Berry phase and topological spin transport in the chiral d-density wave state

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Abstract In this paper we demonstrate the possibility of dissipationless spin transport in the chiral d-density wave state, by the sole application of a uniform Zeeman field gradient. The occurrence of these spontaneous spin currents is attributed to the parity (P) and time-reversal (T) violation induced by the \( d_{xy} + \text{id}_{x^2-y^2} \) density wave order parameter. We calculate the spin Hall conductance and reveal its intimate relation to the Berry phase which is generated when the Zeeman field is applied adiabatically. Finally, we demonstrate that in the zero temperature and doping case, the spin Hall conductance is quantized as it becomes a topological invariant.

Keywords Berry phase · Spontaneous spin Hall effect · chiral d-density wave

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1 Introduction

Manipulating spin currents via the application of electric fields has received notable attention lately, especially in the field of semiconductors \cite{1,2}. In these materials the key ingredient for spin transport is the presence of strong spin-orbit coupling. The arising spin currents may be of intrinsic or extrinsic origin. In both cases, generating spin currents based on spin-orbit coupling is inherently pathological. The spin-orbit term is essentially a spin non-conserving interaction term. As a consequence, the absence of spin conservation prevents us from defining a proper spin current. Nevertheless, Murakami et al. have managed to define dissipationless spin currents, showing in addition, that the related spin Hall conductance depends solely on the curvature of an \( SU(2) \)-holonomy \cite{3}. Actually, this treatment focuses on how to cast out the dissipative part of the spin currents. In another work \cite{4}, it has been shown that the interplay of Rashba and Dresselhaus spin-orbit terms can lead to perfectly dissipationless spin currents. However, the latter case is extremely sensitive to the parameters of the spin-orbit couplings.

In this direction, we propose an alternative way of generating dissipationless spin currents. Specifically, we consider the case of the chiral d-density wave which is an unconventional spin singlet long-range order. Recently the chiral d-density wave state was proposed as a candidate state \cite{5,6}, which can simultaneously explain the enhanced diamagnetic and Nernst signals observed in the pseudogap regime of the cuprates \cite{7}. Moreover, it has also been considered \cite{8} to be the origin of time reversal breaking in YBCO \cite{9}. Apart from the prominent significance of this state in understanding high Tc superconductivity, the chiral d-density wave constitutes a paradigm of a functional state of matter. It has already been shown to exhibit the dissipationless electric charge Hall transport by the sole application of an electric field \cite{10,11}. In fact as we shall demonstrate the topological spin Hall transport is simply the spin analogue of dissipationless charge transport, with the gradient of the Zeeman field playing the role of the electric field \cite{12,13}.

In the case of the chiral d-density wave state, the \( SU(2) \) spin rotational symmetry is totally preserved, which leads to a straightforward definition of a conserved spin current. The dissipationless character of spin Hall transport resides solely on the unconventional structure of the order parameter of the density wave. The chiral d-density wave is a state of two coexisting d-wave type density waves. The \( d_{xy} \) component violates parity (\( P \)) in two dimensions and the \( d_{x^2-y^2} \) component violates time-reversal (\( T \)). As a result, an anomalous magneto-electric coupling arises in the effective action of the charge \( U(1) \) and spin \( SU(2) \) gauge fields, leading to a spontaneous charge and spin Hall response (See e.g. \cite{12}). From another point of view, the adiabatic application of external fields gives rise to a \( U(1) \) holonomy in \( k \)-space and a concomitant Berry connection \cite{14}, that provides an anomalous velocity \cite{15} to the quasi-particles of the system. In fact, the latter situation is similar to a ferromagnetic system \cite{16}. However, in our case there is a finite orbital magnetization \cite{17} in contrast to the usual magnetization.

2 The Model

To demonstrate how the Spontaneous Spin Hall effect arises, we shall consider the chiral d-density wave Hamiltonian \( \mathcal{H} = \sum_k \Psi_k^\dagger \mathcal{H}(\mathbf{k}) \Psi_k \) with

\[
\mathcal{H}(\mathbf{k}) = \begin{pmatrix}
\delta(\mathbf{k}) & g_1(\mathbf{k}) & g_2(\mathbf{k}) \\
 g_3(\mathbf{k}) & \delta(\mathbf{k}) & g_4(\mathbf{k}) \\
 g_5(\mathbf{k}) & g_6(\mathbf{k}) & \delta(\mathbf{k})
\end{pmatrix},
\]

where we have introduced the isospinor \( \Psi_k^\dagger = (c_k^\dagger c_{k+Q}^\dagger) \) and restricted the \( k \)-space summation in the reduced Brillouin zone. The operators \( c_k^\dagger / c_k \) annihilate/create an electron of momentum \( k \). For simplicity we have omitted the spin indices, which will be suitably embodied in our formalism later. Moreover, we employ a single band Bloch electron model with particle-hole asymmetric and symmetric kinetic terms \( \delta(\mathbf{k}) = 4t' \cos k_x \cos k_y - \mu \) and \( g_3(\mathbf{k}) = -2t(\cos k_x + \cos k_y) \). We have also introduced the
dependence of the Berry phase
snapshot eigenstates

This may be effected by considering a time-dependent Hamiltonian in the equivalent form \(\tilde{\mathcal{H}}(k) = \delta(k) + E(k) g(k) \cdot \tau\) with \(g(k) = g(k)/|g(k)|\) and \(\tau\) the isospin Pauli matrices. It is the existence of a isospin vector which can be rotated in isospin space under the adiabatic application of an external field, that generates a Berry phase responsible for the non-dissipative charge and spin Hall response.

3 Application of an electric field

Our next step is to perturb our system with an external electric field and calculate the emergent Berry curvature. This may be effected by considering a time-dependent vector potential of the form \(A_t = -\mathcal{E} t\). This type of perturbation enters our Hamiltonian via the Peierls-Ouonagui substitution \(k \rightarrow k + e A_t\) with \(e > 0\). As a consequence, this minimal coupling constitutes the system’s Hamiltonian time-dependent, \(\mathcal{H}(k) = \mathcal{H}(k, t)\). When this parameter changes adiabatically along a closed path, the ground state of the system remains unaltered and as an outcome the wavefunction of the system acquires a Berry phase. As we have already pointed out, the generation of the Berry phase is strongly related to the \(P - T\) violation originating from the chiral character of the density wave and permits the dissipationless charge and spin pumping.

When the external perturbation is present, the exact eigenstates of the system, \(|\Psi_{\nu}(k, t)\rangle\), satisfy the parametric Schrödinger equation\(\mathcal{H}(k, t)|\Psi_{\nu}(k, t)\rangle = i \partial_t |\Psi_{\nu}(k, t)\rangle\). In the adiabatic approximation, any exact eigenstate of the parametric Hamiltonian, is considered to acquire only a phase factor. This phase factor can be dissociated into two parts, the dynamical part and the Berry phase. Equivalently, one considers the following form for the exact eigenstates

\[
|\Psi_{\nu}(k, t)\rangle = e^{-i \int_0^t E_{\nu}(k, t') dt'} + i \gamma_{\nu}(k, t) |\Phi_{\nu}(k, t)\rangle,
\]

where the first part of the phase denotes the acquired dynamical phase and the second, the Berry phase \(\gamma_{\nu}(k, t)\). The states \(|\Phi_{\nu}(k, t)\rangle\), are the instantaneous (snapshot) eigenstates of the parametric Hamiltonian, satisfying \(\mathcal{H}(k, t)|\Phi_{\nu}(k)\rangle = E_{\nu}(k, t)|\Phi_{\nu}(k)\rangle\). In this equation, \(t\) is introduced only as a parameter. This means that these snapshot eigenstates are not really time-dependent but only parameter dependent, which in our case coincides with \(t\). In our case we deal with a two band system, characterized by the snapshot eigenstates \(|\Phi_{\pm}\rangle\) and the corresponding eigenenergies \(E_{\pm}(k, t) = \delta(k, t) \pm E(k, t)\).

The definition of the exact eigenstates \(|\Psi_{\nu}\rangle\) in terms of the snapshot eigenstates \(|\Phi_{\nu}\rangle\) readily provides the time dependence of the Berry phase

\[
\gamma_{\nu}(k, t) - \gamma_{\nu}(k, 0) = \int_0^t dt' \langle \Phi_{\nu}(k, t') | i \partial_{t'} | \Phi_{\nu}(k, t') \rangle.
\]

Setting \(\gamma_{\nu}(k, t) = 0\) and taking into account that the time dependence of the snapshot eigenstates arises because the crystal momentum becomes time dependent, \(k \rightarrow k + \mathcal{E}_{\nu}(k, t)\), yields \(\Gamma_{\nu}(k, t) = \gamma_{\nu}(k, t)\).

We have also introduced the \(U(1)\) Berry connection \(A_{\nu}(k) = \langle \Phi_{\nu}(k) | \tau | \Phi_{\nu}(k) \rangle\) and the Berry curvature \(\Omega_{\nu}(k) = \mathbf{\nabla}_{k} \times A_{\nu}(k) = \Omega_{\nu}^z \hat{z}\). We observe that the two-dimensional character of our system, forces the Berry curvature to lie along the \(z\)-axis.

4 Dissipationless charge transport

Having obtained the expression for the Berry curvature, we may proceed with studying the dissipationless transport of the system. As a warmup we shall study first the case of dissipationless charge transport. As we shall demonstrate in the next section, the Spontaneous Spin Hall effect will arise as a direct consequence of the Spontaneous Charge Hall effect and the existence of gauge invariance.

In order to demonstrate how the Spontaneous Charge Hall effect arises, we have to define a charge current. This is easily achieved by considering the equation of continuity of the electric charge in momentum space, which dictates that \(\dot{\rho}_c(q) + i q \cdot \mathbf{J}_c(q) = 0\) \(\Rightarrow \mathbf{J}_c(q) = i \lim_{\mathbf{q} \rightarrow 0} \mathbf{\nabla}_q \dot{\rho}_c(q)\). The charge density \(\rho_c(q, t)\) can be expressed using the snapshot eigenstates as \(\rho_c(q, t) = -e \sum_{k, \nu = \pm} \langle \Psi_{\nu}(k + q, t) | \Phi_{\nu}(k, t) \rangle\). To obtain the charge...
current we need the time derivative of the charge density which can be written as

$$\dot{\rho}_c(q, t) = -e \sum_{k,\nu=\pm} \left\{ \langle \partial_t \Phi_\nu(k, t) | \Phi_\nu(k - q, t) \rangle + \langle \Phi_\nu(k + q, t) | \partial_t \Phi_\nu(k, t) \rangle \right\} , \quad (7)$$

where we have used that $\langle \partial_t \Phi_\nu(k + q, t) | \Phi_\nu(k, t) \rangle = \langle \partial_t \Phi_\nu(k, t) | \Phi_\nu(k - q, t) \rangle$. Under these conditions the charge current becomes

$$J_c = -ie \lim_{q \to 0} \nabla_q \sum_{k,\nu=\pm} \left\{ \langle \partial_t \Phi_\nu(k, t) | \Phi_\nu(k - q, t) \rangle + \langle \Phi_\nu(k + q, t) | \partial_t \Phi_\nu(k, t) \rangle \right\}$$

$$= ie \sum_{k,\nu=\pm} \left\{ \langle \partial_t \Phi_\nu(k, t) | \nabla_k \Phi_\nu(k, t) \rangle - h.c. \right\}$$

$$= -ie^2 \sum_{k,\nu=\pm} \sum_{i=x,y} \langle \partial_k \Phi_\nu(k, t) | \nabla_k \Phi_\nu(k, t) \rangle - h.c. \right\}$$

$$= e^2 (\mathbf{E} \times \hat{z}) \int_{RBZ} d^2k (2\pi)^2 n_F[E_\nu(k)] \Omega_\nu(k), \quad (8)$$

where $n_F$ is the Fermi-Dirac distribution. At zero temperature, if the lower and upper bands are separated by a gap, only the lower band is occupied and we obtain $n_F[E_-(k)] = 1$ and $n_F[E_+(k)] = 0$. In this case the charge current becomes $J_c = -\frac{e^2}{2\pi} \hat{N}(\mathbf{E} \times \hat{z})$, where we have introduced the topological invariant $\hat{N}$.

$$\hat{N} = -\frac{1}{2\pi} \int_{RBZ} d^2k \Omega_-(k)$$

$$= \frac{1}{4\pi} \int_{RBZ} d^2k \hat{g}(k) \left( \frac{\partial \hat{g}(k)}{\partial k_x} \times \frac{\partial \hat{g}(k)}{\partial k_y} \right), \quad (9)$$

which is a winding number related to the mapping of the reduced Brillouin zone to the order parameter space.

This winding number is an integer, as it corresponds to the mapping of a torus $T^2$ to an $S^2$ sphere. In our case we obtain $\hat{N} = 1$. This integer equals the angular momentum, in $\mathbf{k}$-space, of the chiral ground state. One would expect that $\hat{N} = 2$, as the order parameter is composed by d-wave functions. However, this contribution is halved as we are restricted to the reduced Brillouin zone.

It is straightforward to obtain the value of the Hall conductance for the dissipationless charge transport from its defining expression $J_c = \sigma_{xy}^c (\mathbf{E} \times \hat{z})$. We observe that the value of the Hall conductance $\sigma_{xy}^c(\mathbf{E} \times \hat{z})$ is universal and equal to (per one spin component)

$$\sigma_{xy}^c = -\frac{e^2}{2\pi} = -\frac{e^2}{h}. \quad (10)$$

We have to underline that this universality originates from the gauge invariance of our system. This should be contrasted to the case of chiral superconductors where the Hall conductance is affected by the existence of the Goldstone mode of the broken $U(1)$ gauge invariance.

5 Dissipationless spin Hall transport

To demonstrate how the Spontaneous Spin Hall effect arises we could embody in our formalism the electron spin and calculate the spin Hall conductance in a manner similar to the previous section. However, we shall follow another derivation that takes advantage of gauge invariance and exhibits the intimate connection of dissipationless charge and spin transport. Specifically, we would like to show that the generation of dissipationless spin currents by applying an external uniform Zeeman field gradient can be mapped to the case of pumping charge with an external electric field. We start from a general real space representation of our chiral d-density...
wave Hamiltonian

\[ S = \int \, dt \, d^2x \, \Psi_\uparrow^\dagger (t, \mathbf{x}) \left\{ i \frac{\partial}{\partial t} - \mathcal{H}(\hat{\mathbf{p}}, \mathbf{x}) \right\} \Psi_\uparrow (t, \mathbf{x}) + \int \, dt \, d^2x \, \Psi_\uparrow^\dagger (t, \mathbf{x}) \mu_z (\mathbf{x} \cdot \nabla B_z) \Psi_\uparrow (t, \mathbf{x}), \tag{11} \]

where \( B_z \) is the external field and \( \mu_z \) the magnetic moment of the electron. Based on the fact that the chiral d-density wave state is characterized by an SU(2) spin invariance we have considered one spin component. The Zeeman interaction term can be eliminated by a phase transformation \( \Psi_\uparrow (t, \mathbf{x}) \rightarrow e^{i\varphi (x)} \Psi_\uparrow (t, \mathbf{x}) \) with \( \varphi (x) = \mu_z (\mathbf{x} \cdot \nabla B_z) t \). This corresponds to a \( U(1) \) gauge transformation, generating a vector potential \( \mathbf{A}_z (t) = \nabla B_z t \). Consequently a constant gradient of a Zeeman field corresponds to an electric field \( \mathbf{E} = - \nabla B_z \) and according to Eq. (10), leads to the spin current \( J_z = \sigma_{xy} (\mathbf{\hat{z}} \times \nabla B_z) \). If temperature and doping are zero the spin Hall conductance is quantized \( \sigma_{xy} = \mu_z^2 / 2\pi \). By substituting \( \mu_z = \hbar / 2 \), we obtain (per one spin component)

\[ \sigma_{xy} = \frac{\hbar}{8\pi}. \tag{12} \]

In the general case, the spin Hall conductance is strongly affected by temperature and doping. As we may see in Fig. (2), both of them tend to suppress the Spontaneous Spin Hall effect. If we take into account that the robustness of dissipationless spin transport is directly related to the robustness of the system’s gap it is natural to expect such a behaviour. A temperature bath gives rise to thermally excited carriers that occupy the upper band of our system which has the opposite Berry curvature of the lower band. The same effect is reproduced by a non zero chemical potential but in a different manner. If the chemical potential crosses the upper band, both bands become occupied yielding conflicting contributions of Berry curvature. However, despite the negative effect that temperature and doping have on dissipationless spin transport they may constitute some of its controlling external parameters.

6 Discussion

Motivated by the necessity of inquiring systems supporting dissipationless spin currents, we have studied the occurrence of topological spin transport in the chiral d-density wave state. The chiral d-density wave is an unconventional spin-singlet state giving rise to a Berry connection in \( k \)-space. We have demonstrated that it exhibits the Spontaneous Spin Hall effect under the adiabatic application of an external Zeeman field gradient. Specifically, spin transport is dissipationless and in the zero temperature and doping case the spin Hall conductance becomes a topological invariant and is quantized. In the general case, spin transport is controlled by the presence of temperature and chemical potential.

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