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Berry Approach to Intrinsic Anomalous Hall Conductivity in Dilute Magnetic Semiconductors (Ga$_{1-x}$Mn$_x$As)

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Abstract

We develop a model Hamiltonian to treat intrinsic anomalous Hall conductivity in dilute magnetic semiconductor (DMS) of type (III, Mn, V) and obtain the Berry potential and Berry curvature which are responsible for intrinsic anomalous Hall conductivity in Ga$_{1-x}$Mn$_x$As DMS. Based on Kubo formalism, we establish the relation between Berry curvature and intrinsic anomalous Hall conductivity. We find that for strong spin-orbit interaction intrinsic anomalous Hall conductivity is quantized which is in agreement with recent experimental observation. In addition, we show that the intrinsic anomalous Hall conductivity (AHC) can be controlled by changing concentration of magnetic impurities as well as exchange field. Since Berry curvature related contribution of anomalous Hall conductivity is believed to be dissipationless, our result is a significant step toward achieving dissipationless electron transport in technologically relevant conditions in emerging of spintronics.

Keywords

1. Introduction

In 1879, Edwin H. Hall discovered that when a conductor carrying longitudinal current was placed in a vertical magnetic field, the carrier would be pressed against the transverse side of the conductor, which led to an observed transverse voltage. This is called the Hall effect (HE) [1]. After almost one century, the quantum Hall effect was discovered by K. von Klitzing in 1982 in a two-dimensional electron gas (2DEG) at low temperature and strong magnetic field [2]. However, in ferromagnetic metals like Fe, Co, and Ni, and newly discovered

DMSs like $Ga_{1-x}Mn_xAs$ the Hall effect is anomalous and controlled more by magnetization than by Lorentz forces [3] [4], called the anomalous Hall resistivity and the phenomenon is known as anomalous Hall effect (AHE). This phenomenon attracted both experimental and theoretical interest due to its potential application in emerging science of spintronics [5]. The origin of anomalous Hall effect is believed to be due to spin-orbit (SO) interaction in the presence of spin polarization [6]. On the other hand, DMS of type (III, Mn, V) spin polarization is due to exchange interaction between localized Mn^{2+} $3d^{5+}$ spins and holes introduced by substitution of Mn^{2+} by Ga^{3+} [7]. There are two popular theories to explain anomalous Hall effect seen in ferromagnetic system, named as intrinsic and extrinsic theories, both of these theories involve the SO interaction. The intrinsic theory was first time proposed by Karplus and Luttinger (KL) [8]. It required no impurity (the intrinsic scenario) and extrinsic theory, which was proposed by Smit and Berger; they pointed out the role of the impurity scatterings in the steady state equilibrium and hence in the AHE [9] [10]. Among others, the intrinsic theory dominantly plays a rule in dilute magnetic semiconductors of type (III, Mn, VI) and the current understanding on intrinsic theories of anomalous hall conductivity allows us to reformulate it with Berry curvature of quasi-particles [11]-[13]. Accordingly, intrinsic AHE results from curvature of electrons below the Fermi surface, as a consequence of the spin-orbit coupling induced topological properties in Bloch bands [13]. Although this anomalous Hall effect (AHE) has become a standard tool to determine the magnetization of ferromagnet and has been known for more than a century, its mechanism is still under debate. Particular attention has been paid to intrinsic mechanisms based on the Berry phase. According to recent experimental result, the intrinsic version of AHC is quantized [14].

In this paper we theoretically study anomalous Hall conductivity. The paper is organized as follows. Firstly we develop model Hamiltonian on basis of above discussion, which obtains analytical expression for Berry potential and Berry curvature; secondly after applying Quantum Kubo formulism the connection between Berry curvature and intrinsic Anomalous Hall conductivity is established.

2. Theoretical Formulation

We consider two dimensional hole gas (2 DhG) in the presence of Spin-orbit coupling taking the form of the usual Rashba term, exchange field, kinetic energy of itinerant holes in the system.

$$\hat{H} = H_{kin} + H_{ex} + H_{so} \tag{1}$$

where

$$H_{kin} = \frac{\hbar^2 K^2}{2m^*} \tag{2}$$

H_{kin} and m^* are usual kinetic energy of carriers (holes) and band mass of charge carriers (holes) respectively

$$H_{ex} = -h_{ex}\sigma_z \tag{3}$$

Here, h_{ex} is exchange field resulting from exchange interaction between localized Mn $3d^5$ spins and valence band holes introduced by substitution of Mn^{2+} by Ga^{3+} Our approach is based on mean field treatment and magnetization along perpendicular to k_x and k_y plane or along z axis(along the direction of quantization). $\hat{H}_{so}$ is spin-orbital interaction term in the form of Rash Hamiltonian which accounts that orbital motion of carriers coupled with its spin is given by

$$\alpha_R \left(\sigma_x k_y - \sigma_y k_x \right) \tag{4}$$

Here, σ_x and σ_y are Dirac spin operators along x and y direction respectively and k_x and k_y are wave vectors along x and y direction respectively and α_R Rashba type of spin-orbit coupling constant. Using Equations (2), (3) and (4) into Equation (1), we rewrite the model Hamiltonian as

$$\hat{H} = \frac{\hbar^2 K^2}{2m^*} + \begin{pmatrix} -h_{ex} & \alpha_R k_y + i\alpha_R k_x \\ \alpha_R k_y - i\alpha_R k_x & h_{ex} \end{pmatrix}. \tag{5}$$

In 2D spin space, application of diagonalization procedures in Equation (5) generates two eigenvalues

$$E_\pm(k) = \varepsilon(k) + s\Im_s(k) = \varepsilon(k) + \sqrt{\alpha_R^2 k^2 + h_{ex}^2} \tag{6}$$

And we have obtained the corresponding normalized eigenvectors for spinor part and its complex conjugate

$$u_s(k)\rangle = \frac{1}{\sqrt{\dfrac{2\Im_s(k)}{h_{ex} + s\Im_s(k)}}} \begin{pmatrix} 1 \\ \dfrac{\alpha_R(k_y - ik_x)}{h_{ex} + s\Im_s(k)} \end{pmatrix} \tag{7}$$

$$\langle u_s(k) = \frac{1}{\sqrt{\dfrac{2\Im_s(k)}{h_{ex} + s\Im_s(k)}}} \begin{pmatrix} 1 & \dfrac{\alpha_R(k_y + ik_x)}{h_{ex} + s\Im_s(k)} \end{pmatrix} \tag{8}$$

2.1. Berry Potential and Berry Curvature

Berry potential in momentum space along α, β and γ where α, β and γ designates x, y and z coordinate system respectively were defined in terms of periodic spinor Bloch state and in bands as [15]

$$A_{\alpha,\beta,\gamma} = i\langle u_s(k)|(\nabla_{\alpha,\beta,\gamma})|u_s(k)\rangle. \tag{9}$$

Here $\nabla_{\alpha,\beta,\gamma} = \dfrac{\partial}{\partial k_{x,y,z}}$ Using Equations (7) and (8) into Equation (9) and after some algebra, we obtained the

Berry potential (connection) along x and y direction in k space as follows

$$A_x = \frac{-\alpha_R^2 k_y}{2\Im_s(k)\left(h_{ex+s\Im_s(k)}\right)}. \tag{10}$$

$$A_y = \frac{\alpha_R^2 k_x}{2\Im_s(k)\left(h_{ex+s\Im_s(k)}\right)} \tag{11}$$

The Berry curvature along perpendicular to α, β and γ plane is defined using analogical expression for real space magnetic field [15].

$$\Omega_{\alpha,\beta,\gamma} = \nabla_{\alpha,\beta,\gamma X} A_{\alpha,\beta,\gamma}. \tag{12}$$

In two dimensional systems we rewrite as,

$$\Omega_{\alpha,\beta} = \left(\nabla_{\alpha,\beta X} A_{\alpha,\beta}\right) e_\gamma \tag{13}$$

$$\Omega_{\alpha,\beta} = \left(\nabla_\alpha A_\beta - \nabla_\beta A_\alpha\right) e_\gamma. \tag{14}$$

Using Equation (9) into Equation (14),

$$\Omega_{\alpha,\beta} = i\langle \nabla_\alpha u_n(k)|\nabla_\beta u_n(k)\rangle + i\langle u_n(k)|(\nabla_\alpha \nabla_\beta)|u_n(k)\rangle - i\left(\langle \nabla_\beta u_n(k)|\nabla_\alpha u_n(k)\rangle\right)$$
$$- \langle u_n(k)|(\nabla_\beta \nabla_\alpha)|u_n(k)\rangle e_\gamma \tag{15}$$

This can be written as compact form after introducing commutation relation and straightforward simplification as

$$\Omega_{\alpha,\beta} = i\langle \nabla_\alpha u_n(k)|\nabla_\beta u_n(k)\rangle e_\gamma - i\left(\langle \nabla_\beta u_n(k)|\nabla_\alpha u_n(k)\rangle\right) e_\gamma - \langle u_n(k)|(\lceil \nabla_\alpha, \nabla_\beta \rceil)|u_n(k)\rangle e_\gamma \tag{16}$$

Since ∇_α and ∇_β commutate each other, we get,

$$\Omega_{\alpha,\beta} = i\left(\left\langle \nabla_\alpha u_n(k) \middle| \nabla_\beta u_n(k) \right\rangle\right) - \left\langle \nabla_\beta u_n(k) \middle| \nabla_\alpha u_n(k) \right\rangle e_\gamma \tag{17}$$

After introducing identity $\hat{I} = \sum_m u_m(k) \rangle \langle u_m(k)$, Equation (17) becomes,

$$\Omega_{\alpha,\beta} = i\left(\sum_{m\neq n} \left\langle \nabla_\alpha u_n(k) u_m(k) \right\rangle \left\langle u_m(k) \middle| \nabla_\beta u_n(k) \right\rangle - \left\langle \nabla_\beta u_n(k) u_m(k) \right\rangle \left\langle u_m(k) \middle| \nabla_\alpha u_n(k) \right\rangle\right) e_\gamma \tag{18}$$

After Series of steps we have obtained analytical expression for k-space Berry curvature as

$$\Omega_{\alpha,\beta} = -2\operatorname{Im} \sum_{m\neq n} \frac{\left\langle u_n(k)(\nabla_\alpha H) u_m(k) \right\rangle \left\langle u_m(k)(\nabla_\beta H) u_n(k) \right\rangle}{\left(\varepsilon_{mk} - \varepsilon_{nk}\right)^2} \tag{19}$$

Here, $\nabla_\alpha = \dfrac{\partial}{\partial k_\alpha}$ and $\nabla_\beta = \dfrac{\partial}{\partial k_\beta}$

Equation (19) is general equation of K-space Berry curvature in 2 DS having periodic part of eigenfunction (Spinor part) $u_{m/k}(k)$ non degenerate case. After applying Equation (19) for 2 DhG in dilute magnetic semiconductor (III, Mn, V) system we rewrite the Berry curvature along z direction in k space as,

$$\Omega_{x,y}(z) = -2\operatorname{Im} \sum_{m\neq n} \frac{\left\langle u_n(k)\left(\dfrac{\partial}{\partial k_x} H(k)\right) u_m(k) \right\rangle \left\langle u_m(k)\left(\dfrac{\partial}{\partial k_y} H(k)\right) u_n(k) \right\rangle}{\left(\Im_{m,k} - \Im_{n,k}\right)^2} e_z. \tag{20}$$

In Equation (20), $\left(\dfrac{\partial}{\partial k_x} H(k)\right)$ and $\left(\dfrac{\partial}{\partial k_y} H(k)\right)$ are the velocity operators along v_x and v_y

which were obtained using our model Hamiltonian in Equation (5)

$$v_x = \frac{\partial H(k)}{\hbar \partial k_x} = \frac{\hbar k_x}{m^*} - \alpha_R \sigma_y \tag{21}$$

$$v_y = \frac{\partial H(k)}{\hbar \partial k_y} = \frac{\hbar k_y}{m^*} + \alpha_R \sigma_x. \tag{22}$$

Introducing three dimensional unit vector along x, y and z direction, in two dimensional plane in k space in terms Eigen values as follows

$$\hat{n}(k) = \left\{\frac{\alpha_R k_y}{\Im_{\pm,k}}, -\frac{\alpha_R k_x}{\Im_{\pm,k}}, \frac{h_{ex}}{\Im_{\pm,k}}\right\} \tag{23}$$

where $\Im_\pm(k) = \pm\sqrt{\alpha_R^2 k^2 + h_{ex}^2}$, using Equations (21)-(23) into Equation (20) and after straightforward manipulation, we have obtained expression for the Berry curvature in k-space for upper and lower band ($\pm$), for system of hole gas subjected to spin-orbital coupling and exchange splitting in dilute magnetic semiconductor of type (III, Mn, V) as shown in Equation (24)

$$\Omega_{x,y}^\pm(z) = \pm\frac{\alpha_R^2 h_{ex}}{2\left(\alpha_R^2 k^2 + h_{ex}^2\right)^{3/2}}. \tag{24}$$

The Berry curvature in Equation (24) is responsible for intrinsic Anomalous Hall Conductivity seen in system under consideration.

The connection between Berry curvature and Anomalous Hall conductivity is obtained using Quantum Kubo formalism in the following section.

2.2. Quantum Kubo Formalism and AHC

The Kubo formula for Hall conductivity for current-current correlated system is given by [16]

$$\sigma_{\alpha,\beta}(\omega) = \lim_{\delta \to 0} \frac{\hbar}{V} \sum_{nm} \frac{(f_n - f_m)}{\varepsilon_m - \varepsilon_n} \cdot \mathrm{Im} \frac{\langle n|J_\alpha|m\rangle\langle m|J_\beta|n\rangle}{(\varepsilon_n - \varepsilon_m + \hbar(\omega+\delta))}. \tag{25}$$

V is volume of system, $|n\rangle$ is basis of eigenvectors of the one particle Hamiltonian $\hat{H}$ of Eigenvalues ε_n, f_n and f_m are Fermi Dirac distribution function for band n and m respectively.

J_α and J_β are single particle current operators given by $J_\alpha = -qv_\alpha$ and $J_\beta = -qv_\beta$, here α and β are the direction of current density. Considering Equation (26) in static limit ($\omega = 0$) and in clean sample and after applying for system of 2D spin polarized hole gas in DMSs after some manipulation we have obtained the flowing expression for AHC.

$$\sigma_{\alpha,\beta} = \frac{q^2}{\hbar V} \sum_k (f_{\varepsilon km} - f_{\varepsilon kn}) \cdot \left(\mathrm{Im} \sum_{m \neq n} \frac{\langle u_n(k)(\nabla_\alpha H(k))u_m(k)\rangle\langle u_m(k)(\nabla_\beta H(k))u_n(k)\rangle}{(\varepsilon_{km} - \varepsilon_{kn})^2} \right). \tag{26}$$

On view of Equation (20), right side of Equation (26) inside the bracket gives $-\dfrac{\Omega_{\alpha,\beta}}{2}$. Hence, we can rewrite Equation (26) as

$$\sigma_{\alpha,\beta(\gamma)} = -\frac{q^2}{2\hbar V} \sum_k (f_{\varepsilon k-} - f_{\varepsilon k+})\Omega_{\alpha,\beta}e_\gamma \tag{27}$$

Here we have replaced the band indices n and m via ± which designates lower occupied (−) and upper empty band (+). In continuous limit it is convenient to replace summation into integration. Therefore, Equation (27) becomes

$$\sigma_{\alpha,\beta}(\gamma) = -\frac{q^2}{8\pi^2\hbar} \int_0^{k_F} d^2k (f_{\varepsilon k-} - f_{\varepsilon k+})\Omega_{\alpha,\beta} \tag{28}$$

Plugging Equation (24) into Equation (28), after some algebra we obtained AH conductivity for lower occupied states at T = 0,

$$\sigma_{x,y}(z) = \frac{\alpha_R^2 q^2 h_{ex}}{4\pi\hbar} \int_0^{k_F} (f_{\varepsilon k-}) \frac{k\,dk}{(\alpha_R^2 k^2 + h_{ex}^2)^{3/2}}. \tag{29}$$

In Equation (29) we have considered that at Temperature ($T = 0$) upper band (+) is empty and has nothing contribution to Hall conductivity. Equation (29) integrated to give

$$\sigma_{AH}(z) = -\frac{\alpha_R^2 q^2}{4\hbar} \left(1 - \frac{h_{ex}}{\sqrt{\alpha_R^2 k^2 + h_{ex}^2}} \right) \tag{30}$$

3. Discussion and Conclusions

From Equation (8) and Equation (9) we can observe that in absence of spin-orbital coupling ($\alpha_R = 0$) Berry potential along x and y direction in k-space goes to zero and in similar manner the Berry curvature in Equation (24) also vanishes as ($\alpha_R = 0$) Or/and ($h_{ex} = 0$). Therefore, the origin of Berry potential (connection) as well as Berry curvature in a DMS of type (III, Mn, V) is spin-orbital interaction and exchange field (h_{ex}). As seen in **Figure 1**, the Berry curvature is peaked at $k = 0$, and from Equation (27) the curvature is proportional to AHC; hence the maximum anomalous Hall conductivity can be attained for $k = 0$.

From Equation (30), if $\alpha_R k_F \gg h_{ex}$, for strong spin orbit coupling limit, we have approximate value anomalous Hall conductivity as
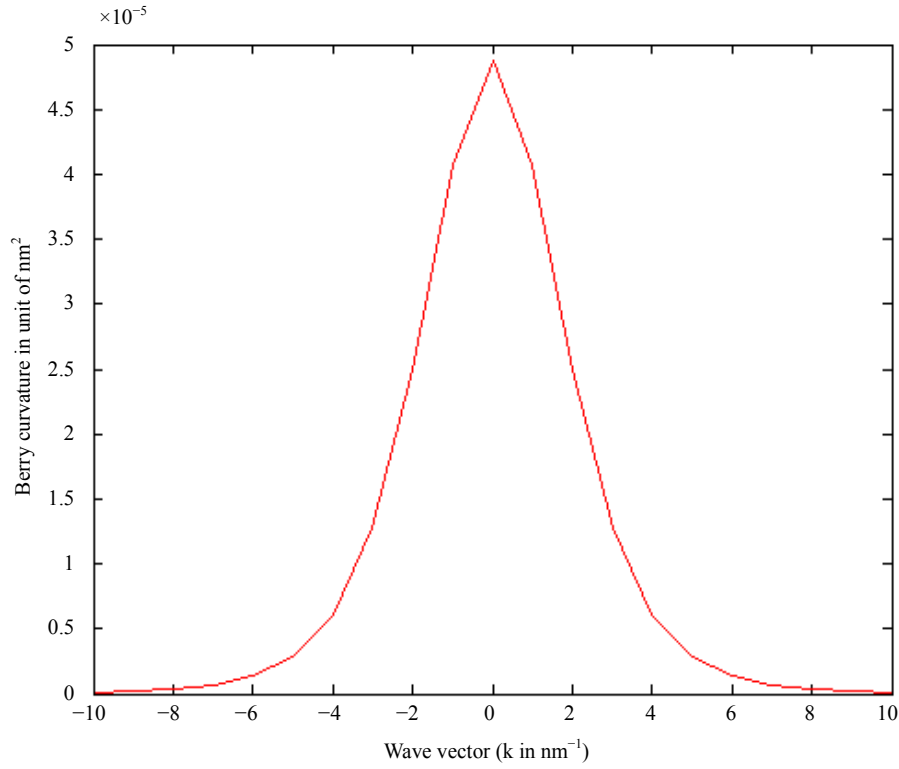
$$\sigma_{AH}(z) = -\frac{q^2}{2\hbar} \tag{31}$$

Figure 1. The variation of Berry curvature as function of wave vector k for material constant of intrinsic Rashba spin-orbit coupling constant ($\alpha_R = 10$ ÅeV) and exchange field ($h_{ex} = 40$ meV).

Equation (31) reveals that intrinsic anomalous Hall conductance is almost quantized which is also supported by recent experimental results [14] [17] [18]. On the other hand, from Equation (27), the intrinsic anomalous Hall conductance is simply the sum of the Chern numbers (the total Berry flux through the BZ) for all the occupied band.

From Case II, integrating Equation (29) from k_{F-} to upper empty band k_{F+}, we obtain anomalous Hall conductivity for lower occupied band is

$$\sigma_{AH}(z) = \frac{q^2}{2h} \frac{h_{ex}}{\sqrt{\alpha_R^2 k_F^2 + h_{ex}^2}} \ . \tag{32}$$

Our analytical results obtained from Equation (30) are similar to result obtained for intrinsic contribution of anomalous hall conductance by classical approach [19].

In **Figure 2**, we have plotted the variation anomalous Hall conductivity as function exchange field. As can be seen in **Figure 1**, when there is no magnetic interaction ($h_{ex} = o$), the spin lies in the xy plane but there is no spin polarization along z axis. As a result, intrinsic Hall conductivity is zero. However, As h_{ex} increases the spin is tilted out of the plane by larger amounts, increasing the phase acquired by the wave function (Berry curvature); as a result anomalous hall conductivity increases a until it reaches a maximum and gradually saturates.

In **Figure 3**, anomalous Hall conductivity increases monotonically as composition of magnetic dopant (x) increases. Hence, it is possible to control intrinsic anomalous Hall conductivity by changing the concentration of magnetic impurities.

In conclusion we say that, at low temperature, in the presence of strong spin-orbit interaction, the anomalous Hall conductivity is quantized. The interplay between spin-orbit interaction and exchange field introduces Berry curvature which is responsible for intrinsic anomalous Hall effect in dilute magnetic semiconductors ($Ga_{1-x}Mn_xAs$). Anomalous Hall conductivity increases monotonically as composition of magnetic dopant (x) increases in mean field theory treatment
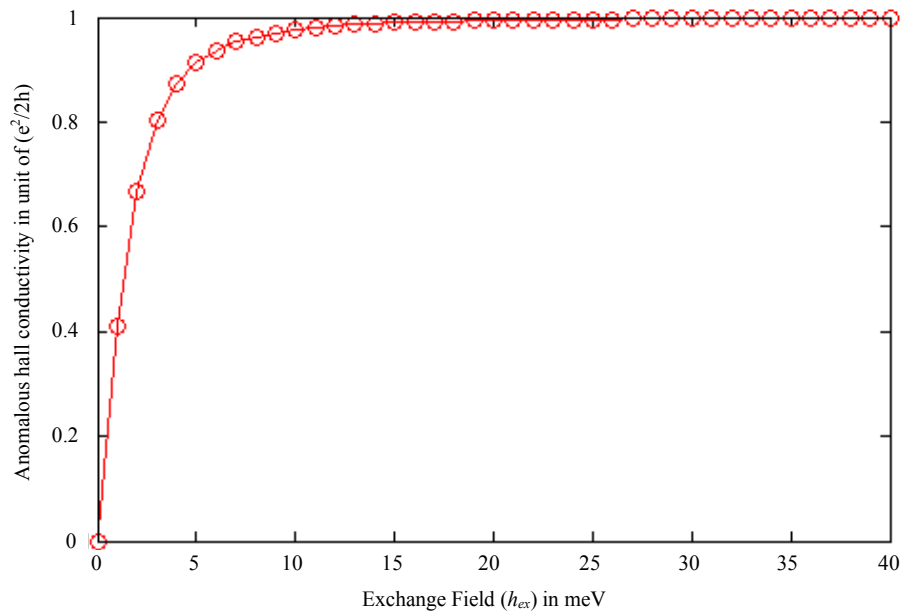
Figure 2. The Variation of Anomalous Hall conductivity as function of exchange field for material constant of spin-orbit splitting ($\nabla_{so} = 5\,\text{meV}$) and exchange field h_{ex} 0 to 40 meV.
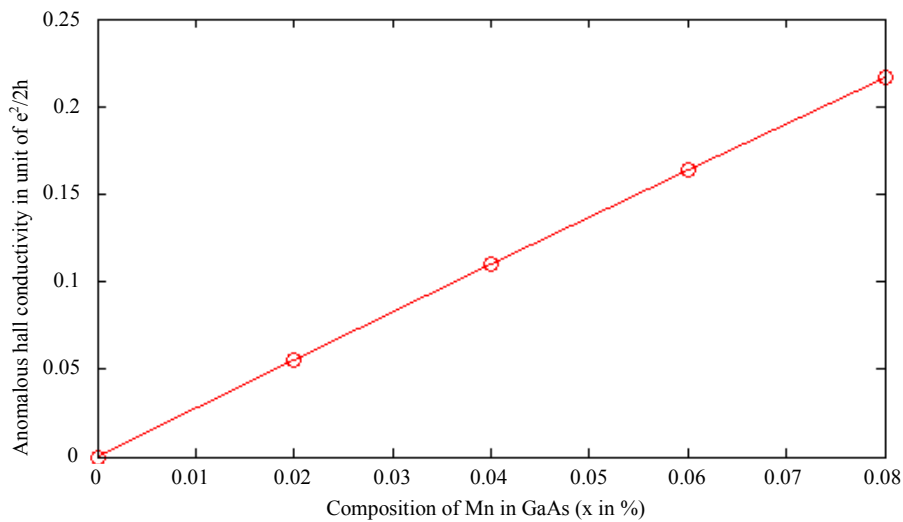

Figure 3. Anomalous Hall conductivity as function of composition of magnetic dopant for material constants of spin-orbit splitting ($\nabla_{so} = 1\,\text{meV}$) and composition of Mn in GaAs ($x =$ 0 to 0.08).

Acknowledgements

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