Anomalous Hall Effect in Ferromagnetic Semiconductors

T. Jungwirth,[1,2] Qian Niu,[1] and A. H. MacDonald[1]
[1]*Department of Physics, The University of Texas, Austin, Texas 78712*
[2]*Institute of Physics ASCR, Cukrovarnická 10, 162 53 Praha 6, Czech Republic*
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We present a theory of the anomalous Hall effect in ferromagnetic (III, Mn)V semiconductors. Our theory relates the anomalous Hall conductance of a homogeneous ferromagnet to the Berry phase acquired by a quasiparticle wave function upon traversing closed paths on the spin-split Fermi surface. The quantitative agreement between our theory and experimental data in both (In, Mn)As and (Ga, Mn)As systems suggests that this disorder independent contribution to the anomalous Hall conductivity dominates in diluted magnetic semiconductors. The success of this model for (III, Mn)V materials is unprecedented in the longstanding effort to understand origins of the anomalous Hall effect in itinerant ferromagnets.

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In recent years the semiconductor research community has enjoyed a remarkable achievement, making III-V compounds ferromagnetic by doping them with magnetic elements. The 1992 discovery [1] of hole-mediated ferromagnetic order in (In, Mn)As has motivated research [2] on GaAs and other III-V host materials. Ferromagnetic transition temperatures in excess of 100 K [3,4] and long spin-coherence times in GaAs [5,6] have fueled hopes that a new magnetic medium is emerging that could open radically new pathways for information processing and storage technologies. Recent reports [7] of the room temperature ferromagnetism predicted [8] for (Ga, Mn)N have added to interest in this class of materials. In both (In, Mn)As and (Ga, Mn)As systems, measurements of the anomalous Hall effect have played a key role in establishing ferromagnetism in the studied samples, and in providing evidence for the essential role of hole-mediated coupling between Mn local moments in establishing long-range order [1,2,9]. Despite the importance of the anomalous Hall effect (AHE) [10–15] for sample characterization, a theory which allows these experiments to be interpreted quantitatively has not been available. In this article we present a theory of the AHE in ferromagnetic III-V semiconductors that appears to account for existing observations.

The Hall resistivity of ferromagnets has an ordinary contribution, proportional to the external magnetic field strength, and an anomalous contribution often assumed to be proportional to the sample magnetization. Theories of the anomalous Hall effect (AHE) in a metal [13] usually start from a mean-field theory description of its ferromagnetic state, in which current is carried by quasiparticles in spontaneously spin-split bands. Recent theoretical studies of the AHE in colossal magnetoresistance manganites [16], pyrochlore ferromagnets [17], or noncoplanar antiferromagnets [18] relate the AHE to Berry phase effects caused by carrier hopping in a *noncollinear* spin-splitting effective field produced by a spin-lattice background. Noncollinear magnetic order is, however, not required to produce an anomalous Hall effect and indeed it is not present in most materials in which the effect has been measured, including those of interest to us here. In this paper we relate the AHE in collinear ferromagnets to a Berry phase in momentum space, rather than real space. The AHE we evaluate is a ground state property which depends on the way in which spin-orbit coupled Bloch band wave functions evolve with wave vector [19]. Our theory of the Hall effect is not without precedent. It is related to the Kubo formula for the Hall conductance derived by Thouless and co-workers [20] in their analysis of the quantum Hall effect, and to the master-equation quantum-transport analysis of Luttinger [11]. What is without precedent in this work, is the demonstration that it quantitatively explains the large anomalous Hall effect observed in this new class of magnetic materials.

Our theory of the anomalous Hall effect in (III, Mn)V ferromagnets is built on a mean-field description that has recently been developed [21–25] and used successfully to interpret many magnetic and transport properties. In this mean-field theory the host semiconductor valence bands are split by an effective field that results from exchange interactions with polarized Mn moments. The field makes a wave vector independent contribution,

$$H_{\text{split}} = h\hat{m} \cdot \vec{s} \tag{1}$$

to the band Hamiltonian. Here $\hat{m}$ is the polarization direction of the local moments and $\vec{s}$ is the electron spin operator. The effective field h is proportional to the average local moment magnetization and is nonzero only in the ferromagnetic state. The antiferromagnetic interaction [26,27] between localized and itinerant spins implies that $h > 0$. When Mn spins are fully polarized, $\hat{m}$ is *uniform* and $h = N_{\text{Mn}} S J_{pd}$, where N_{Mn} is the density of Mn ions with spin $S = 5/2$, and $J_{pd} = 50 \pm 5$ meV nm^3 is the strength of the exchange coupling between the local moments and the valence band electrons [9]. In the (In, Mn)As and (Ga, Mn)As AHE measurements, [1,2] $\hat{m}$ is in the $\langle 00\bar{1}\rangle$ direction for positive external magnetic fields.

From a symmetry point of view, the AHE is made possible by this effective magnetic field, and by the spin-orbit coupling present in the host semiconductor valence band.

In the standard model of the AHE in metals, skew-scattering [10] and side-jump [12] scattering give rise to contributions to the Hall *resistivity* proportional to the diagonal resistivity ρ and ρ^2, respectively, with the latter process tending to dominate in alloys because ρ is larger. We present our anomalous Hall effect theory using the language of semiclassical transport theory, namely the expressions for wave-packet dynamics developed previously by one of us [28,29]. These imply a contribution to the Hall *conductivity* independent of the kinetic equation scattering term. Identical expressions can be derived using theoretical approaches of Thouless and co-workers [20] or Luttinger [11]. In the early stages of the development of AHE theory disagreements arose between Smit [10] and Luttinger [11], that do not appear to have ever been fully resolved, on whether AHE can occur in a perfectly periodic lattice. While Smit [10] argued that the explanation has to be based on the anisotropic scattering we follow Luttinger [11] in taking the view that there is a contribution to the AHE due to the change in wave packet group velocity that occurs when an electric field is applied to a ferromagnet.

Our focus on this anomalous wave-pocket velocity contribution is motivated in part by practical considerations, since our current understanding of (III, Mn)V ferromagnets is not sufficient to permit confident modeling of quasiparticle scattering, and in part by estimates [30] of a typical disorder spectral broadening which is smaller than the spin-orbit coupling strength. Since the Hall resistivity is invariably smaller than the diagonal resistivity, a temperature independent value of the Hall conductivity corresponds to a Hall resistivity proportional to ρ^2, usually interpreted as evidence for dominant side-jump scattering. As we explain below, we find quantitative agreement between our Hall conductance values and experiment.

The Bloch electron group velocity correction is conveniently evaluated using expressions derived by Sundaram and Niu [28,29]:

$$\dot{x}_c = \frac{\partial \epsilon}{\hbar \partial \vec{k}} + (e/\hbar)\vec{E} \times \vec{\Omega} . \qquad (2)$$

The first term on the right-hand side of Eq. (2) is the standard Bloch band group velocity. Our anomalous Hall conductivity is due to the second term, proportional to the $\vec{k}$-space Berry curvature $\vec{\Omega}$. It follows from symmetry considerations that for a cubic semiconductor under lattice-matching strains and with $\hat{m}$ aligned by external fields along the $\langle 001 \rangle$ growth direction, only $\Omega_z \neq 0$:

$$\Omega_z(n, \vec{k}) = 2\,\mathrm{Im}\left[\left\langle \frac{\partial u_n}{\partial k_y} \middle| \frac{\partial u_n}{\partial k_x} \right\rangle\right]. \qquad (3)$$

Here $|u_n\rangle$ is the periodic part of the nth Bloch band wave function with the mean-field spin-splitting term included in the Hamiltonian. The anomalous Hall conductivity that results from this velocity correction is

$$\sigma_{AH} = -\frac{e^2}{\hbar} \sum_n \int \frac{d\vec{k}}{(2\pi)^3} f_{n,\vec{k}} \Omega_z(n, \vec{k}), \qquad (4)$$

where $f_{n,\vec{k}}$ is the equilibrium Fermi occupation factor for the band quasiparticles. We have taken the convention that a positive σ_{AH} means that the anomalous Hall current is in the same direction as the normal Hall current.

This Berry phase contribution occurs for any itinerant electron ferromagnet. To assess its importance for (III, Mn)V compounds, we first explore a simplified model that yields parabolic dispersion for both heavy-hole and light-hole bands and a spin-orbit coupling [23,31] strength that is much larger than the hole Fermi energy. Detailed numerical calculations that account for mixing of the spin-orbit split-off bands, and warping of the occupied heavy-hole and light-hole bands [23,31] in (In, Mn)As and (Ga, Mn)As samples [1,3] will follow this general and qualitative discussion. Within a 4-band model, the spin operator $\vec{s} = \vec{j}/3$ in Eq. (1), and the spherical model Hamiltonian for holes in III-V host semiconductors can be written as

$$H_0 = \frac{\hbar^2}{2m}\left[\left(\gamma_1 + \frac{5}{2}\gamma_2\right)k^2 - 2\gamma_2(\vec{k} \cdot \vec{j})^2\right], \qquad (5)$$

where $\vec{j}$ is the total angular momentum operator, γ_1 and γ_2 are Luttinger parameters [31,32]. In the unpolarized case ($h = 0$), the total Hamiltonian, $H = H_0 + H_{\mathrm{split}}$, is diagonalized by spinors $|j_{\hat{k}}\rangle$ where, e.g., $j_{\hat{k}} \equiv \vec{j} \cdot \hat{k} = \pm 3/2$ for the two degenerate heavy-hole bands with effective mass $m_{hh} = m/(\gamma_1 - 2\gamma_2)$. The Berry curvature (3), which can be rewritten as $\vec{\nabla}_{\vec{k}} \cdot [\hat{z} \times \langle u_n | \partial u_n / \partial \vec{k} \rangle]$, is familiar in this case since the Bloch eigenstates are $j = 3/2$ spin coherent states [33]. Integrating over planes of occupied states at fixed k_z we find that $\int d^2k f_{n,\vec{k}} \Omega_z(n, \vec{k}) = \pm 3/2(\cos\theta_{\vec{k}} - 1)$ where $\cos(\theta_{\vec{k}}) \equiv k_z/k_{hh}$ and k_{hh} is the Fermi wave vector. The anomalous Hall conductivity (4) vanishes in the $h = 0$ limit because the contributions from the two heavy hole bands, and also from the two light hole bands, cancel. In the ferromagnetic state, on the other hand, majority and minority spin heavy and light hole Fermi surfaces differ and also the Berry phases are modified when $h \neq 0$. Both effects contribute to σ_{AH}. Up to linear order in h we obtain that $k_{hh}^{\pm} = k_{hh} \pm \cos\theta_{\vec{k}} h m_{hh}/(2\hbar^2 k_{hh})$ and the Berry phase is altered by the factor $1 \mp 2mh/(9\gamma_2 \hbar^2 k_{hh}^2)$. A similar analysis for the light-hole bands leads to a total net contribution to the AHE from the four bands whose lower and upper bounds are the following:

$$\frac{e^2}{2\pi\hbar}\,\frac{h}{2\pi\hbar^2}\,(3\pi^2 p)^{-1/3} m_{hh} < \sigma_{AH} < \frac{e^2}{2\pi\hbar}\,\frac{h}{2\pi\hbar^2}\,(3\pi^2 p)^{-1/3} 2^{2/3} m_{hh} . \qquad (6)$$

Here $p = k_{hh}^3/3\pi^2[1 + (m_{lh}/m_{hh})^{3/2}]$ is the total hole density and $m_{lh} = m/(\gamma_1 + 2\gamma_2)$ is the light-hole effective mass. The lower bound in Eq. (6) is obtained assuming $m_{lh} \ll m_{hh}$ while the upper bound is reached when $m_{lh} \approx m_{hh}$.

Based on the above analysis we conclude that the Berry phase anomalous velocity can yield a sizable AHE in (III, Mn)V ferromagnets. The dot-dashed line in Fig. 1 shows our analytic results for GaAs effective masses $m_{hh} = 0.5m$ and $m_{lh} = 0.08m$. Note that in experiment, anomalous Hall conductances are of order 1–$10\ \Omega^{-1}\,\mathrm{cm}^{-1}$ and the effective exchange field $h \sim 10 - 100$ meV. According to Eq. (6) *larger σ_{AH} values should be expected in systems with larger heavy-hole effective masses and in systems with the ratio m_{lh}/m_{hh} close to unity.*

So far we have discussed the limit of infinitely strong spin-orbit coupling with an exchange field that is small relative to the hole Fermi energy. In the opposite limits of zero spin-orbit coupling or large h, σ_{AH} vanishes. This implies that the anomalous Hall conductivity is generally nonlinear in the exchange field and the magnetization. To explore the intermediate regime we numerically diagonalized the 6-band Luttinger Hamiltonian [23,31] with the spin-orbit gap $\Delta_{so} = 1$ eV, and for the GaAs value $\Delta_{so} = 341$ meV. The results shown in Fig. 1 confirm that *a smaller σ_{AH} is expected in systems with smaller Δ_{so} and suggest that both positive and negative signs of σ_{AH} can occur in general.*

The curves in Fig. 1 are obtained by neglecting band warping in III-V semiconductor compounds. The property that the valence bands in these materials are strongly nonparabolic, even in the absence of the field h and even in the large Δ_{so} limit, is accurately captured by introducing the third phenomenological Luttinger parameter γ_3 [23,31]. Our numerical results indicate that *warping ($\gamma_2 \neq \gamma_3$) leads to an increase of σ_{AH},* as seen when comparing the solid curves in Fig. 1 and in the top panel of Fig. 2. The hole-density dependence of σ_{AH}, illustrated in Fig. 2, is qualitatively consistent with the spherical model prediction (6). The numerical data in Fig. 2 are also consistent with the trends for dependence on host parameters, highlighted in italics in the preceeding paragraphs, suggesting a large positive AHE coefficient for (Al, Mn)As ($m_{hh} = 0.66m, m_{hh}/m_{lh} = 3.96, \gamma_2/\gamma_3 = 1.73$), an intermediate positive σ_{AH} in (Ga, Mn)As ($m_{hh} = 0.5m, m_{hh}/m_{lh} = 6.05, \gamma_2/\gamma_3 = 1.42$), and a relatively weak AHE in (In, Mn)As ($m_{hh} = 0.43m, m_{hh}/m_{lh} = 21.5, \gamma_2/\gamma_3 = 1.08$) with a sign that may be sensitive to strain and other details of a particular sample.

We now compare our σ_{AH} theory with the experimental data available in (In, Mn)As and (Ga, Mn)As

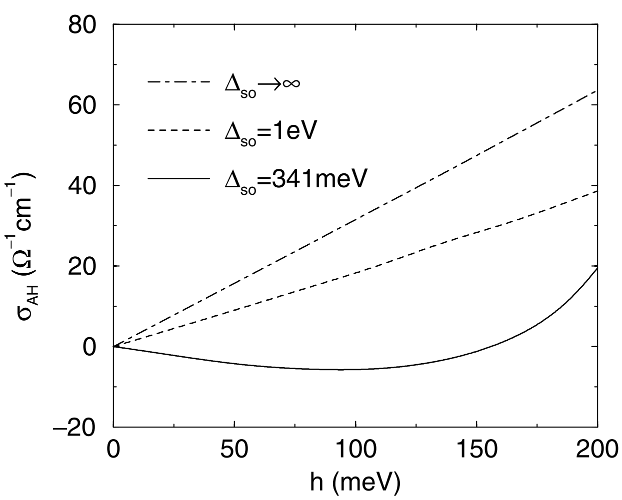

FIG. 1. Illustrative calculations of the anomalous Hall conductance as a function of polarized Mn ions field for hole density $p = 0.35$ nm^{-1}. The dot-dashed curve was obtained assuming infinitely large spin-orbit coupling. The decrease of theoretical σ_{AH} with decreasing spin-orbit coupling strength is demonstrated for $\Delta_{so} = 1$ eV (dashed line) and $\Delta_{so} = 341$ meV (solid line).

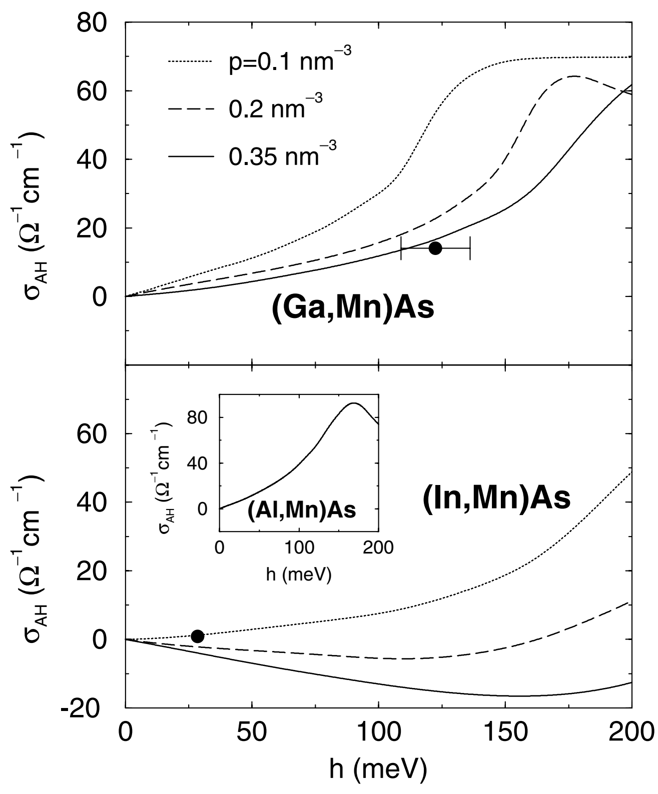

FIG. 2. Full numerical simulations of σ_{AH} for GaAs host (top panel), InAs host (bottom panel), and AlAs host (inset) with hole densities $p = 0.1$ nm^{-1} (dotted lines), $p = 0.2$ nm^{-1} (dashed lines), and $p = 0.35$ nm^{-1} (solid lines). Luttinger parameters of the valence bands were obtained from Ref. [32]. Filled circles in the top and bottom panels represent measured AHE [1,3,9]. The saturation mean-field h values for the two points were estimated from nominal sample parameters [1,3,9]. Horizontal error bars correspond to the experimental uncertainty of the J_{pd} coupling constant. Experimental hole density in the (Ga, Mn)As sample is $p = 0.35$ nm^{-1}; for (In, Mn)As, $p = 0.1$ nm^{-1} was determined indirectly from sample's transition temperature.

samples, studied extensively by Ohno and co-workers [1,3,4,9]. The nominal Mn densities in these two systems are $N_{\mathrm{Mn}} = 0.23\ \mathrm{nm}^{-3}$ for the InAs host and $N_{\mathrm{Mn}} = 1.1\ \mathrm{nm}^{-3}$ for the GaAs host, yielding saturation values of the effective field $h = 25 \pm 3$ meV and $h = 122 \pm 14$ meV, respectively. The low-temperature hole density of the (Ga, Mn)As sample, $p = 0.35\ \mathrm{nm}^{-3}$, was unambiguously determined [9] from the ordinary Hall coefficient measured at high magnetic fields. Since similar experiments have not been reported for the (In, Mn)As sample, we estimated the hole density, $p = 0.1\ \mathrm{nm}^{-3}$, by fitting the density-dependent mean-field theory T_c to the measured value $T_c = 7.5$ K. The use of a mean-field theory description of the ferromagnetic state in both samples is justified [34,35] by the homogeneity of the samples and by the relatively small Fermi energy density of states. Indeed, the measured ferromagnetic transition temperature for the (Ga, Mn)As sample, $T_c = 110$ K, is in an excellent agreement with the calculated transition temperature [22,25,36], and mean-field theory also successfully explains the magnetic anisotropy of both systems [22,23]. Luttinger parameters for the two host semiconductors are well known [32] and are listed in the caption of Fig. 2. As demonstrated in Fig. 2, our theory explains the order of magnitude difference between AHE's in the two materials [$\sigma_{AH} \approx 1\ \Omega^{-1}\,\mathrm{cm}^{-1}$ in (In, Mn)As and $\sigma_{AH} \approx 14\ \Omega^{-1}\,\mathrm{cm}^{-1}$ in (Ga, Mn)As]. The calculations are also consistent with the positive sign and monotonic dependences of σ_{AH} on sample magnetizations [9].

We take the agreement in both magnitude and sign of the AHE as a strong indication that the anomalous velocity contribution dominates AHE in homogeneous (III, Mn)V ferromagnets. This Berry phase conductivity, which is independent of quasiparticle scatterers, is relatively easily evaluated with high accuracy. According to our theory, comparison of theoretical and experimental Hall conductivity values provides information not only on the magnetization but also on the character of the itinerant electron wave functions that participate in the magnetism. For example, we predict that size quantization effects in quantum wells that inhibit heavy-light hole mixing will reduce the $\vec{k}$-space Berry curvatures and hence anomalous Hall conductivities. The extreme strength of the spin-orbit interaction compared to other characteristic energy scales in DMS ferromagnets, may be responsible for the relatively simple physics that evidently determines their AHE. Nevertheless, the success reported here motivates a reexamination of this effect in all itinerant electron ferromagnets.

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