Influence of the Fermi surface shape on magnetotransport: the MnAs case

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We analyze the effects of the Fermi surface (FS) shape on magnetotransport properties, especially the Hall effect in the MnAs compound. Inspired by previous measurements of MnAs on GaAs substrates which show simultaneously electron and hole conduction, we develop a model based on the semiclassical equations of magnetotransport. In our model, we take into account both, the applied magnetic field as well as the Fermi surface shape. By means of density functional theory, we obtain the FS sheets where there is a clear dominance of the hyperboloid shape. We prove that this shape of the FS is the cause of the simultaneous electron/hole conduction. Our model is corroborated by performing measurements of MnAs epitaxially grown on GaAs(001) and GaAs(111), both substrates allow us to study the magnetoresistance, the magnetization, and the Hall resistance for different crystal direction of the compound. Our study provides guidelines for clarifying the magnetotransport properties in a broad range of materials with similar Fermi surfaces.

I. INTRODUCTION

The shape of the Fermi surface (FS) has been used to describe transport properties since the early days of material science. Pioneering works by Pippard [1] and Lifshitz [2] theoretically prove that the magnetotransport behavior depends on the type of orbits that the wave vector performs in momentum space. The orbits are classified as open or close only between two scattering events, with the characteristic time. For these cases, the magnetoresistance (MR) and especially the Hall resistivity present different behaviors with the magnetic field. On one hand, close orbits lead to a linear dependence of the Hall resistivity and a saturating MR with increasing applied magnetic field. If these orbits on the FS enclose a region with lower energy, then positive values are expected for Hall resistivity (hole-type) and negative values on the opposite case (electron-type). On the other hand, open orbits lead to a quadratic dependence of the Hall resistivity (hole type) and non-saturating magnetoresistance with the applied magnetic field.

The above-mentioned behavior of close/open orbits in momentum space are usually recovered from the FS modeled as an ellipsoid connected with a neck that reaches the boundary of the Brillouin zone (BZ) [1, 3, 4]. Other attempts to describe the magnetotransport properties using a tubular-like FS model, but the analysis emphasizes the connectivity of the surface more than the concavity [1, 5]. Recently, He et al. [6] expose that the concavity of the FS leads to simultaneous electron and hole-like magnetotransport properties, especially when existing open orbits. Hence, for different crystal directions, the transport properties show opposite conduction polarities. This effect, denominated goniopolar by the authors, is theoretically and experimentally described in the NiSn$_2$As$_2$ compound [6, 7]. The origin of this phenomenon is straightforward in the case of a single band FS when it is singly connected with open orbits in one crystal direction and close orbits in other direction. These differences in the orbits give rise to a noticeable different behavior in electron transport measurements for different crystal directions [8]. In the case of the Hall effect (HE), the goniopolarity is manifested when the Ordinary Hall coefficient $R_H$ has the opposite sign when measuring it with respect to different crystal directions as a function of the applied magnetic field. Similar behavior is also observed in the case of the Seebeck effect as the thermopower has the opposite sign for different crystalline directions[6].

Manganese Arsenide (MnAs) compound is a good candidate to be classified as a goniopolar material because it presents simultaneously electron- and hole-like transport behavior, as earlier observed by Berry et al. [9]. They presented measurements of the MR and the HE in MnAs/GaAs(001) epilayers that reveal the presence of both, electron and holes in the magnetotransport, with a contribution that varies with temperature and magnetic field. Also, Friedland et al. [10] observed mainly the same characteristics in the MnAs/GaAs magnetotransport, adding that the carrier type strongly depends on the crystal orientation: MnAs/GaAs(001) samples exhibit mixed hole-like to electron-like conductivity already at zero magnetic field, while in MnAs/GaAs(111) the low-temperature transport is dominated by holes at zero magnetic fields.

To explain their results Ref. [9] propose a two carrier model, while Ref. [10] use a model based on spherical bands with a small number of impurities [11]. Nowadays, we know that MnAs compound shows complex Fermi surfaces topologically different from spherical models, and...
the good quality of the MnAs/GaAs epilayers [12–14] diminishes the role of impurities and domains in low-temperature transport phenomena.

In this work, we analyze the magnetotransport properties of MnAs from both experimental and theoretical points of view. In Sec. II we present the necessary theoretical background to explain our transport measurements. Then Sec. III A describes the MnAs compound using the ab initio calculations and presents the FSs from which we do a model to predict the magnetotransport behavior and Sec. III B presents our measurements (MR, HE and magnetization) on MnAs/GaAs for different crystal orientations. In Sec. IV there is a discussion on the theoretical model presented and its accuracy to describe the experimental measurements.

II. THEORETICAL BACKGROUND

In order to describe the transport behavior with magnetic field we restrict ourselves to a semiclassical treatment, in which the electrons can be thought as classical particles obeying Fermi–Dirac statistics. At low temperature the features of the FS rule the electronic properties of metals, where the mean free time \( \tau \) can be assumed to be large and only band dependent. This extreme case in temperature can be achieved in our theoretical approach by tending to zero the smearing of the FS occupation. This extreme case in temperature transport phenomena.

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Many semiclassical transport calculations have been done taking into account spherical-like FS, with or without open orbits [1–4, 8, 15]. In this section we analyse the case of a FS that is concave in one direction and convex in other direction. More precisely, a circular hyperboloid of one sheet or an hyperboloid of revolution, which leads to a noticeably different behaviour in conductance (or resistivity), as we discuss next.

**Hyperboloid Fermi surface**

![Hyperboloid Fermi surface](image)

**FIG. 1.** Hyperboloid of revolution as a FS model from Eq. 4. The applied magnetic field is perpendicular to the gray planes and the intersection with FS is in red. (a) \( H \parallel z \), only close orbits are possible. (b) \( H \parallel \bar{z} \), where open orbits are allow.
Assuming a FS parameterised as
\[ \varepsilon(k) = \frac{\hbar^2}{2} \left( \frac{k_x^2}{m_x} + \frac{k_y^2}{m_y} - \frac{k_z^2}{m_z} \right) = E_F, \]  
(4)
where \( m_i \) are the effective masses. The minus sign of the \( k_z^2 \)-term indicates that the rotation symmetry axis is parallel to \( z \)-axis, while \( m_x = m_y \) is the condition to be a hyperboloid of revolution. For our future analysis is convenient to define the quantity \( \alpha = \frac{m_z}{m_x} \) that is always a real positive number. If \( \alpha \gg 1 \), the hyperboloid surface approaches to a cylinder with small concave curvature, while for \( \alpha \approx 0 \), the surface has two parabolic sheets joined by a small neck. It is well known that bands must be perpendicular to the BZ boundaries. To fulfill this requirement, we can define energy as a continuous and piece-wise function. However, the change in the energy function from convex to concave is very small and its effect on the orbits is negligible [6].

In order to obtain \( \psi^{(n)} \), we need the time-dependent wave-vector expression \( k(t) \), which describes the orbits on the FS. Since \( z \)-axis is a center of rotational symmetry, only two cases are important to analyse: One where the magnetic field \( \mathbf{H} \parallel \mathbf{z} \)-axis and the other one is when \( \mathbf{H} \) lies in the hexagonal planes, i.e. \( \mathbf{H} \parallel \mathbf{y} \)-axis. The previously mentioned conservation law can help us to have an insight on the solution of the set of Eq. (3). For the \( \mathbf{H} \parallel \mathbf{z} \) case, the obtained orbits are closed circles, as shown in Fig. 1(a), where the time dependent solution has the characteristic frequency \( \omega_z = \frac{\varepsilon}{m_z} \). Instead, for the \( \mathbf{H} \parallel \mathbf{y} \) case, the orbits are open hyperboloid, as shown in Fig. 1(b), with characteristic frequency \( \omega_y = \frac{\varepsilon}{m_y} \sqrt{\frac{m_z}{m_y}} = \omega_z / \sqrt{\alpha} \). For simplicity we use \( \omega_{z,y} \) instead magnetic field \( \mathbf{H} \). In the case of close orbits, the physical meaning of \( \omega \) is the inverse of the time to do one cycle. Hence, for higher magnetic field the wave-vector can perform more cycles. A similar concept can be induced in the case of open orbits, a larger length of the orbit in the extended BZ is covered with an increasing magnetic field. In our approach, the RTA and low field condition happens when \( \omega \tau < 1 \), which is the main difference with previous works of Ref. [1, 2] and more recently [5], where they analyse the high field limit \( (\omega \tau \gg 1) \).

The expression of \( \psi^{(n)} \) depends on \( \omega \tau \), the effective mass \( m_z \), the mass parameter \( \alpha \), and the initial position of the wave-vector \( \mathbf{k}_0 \), which could be any point on the FS as pointed in Eq. (3c). In order to obtain the final expression of the conductivity we must integrate over the FS. In this process the vector \( \mathbf{k}_0 \) becomes an integration variable and the final expression takes into account the history of all possible orbits on the FS.

The resistivity tensor for the \( \mathbf{H} \parallel \mathbf{y} \)-configuration can be expressed as a function of \( \alpha \) and \( \omega \tau \) (for simplicity we omit the index \( z \) ),
\[ \rho_{\text{open}} = \rho_0 \left( \begin{array}{ccc} \alpha - (\omega \tau)^2 & 0 & \alpha - (\omega \tau)^2 \\ \alpha - (\omega \tau)^2 & 0 & \alpha - (\omega \tau)^2 \\ 0 & 1 & 0 \end{array} \right) . \]  
(5)
In this configuration the current is perpendicular to the applied magnetic field and can be in directions \( \hat{x} \) or \( \mathbf{z} \). Instead, the \( \mathbf{H} \parallel \mathbf{z} \)-case the resistivity tensor is the expected for close orbits;
\[ \rho_{\text{close}} = \rho_0' \left( \begin{array}{ccc} 1 & \omega \tau & 0 \\ -\omega \tau & 1 & 0 \\ 0 & 0 & g_4 \end{array} \right) . \]  
(6)
Both tensors are antisymmetric and respect the Onsager’s relations. We group most of the constant in \( \rho_0 \) and magnetoresistance (inset) assume current in \( \mathbf{z} \)-direction. The different curves correspond to values of \( g_2/\alpha \) with \( \alpha = \frac{m_z}{m_x} \) and \( g_2 \) is a geometric factor that comes from integral of Eq.(1).

For the case \( \mathbf{H} \parallel \mathbf{y} \), we plot in Fig. (2) the ordinary Hall resistivity \( \rho_{\text{open}}^{\text{Hall}} \) and the MR (inset) for different values of the parameter \( g_2/\alpha \). The ordinary Hall has a root when \( \omega \tau = 1 \) or equivalently \( \omega \tau = \sqrt{\alpha} \), and then it changes the sign, which can be interpreted as a switch of the carrier type, from holes to electron. In all cases of \( g_2/\alpha \), the ordinary Hall \( \rho_{\text{open}}^{\text{Hall}} \), presents a mixed behavior with applied magnetic field. For values of \( \omega \tau < 1 \), the Hall resistivity is positive and reaches a maximum value that depends on \( \alpha \). If \( g_2/\alpha = 1 \), then the maximum of \( \rho_{\text{Hall}} \) is reached for \( \omega \tau \approx 0.5 \), higher values of \( g_2/\alpha \) displace the maximum to zero, and for smaller values the maximum approaches 1. The MR defined as \[ |\rho_{\alpha}(\mathbf{H}) - \rho_{\alpha}(0)| / \rho_{\alpha}(0) \], saturates for values of \( \omega \tau \) where the RTA and low field condition are no longer valid (\( \omega \tau \gg 1 \)). In all the cases of \( g_2/\alpha \), the MR presents a quadratic-like behaviour for \( \omega \tau < 1 \), as expected for open orbits.

The gonio-polar behavior is manifested by comparing Eq. (5) and (6), where a different magnetotransport behaviour should be expected for this kind of FS. When the magnetic field is parallel to the \( y \)-axis (\( \mathbf{H} \parallel \mathbf{y} \)), the ordinary Hall resistivity as a function of the applied magnetic field

![FIG. 2. Curves corresponding to Eq.(5) as a function of \( \omega \tau \), where \( \mathbf{H} \parallel \mathbf{y} \)-axis (see Fig.1). Ordinary Hall is in units of \( \rho_0 \) and magnetoresistance (inset) assume current in \( \mathbf{z} \)-direction. The different curves correspond to values of \( g_2/\alpha \) with \( \alpha = \frac{m_z}{m_x} \) and \( g_2 \) is a geometric factor that comes from integral of Eq.(1).](Image)
TABLE I. Relation among components of the resistivity for the $P63/mmc$ space structure. The figure shows the atomic arrangements as well as the lattice parameters.

| Structure | Direction | Relation |
|-----------|-----------|----------|
| $H \parallel c$-axis | $\rho_{zz} = \rho_{yy} = 0$ | (H$\parallel z$) $\rho_{yy}(H) = -\rho_{yy}(-H)$ |
| $H \parallel ab$-plane | $\rho_{xy} = 0$; $\rho_{xx} = \rho_{yy}$ | (H$\parallel y$) $\rho_{xx}(H) = -\rho_{xx}(-H)$ |

presents a non-monotonic behavior, having positive slope for lower $\omega_3 \tau$ values and negative slope for higher ones. Instead, when the magnetic field is parallel the $z$-axis ($H\parallel z$), the ordinary Hall resistivity presents a linear behavior with increasing field.

Nevertheless, the present analysis is for a single band and simply connected FS sheet. In the case of multiband transport, the effects that come from other FS sheets should be taken into account in order to reproduce experimental results. However, the curves obtained for the hyperboloid model, specially for $g_z/\alpha \approx 1$, present the same behaviour with applied magnetic fields as the ones experimentally obtained in Ref. [9, 10, 17]. Our results indicate that the direction of the magnetic moments do not affect the shape of the FSs. Nevertheless, one situation has to be mentioned: the FS in Fig. 3(a) has a small ellipsoid around $\Gamma$ and a “flat flower” close to the $\Delta$ symmetric point. This band is affected by the SOC in the $H\parallel z$-case, producing a small splitting around $\Gamma$-point, leaving the Fermi level inside the gap. As a consequence the ellipsoid sheet around $\Gamma$ disappears for the $H\parallel z$ configuration. The area of this ellipsoid is small compared with other FS sheets and, as a consequence, its contribution to the MR and Hall conductivity at low temperatures is negligible.

The surface shown in Fig. 3(b) has two not-connected sheets, where the red part indicates the face of the surface with occupied-states. One of them has the shape of a "nut" when is draw in an extended BZ, but does not connect opposite borders, thus only close orbits are allowed. The other one has an "X" shape made with a folded sheet on itself, but it does not reach the top and bottom borders. To visualize one possible orbit on this surface, we plot in Fig. 3(e) the cross section in the repeated-zone of a plane perpendicular to $k_y$-axis that contains the $\Gamma$ point; it is clear that there is no possibility to hold open orbits. Moreover, the sheet with the "X" shape has a small contribution to the Hall transport due to the folded sheet. The normal vectors of the folded sheet have opposite direction for very close points in the reciprocal space, although they do not cancel each other. They considerably reduce their contribution to the Hall conductivity.

The FSs of interest are those shown in Fig. 3(c) and 3(d). Both surfaces are hyperboloid-like along the $k_z$-axis which is parallel to the $c$-crystal axis. Now it becomes clear the association of these surfaces with the model presented in Sec. II: When the magnetization is parallel to the $c$-axis, it is related to the case where the magnetic field is parallel to the $z$-axis of the hyperboloid model ($H\parallel z$ configuration). On the other hand, when magnetization is parallel to the hexagonal planes, it is related to the $H\parallel y$ configuration. In Fig. 3(f) we present the cross section of the bands plotted in Figs. 3(c) and 3(d) at the repeated-zone in a plane perpendicular to $k_z$-axis that...
FIG. 3. (a-d) Fermi surfaces obtained for the $Hpz$ case. (a) There is a flat flower around $\Delta$-point while the ellipsoid around $\Gamma$ is not appreciated on this scale. (b) For this band, the FS is not simply connected and possesses two independent sheets, one has a "nut"-shape in the extended zone, while the other has an "X"-shape centered in $K$-point, folded on itself and do not reach the top and bottom boundaries. (c) and (d) are FS having hyperboloid-like shape. (e) Cross section of the band plotted in (b) in a extended plane that contains $\Gamma - K - M$ points, only close orbits are allowed. (f) Cross section of the band plotted in (c)-yellow and (c)-green in a extended plane that contains $A - L - H$ points. The connections among yellow lines indicates that this surface holds open orbits in directions perpendicular to $c$-axis. (g) Cross section of the bands plotted in (b) and (c) in a plane that contains $\Gamma - H - K$ points, it presents open open orbits along the $c$-axis and a curvature that can be extrapolate to an hyperboloid-like surface cut. (h) First Brillouin zone and its symmetric points used as reference.

contains the $A$-point. Interestingly, it is observed a path that contain open orbits in a direction perpendicular to the $k_z$-axis.

The last two mentioned FSs have hyperboloid-like surface, which as we describe in previous section lead to a goniopolar magnetotransport behavior that we verify in the following section.

B. Magnetotransport measurements

The MnAs samples are epitaxially grown on GaAs(001) and GaAs(111) substrates [22, 23], as depicted in the first column of Fig. 4. These samples allow us to study the magnetotransport phenomena at two different MnAs-crystal direction, one where the applied magnetic field is parallel to the plane of the hexagon (H||$y$) and the other where is perpendicular to it (H||$z$) as indicated in Fig. 4. Magnetotransport data and magnetization measurements as a function of external magnetic field and temperature were done in a physical property measurement system (PPMS) using the Van der Pauw electric contact configuration [24].

The results on the MnAs/GaAs(001) sample (H||$y$) are displayed in the upper row of Fig. 4. The MR presented in Fig. 4(c) is positive with positive slope for all temperatures, presents a quasi-parabolic behavior and does not saturate for the maximum applied field of 9T. In Fig. 4(d) we present the Hall resistivity as a function of the applied magnetic field, where is observed an inverted parabola with a root at 8.6 T and reach a maximum value for 4 T, in both 5 K and 10 K curves. The same behaviour is observed for T=30 K, with a maximum at 6 T, and a possible root outside of the maximum applied field range of 9 T. These results were already reported by Berry[9], relating them to a change on the type of carriers. However, this behavior is expected for FSs with hyperboloid shapes and magnetic field perpendicular to the its symmetry axis as predicted in previous sections and show in Fig. 2. The magnetization vs. field shown in Fig. 4(e) rises until $\sim$1T and gradually saturates upon increasing the magnetic field. The shoulder at $\sim$1 T in the Hall resistivity is related to the magnetization saturation at this field value, and indicates the saturation of the anomalous Hall effect [25].

For the MnAs/GaAs(111) sample (H||$z$-case), the MR presented in Fig. 4(f) has negative value with negative slope and saturates for increasing applied magnetic field for 5 K and 10 K, instead for 30 K the saturation is not reached for the maximum applied field of 9 T. This sat-
FIG. 4. Magnetotransport measurements in MnAs/GaAs(001) (H∥y), upper row, and MnAs/GaAs(111) (H∥z), lower row, showing Magnetoresistance (c/f), Hall resistivity (d/g) and magnetization (e/h) for both epitaxies as a function of the applied magnetic field and for different low temperature (5K, 10K and 30K). H is the applied magnetic field direction. In (c) the MR is positive and does not saturate, while for (f) is negative and saturates for low temperatures. For the Hall resistivity (d) a change in the polarized charge is observed for magnetic fields larger than 8.6T, not observed in (g), which has a linear behavior. In (e) and (h) the magnetization saturates at 1.5T and 4T respectively, and it is related to the shoulder observed at ∼1.5T in (d) and the change in slope around ∼4T in (e).

uration is observed in a low field regime, which indicates dominance of close orbits in momentum space at low temperatures. The Hall resistivity for MnAs/GaAs(111) sample displayed in Fig. 4(g) presents a monotonously increasing behaviour with magnetic field, as expected for the hyperboloid-like FS with magnetic field parallel to symmetry axis. There is a subtle change of slope at 4 T, which is the same filed where the magnetisation saturates as shown in Fig. 4(h), suggesting the saturation of the anomalous Hall contribution to the Hall resistivity.

MBE growth ensures an excellent crystal quality as well as sharp interfaces between the MnAs layer and the GaAs substrate [12], allowing to rule out any significant role of the impurities at low temperatures. Also, possible magnetic domains disappear when magnetic saturation is reached.

To summarize the experimental results for different crystalline orientations, MnAs/GaAs(001) shows a change of carrier type with increasing magnetic field, but for MnAs/GaAs(111) the carrier type is conserved. This means that the ordinary Hall behavior with magnetic field is in agreement with the model discussed in Sec. II for FSs like the ones presented in Sec.III A. This is the main issue we addressed in this work.

IV. APPLIED MODEL

In order to reproduce the experimental results with the modeled FS, it is necessary take into account that

the Hall measurement include two effects, the so-called ordinary Hall effect and the anomalous Hall effect. They are related with the total Hall resistivity by [25, 26]

\[ \rho(H) = \rho_{ord}(H) + R_A \rho_0 M(H). \]  

(7)

Where H and M are the applied magnetic field and magnetization of the sample, respectively. Also, \( \rho_{Hall} \) is the measured resistivity, \( R_A \) is the anomalous Hall and \( \rho_{ord} \) is the ordinary Hall, which, in our case, are the non-diagonal elements of the Eq. (5) and (6).

In the case of the sample MnAs/GaAs(111), the Hall

FIG. 5. Experimental measurement at 5 K of the Hall resistivity for sample MnAs/GaAs(001) and the fitted curve using Eq.(7), where \( \rho_{ord} = \rho_{Hk} \). At the inset the magnetization is fitted by a Langevin function.

The magnetization saturates at 1.5T and 4T respectively, and it is related to the shoulder observed at ∼1.5T in (d) and the change in slope around ∼4T in (e).
measurement present a linear behavior with applied magnetic field, see Fig. 4(g). This result is expected since we prove that in this configuration the possible orbits in reciprocal space are closed. From Eq. (6) we obtain the linear behaviour for this case, where $\rho_{\text{ord}} = \rho_0 H$. Instead, for the sample MnAs/GaAs(001), we found open orbits for this configuration and experimental result on Hall resistivity show a non linear behavior. For the later case, we use $\rho_{x,y}^2$ from Eq. (5) as $\rho_{\text{ord}}$ in the Eq. (7) to reproduce the experimental results.

For the case MnAs/GaAs(001), we found an excellent agreement between the model and experimental Hall measurements as shown in Fig.5. We obtain for this case that $g_2/\alpha \approx 2.10$, which is comparable with the values 4.09 and 1.41 obtained for the FS of Figs. 3(d) and 3(c), parameterised using Eq.(4). Also, for the same case the $R_A = 0.1 \text{nm}^2\text{cm}$ has the order of magnitude for similar reported metallic systems [27].

V. CONCLUSION

Epitaxial grown conditions of MnAs on different substrates allow us to explore the magnetotransport properties for different crystal directions, such as Hall resistivity. For the MnAs/GaAs(001) (H||y configuration) the carrier polarity changes when the system goes from low field state ($\omega T < 1$) to high field state ($\omega T > 1$). This change of carrier polarity is not observed in MnAs/GaAs(111) (H||z configuration). The experimental results evidences the different behaviour of the charge carriers depending on the crystal direction, this fact allow us to classified the MnAs as goniopolar material.

Results from the electronic structure calculation presented in Sec. III A show a multiband contribution to the electron transport with four bands crossing the Fermi level. However, one of the bands presented in Fig. 3(a) has a negligible number of states compared with the other bands, which diminishes its contribution to conductivity. Another band presented in Fig. 3(b) are not simply connected surface and it is made of two sheets that contribute with close orbits, although one of the sheets is folded on itself and its contribution to the conductivity is also negligible. Finally, the remain two bands have an hyperboloid-like shape along the $z$-axis in reciprocal space and they made the main contribution to the resistivity dependence with magnetic field at low temperatures. The good agreement between measurements and our model is a strong evidence of the phenomena involved.

In conclusion, we use the shape of the Fermi surface of the MnAs to explain low temperature magnetotransport measurements. The specific topology of the dominant Fermi surface sheets with an hyperboloid shape allow us to classify this material as goniopolar and also understand the ordinary Hall behavior with magnetic field, that remained unclear for more than a decade. We believe our study provides guidelines to clarifying the magnetotransport properties in a broad range of materials with similar Fermi surfaces.

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