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It is investigated how a Berry phase is created in polycrystalline nanomagnets and how the phase translates into an emergent magnetic field and into a topological Hall-effect contribution. The analysis starts directly from the spin of the conduction electrons and does not involve any adiabatic Hamiltonian. Completely random spin alignment in the nanocrystallites does not lead to a nonzero emergent field, but a modulation of the local magnetization does. As an explicit example, we consider a wire with a modulated cone angle. [http://dx.doi.org/10.1063/1.4972804]

I. INTRODUCTION

The Berry phase, $|\psi\rangle \rightarrow \exp(i\gamma)\,|\psi\rangle$, which is unrelated to the dynamical phase $\exp(-i\mathfrak{H}t/\hbar)$, has revolutionized quantum mechanics and permeated many areas of physics.[1] In particular, it is important for the understanding of many magnetic phenomena, such as orbital magnetic moment, anomalous Hall effect, and quantum Hall effect.[1–3] An intriguing aspect of the Berry phase is its relation to topological invariants, which indicate robustness against small and moderate perturbations.[3] For example, the Dirac points of graphene are topologically protected, which manifests itself as a Berry curvature.[3] The invariants often have the character of integrals over curvatures (Gaussian curvature in geometry, Berry curvature in quantum mechanics) are global rather than local.

The Berry phase was originally associated with an adiabatically slow parametric change in the spin wave function,[1] and adiabacity has continued to play a big role in the discussion of Berry-phase effects.[4,5] However, the involvement of an adiabatically varying Hamiltonian $\mathfrak{H}(t)$ is rather secondary from a fundamental viewpoint. One example is that Berry-phase effects exist even for $\mathfrak{H} = 0$ so long as the Lagrangian $\mathcal{L} = \mathbf{p}\cdot\mathbf{q} - \mathfrak{H}$ entering the action $\mathcal{S} = \int \mathcal{L}\,\mathrm{dt}$ involves conjugate quantities $\mathbf{p}$ and $\mathbf{q}$ that form a curved space rather than a "flat" Euclidian space.[6] In fact, considering the Berry phase as a wave-function property, without any reference to Hamiltonians, is not only possible but also convenient for many purposes.

In this paper, we analyze the topological Hall effect, that is, the Berry-phase contribution to the anomalous Hall effect,[7,8] in terms of itinerant wave functions in granular nanostructures. In Sect. II, we outline our approach and show that it is equivalent to previous approaches. Section III, we determine the "emergent" or effective Hall magnetic fields for a thin-film Hall geometry.

II. BACKGROUND

In his original paper, Berry considered an adiabatically slow spin rotation in a strong field of constant magnitude H. Figure 1 shows the corresponding geometry. The change in the wave vector is

$$|\psi\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \quad \rightarrow \quad |\psi\rangle = \begin{pmatrix} \cos\frac{\theta}{2} \\ e^{-i\varphi}\sin\frac{\theta}{2} \end{pmatrix}. \tag{1}$$

The Hamiltonian used by Berry[1] is $\mathfrak{H} = -\mu_o\,\mu_B\,\mathbf{H}\cdot\mathbf{s}$ or, due to adiabacity, $\mathfrak{H} = -\mu_o\,\mu_B\,H = const.$ Shifting the energy zero by a unitary operator $\mathcal{U}$ yields $\mathfrak{H} = 0$ and the Schrödinger equation

$$i\,\partial|\psi\rangle/\partial t = \mathfrak{H}\,|\psi\rangle = 0 \tag{2}$$

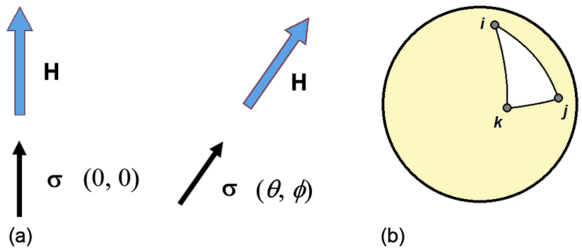

FIG. 1. Berry phase: (a) adiabatically rotating spin $\boldsymbol{\sigma}$, as considered in Berry's original paper, and (b) visualization of a nonzero Berry phase as closed-loop area on the Bloch sphere (θ, ϕ). In a typical solid-state situation, an itinerant electron exchange-interacts with atomic spins $\mathbf{S}_i$ and undergoes a spin change to $\boldsymbol{\sigma}_i$. In the adiabatic limit, $\boldsymbol{\sigma}_i = \mathbf{S}_i$, but in general only the $\boldsymbol{\sigma}_i$ matter.

where $|\psi(\theta, \phi)\rangle = (0, 1)^T$. Equation (2) is paradoxical, because it means that $|\psi\rangle$ does not change, in contradiction the involved physics, which is outlined in Fig. 1(a).

Berry solved this paradox by considering the Berry phase $|\psi\rangle \rightarrow e^{i\gamma}|\psi\rangle$. The phase is often negligible, because $e^{-i\gamma}\, e^{i\gamma} = 1$ in averages of the type $\langle\psi|...|\psi\rangle$, but important if it involves time-dependent parameter sets, such as $\mathbf{b} = (b_1, b_2, ... b_N)$. In the example of Fig. 1, these parameters form the vector $\mathbf{b} = (\theta, \phi)$.

A. Berry connection

The Berry phase of a closed loop C is $\gamma = \int_C \mathbf{A} \cdot \mathrm{d}\mathbf{b}$, where $\mathbf{A} = \langle\psi|\partial/\partial\mathbf{b}|\psi\rangle$ is the Berry connection. In the example of Fig. 1, the Berry connections are $A_\theta = \langle\psi|\partial/\partial\theta|\psi\rangle$ and $A_\phi = \langle\psi|\partial/\partial\phi|\psi\rangle$, or explicitly $A_\theta = 0$ and $A_\phi = \sin^2(\theta/2)$. The corresponding Berry-phase integral $\gamma = \int \mathbf{A} \cdot \mathrm{d}\mathbf{b}$ is equal to

$$\gamma = \int \sin^2(\theta/2)\, \mathrm{d}\phi \tag{3}$$

The Berry phase has a direct physical meaning for closed loops C only, so it is often useful to consider the Berry curvature $\Omega_{mn} = \partial A_n/\partial b_m - \partial A_m/\partial b_n$. In the example of Fig. 1, $\Omega = {}^1/_2\sin\theta$.[3] For closed loops, the Berry phase is $\gamma = \int_C A_\phi\, \mathrm{d}\phi = {}^1/_2\Omega_S$, which can be visualized as an area on the unit sphere, Fig. 2. Integration over the whole sphere yields $\gamma = 2\pi$. This phase is a topological invariant, equivalent to the integral 4π over the Gaussian curvature (Euler characteristic $\chi = 2$ of an ideal or distorted sphere).

B. Berry phase and electromagnetism

There is a close analogy between the Berry connection and the electromagnetic vector potential, both commonly denoted by $\mathbf{A}$, and between the Berry curvature Ω_{mn} ($\boldsymbol{\Omega} = \nabla \times \mathbf{A}$ in three-dimensional parameter space) and the magnetic field $\mathbf{B} = \nabla \times \mathbf{A}$. In fact, the Aharonov-Bohm effect (electron motion in zero $\mathbf{E}$ and $\mathbf{B}$ fields) can be interpreted as an electromagnetic Berry-phase effect.

The analogy carries over to the Lorentz force $\mathbf{F} = -\mathrm{e}\, \mathbf{v} \times \mathbf{B}$ acting on an electron and thereby affects the Hall effect, which is known as the topological Hall effect).[7] The relation between mechanical motion and electromagnetism is provided by the gauge # transformation $\mathbf{p} \rightarrow \mathbf{p} + \mathrm{e}\, \mathbf{A}$. Quantum-mechanically, the kinetic motion of an electron obeys $\mathfrak{H} = \mathbf{p}^2/2m$ and $\mathbf{p} = -i\hbar\nabla$, so that we need to

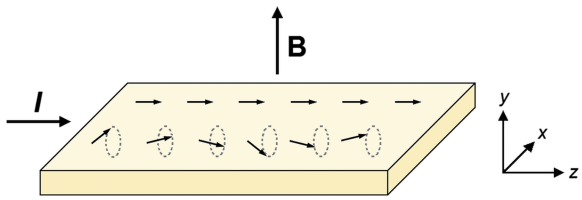

FIG. 2. Example of a nanostructure exhibiting a topological Hall effect due to a Berry-phase-induced emergent B-field.

explore the effect of ∇^2 on the complete wave function $e^{i\gamma}\psi$. It is straightforward to show that

$$\nabla^2(e^{i\gamma}\psi) = e^{i\gamma}(\nabla + i\nabla\gamma)^2\psi \tag{4}$$

The term $e^{i\gamma}$ is now on the left of the nabla operator, where it is "annihilated" through $e^{-i\gamma}e^{i\gamma} = 1$ in quantum-mechanical averages. Equation (4) confirms the equivalence of vector potential and Berry connection, both proportional to $\nabla\gamma$. The corresponding emergent magnetic field $\nabla \times \mathbf{A}$ (or Berry curvature $\mathbf{\Omega}$) contributes to Hall effect,[3] which is the above-mentioned topological Hall effect.

The argumentation in this section reproduces well-known findings but is exclusively based on wave functions and no assumptions were made about the adiabacity or nonadiabacity of the involved Hamiltonians. This is practically important, because the Hamiltonians describing solid-state phenomena are often complicated and difficult to solve.

III. RESULTS

Let us assume that an electron travels through a magnetic lattice (spins $\mathbf{S}_i$), so that the spin angles of the itinerant electron vary along the path, that is, $\theta(\mathbf{r})$ and $\phi(\mathbf{r})$ in Eq. (1). The Berry connection of Eq. (3) then corresponds to the emergent magnetic field,[3,7,9] which has frequently been considered in the context of lattices with non-collinear spins $\mathbf{S}_i$,[8,10] composite thin-film nanostructures,[5] and skyrmion-like micromagnetic spin structures.[7] Atomic-scale examples are $Nd_2Mo_2O_7$ pyrochlore ferromagnets[10] and γ-FeMn,[8] where a Berry phase is created by nonzero scalar spin chirality $c_{ijk} = \mathbf{S}_i \cdot (\mathbf{S}_j \times \mathbf{S}_k)$. Note that noncollinearity of the atomic spins i, j, and k is a necessary but not sufficient condition, because coplanar noncollinearities yield a zero Berry phase.

However, as we will discuss in this section, emergent magnetic fields are very common, and any granular magnetic nanostructure exhibit such fields. The magnitude and direction of the emergent magnetic field follows from the Berry phase of Eq. (3),

$$\mathbf{B} = \frac{\hbar}{2e}\sin\theta\,(\nabla\theta \times \nabla\phi) \tag{5}$$

The B-field scales as $\Phi_o/2\pi R^2$, where $\Phi_o = 2.067$ fTm^2 is the magnetic flux quantum and R is the distance over which the electron changes its spin directions. On a truly macroscopic scale, the fields are weak, but they are fairly large when R is smaller than one micrometer.

The simplest way to introduce the θ and ϕ variations necessary to create the field of Eq. (4) is to consider a fixed or 'frozen' spin structure in the magnet. Granular nanostructures, which can be produced by a variety of methods, such as melt-spinning or cluster deposition, exhibit noncollinear spin structures.[11] First, inversion symmetry is broken at grain boundaries and therefore leads to noncollinear spin structures due to Dzyaloshinski-Moriya (DM) interactions.[11] However, the corresponding angular variations are relatively small, due to the higher-order relativistic character of the DM interactions. A second mechanism is noncollinearities due to competing exchange. These interactions are sometimes rather weak (a few K in temperature units), as exemplified by RKKY interactions in dilute alloys,[12] but values in excess of 100 K are possible in heavy rare earth (Dy) and frustrated magnets.[13]

Our focus in on artificially created spin structures in granular nanostructures. This includes both nanocrystalline single-phase magnets and magnetic nanoparticles embedded in a nonmagnetic metallic matrix, which can be produced by methods such as melt-spinning and cluster deposition.[14,15] If the magnetization orientations of the grains (or crystallites) are random, then Eq. (4) creates locally strong emergent fields. These fields average to zero but contain a $1/\sqrt{N}$ noise component, where N is the number of involved grains. To create a well-defined macroscopic emergent field, one needs a spin structure where $\nabla\theta$ and $\nabla\phi$ do not average to zero. Such spin structure can be produced, in principle, by magnetizing grains or crystallites of a semihard nanostructure. The important point is the *averages* of $\theta(\mathbf{r})$ and $\phi(\mathbf{r})$ vary over a distance of several grains. For individual grains, the angles θ and ϕ are strongly affected by the local anisotropy axis.

The experimental control of the locally averaged angles $\theta(\mathbf{r})$ and $\phi(\mathbf{r})$ is a challenge to future experimental research, and there are many scenarios where Eq. (4) yields a nonzero global B-field. Since the field is monitored through the Hall voltage, it is appropriate to choose a geometry where a

long flat wire of thickness t and width w carries a current in the z-direction. The voltage is measured in the x-direction across the width of the wire, so that the emergent field must point in the y-direction perpendicular to the wire. However these restrictions do not fix $\theta(\mathbf{r})$ and $\phi(\mathbf{r})$, and further choices needs to be made. Figure 2 shows one of these choices. First, we assume that $\phi(\mathbf{r}) = \cos(k\ z)$, which corresponds at a cone angle spiraling in the wire direction. Second, we assume that the cone angle varies across the wire, so that $\theta(\mathbf{r}) = (\pi/2)\ (1 - x/w)$. Since $<\sin\theta> = 2/\pi$, this choice yields

$$\mathbf{B} = -\frac{\hbar}{2e}\frac{k}{w} \tag{6}$$

Note that k and w refer to the spin $\boldsymbol{\sigma}(\mathbf{r})$ of the itinerant electrons, not to the locally "fixed" spins $\mathbf{S}(\mathbf{r})$ of the granular crystallites. The two sets of spins are parallel in the adiabatic limit only, although adiabacity is probably a good approximation for nanostructures.

Note that the spin structure of Fig. 2 is noncollinear and noncoplanar but not of the skyrmion type. The relation between skyrmions and Fig. 2 is analogous to the relation between spin-orbit coupling in atoms and general spin-orbit coupling, for example in thin films (Rashba effect). Skyrmions and atomic spin-orbit coupling are special cases of the more general cross-product-containing description.

IV. CONCLUSIONS

In summary, we have analyzed how itinerant electron in polycrystalline nanomagnets yield an emergent magnetic field and a topological contribution to the anomalous Hall effect. Our analysis is based exclusively on the spin wave functions of the itinerant electrons, which are assumed to reflect the spin structure of the nanomagnet in an adiabatic or nonadiabatic way. Random nanocrystallinity does not yield a net emerging field, but a modulation of the spin structure does, as explicitly shown for one structure. This modulation is not necessarily of the skyrmion type, and other nonskyrmionic spin structures with similar Berry-phase effects are likely to exist.

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