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Theory of the piezo-spintronic effect

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ABSTRACT

The theoretical prediction that some materials might develop pure spin currents in response to strain is presented. Such piezo-spintronic effect is studied and shown to be allowed by symmetry in several systems. This mechanism opens up a way to obtain and measure pure spin currents. From a close analogy with the theory of electric polarization and the piezoelectric effect, we show that such piezo-spintronics response can be represented in a geometrical form in terms of spin Berry phases. Additionally, we illustrate the ideas by the use of two toy models that displays a non-trivial piezo-spintronic response and discuss on possible experimental realizations on antiferromagnetic insulators.

1. Introduction

The phenomenon that certain kind of materials respond to elastic deformations by becoming electrified is named piezoelectricity. Piezoelectricity became an essential part of several applications within a few years after its discovery. Nowadays, the effect plays a fundamental role in a great variety of applications ranging from domestic electronics [1,2] to advanced microscopy measurements on the atomic scale [3]. In this paper we show a prediction of an analogous effect in the context of spintronics [4]. By means of this effect, spin currents are expected to arise in response to strain in structures lacking inversion symmetry. Additionally, we characterize the main properties of this piezo-spintronic response and discuss the basic features of the family of materials expected to display the effect.

The intuitive notion of spin current is based on a picture with different spin species flowing at different speeds. To accommodate this notion within the formalism of quantum mechanics is a well defined problem only in systems where the spin is a good quantum number. In cases in which spin is not conserved such as, for example, when the effects of spin orbit interaction are not negligible, the problem is more subtle. In this work we shall use the definition [7] given by

$$\mathbf{J}^S_{i;j} = \frac{\mathrm{d}(\hat{S}_i \hat{R}_j)}{\mathrm{d}t}, \qquad (1)$$

where $\vec{R}$ corresponds to the electronic position operator. This definition has several advantages. Naturally, it reduces to the intuitive notion of spin current, $\mathbf{J}^S_{z,j} = \hbar(\vec{v}_\uparrow - \vec{v}_\downarrow)_j$, when the spin is conserved. Additionally, it is linked directly to a thermodynamical conjugated variable [7]. It can be noticed that the above definition links the spin current to the time derivative of the spin dipolar moment $\mathbf{p}^S_{i;j}$. In the context of this paper all such properties will be used.

With a precise definition of spin current we proceed to analyze the basic symmetry requirements imposed on the systems in order to have a piezo-spintronic effect.

2. Macroscopic analysis

Interestingly, the spin current defined in Eq. (1) has a peculiar behavior under space reflections. As shown in Fig. 1a, the axial nature of the spin operator [10] enforces the spin current to transform as a pseudo-tensor under reflections. On the other hand, the spin current defined in Eq. (1) is even under time reversal. This is in contrast with charge currents that transform as an odd operator under time reversal. With these two properties in mind we will analyze the symmetry features that a system must display in order to have a piezo-spintronic effect.

Let us suppose that under strain a spin current is generated in a generic system (see Fig. 1b). Under distortion spin currents should be expected, within the linear regime whenever there is a change in the spin dipolar moment. For small enough deformations we can generally expect a relation of the form:

$$\mathbf{p}^S_{i;j} = \lambda_{i;jkl} \mathbf{u}_{lk}. \qquad (2)$$

This equation constitutes the definition of the "piezo-spintronic" tensor λ. In this equation, $\mathbf{u}_{lk} = (\partial_k u_l + \partial_l u_k)/2$ corresponds to the strain tensor [9], where u is the deformation field, and $\mathbf{p}^S_{i;j}$ the spin dipolar moment. Since the spin current is a pseudo-tensor, λ must also behave as a pseudo-tensor [10]. Under an inversion transformation $\vec{x} \longrightarrow -\vec{x}$, λ must change sign. Therefore, like the

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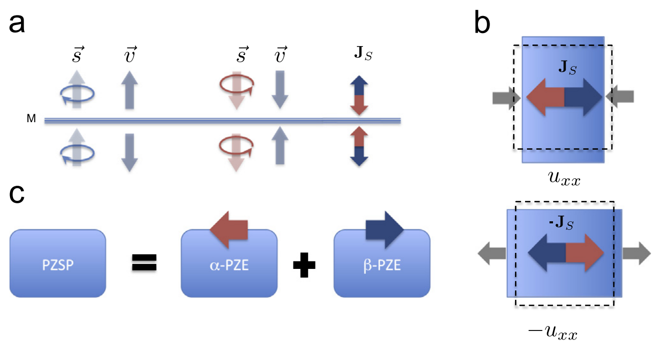

Fig. 1. (Color online) (a) Axial vector properties of the spin are reflected in the spin current tensor $\mathbf{J}^S$. The axial nature of the spin operator s_z renders it invariant under reflection on a mirror (M) in the *xy*-plane. In contrast, the velocity operator v_z changes sign, (b) illustration of the piezo-spintronic effect, distortion of the sample, u_{xx} (greatly exaggerated), from the equilibrium configuration (dashed lines) lead to a spin current $\mathbf{J}^S$. Opposite distortions lead to opposite spin currents and (c) the pure piezo-spintronic (PZSP) effect can be understood as two separated piezo-electric effects (PZE), α and β, for each spin channel. This leads, under strain, to opposite currents and a net spin current.

piezoelectric [1,11] and piezomagnetic effects [8,11], the piezo-spintronic effect is restricted only to crystals classes lacking a center of inversion. In addition to inversion symmetry breaking it is important to emphasize that time reversal symmetry breaking is required for a crystal to display piezo-spintronic effects. In principle, a crystal might display simultaneously the piezoelectric, piezomagnetic and piezo-spintronic effects. However, in the remaining parts of the paper, we shall focus on a special form of the effect. It is easy to realize that it is possible for certain structures under strain to display exclusively the piezo-spintronic effect without giving rise to charge currents. Let us denote by $\mathcal{R}$ and $\mathcal{I}$ the spin reversal and the spatial inversion operators, respectively. Crystals invariant under the consecutive action of $\mathcal{R}$ and $\mathcal{I}$ cannot have a piezoelectric response. We expect, therefore, that crystals classes invariant under $\mathcal{RI}$ will respond with a pure spin-current to an external strain. This effect is very similar to the piezospin polarization of charge currents that arises due to strain-induced spin orbit interactions [5,6]. However there are two main differences: first, as we shall see in the examples the presence of spin-orbit interaction is not necessary in order to the piezo-spintronic effect to be displayed, and second, there is no need to have charge currents, indeed the prediction is made that in systems with certain symmetries pure spin currents might be generated by strain.

A natural way to understand the effect is to regard each spin component manifesting opposite piezoelectric effects as shown in Fig. 1c. Following standard notation that refers to the opposite piezoelectric effects displayed by enantiomeric versions of quartz crystals [1] as α- and β-like opposite responses, we say that the pure piezospintronic effect can be understood as nothing more than an α-like response for one spin polarization and the opposite β-like response for the other spin polarization. The direction of each piezoelectric effect is reversed under inversion, while the spin labels remain equal. Therefore, there is a reversal of the piezo-spin current. An additional spin reversal will restore the original current.

3. Microscopic theory

Having shown the symmetry features that are needed for a system to display the piezospintronic effect, we proceed to explain how the piezospintronic response might be calculated in general. The most convenient interpretation of Eq. (1) is obtained in terms of the Berry phase theory of polarization [12,13]. Instead of calculating the spin current directly, we proceed to evaluate it in terms of the changes of spin current associated with an arbitrary adiabatic deformation. Let the elastic strain be parametrized through the dependence of electric potentials over some parameters Q. We regard the strain tensor as a function of the Q parameters, $u_{ij}=u_{ij}(Q)$ as well as the electronic Hamiltonian $\mathcal{H}=\mathcal{H}(Q)$. The change in spin dipolar moment density in response to a change in the external parameters $Q\to Q+dQ$, is

$$\mathrm{d}\mathbf{p}^S_{i;j}=\mathbf{A}^{\mu}_{i;j}\mathrm{d}Q^{\mu}. \tag{3}$$

where

$$\mathbf{A}^{\mu}_{i;j}=-\sum_{\nu}\int\frac{\mathrm{d}^dk}{(2\pi)^d}n_{\nu}(k)Im\left\langle\frac{\partial\phi_{\nu}}{\partial k_j}\middle|\hbar\sigma_i\middle|\frac{\partial\phi_{\nu}}{\partial Q^{\mu}}\right\rangle \tag{4}$$

These formulae are analogous to the one used in the theory of polarization [13], the crucial difference being the Pauli matrix lying in between brackets. This difference makes them appropriate to evaluate changes in spin dipolar moments instead of changes in polarization. Eqs. (3) and (4) are the basis for all the results of this paper. Starting from them we can calculate the piezo-spintronic response of any material. Such task is achieved by integrating Eq. (3) over the path, γ in parameter space (Q-space) that is swept by the system due to the strain:

$$\delta\mathbf{p}^S_{i;j}=\int_{\gamma}\mathbf{A}^{\mu}_{i;j}\,\mathrm{d}Q^{\mu}. \tag{5}$$

The symbol $\delta\mathbf{p}^S$ stands for the accumulated spin dipolar moment during the process of distorting the system from a reference configuration into any other configuration. As shown in Eq. (1) changes in the configuration are accompanied by spin currents whenever $\delta\mathbf{p}^S$ is non-zero. In order to show the validity of Eqs. (3) and (4), we need to calculate the change in the spin dipolar moment associated with infinitesimal and adiabatic changes in the Hamiltonian. Following Eq. (1) the rate of change of $\mathbf{p}^S$ with time corresponds directly to the spin current: $\mathbf{J}^S=\mathrm{d}\mathbf{p}^S/\mathrm{d}t$. The change in the expectation value of the operator $\mathbf{p}^S$ can be evaluated using a corresponding Kubo formula:

$$\mathrm{d}\mathcal{A}_{\mu}=\mathrm{Im}\left(i\hbar\sum_{\nu\neq\mu}\frac{\langle\psi_{\mu}|\mathbf{p}^S|\psi_{\nu}\rangle\langle\psi_{\nu}|\mathrm{d}\mathcal{H}|\psi_{\mu}\rangle}{(\mathcal{E}_{\mu}-\mathcal{E}_{\nu})^2}\right) \tag{6}$$

Standard matrix element manipulations [7] lead to Eqs. (3) and (4).

In the remainder of this work, we illustrate the basic ideas discussed so far with the aid of two toy models.

4. Antiferromagnetic toy model in 1D

The first system we consider is the case of an insulator with electrons hopping along a dimerized antiferromagnetic spin chain as shown in Fig. 2.

Let us consider a 1D tight binding Hamiltonian with a dimerized structure.

$$\mathcal{H}_1=\sum_{\ell,\mu}t_{\ell}(c^{\dagger}_{\ell\mu}\,c_{\ell+1\mu}+c^{\dagger}_{\ell+1\mu}\,c_{\ell\mu})+\Delta\sum_{\ell,\mu,\nu}(-1)^{\ell}\,c^{\dagger}_{\ell\mu}\,\sigma^z_{\mu\nu}\,c_{\ell\nu} \tag{7}$$

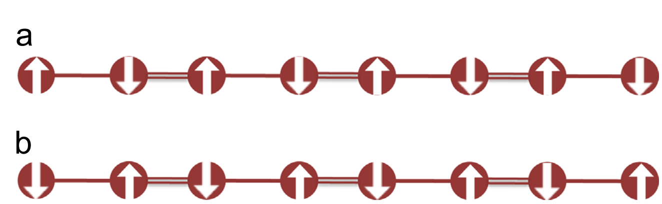

Fig. 2. (Color online) (a) Cartoon of a spin-Peierls chain. Electrons hop through an alternating arrangement of local moments in a dimerized chain, (b) the non-equivalent image of the system under $\mathcal{R}$ and $\mathcal{I}$ (Note that the system is invariant under $\mathcal{RI}$). A pure spin-current is expected to arise from strain.