Hidden Ferromagnetism of Centrosymmetric Antiferromagnets

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Time-reversal symmetry ($\mathcal{T}$) breaking is a signature of ferromagnetism, giving rise to such phenomena as the anomalous Hall effect (AHE), orbital magnetism, and magneto-optical response. Nevertheless, $\mathcal{T}$ can be also broken in certain classes of antiferromagnets, which remain invariant under the spatial inversion [1,2,3]. In the light of this similarity with ferromagnetism, it is tempting to ask whether such unconventional antiferromagnetic state can be represented as the simplest ferromagnetic one, i.e. within the minimal unit cell containing only one magnetic site. I will show that such representation is possible due to special form of the spin-orbit interaction in an antipolar lattice hosting this antiferromagnetic state. There are two important aspects of the problem:

(1) The spin-orbit interaction in the bonds surrounding each magnetic site has the same-sign components as well as sign-alternating components. While the former are responsible for the weak spin ferromagnetism (and can be eliminated in the simplest one-orbital model), the latter give rise to AHE. Thus, these two phenomena are fundamentally different from the microscopic point of view [4];

(2) The inversion symmetry constrains the form of the spin-orbit interaction, which becomes invariant under the symmetry operation $\{\mathcal{S}|\mathbf{t}\}$, combining the 180° rotation of spins ($\mathcal{S}$) with the lattice shift $\mathbf{t}$, connecting two antiferromagnetically coupled sublattices. This is the fundamental symmetry property of centrosymmetric antiferromagnets, which justifies the use of the generalized Bloch theorem [5] and transformation to the local "ferromagnetic" coordinate frame with one magnetic site per cell [6].

It naturally explains the emergence of AHE and net orbital magnetization and provides transparent expressions for these properties in terms of the electron hoppings and spin-orbit interaction operating between antiferromagnetic sublattices, as well as the orthorhombic strain, controlling the piezomagnetic response.

This idea will be illustrated on a number of examples, using for these purposes realistic models derived from first-principles electronic structure calculations.

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