_1 \) can be found from the relaxation curve of \( k = 6 \) resonance provided that the initial magnetization of \( k = 7 \) resonance is known. Although the experimental data for \( M_{\theta}(k = 7) \) is not available, one can approximately estimate it from the relaxation curve in the low transition rate limit. Low transition rate means that sweeping over the \( k = 7 \) resonance 1 time does not lead to observable change of the magnetization, this implies that \( M_{\theta}(k = 7) \approx M(k = 7, n = 1) \). For fitting the relaxation curve, this approximation is reasonable since the main contribution of the relaxation curve is from \( n > 1 \). As illustrated in Figure 4, if we take \( \alpha = 3.33 \times 10^{-3} \text{ T/s} \), we have \( n_1 \approx 8 \), then one can find out from equation (10) that \( E_c \approx 0.0207 \text{ using the tunnel splitting formula in equation (5)} \). However, if we take \( \alpha = 1.33 \times 10^{-2} \text{ T/s} \), then \( n_1 \approx 148 \), the estimated \( E_c \) is 0.01825 which is very close to what we have found (i.e., \( E_c \approx 0.018 \)). As a conclusion, we can say that the extracted \( P(E) \) of \( k = 7 \) resonance shown in Figure 3 is reasonable.

We have presented a detail analysis on extracting the second-order transverse anisotropic parameters \( P(E) \) from the relaxation curve in Mn_{12} acetate molecule. It is found that the pre-relaxation of the spins with larger \( E \) before the relevant resonance point is reached will lead to
on the solvent-disorder theory, i.e., by adapting a discrete distribution center of \( \sigma_0 \) to \( E \) can be fitted by \( 3 \) resonance which is the prediction of solvent-disorder theory [4,12]. Probably the origin of the second-order transverse anisotropic parameters is a “mixed result”, i.e., both dislocation and disorder contribute to the distribution [6], but further analysis is necessary for confirming this point.

The work was supported by a grant from the Research Grants Council of the Hong Kong, China under Grant No. 7023/03P.

References

22. The obtained \( E_0 \) and \( w \) are smaller than that of experimental analysis from reference [6] (i.e., \( E_0 \approx 0.02673 \) K and \( w \approx 0.003525 \) K), this is because that the local stray field distribution is included in the present case
24. Physically \( M_{eq} \) will oscillate around zero following the sweeping field

\[ R_k = \sum_{i=1}^{3} b_i \int W(h) dh \exp \left\{ -\alpha k(n/\gamma) \Delta h_0(E_i) \gamma k(E_i, h) \right\}, \]
Quantum dynamics of a vortex in a Josephson junction

Hong Li,1 Shun-Qing Shen,2 Jiu-Qing Liang,3 and Wu-Ming Liu1
1Joint Laboratory of Advanced Technology in Measurements, Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China
2Department of Physics, University of Hong Kong, Pokfulam Road, Hong Kong, China
3Institute of Theoretical Physics, Shanxi University, Taiyuan, Shanxi 030006, China

(Received 20 April 2005; published 29 July 2005)

We investigate the tunneling character of vortex in an asymmetrical potential well with a finite barrier by using the periodic instanton method. We obtain the total decay rate which is valid for the entire range of temperatures and show how it reduces to the appropriate results for the classical thermal activation at high temperatures, the thermally assisted tunneling at intermediate temperatures, and the pure quantum tunneling at low temperature. We can even give the exact definition of the “crossover” temperature and find experimental data to support our theoretical analysis.

DOI: 10.1103/PhysRevB.72.014546 PACS number(s): 67.40.Vs, 03.75.Lm, 05.30.Jp, 64.60.My

I. INTRODUCTION

The question of particlelike collective excitations, like domain walls, solitons, vortices, or fluxons, exhibiting quantum behavior has attracted much attention. Especially the escaping process of a particle from a potential well is a problem of great importance in almost all areas of physics.1–7

Vortices occur naturally in a wide range of gases and fluids, from macroscopic to microscopic scales.8–10 Two kinds of vortices can develop in superconductors. The first, the Abrikosov vortex, penetrates certain (type II) superconductors above a critical value of applied magnetic field. It can hop between pinning sites under thermal activation, causing dissipation in current-carrying wires and generating noise in sensors such as superconducting quantum interference devices (SQUIDs). Quantum tunneling of Abrikosov vortices remains controversial. The second vortex, the Josephson vortex, exists in a Josephson junction, formed by a sandwich of two superconducting layers and a thin insulating layer, through which electrons in the form of Cooper pairs can tunnel coherently. In a current-biased Josephson junction, swirling currents generate vortices of flux. Vortex motion in current-biased Josephson junction systems has been the subject of much theoretical and experimental work.11–14

Recently, Wallraff et al.9 showed that a single pinned vortex in a current-biased annular junction subject to an in-plane field can undergo macroscopic quantum tunneling to escape from a potential well; they also showed that the vortex’s energy in the controllable well is quantized. In their experiment, they made an annular junction between two narrow rings of the superconductor niobium, stacked one on top of the other. The flux in each ring is quantized in units of $\hbar/2e$ (where $\hbar$ is Plank’s constant and $e$ is the charge on an electron); when this flux quantum number differs between the two rings by one unit, the difference is manifested as a single vortex in the junction. If a magnetic field is applied in the plane of the annulus, at an angle to the magnetic moment of the vortex, the potential energy of the system is proportional to the cosine of the angle. If an external current is then applied to the junction, across the two superconducting layers, the resulting imbalance in the tunneling currents produces a force on the vortex to escape and move along the barrier.

In this paper we investigate the quantum tunneling of a vortex in a long Josephson junction by using the periodic instanton method which is well known as a powerful tool for dealing with quantum tunneling phenomena.15,16 In our model, we simplify a single vortex behavior in an annular junction subject to an in-plane field as a particle in a tilted washboard potential. We first calculate the total decay rate for all temperatures and show how it reduces to the appropriate results for the classical thermal activation at high temperatures, the thermally assisted tunneling at intermediate temperatures, and the pure quantum tunneling at low temperatures.

The rest of the paper is as follows: In Sec. II we gain the base mode of our path-integral approach from the master equation. In Sec. III we recall from Ref. 16 the bounce with nonzero energy and again give the main process of the calculation. Results and comparison with experiments are discussed in Sec. IV. The analysis of quantum-classical transition property is in Sec. V.

II. THE MASTER EQUATION IN CURRENT-BIASED JOSEPHSON JUNCTION

The dynamics of a current-biased Josephson tunnel junction can be described by the master equation.17,18 The behavior of the superconducting tunnel junction is described by the Josephson relations

$$I_J = I_c \sin \phi, \quad V = \frac{\Phi_0}{2\pi} \frac{d\phi}{dt}. \quad (1)$$

Here $I_J$ is the tunneling current of Cooper pairs flowing through the junction, $I_c$ the critical current, $V$ the voltage across the junction, $\phi$ the phase difference of the superconducting order parameter, and $\Phi_0 = \hbar/2e = 2.07 \times 10^{-15}$ Wb the flux quantum. The classical equation describing the system is
\[ I = C \frac{dV}{dt} + \frac{V}{R} + I_J, \]  

where \( I \) is the bias current, \( C \) the capacitance, and \( R \) the resistance characterizing the dissipation. Inserting the Josephson relations into the classical equation one obtains

\[
C \left( \frac{\Phi_0}{2\pi} \right)^2 \frac{d^2 \phi}{dt^2} + \frac{1}{R} \left( \frac{\Phi_0}{2\pi} \right)^2 \frac{d\phi}{dt} = -\frac{\partial}{\partial \phi} \left[ -I_c \left( \frac{\Phi_0}{2\pi} \right) \left( \cos \phi + \frac{I}{I_c} \phi \right) \right].
\]

This equation is identical with the equation of motion of a particle with mass \( M = (\Phi_0/2\pi)^2 C \), subject to damping and a fluctuating force, and move in the one-dimensional potential \( \tilde{U}(\phi) \), commonly known as the washboard potential: \( \tilde{U}(\phi) = -I_c (\Phi_0/2\pi) \cos \phi + I/I_c \phi \).

The component of the potential periodic in the vortex coordinate \( \phi \) is due to the interaction of the vortex magnetic moment with the external magnetic fields. The tilt of the potential is proportional to the Lorentz force acting on the vortex which is induced by the bias current applied to the junction. The rate at which the particle escapes from the potential depends on details of the shape of the potential.

Experimentally, the escape rate of a vortex from the zero-voltage state to the finite-voltage state was measured. In the mechanical analog this corresponds to measuring the escape of the particle from one of the washboard potential wells. The escape might occur either by thermal fluctuations or by quantum tunneling. Since in the weak-damping limit the particle is unlikely to be retrapped in another well, we are interested in only one potential well of the washboard potential. We can approximate it very well, for bias currents close to the critical current, by a cubic parabola,

\[ U(\phi) = 3U_0 \left( \frac{\phi}{\phi_0} \right)^2 \left( 1 - \frac{2\phi}{3\phi_0} \right). \]

The height \( U_0 \) and the position of the maxima \( \phi_0 \) are given in terms of the parameters of the junction by \( U_0 = 2I_c [\Phi_0/2\pi] [(1 - I^2)^{1/2} - I'] \arccos I' \), \( \phi_0 = 2\sqrt{3}[1 - I'] \arccos I' / (1 - I^2)^{1/2} \), where \( I' = I/I_c \). Increasing the bias current \( I \) through the junction corresponds to reducing the height \( U_0 \) of the barrier.

The existence of tunneling results in a complex vortex energy \( E \) (see Fig. 1). The decay rate \( \Gamma \) of the vortex states is defined as the imaginary part of the complex energy, \( \Gamma = 2/\hbar \Im E \). If \( |\Psi\rangle \) denotes an eigenstate of the Hamiltonian \( H \) with energy \( E \), the transition amplitude \( A \) from the state \( |\Psi\rangle \) to itself—the “survival probability” of \( |\Psi\rangle \)—in the presence of quantum tunneling over Euclidean time \( 2\beta \) reads

\[ A = \langle \Psi | e^{-2\beta H} |\Psi\rangle = e^{-2\beta E}. \]

The amplitude \( A \) can also be calculated with the help of the path-integral method. Comparing the defined transition amplitude \( A \) from Eq. (5) with the path-integral result in the next section, we can find the decay rate \( \Gamma \).

**III. TUNNELING OF VORTEX**

The Lagrangian for a 0+1 dimension scalar field \( \phi(t) \) is

\[ L = \frac{1}{2} M \left( \frac{d\phi}{dt} \right)^2 - U(\phi). \]

By using Euclidean time \( \tau = it \) we can rewrite \( L \) as

\[ L_E[\phi(\tau),\phi(\tau)] = -L = \frac{1}{2} M \left( \frac{d\phi}{d\tau} \right)^2 + U(\phi), \]

and the classical action is

\[ S_E(\phi) = \int_{\tau_i}^{\tau_f} L_E[\phi(\tau),\phi(\tau)] d\tau. \]

The classical solution \( \phi_{cl} \) which minimizes the action with Euclidean time \( \tau \) satisfies the equation

\[ \frac{1}{2} M \left( \frac{d\phi_{cl}}{d\tau} \right)^2 - U(\phi_{cl}) = -E. \]

The periodic instanton represents the pseudoparticle configuration responsible for tunneling under the barrier at energy \( E \). Tunneling out of a vortex state in a potential \( U(\phi) \) can be treated as motion with imaginary time \( \tau = it \) in the corresponding inverted potential. The corresponding “periodic instanton” solution

\[ \phi_\tau(\tau) = \phi_1 - (\phi_1 - \phi_2) \sn^2(u|k) \]

is periodic with period \( T \), \( \chi(k^\prime)T = n2K(k) \), \( n = 1, 2, 3, \ldots \), and \( \phi_\tau(\tau + T) = \phi_\tau(\tau) \), where \( \phi_1(E) > \phi_2(E) > \phi_3(E) \) denote three roots of the equation \( U(\phi) = E \). \( \phi_1 \) and \( \phi_2 \) denote the turning points of the instanton motion in inverted potential. \( \sn(u|k) \) denotes a Jacobian elliptic function with the modulus \( k = \sqrt{(\phi_1 - \phi_2)/(\phi_1 - \phi_3)} \), where \( u = \chi(k^\prime) \), \( \chi(k^\prime) = \sqrt{U_0(\phi_1 - \phi_3)/M \phi_0^2} \), \( k^\prime = \sqrt{1-k^2} \) is the complementary modulus of \( k \).

Considering the small fluctuation about the classical solution \( \phi_\tau(\tau) \) is

\[ \phi(\tau) = \phi_\tau(\tau) + \eta(\tau), \]

and correspondingly

![FIG. 1. A particle with energy E moving in the cubic potential given by Eq. (4); trajectories of the nonvacuum instantons (the case \( n=1 \) and \( n=2 \)) given by Eq. (9).](image)
with the ground state to the first excited state. The occupation of the excited state is very small. In fact, the results of the microwave frequency versus normalized bias current in Fig. 2 with Wallraff experimental parameters. In fact, the results of the microwave frequency versus normalized bias current in Fig. 2 with Wallraff experimental parameters. In Fig. 2, the microwave frequency $\omega/2\pi$ is plotted against the normalized bias current $I/I_c$. The amplitude $A$ can also be calculated with the help of the path integral method. We rewrite it

$$ A = \int \psi_{E}^{*} (\phi_f) \psi_{E} (\phi_i) K(\phi_f, \phi_i) d\phi_f d\phi_i, \quad (12) $$

with $\phi_f = (t_f)$, $\phi_i = (t_i)$, and $t_f - t_i = 2\beta$. The Feynman propagator from $\phi_i$ to $\phi_f$ resulting from the instanton motion is defined by

$$ K(\phi_f, \phi_i) = \sum_{n=0,1,2\ldots} K_n(\phi_f, \phi_i), \quad (13) $$

The zero bounce contribution, $n=0$ means there is no tunneling occurring which equals the harmonic oscillator in infinite barrier, i.e., $\frac{1}{2}M\omega_0^2\phi_0^2 = 3U_0$ and the zero bounce contributes to the real part of the complex energy $A_0 = e^{-2Ei\beta}$, where $E_i = (m+\frac{1}{2})/h\omega_0$, $m=0,1,\ldots$ and $\omega_0 = \sqrt{6U_0/M\phi_0^2}$. Both bias current and applied magnetic field scale the energy level separation $\Delta E = \hbar\omega_0 \times [1 - 1/(1/2\omega_0)]^{1/4}$. We draw the microwave frequency versus normalized bias current in Fig. 2 with Wallraff experiment parameters. In fact, the results of Fig. 2 just give the theoretical dashed lines in Fig. 3(b) of Ref. 8. At low temperature and in the absence of microwave radiation, the occupation of the excited state is very small. By irradiating the sample with microwaves, the vortex can be excited resonantly from the ground state to the first excited state. Then obviously a lower bias current corresponding to the tunneling out to the first excited state will be detected [see Fig. 3(a) in Ref. 8].

The one bounce contribution. Setting $T = 2\beta$ and taking $n=1$, we have $\gamma(k') \beta = K(k)$, where $\beta$ is half the period of the motion of the pseudoparticle as indicated in Fig. 1. As the energy tends to zero with $k\to 1$, the periodic instanton solution reduces the usual vacuum bounce. On the other hand, as the energy approaches the top of the barrier $E - U_0$ with $k \to 0$, the solution becomes the trivial configuration $\phi_f = \phi_i$. This trivial solution is called a spherelon. The nonvacuum bounce thus interpolates between the vacuum bounce and this spherelon.

The necessary boundary conditions for $\eta(\tau)$, where $\eta(\tau)$ denotes the small deviation of $\phi$ from the classical trajectory with end points held fixed, are $\eta(\tau_f) = \eta(\tau_i) = 0$. From the expressions of $K_n$ in Eq. (13) and $S_E$ in Eq. (11) we obtain

$$ K_1 = e^{-\Delta E/\hbar} I_{\pi}, \quad (14) $$

where $I_{\pi}$ is the functional integral $I_{\pi} = \int_{[\pi, \pi]} \rho e^{-iS_E}$. We can evaluate the expression with the help of tables of integrals in Ref. 20 and find with $\tau_f = \beta$, $\tau_i = -\beta$, and $\beta = (K/k)/\gamma(k')$, $S_n(\phi_i, \phi_f, \phi_i, \phi_f, E, \beta) + 2\pi E\beta$, where $W = \frac{\pi}{16} \sqrt{6U_0/\phi_0^2} (\phi_i - \phi_f)^{3/2}[1 - (k^2 - 2)^2K(k) + 2(k^2 - k^2 + 1)E(k)]$, where $K(k)$ and $E(k)$ are the complete elliptic integrals of the first and second kinds.

The Feynman propagator of the path integral is divergent because the velocity of instanton $\eta(\tau) = d\phi_i/d\tau$ 

$= -2\sqrt{U_0/M}(\phi_i - \phi_f)/d\tau/\eta = d\phi_i/d\tau - d\phi_i\delta n(u(k))/d\tau\eta$ vanishes at the turning points, i.e., $c/n(\pm K(k)/k) = 0$. The transition amplitude has to be finite and this singularity must be smoothed out by turning point integrations of $d\phi_i$ and $d\phi_f$. We use the following relations established in Ref. 16: $I_{\pi} = [1/2\pi]^{1/2} [N(\phi_i)/N(\phi_f)]^{1/2} [\phi_f/\phi_i]^{1/2}$. The WKB approximations of the wave functions are given by $\psi_{E}(\phi_f)$

$$ \psi_{E}(\phi_f) = [\eta]^{1/2} \left[ N(\phi_i)/N(\phi_f) \right]^{1/2} \left[ \phi_f/\phi_i \right]^{1/2}. $$

The normalization constant $C$ is defined by $C = [2\pi \phi_f/\psi_{E}(\phi_f) - 2\sqrt{M(I - U(\phi_f))}]^{-1/2}$, where the integration extends from turning point to turning point across the nontunneling domain (i.e., the region of the harmonic-oscillator approximation). Evaluating $C$ one obtains $C = [\{U_0/M\phi_0^2\} \phi_f/\phi_i]/2K(k')]^{1/2}$. Using one loop expansion of the action and completing the turning point integration, we can obtain one instanton contribution

$$ A_1 = -2i\beta e^{-2E\beta} \sqrt{U_0/M\phi_0^2} \phi_f/\phi_i/2K(k') \quad (15) $$

The one instanton contribution is that of the classical configuration with period $T = n2K(k)/\gamma(k')$ with $n=1$. For $n=2$ there are two instantons moving from $-\beta$ to $\beta$ with "positions" $\tau_0 = \pm K(k)/\gamma(k')$ (see Fig. 1). The contribution $A_0$ to the transition amplitude arising from $n$ instantons can be calculated analogously.
\[ A_n = (-i)^n \frac{(2\beta)^n}{n!} e^{-nW-2E\beta} \left( \frac{U_0}{M\phi_0^3} \left( \phi_1 - \phi_3 \right)^n \right). \]  

The total transition amplitude \( A \) is obtained by summation, 
\[ A = \sum_n A_n = e^{-2E\beta} \exp \left( -i2\beta \sqrt{\frac{U_0}{M\phi_0^3}} \left( \phi_1 - \phi_3 \right) e^{-W} \right). \]

We can get the imaginary part of energy \( E \) by comparing the above amplitude \( A \) in Eq. (17) with defined amplitude \( A \) in Eq. (5). The decay rate of vortex state with energy \( E \) can be written as
\[ \Gamma = \frac{\omega_E}{2\hbar k(T')} e^{-W}, \]  
where \( \omega_E = \sqrt{(2\phi_1 - \phi_3)/3\phi_0\omega_0} \) is the energy dependent frequency. We emphasize that this compact formula is valid for the entire region of energy \( 0 < E < U_0 \). It can be applied to any excited states from bottom to top of the well.

In low energy limit \( E \ll U_0 \), introducing a harmonic approximation \( E_m = m\hbar\omega_0 + E_0 \), we can evaluate the decay rate \( \Gamma_m \) of \( m \)th excited state, 
\[ \Gamma_m = \frac{1}{m!} \left( \frac{432U_0}{\hbar\omega_0} \right)^m \Gamma_0. \]

When \( m = 0 \), \( \Gamma_m \) reduces to the decay rate \( \Gamma_0 \) of the vortex state with energy \( E_0 \) and \( \Gamma_0 = 12\omega_0 \sqrt{6U_0/\pi\hbar\omega_0} e^{-36U_0/\hbar\omega_0} \).

We can find that the decay rate depends on the well depth. In a future experiment, we can increase the bias current through the junction corresponding to reducing the height of the barrier. The tunneling rate could be increased by lowering the well depths.

### IV. TEMPERATURE DEPENDENCE

Taking a statistical average of the decay rates of different vortex states, \( \Gamma(T) = 1/\sum_m \Gamma_m e^{-E_m/k_BT} \), where \( Z_0 = \sum_m e^{-E_m/k_BT} \), we can obtain the decay rate of temperature dependence
\[ \Gamma(T) = \Gamma_0 (1 - e^{-\hbar\omega_0/k_BT}) e^{432U_0/\hbar\omega_0} e^{-36U_0/\hbar\omega_0} T, \]
where \( k_B \) is the Boltzmann constant. With experimental parameter \( \omega_0 = 2\pi v_0 = 75 \text{ GHz} \) for \( v_0 \) between 10 and 13 GHz given in Ref. 8 and \( U_0 = 2.5\hbar\omega_0 \) for two energy levels in the well, Fig. 3 shows three distinct regions with different behavior for \( \Gamma(T) \). At high temperature, the decay is thermally activated and exhibits the expected Arrhenius law, \[ \Gamma_{AP} = \omega_0/2\pi e^{-U_0/k_BT}. \]  
At intermediate temperature, we observe “thermally assisted” tunneling, in which atoms are thermally activated to excited quantum state in the well, and then decay out from the well by quantum tunneling. At lower temperature, pure quantum tunneling from the trapped ground state is dominant, which is controlled by the “vacuum” instanton trajectory. Hence the ordinarily definition of the “crossover” temperature is \( T_{cr} = \hbar\omega_0/2\pi k_B \), below which quantum tunneling dominates. The decay rate is independent on temperature if \( T < T_{cr} \), whereas it will increase appropriately with temperature if \( T > T_{cr} \). We find \( T_{cr} = 92 \text{ mK} \) which is consistent with the “crossover” temperature extracted from the temperature dependence of the switching current distributions in Ref. 8. In the following section, we will give another definition of the \( T_{cr} \) using our method, which will help in getting a deeper understanding of the conception.

In order to make clearer the meaning of \( \Gamma(T) \), we repeat the process of the experiment. Wallraff et al. investigate the escape process by ramping up the current that is flowing through the annular junction until they see a jump in the voltage across the junction, which corresponds to the vortex beginning to rotate rapidly around the annulus (the voltage is proportional to the vortex velocity). This depinning of the vortex and its subsequent escape from the well is a stochastic process, so repeated measurements yield a distribution of switching currents at which depinning occurs. As the temperature is lowered, the width of this distribution shrinks, indicating a crossover from the classical region to macroscopic quantum tunneling in the quantum regime. We assume that we have an initial thermal distribution of the vortices (the decay principle will be consistent with the statistical experimental results); the population should decay as
\[ N(t) = \frac{N_0}{Z_0} \sum_m e^{-E_m/k_BT}, \]  
where \( N_0 \) is the initial population of trapped vortices. Since \( N(t) \) is a sum of exponential decay factors, it does not decay exponentially itself, i.e., \( N(t) \) is not a straight line if we plot \( \log N(t) \) as a function of time. There is not a single slope, and therefore it cannot be assigned a single decay rate. At long times, the curve approaches a straight line, with the corresponding rate given by \( \Gamma_0 \), i.e., the slowest channel dominates the long time behavior. In fact, the initial slope at time \( t = 0 \) corresponds to a rate of \( \Gamma(T) \) as calculated, meaning that \( \Gamma(T) \) is simply the initial rate of decay of the population. The above discussion is valid if there is no thermalization of the population during decay, which is a situation that the experimentalist can realize. On the other hand, it is also possible to intentionally introduce intrawell transitions between the dif-
different levels, such that thermalization can be established in a
time $t_c$. In this case, if $t_c$ is short compared to $1/\Gamma(t)$, the
population will decay at $\Gamma(t)$ at all times. If it is larger than
$1/\Gamma(t)$, the population will decay initially nonexponentially
until time $t_c$, after which the population will decay at $\Gamma(t')$, where
$T'$ is some temperature below $T$. There is a cool down of
the population due to the initial decay.

To probe the $\Gamma(T)$ versus the temperature for a different
external condition we draw Fig. 4. In order to have a qualitative analysis about Fig. 2(b) in Ref. 8, we use the experiment parameters $I_1(H)$. From our Fig. 4, we can find a value of $T_{cr}$ about 90 ± mk, which is consistent with the saturation temperature in Fig. 2 of Ref. 4. In Fig. 4, we can see in a higher field the quantum region corresponds to a higher decay rate. That indicates the quantum tunneling is also dominated by the potential. If a higher field is applied to the junction, which corresponds to the vortex having a higher harmonic oscillator frequency and less shallow effective potential, the quantum tunneling will get a higher decay rate. This is the reason for Fig. 2(b) in Ref. 8 having two branches in the quantum region.

V. QUANTUM-CLASSICAL TRANSITION

The second derivative of the action, which is proportional to $dE/dT$, can be interpreted as the specific heat of the system. Our model, allowing explicit calculation of periodic instantons and the corresponding evaluation of the action, can be studied with regard to phase transitions from classical to quantum behavior. When the vortex escape from the potential under certain in-plane field, the second-order transition from thermal activation to macroscopic quantum tunneling should be observed as the temperature is lowered. The thermodynamic action, i.e., that of the sphere-ron at the top of the barrier, and the action are correspondingly given by $S_0=(U_B)/(kbT)$ and $S=T/(T+W)$. Figure 5 displays the behavior of $S_T$ and $S_0$ versus temperature $T$. We emphasize that the temperature of the point of intersection is the “cross” temperature $T_{cr}$. In Fig. 5(b), arrows show the actual dependence of $S(T)$ as the temperature is lowered and one can clearly see the typically smooth behavior of a second order transition from the thermal to the quantum regime as the temperature is lowered.

In conclusion, we have calculated the total decay rate over the entire range of temperature of the vortex, which is confined in a current-biased annular junction subject to an in-plane field. We also pointed out that the system acquires a second order transition.

ACKNOWLEDGMENT

This work was supported by the NSF of China under Grants 60490280, 90403034, and 90406017. This work was also supported by the Research Grant Council of Hong Kong under Grant No. HKU 7023/03P.

Charge Hall effect driven by spin-dependent chemical potential gradients and Onsager relations in mesoscopic systems

E. M. Hankiewicz,1 Jian Li,2 Tomas Jungwirth,3,45 Qian Niu,5 Shun-Qing Shen,2 and Jairo Sinova1
1Department of Physics, Texas A&M University, College Station, Texas 77843–4242, USA
2Department of Physics, The University of Hong-Kong, Pokfulam Road, Hong-Kong, China
3Institute of Physics ASCR, Cukrovarnická 10, 162 53 Praha 6, Czech Republic
4School of Physics and Astronomy, University of Nottingham, Nottingham NG7 2RD, United Kingdom
5Department of Physics, University of Texas, Austin, Texas 78712-0264, USA
(Received 25 May 2005; published 7 October 2005)

We study theoretically the spin-Hall effect as well as its reciprocal phenomenon (a transverse charge current driven by a spin-dependent chemical potential gradient) in electron and hole finite size mesoscopic systems. The Landauer-Buttiker-Keldysh formalism is used to model samples with mobilities and Rashba coupling strengths which are experimentally accessible and to demonstrate the appearance of measurable charge currents induced by the spin-dependent chemical potential gradient in the reciprocal spin-Hall effect. We also demonstrate that within the mesoscopic coherent transport regime the Onsager relations are fulfilled for the disorder averaged conductances for electron and hole mesoscopic systems.

DOI: 10.1103/PhysRevB.72.155305

PACS number(s): 73.23.—b, 72.25.Dc, 72.25.Hg, 85.75.—d

INTRODUCTION

In the very active field of semiconductor based spintronics the control of spin can be achieved by the manipulation of the strength of spin-orbit (SO) interactions in paramagnetic systems. Within this context, the newly proposed intrinsic spin-Hall effect (SHE) in p-doped semiconductors by Murakami et al.1 and in a two-dimensional electron system (2DES) by Sinova et al.2 offers new possibilities for spin current manipulation and generation in high mobility paramagnetic semiconductor systems. In contrast to the earlier proposed extrinsic spin-Hall effect,3–5 which is associated with scattering from impurities, the intrinsic spin-Hall arises purely from host semiconductor band structure and represents a spin-current response generated perpendicular to the driving electric field.

Recently, the spin Hall effect was experimentally observed by Kato et al.6 in n-doped GaAs using the Kerr effect and by Wunderlich et al.7 in the p-n junction light-emitting diodes based on two-dimensional hole gas (2DHG) (Al,Ga)As. Although the experiment by Wunderlich et al. seems to be in the regime where the intrinsic effect in 2DHG is dominant, the main theoretical focus has been concentrated so far on 2DEG with Rashba SO interactions, where Rashba term is linear with k.28–21 The influence of disorder on infinite 2DEG is still unclear (for a recent review see Ref. 21). For δ-function impurities the analytical calculations of vertex corrections in the ladder approximation seem to cancel the intrinsic spin-Hall effect in a weak scattering regime.12,14 However, these calculations have been challenged recently.20 Further, the numerical calculations for 2DEG based on Kubo formula using continuum model in momentum space show the finite value of SHE in a weak scattering regime which goes to constant in the thermodynamic limit.23

The calculations within the Landauer-Buttiker (LB) formalism on finite size systems17–19,26 model a sample of micro/nanosize attached to contacts. The calculations on electron mesoscopic systems show that spin Hall conductance is a fraction of e/8π in a weak scattering regime.17–19 Moreover, a mesoscopic spin-Hall conductance is robust against the disorder.17–19 Very recently Wu and Zhou considered the Luttinger model,27 showing as expected that SHE can be much larger in hole systems in comparison with the electron ones. Although the experimental measurement by Wunderlich et al.7 concern 2DHG systems with broken inversion symmetry, the pure cubic Rashba term was not considered in detail within the LB formalism so far.

The observation of spin-Hall effect through transport measurements is one of the urgent experimental challenges facing this spin-transport physics. Recently, an H-probe structure has been proposed to measure the effect where the spin-Hall effect could be measured indirectly by detecting charge voltages induced by the reciprocal spin-Hall effect (RSHE).19 This RSHE, where transverse charge current is driven by spin dependent chemical potential, was proposed in a context of extrinsic spin-Hall effect by Hirsch4 and formulated in a semiclassical approach by Zhang and Niu.28 Also, the Onsager relation between the spin-Hall conductivity and reciprocal charge-Hall conductivity was established within a wave packet model through a redefinition of the spin-current including spin-torque terms in the bulk.28

We show here that within the mesoscopic regime, and more specifically within the Landauer-Buttiker-Keldysh formalism, the Onsager relations are satisfied within the models studied for the disorder averaged conductances. Because the conductances are formulated with respect to the leads which have no spin-orbit coupling, it is not necessary nor consequential to introduce the spin current redefinition in our problem.28
In this paper we compare the magnitude of the SHE as well as the RSHE in finite electron and hole mesoscopic systems within the LB formalism. We show that the conductances associated with both effects are significantly larger in the hole systems. Furthermore, we analyze the possible experimental setup to measure the RSHE. We show that the charge current driven by a spin-dependent chemical potential gradient is on the order of hundred nano-ampers for typical voltages in hole systems and should be experimentally measurable.

MODEL HAMILTONIAN FOR HOLE SYSTEM AND LB TREATMENT OF THE SPIN-HALL EFFECT AND ITS RECIPROCAL CORRESPONDENT

The observation of the spin-Hall effect and its reciprocal phenomenon in transport is the next experimental challenge in the subfield of spintronics using spin-orbit interactions to manipulate the spin.

The continuum effective mass model for 2DHG in a narrow inversion asymmetrical well is given by:

$$H = \sum_{j,\sigma} \varepsilon_j c_{j,\sigma}^\dagger c_{j,\sigma} - t \sum_{j,\delta,\sigma} c_{j,\delta,\sigma}^\dagger c_{j+\delta,\sigma} + \alpha_0^2 \sum_{j} \left( \sum_{1} c_{j,1}^\dagger c_{j+2a_y,1} + c_{j,1}^\dagger c_{j-2a_y,1} \right) - c_{j,1}^\dagger c_{j-2a_y,1} + 3(1-i) \sum_{j} c_{j,1}^\dagger c_{j-a_y,1}^\dagger c_{j+a_y,1} - c_{j,1}^\dagger c_{j-a_y,1} c_{j+a_y,1} + 4 \sum_{j} c_{j,1}^\dagger c_{j+a_y,1}$$

where $t=\hbar^2/2m^* a_0^2$ and $\delta=\pm a_0 \delta_j$, $a_0$ is the mesh lattice spacing, and $\delta_j=\pm a_0 \delta_j$. The first term represents a quenched disorder potential and disorder is introduced by randomly selecting the on-site energy $\varepsilon_j$ in the range $[-W/2, W/2]$. The continuum effective mass model for 2DES and its tight-binding correspondent can be found elsewhere.

Within the leads the SO coupling is zero and therefore each lead should be considered as having two independent spin-channels. Moreover, in leads without the SO coupling, the spin current is measured in a medium where spin is conserved removing the ambiguity of spin-current definition. For SHE, leads constitute reservoirs of electrons at chemical potential $\mu_1, \ldots, \mu_N$, where $N$ is the number of leads that we consider to be four [see Fig. 1(b)]. For RSHE, the chemical potential is spin dependent in leads 1 and 2 allowing the generation of spin-force in the $x$ direction [see Fig. 1(a)].

In the low temperature limit $k_B T \ll E_F$ and for low bias-voltage, the particle current going through a particular channel is given within the LB formalism by:

$$I_{p,\sigma} = (e/\hbar) \sum_{q,\sigma'} T_{p,q,\sigma,\sigma'} [V_{p,q} - V_{q,\sigma'}],$$

where $p$ labels the lead and $T_{p,q,\sigma,\sigma'}$ is the transmission coefficient at the Fermi energy $E_F$ between the $(p, \sigma)$ channel and the $(q, \sigma')$ channel. This transmission coefficient is obtained by $T_{p,q,\sigma,\sigma'} = \text{Tr} \left[ \Gamma_{p,\sigma} G^R \Gamma_{q,\sigma'} G^A \right]$ where $\Gamma_{p,\sigma}$ is given by $\Gamma_{p,\sigma}(i,j) = \hat{S} \Gamma_{p,\sigma}(i,j) \hat{S}$. The retarded and advanced Green’s function of the sample $G^{RA}$ with the leads taken into account through the self energy $\Sigma^{RA}(i,j)$ has a form $G^{RA}(i,j) = \left[ E \delta_{ij} - H_{ij} - \Sigma^{RA}(i,j) \right]^{-1}$. Here the position representation of the matrices $\Gamma_{p,\sigma}$, $G^R$, $H_{ij}$, and $\Sigma^R$ are in the subspace of the sample. Within the above formalism the spin current through each channel is given by:

$$I_{p,\sigma} = (e/4\pi) \sum_{q,\sigma'} T_{p,q,\sigma,\sigma'} [V_{p,q} - V_{q,\sigma'}].$$

The spin force driven charge-Hall conductance, $G_{CS}^{yx}$, is defined as the ratio of charge current in the $y$ direction induced by the spin-dependent chemical potential along the $x$ axis to this spin-dependent chemical potential difference [see Fig. 1(a)].

$$G_{CS}^{yx} = \frac{(I_{1}^{3} + I_{2}^{3})}{V_{2} - V_{1}}.$$  

where $V_{i} = \mu_{i}/e$. The spin-Hall conductance, $G_{SC}^{xy}$, is defined as the ratio of spin-current in the $x$ direction induced by charge voltage difference in $y$ direction to this voltage difference

$$G_{SC}^{xy} = \frac{(I_{1}^{1} - I_{2}^{1})}{V_{4} - V_{3}},$$

where $V_{i} = \mu_{i}/e$, and the labels are indicated in Fig. 1(b). $G_{SC}^{xy}$ and $G_{CS}^{yx}$ are defined by analogy. We set the absolute value of voltage for spin and spin force driven charge-Hall effects as $V = \mu/e = 2.5$ mV.

RESULTS AND DISCUSSION

In order to address the key issue of experimental observation of spin force driven charge-Hall effect as well as to establish the Onsager relation between spin-Hall effect and it
reciprocal correspondent we choose realistic parameters for our calculations which model currently attainable systems. We consider an effective mass of $m^* = 0.05 m_e$ for electron systems and $m^* = 0.5 m_e$ for hole ones. The disorder strength $W = 0.09 \text{ meV}$ corresponds to the mobility of $250,000 \text{ cm}^2/\text{Vs}$, which is typical for a semiconductor like In,Ga$_{1-x}$As. We take the Rashba parameter in the range from 0 to 100 meV nm, easily obtained in experiments, and we choose the electron concentration $n_{2D}$ in a range between $3 \times 10^{11}$ cm$^{-2}$ and $1.3 \times 10^{12}$ cm$^{-2}$. The Fermi energy is obtained from the chosen carrier concentration assuming an infinite two-dimensional (2D) gas. Parameters considered here correspond to $t = 0.2t$, $E_F/W \approx 500–800$ in other theoretical studies with small variation due to mesh scaling as physical system size and effective masses for hole and electron systems are kept constant. The Fermi energy is close to the bottom of the band and $E_F$ changes from $-3.9t$ to $-3.5t$ in units of Refs. 17 and 18 dependent on electron concentration.

In the detection of spin force driven charge-Hall effect the first task is to generate a spin force which can be realized by spin dependent chemical potential in the leads. The ferromagnetic leads are not the good candidates because although magnetization exists in ferromagnetic leads, the chemical potential is the same for both spin directions. Here, we propose the optical method of spin-dependent chemical potential generation by shining the beam of circularly polarized light on the leads (see Fig. 2). The right-circularly polarized beam shines on the right lead and the left circularly polarized beam on the left one. The sample as well as the transverse leads should be covered by mask, preventing the light absorption anywhere except the small part of longitudinal leads as shown in Fig. 2. Choosing semiconductor leads for this setup, e.g., GaAs, will cause the opposite spin polarizations in left and right leads through optical selection rules. Using the beam splitter should produce the same light intensity in each leads providing simultaneously the spin-dependent chemical potential between leads 1 and 2 and the total charge current across a sample equal zero. Having produced the spin-dependent chemical potential in the leads, we perform calculations using nonequilibrium Green function method presented in previous section. Figures 3 and 4 present the charge current $I_3 = I_{3\uparrow} + I_{3\downarrow}$ as a function of SO coupling $\lambda$ and electron or hole concentrations, respectively. The charge current for electron systems show oscillations with respect to the electron density and SO coupling.

**FIG. 2.** (Color online) Proposal of experimental setup to measure the reciprocal spin-Hall effect. (a) Mask (light-gray) covers a sample and leads except for two holes in the longitudinal leads where circularly polarized light shines. (b) Full schematics of the experimental setup.

**FIG. 3.** (Color online) The spin-force driven charge current as a function of electron concentration and Rashba coupling, $\lambda$, for mesoscopic square sample 100 nm by 100 nm and $\mu = 250,000 \text{ cm}^2/\text{Vs}$.

**FIG. 4.** (Color online) The spin-force driven charge current as a function of hole concentration and Rashba coupling, $\lambda$, for mesoscopic square sample 100 nm by 100 nm and $\mu = 250,000 \text{ cm}^2/\text{Vs}$. 
The period of current oscillations depends on the system size, however, its maximal value seems to be around 40 nA for systems sizes achievable in our calculations. For hole mesoscopic systems (see Fig. 4), the charge current also oscillates with λ and for system sizes on the order of 100 nanometers is on the order of hundred nanoamperes in a wide range of densities starting from $6 \times 10^{11}$ cm$^{-2}$. Hence the charge current is much larger in hole systems and shall be detectable in experiments.

Figure 5 presents the spin-Hall conductance $G_{SC}$ as a function of λ for electron and hole systems. One can see that spin-Hall conductances (Fig. 5) and spin-force driven charge conductances (see Figs. 3 and 4) behave similarly. Spin-Hall conductances for electron systems oscillate with SO coupling and have values of the fraction of conductances for electron systems oscillate with SO coupling as a function of spin-Hall conductances $G_{CS}/H^2$.

On the $x$-$y$ plane which relate $T_{\sigma m;\sigma n} = T_{\sigma m;\sigma n}^{\alpha}$ and $T_{\sigma m;\sigma n} = T_{\sigma m;\sigma n}^{\alpha}$, respectively, where $\sigma, \alpha$ and $n, m$ are the spin and lead labels and a bar represents the opposite direction. Within the SHE $V_{1}^{\sigma} = V_{2}^{\sigma} = 0$ and $V_{3}^{\sigma} = V_{4}^{\sigma} = V_{0}/2$ following the labels of Fig. 1. Within the RSHE $V_{1}^{\sigma} = V_{2}^{\sigma} = 0$ and $V_{3}^{\sigma} = V_{4}^{\sigma} = s(\sigma)V_{0}/2$ where $s(\uparrow) = +1$ and $s(\downarrow) = -1$. Within the LB formalism and these boundary conditions we obtain for the spin-current associated with the SHE:

$$I_{1}^{\text{spin}} = I_{1} - I_{1}^{\text{open}} = V_{0} \sum_{\sigma, \alpha} s(\sigma)(T_{\sigma 1;\alpha 3} - T_{\sigma 1;\alpha 4})/2,$$

and for the charge current associated with the RSHE:

$$I_{3}^{\text{charge}} = I_{3} + I_{3}^{\text{open}} = V_{0} \sum_{\sigma, \alpha} s(\alpha)(T_{\sigma 3;\alpha 1} - T_{\sigma 3;\alpha 2})/2.$$

The above symmetries imply that $T_{\sigma 1;\alpha 4} = T_{\sigma 2;\alpha 3} = T_{\sigma 3;\alpha 2}$. This then yields $I_{1}^{\text{spin}} = -I_{3}^{\text{charge}}$ which implies the Onsager relation

$$G_{SC}^{\text{xy}} = -G_{CS}^{\text{xy}}.$$

This is verified numerically in Fig. 6 which presents the disorder averaged spin-Hall conductance and charge Hall conductance for hole systems of different sizes. For a specific disorder realization this relation does not hold and is only approximate depending on the strength of the fluctuations induced by disorder. This relation between $G_{SC}$ and $G_{CS}$ is consistent with predictions of semiclassical wave-packet theory, where standard definition of spin-current was modified by a spin-torque term. However, as seen from the above derivation and noted in the introduction, our finding of an Onsager relations in mesoscopic coherent systems do not involve such spin-torque term since all spin-currents are defined in the non-spin-orbit coupled leads.

**SUMMARY**

We have analyzed the spin Hall effect as well as its reciprocal effect in mesoscopic hole and electron systems. We have shown that the spin-Hall as well as the spin-dependent...
chemical potential gradient driven charge-Hall conductances are several times larger for hole systems. Further we have proposed the experimental setup to detect the transverse charge current driven by the spin-dependent chemical potential gradient through transport measurements. We have shown that this charge current is of the order of hundred nano-amperes in hole systems and should be detectable. Also, we have established a direct relation between the disorder average spin-Hall and spin-dependent chemical potential driven charge-Hall conductances in the mesoscopic systems.

ACKNOWLEDGMENTS

We thank A. H. MacDonald for stimulating discussions. The work was partly supported by the Research Grant Council of Hong Kong under Grant No. HKU 7039/05P (S.Q.S.) and DOE Grant No. DE-FG03-02ER45958 (Q.N.) as well as The Grant Agency of the Czech Republic under Grant No. 202/05/0575 (T.J.).

\[\text{1} S. \text{Murakami, N. Nagaosa, and S.-C. Zhang, Science 301, 1348 (2003).}\]
\[\text{5} S. Zhang, Phys. Rev. Lett. 85, 393 (2000).}\]
\[\text{10} E. I. Rashba, Phys. Rev. B 70, 161201(R) (2004).}\]
\[\text{11} O. V. Dimitrova, cond-mat/0405339 (unpublished); cond-mat/0407612 (unpublished).}\]
\[\text{15} O. Chalaev and D. Loss, cond-mat/0407342 (unpublished).}\]
\[\text{16} A. Khaetskii, cond-mat/0408136 (unpublished).}\]
\[\text{17} B. K. Nikolić, L. P. Zaro, and Z. Souma, cond-mat/0408693 (unpublished).}\]
\[\text{20} N. Sugimoto, S. Onoda, S. Murakami, and N. Nagaosa, cond-mat/0503475 (unpublished).}\]
\[\text{21} S. Murakami, cond-mat/0504353 (unpublished).}\]
\[\text{22} D. N. Sheng, L. Sheng, Z. Y. Weng, and F. D. M. Haldane, cond-mat/0504218 (unpublished).}\]
\[\text{23} K. Nomura, J. Sinova, N. A. Sinitsyn, and A. H. MacDonald, cond-mat/0506189 (unpublished).}\]
\[\text{24} S. Murakami, Phys. Rev. B 69, 241202(R) (2004).}\]
\[\text{25} B. A. Bernevig and S.-C. Zhang, cond-mat/0412550 (unpublished).}\]
\[\text{26} J. Li, L. Hu, and S.-Q. Shen, cond-mat/0502102 (unpublished).}\]
\[\text{27} M. W. Wu and J. Zhou, cond-mat/0503616 (unpublished).}\]
\[\text{28} P. Zhang and Q. Niu, cond-mat/0406436 (unpublished).}\]
\[\text{29} J. Schliemann and D. Loss, Phys. Rev. B 71, 085308 (2005).}\]
\[\text{33} P. Zhang, J. Shi, D. Xiao, and Q. Niu, cond-mat/0503505 (unpublished).}\]