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AFFILIATIONS

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ABSTRACT

Magnetic flux densities (*B*-fields) and field intensities (*H*-fields) in thin films are investigated from the viewpoints of Berry phase and topological Hall effect. The well-known origin of the topological Hall effect is an emergent *B*-field originating from the Berry phase of conduction electrons, but Maxwell's equations predict the relevant perpendicular component B_z to be zero. This paradox is solved by treating the electrons as point-like objects in Lorentz cavities. These cavities can also be used to interpret magnetization measurements in the present and other contexts, but structural and magnetic inhomogeneities lead to major modifications of the Lorentz-hole picture.

I. INTRODUCTION

The topological Hall effect (THE) in thin films has recently attracted much attention.[1,2] The effect is caused by a phase factor in the conduction-electron wave function known as the Berry phase.[3] Conduction electrons undergoing spin rotation due to exchange interaction with atomic moments develop an emergent flux density $B^{em}{}_z$, and this *B*-field contributes to the Hall effect. Paradoxically, Maxwell's equations predict the relevant perpendicular *B*-field in laterally homogeneous thin films to be *zero*, so the THE should not exist in real thin films, in contrast to experiment.

The flux density obeys $\boldsymbol{B} = \mu_o(\boldsymbol{M} + \boldsymbol{H})$, where M is the magnetization and H is the magnetic field. One experimental method to investigate the THE is to measure the magnetization M and the Hall resistivity ρ_{xy} in the film plane (*x-y* plane) as a function of the magnetic field applied perpendicular to the film[4,5]

$$\rho_{xy} = R_o B_z + \mu_o R_s M_z + \rho_{xy}{}^{THE}. \tag{1}$$

Here R_0 is the ordinary Hall coefficient and R_s describes the anisotropy contribution to the anomalous Hall effect. The question arises how B_z relates to the external magnetic field $H_{z,ext}$. According to Maxwell's equations, perpendicular *B*-components are continuous, so one may expect that $B_z = \mu_o H_{z,ext}$ inside the film, irrespective of the magnetization. This is not the case experimentally, with implications especially in the low-field region. Similarly, the question arises whether the magnetization should be plotted and analyzed as $M(B)$, $M(H_{ext})$, or $M(H)$, where H is the total magnetic field. It has long been known that the answer to this question involves Lorentz cavities. These cavities were first investigated in the context of dielectric interactions but are equally relevant in magnetism.[6]

A second important consideration is the point-like character of the electrons. In a fairly good approximation, correlation effects can be ignored in itinerant magnets, which makes it possible to treat electrons on a quantum-mechanical mean-field level. In this approximation, exemplified by first-principle calculations using the local spin density approximation (LSDA), individual electrons move in an effective electrostatic field created by the nuclei and by all other electrons.[7] This excludes, for example, the fractional-quantum-Hall effect, where electron-electron interactions give rise to Laughlin-type wave functions.[8]

II. SCIENTIFIC BACKGROUND

$\boldsymbol{B}$ and $\mu_o\boldsymbol{H}$ are equivalent in some contexts, but in general, they need to be distinguished properly. For example, $\boldsymbol{B} = \nabla \times A$, where the vector potential $\boldsymbol{A}$ has the character of a Berry connection and $\boldsymbol{B}$ is the corresponding Berry curvature. In contrast to the source-free

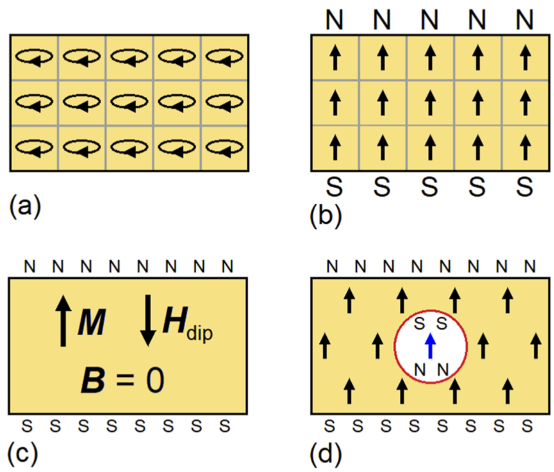

FIG. 1. Currents and magnetic fields in thin films: (a) 19th-century explanation in terms of currents, (b) 20th-century explanation in terms of spin, (c) Maxwell prediction for infinite thin films in zero external field, and (d) magnetic Lorentz hole.

B-field, the H-field has a source, namely the magnetic pole density. It is convenient to divide the H-field into two parts: $\boldsymbol{H} = \boldsymbol{H}_{ext} + \boldsymbol{H}_{dip}(\boldsymbol{r})$. The external or applied field H_{ext} has its source outside the sample (e.g. an electromagnet in the laboratory), whereas the demagnetizing field (dipolar interaction field) H_{dip} is the dipolar field created by the sample itself. The question of B-fields acting on conduction electrons is somewhat different from inherently micromagnetic effects such as the sample-shape dependence of the energy product of permanent magnets.[9] In the latter case, one can use the demagnetizing factor to determine H and B, and no further considerations are necessary.

Figure 1 summarizes the basic situation in homogeneous thin films. Maxwell's equations (Ampère's law) show that currents create a B-field, and this mechanism includes atomic current loops (a). The loops correspond to orbital moments m_L and, on a continuum level, to a magnetization $M = m_L/V_{at}$, where V_{at} is the atomic volume. While the magnetization M is traditionally associated with bound currents (a), the orbital-moment contribution in most transition-metal magnets is very small, only about 5% in bcc Fe. The reason for this orbital-moment quenching is the interaction with the crystalline environment (crystal-field or ligand-field interaction), which disrupts the orbital motion of the spins.[10] The majority of the magnetization originates from the spin (b). The spin is a relativistic quantum effect that cannot be explained in terms of any real-space motion. In fact, if an electron was a rotating or spinning charge cloud, then it would correspond to a velocity much large than the velocity of light.[9] However, from the viewpoint of atomic moments and magnetization, no distinction is necessary between orbital and spin magnetism, and it is convenient to visualize atomic moments as spin moments m_s, as in Fig. 1(b).

The magnetization gives rise to magnetic poles, which occur in pairs (N, S) and operate as the sources of the H-field. Figure 1(c) illustrates the situation in the absence of an external magnetic field. The H-field and the magnetization are of equal magnitude but opposite sign, so that $\boldsymbol{B} = \mu_o(\boldsymbol{M} + \boldsymbol{H})$ yields $B = 0$. This finding is a well-known textbook result, derived by using $\nabla \cdot B = 0$ or, slightly more cumbersome, by integration over all magnetic surface charges. The B-field in the film plane is generally nonzero but does not contribute to Eq. (1).

Figure 1(d) shows the Lorentz hole in a thin film. The blue spin in the hole may represent a local atomic moment or a conduction electron. In the simplest interpretation, the spin is embedded in vacuum, as exemplified by atomic moments in oxides and electrons in their own exchange and correlation holes. Note that electrons are point-like objects that undergo magnetostatic interaction. The Lorentz-hole approach deals with macroscopic magnetostatic interactions only and does not address, for example, short-range exchange interactions.

III. MAGNETIC FIELDS IN LORENTZ CAVITIES

The (spherical) Lorentz hole is a missing piece of magnetic material and therefore characterized by the demagnetizing factor $-1/3$.[6] The B-field acting on the electrons, namely the field in the Lorentz cavity, is therefore

$$\boldsymbol{B} = \mu_o(\boldsymbol{H}_{ext} - 2\boldsymbol{M}/3). \quad (2)$$

This expression is exact for cubic and spherical symmetry and reasonably accurate for most dense-packed magnets, including, for example, hexagonal Co. However, some materials, such as hexagonal RT_5 intermetallics[9] are structurally very anisotropic and need somewhat different demagnetizing factors. Equation (2) can also be used for other phenomena reflecting internal B- and H-fields.

The Lorentz hole can be chosen to contain several atoms so long as the radius of the hole remains much smaller than the film thickness. In particular, the topological Hall effect is caused by the exchange interactions of conduction-electron spins with atomic magnetic moments. The macroscopic sample shape (for example thin film vs. bulk) is included in the Lorentz hole, but the interactions inside the cavity need to be considered explicitly.

To see that the emergent B-field is very different from the magnetostatic fields in Fig. 1, we use a modified version of Berry's original argumentation. We consider a single electron spin in a rotating external magnetic field of constant flux magnitude B_o and describe the system by the Hamiltonian

$$\mathcal{H} = E_o - 2\,\mu_B\,\boldsymbol{S}\cdot\boldsymbol{B} \quad (3)$$

The zero-point energy E_o is physically unimportant, but it is convenient to choose $E_o = \mu_B B_o$. The evolution of the wave function is described by the Schrödinger equation $i\hbar\,\partial\psi/\partial t = \mathcal{H}\,\psi$. For adiabatically slow field rotation, $\boldsymbol{S}$ remains parallel to $\boldsymbol{B}$, so that $\boldsymbol{SB} = B_o/2$ and $\mathcal{H} = 0$. This zero-Hamiltonian property is remarkable, because it means that the Schrödinger equation predicts $\psi(t) = \psi(0)$, in contradiction to the original assumption of a rotating spin. The paradox is solved by the introduction of the Berry phase,

$$\psi \to e^{i\gamma}\,\psi. \quad (4)$$

Throughout most of the 20th century, scientists believed that such phases are unimportant, because quantum-mechanical averages involve $\psi^*\,\psi$, which corresponds to a factor $e^{-i\gamma}\,e^{i\gamma} = 1$.

How does the Berry phase γ of the conduction electrons produce a B-field? It is well-known that the B-field amounts to the introduction of a vector potential $\boldsymbol{A}$, realized by the transformation $\boldsymbol{p}^2 \rightarrow (\boldsymbol{p} + \mathrm{e}\,\boldsymbol{A})^2$ or, due to $p = -i\hbar\,\nabla$,

$$\nabla^2 \rightarrow (\nabla + \mathrm{i}\,e/\hbar\,A)^2 \tag{5}$$

Application of ∇^2 onto the wave function $\mathrm{e}^{\mathrm{i}\gamma}\,\psi$ in Eq. (4) yields

$$\nabla^2\left(\mathrm{e}^{\mathrm{i}\gamma}\quad\psi\right) = \mathrm{e}^{\mathrm{i}\gamma}(\nabla + \mathrm{i}\nabla\gamma)^2\psi \tag{6}$$

The factor $\mathrm{e}^{\mathrm{i}\gamma}$ on the right-hand side of this equation undergoes compensation ($\mathrm{e}^{-\mathrm{i}\gamma}\,\mathrm{e}^{\mathrm{i}\gamma} = 1$) and is therefore inconsequential. By contrast, the quadratic term on the right-hand side of Eq. (6) produces quantum averages different from $\nabla^2\psi$. Equations (5) and (6) are equivalent for the Berry connection $\nabla\gamma = e\boldsymbol{A}/\hbar$, which yields

$$\nabla^2\left(\mathrm{e}^{\mathrm{i}\gamma}\quad\psi\right) = \mathrm{e}^{\mathrm{i}\gamma}(\nabla + \mathrm{i}\,e/\hbar\,\boldsymbol{A})^2\psi \tag{7}$$

Two points are worthwhile noting here. First, $\hbar/\mathrm{e}$ is essentially the magnetic flux quantum. Second, $B = \nabla \times A$ requires a closed path to be nonzero,[2] because $\nabla \times \nabla\gamma = 0$ in flat spaces. This is an example of a bulk-boundary correspondence and the closed path may be rationalized as an circular current.

The above $\mathcal{H} = 0$ feature, realized by a physically unimportant shift of the energy zero, is crucial for the understanding of the Berry phase and of the role of fields in magnetism. Traditional quantum mechanics focusses on the Hamiltonian $\mathcal{H}$, but the Lagrangian $\mathcal{L} = \boldsymbol{p}\cdot\mathrm{d}\boldsymbol{q}/\mathrm{d}t - \mathcal{H}$ is the more fundamental quantity, because both classical and quantum physics are determined by the action $\mathcal{S} = \int \mathcal{L}\,\mathrm{d}t$. The term $\boldsymbol{p}\mathrm{d}\boldsymbol{q}/\mathrm{d}t$ can be ignored in flat coordinate frames but is important in curved and periodic spaces.[8] The zero-Hamiltonian character of the magnetic interaction can also be rationalized by looking at the equations of motion for the orbital and spin degrees of motion. The Lorentz force $\boldsymbol{F} = e\,\boldsymbol{v} \times \boldsymbol{B}$ is always perpendicular to $\boldsymbol{v}$, which leaves $\boldsymbol{v}^2$ and E unchanged, and the Landau-Lifshitz equation $\mathrm{d}\boldsymbol{S}/\mathrm{d}t = \Gamma_\mathrm{o}\ \boldsymbol{S} \times \boldsymbol{B}$ yields a spin precession that does not change the field energy $-\mu_\mathrm{B}\ \boldsymbol{SB}$.

IV. FLUX DENSITY IN INHOMOGENEOUS MAGNETS

Equation (1) is limited to homogeneous thin films. The basic idea behind Eq. (1) is to separate the THE, caused by spin rotations, from the R_o and R_s terms. In particular, the R_s term is proportional to the magnetization. In inhomogeneous materials, this separation is not straightforward, because the magnetization and Hall-effect signals may come from different regions in the film. An extreme case would be regions that switch easily in a magnetic field but are unconnected by conduction paths to the remainder of the films. Such 'multichannel' inhomogeneity effects are likely to yield systematic errors.[11,12] In this paper, we are primarily interested in the magnetostatic aspect of this constellation. It is important at this point to recall that magnetostatic effects are scale-invariant. For instance, a spherical cavity has a demagnetizing field of $-M/3$, irrespective of whether the cavity is atomic, nanoscale, or macroscopic. The only condition is that the cavity is sufficiently far away from the surface of the magnetic material, that is, the distance R_o between a cavity of radius R and the surface should be bigger the than R. The corresponding corrections scale as R^3/R_o^3 and cannot be ignored, for example, in atomic-scale ultrathin-film cavities.

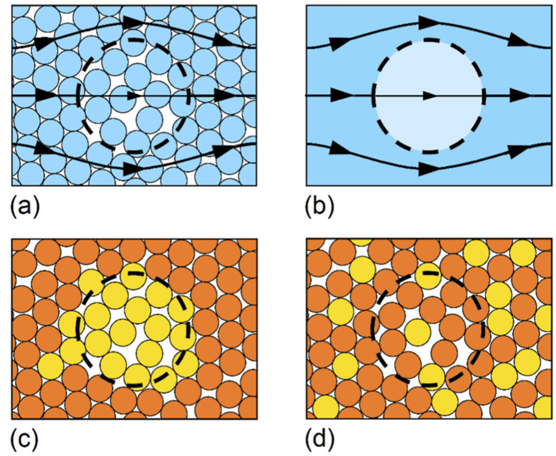

FIG. 2. Effect of structural inhomogeneities on the topological Hall effect: (a) current density in a nanoparticulate thin film, (b) Bruggeman description of the current, (c) spin-structure in the interaction-domain limit, and (d) spin structure in the noncooperative micromagnetic limit. The yellow region in (c) fully contributes to the magnetization but only partially to the Hall effect.

A particularly interesting class of materials are nanogranular materials produced by rapid quenching and cluster deposition. Figure 2 shows one example, namely ensembles of interacting nanoparticles. Ensembles of this type can be produced by cluster deposition[14,15] and exhibit nonzero topological Hall signatures. Macroscopic magnetization measurements capture the average magnetization $\langle M\rangle$ but the local magnetization $\boldsymbol{M}(\boldsymbol{r})$ and the local current density $\boldsymbol{j}(\boldsymbol{r})$ are not necessarily proportional. For instance, in nanogranular structures, magnetization changes may be dominated by loosely coupled regions (inside the dashed circles) where the conductivity and therefore the Hall-effect contribution are disproportionally small.

Inhomogeneous currents are fairly well described by the self-consistent mean-field-type Bruggeman approximation.[10,13] In the specific example of Fig. 2(b), the THE effect comes predominantly from the dark blue matrix region, because the Hall voltage is proportional to the current density. The description of the magnetization is more complicated and goes beyond the consideration of the cavity fields associated with local magnetizations. A crucial aspect is the distinction between cooperative and noncooperative magnetization processes. Figure 3 shows how these two mechanisms affect the cavity field during magnetization reversal. In the noncooperative regime (a), individual regions switch independently while being subject to a Lorentz field $\boldsymbol{B} = \mu_\mathrm{o}(H_\mathrm{ext} - 2\langle M_\mathrm{z}\rangle/3)$. In the cooperative regime, the regions are strongly coupled and the field in the Lorentz cavity rotates with the magnetization:

$$\boldsymbol{B} = \mu_\mathrm{o}\left(H_\mathrm{ext}\mathrm{e}_\mathrm{z} - \langle M_\mathrm{z}\rangle\mathrm{e}_\mathrm{z} + \boldsymbol{M}/3\right). \tag{8}$$

Cooperativity is realized through interatomic interactions, often exchange interactions and sometimes magnetostatic interactions. Exchange ensures almost perfect spin parallelity on atomic length scales, but the effective coupling breaks down above length scales of the order of $a_\mathrm{o}/\alpha = 7.53$ nm even in structurally homogeneous magnets.[16,17] However, in practice, the cooperativity depends on

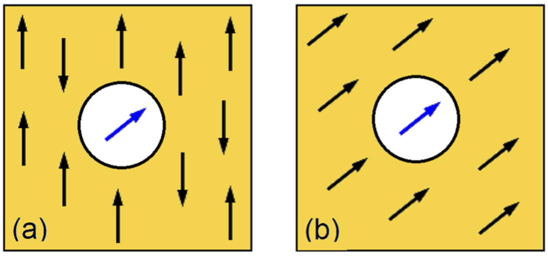

FIG. 3. Magnetization reversal and Lorentz cavity field: (a) noncooperative reversal and (b) cooperative reversal.

the strength and size of the structural inhomogeneities, homogeneous systems being more cooperative.[17] For instance, nonmagnetic regions can strongly reduce cooperativity, as exemplified by nonmagnetic spacer layers in magnetic tunneling junctions. A well-investigated case is anisotropy inhomogeneities in granular materials, which cause the reversal modes to become localized, similar to Fig. 3(a). In the context of magnetic anisotropy, these two cases are known as anisotropy-field (a) and shape-anisotropy (b) limits, which need to be carefully distinguished during magnetization reversal.

V. CONCLUSIONS

In summary, we have investigated the relationship between Berry phase and magnetostatic fields in homogeneous and inhomogeneous magnetic thin films. Treating the electrons as point-like particles in a quantum-mechanical mean-field approximation yields a picture in terms of magnetic Lorentz cavities. This picture reconciles field predictions from Maxwell's equations with those from the Berry connection and from the experiment. The corresponding magnetic flux densities also describe magnetization measurements and are easy to estimate for homogeneous thin films. Future work is necessary to achieve a quantitative understanding of inhomogeneous thin films.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

DATA AVAILABILITY

The data that support the findings of this study are available within the article.

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