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Electron states of a magnetic/non-magnetic layered structure

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Abstract. We consider the electronic structure of a magnetic film inserted between distinct non-magnetic materials. Assuming a particular functional form for the electrostatic and magnetic interactions, we obtain an exact solution to the energy spectrum. Several static and transport properties of the solution are discussed.

Recent advances in experimental techniques have provided an extraordinary tool to investigate the behaviour of electrons in heterostructures created by alternating magnetic and non-magnetic films. The giant magnetoresistance observed for very thin layered systems has attracted a great deal of attention in recent years [1]. It has been established that this extraordinary magnetotransport effect rapidly decreases as the film thickness increases beyond the range of 100 Å and becomes quite small (typically a few per cent). (For an updated review on giant magnetoresistance in magnetic multilayers and related structures, see review lecture by Parkin [2].) The theoretical approaches that have been proposed to explain this phenomenon [3, 4] correctly assume that for thin films the magnetic field plays no role in the dynamics of the electrons, and its only effect is to provide a mechanism to overturn the antiferromagnetic layers.

It is the purpose of this work to study the electron states under different conditions. Here we assume that the film thickness is much larger, and we will find that, in such a case, the magnetic field plays an important role in the electron dynamics. We shall derive for this regime some interesting and unusual physical effects. Our system will consist of a single ferromagnetic layer surrounded by two different non-magnetic materials, which may be metals or semiconductors (figure 1). The electrons will be subject to the following interactions: an electrostatic potential, $V(x)$, which changes at the interfaces of the system; a magnetic field, $B(x)$, present inside the film and which results from the spontaneous magnetization of the ferromagnetic layer; and an exchange field, $B'(x)$, which couples to the electron spin and is also confined to the film. In figure 1 we have depicted schematically an idealized form of these interactions. In our analysis, we will assume diffuse surfaces characterized by an average width ξ. This parameter can be varied experimentally. As a first approximation we ignore surface roughness. The typical strength of these interactions can be characterized by the asymptotic potential differences, parametrized as $V_\pm = V_0(1 \mp \Delta/4)^2$. The magnetic interaction is given by $(eA/c)^2/2m$, where $A = B_0 d$, with B_0 being the magnetic field in the interior of the film and $2d$ its width. Finally, the exchange energy is

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$e\hbar B'/2mc$, with B' the exchange field inside the layer. We introduce dimensionless scales for these interactions by dividing them by $\hbar^2/2md^2$. Let

$$\alpha^2 = (ed^2B_0/\hbar c)^2 = (p_0 d/\hbar)^2 \qquad \beta = 2md^2V_0/\hbar^2 \qquad \alpha' = ed^2B'/\hbar c \tag{1}$$

with $p_0 = edB_0/c$. An estimate of these parameters can be obtained by assuming $V_0 = 1$ eV, $B_0 = 10^4$ G and $B' = 10^6$ G. In this case we find $\alpha'/\beta = 0.1$ and $\alpha^2/\beta = 10^7 d^2$ (cm). Thus for $d \lesssim 10^{-5}$ cm, the potential term is dominant; but for $d \gtrsim 10^{-4}$ cm, the magnetic term may be comparable or larger. In addition, we see that α^2, β and $\alpha' \gg 1$ in all this range.

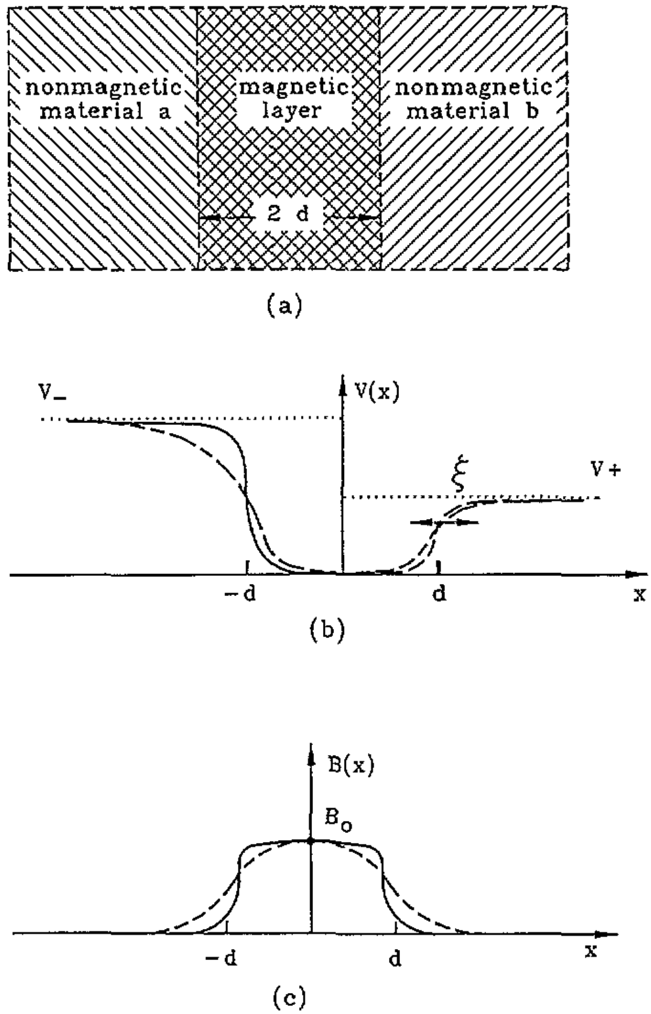

Figure 1. (*a*) Schematic diagram of magnetic/non-magnetic structure. Typical profiles of the electrostatic potential and the magnetic field are plotted (——), as functions of x, in (*b*) and (*c*), respectively. Except for the strength, the exchange field is similar to (*c*). The length ξ measures the width of the interface region. The broken curves in (*b*) and (*c*) represent, schematically, the functional forms for which the exact solution is derived, equation (2). Note that in this case $\xi = d$ so that the interface is rather diffuse.

In the following we shall consider an exact solution to the one-electron eigenvalue problem by choosing a particular functional form for these interactions, which qualitatively reproduces the forms depicted in figure 1. Our choice is

$$\begin{aligned} V(x) &= V_0[\tanh(x/d) - \Delta/4]^2 \\ \boldsymbol{B}'(x) &= B'[1 - \tanh^2(x/d)]\hat{z} \\ \boldsymbol{B}(x) &= B_0[1 - \tanh^2(x/d)]\hat{z} \end{aligned} \tag{2}$$

for which the corresponding vector potential is

$$\boldsymbol{A}(x) = B_0 d \tanh(x/d)\hat{y}. \tag{3}$$

The graphical representation of these functions is shown in figure 1. In addition, we assumed $\Delta \lesssim 2$ so that the minimum of $V(x)$ occurs within $|x| \leqslant d/2$. The resulting Schrödinger equation becomes

$$H\psi = E\psi$$

with

$$\begin{aligned} H = &-(\hbar^2/2m)\mathrm{d}^2/\mathrm{d}x^2 + [p_y + (eB_0 d/c)\tanh(x/d)]^2/2m + p_z^2/2m + V_0[\tanh(x/d) - \Delta/4]^2 \\ &\pm \mu B'[1 - \tanh^2(x/d)] \end{aligned} \tag{4}$$

where p_y and p_z are the conserved components of the momentum. This equation is readily converted into dimensionless form

$$(-\mathrm{d}^2/\mathrm{d}z^2 + A_\pm^2(\tanh z + \tanh z_0^\pm)^2 + C_\pm)\phi_\pm(z) = 0 \tag{5}$$

where

$$z = x/d \qquad A_\pm^2 = \alpha^2 + \beta \pm \alpha' \qquad \tanh z_0^\pm = \alpha^2 p_y / A_\pm^2 p_0 - \beta\Delta/4A_\pm^2$$

and

$$C_\pm = \alpha^2\left(\frac{p_y}{p_0}\right)^2 + \frac{\beta\Delta^2}{16} \mp \alpha' - \left(\frac{\alpha^2 p_y}{A_\pm p_0} - \frac{\beta\Delta}{4A_\pm}\right)^2 + \frac{2md^2}{\hbar^2}\left(\frac{p_z^2}{2m} - E\right). \tag{6}$$

The solutions of equation (5) are well known [5]. We shall reproduce here only its most relevant aspects. Depending on the value of p_y, the spectrum consists of a finite set of discrete bound states, localized inside the film about the point $-z_0$, plus a set of continuum extended states. For larger values of p_y, and depending on their energy, there will only be extended states on one side of the film, or throughout all space. Extended states behave asymptotically as free particles, which either bounce specularly from the film, as in the former case, or cross it, as in the latter case. The bounded spectrum is

$$\begin{aligned} E_n(p_y) = &\frac{1}{2m}\left(1 - \frac{\alpha^2}{b_n^2}\right)\left(p_y + p_0\frac{\beta\Delta}{4(b_n^2 - \alpha^2)}\right)^2 - \frac{\hbar^2}{2md^2}\frac{(\beta\Delta/4b_n)^2}{(b_n^2/\alpha^2 - 1)} \\ &+ \frac{\hbar^2}{2md^2}\left[A_\pm^2 - b_n^2 + \frac{\beta\Delta^2}{16}\left(1 - \frac{\beta}{b_n^2}\right) \mp \alpha'\right] \end{aligned} \tag{7}$$

with $n = 0, 1, 2, \ldots, n_{\max}(p_y)$, and where

$$b_n = (A_\pm^2 + \tfrac{1}{4})^{1/2} - n - \tfrac{1}{2}.$$

In addition, the states $E_n(p_y)$ only exist if p_y is within the interval

$$|p_y/p_0 - \beta\Delta/4\alpha^2| < b_n^2/\alpha^2. \tag{8}$$

For the extended states the spectrum is

$$E(p) = [p_{x,\pm}^2 + (p_y \pm p_0)^2 + p_z^2]/2m + V_0(1 \pm \Delta/4)^2. \tag{9}$$

Here $-/+$ indicates the asymptotic limits $x \gg d$ or $x \ll d$, respectively. We saw above that typically $\alpha^2, \beta \gg \alpha'$, so let us simplify our analysis and drop α'.

The discrete spectrum is plotted as a function of p_y in figure 2. We note that, for fixed n, the resulting curves are parabolae with their centres and their curvatures depending on n. Let us define an effective mass as

$$m_n^* = m/(1 - \alpha^2/b_n^2). \tag{10}$$

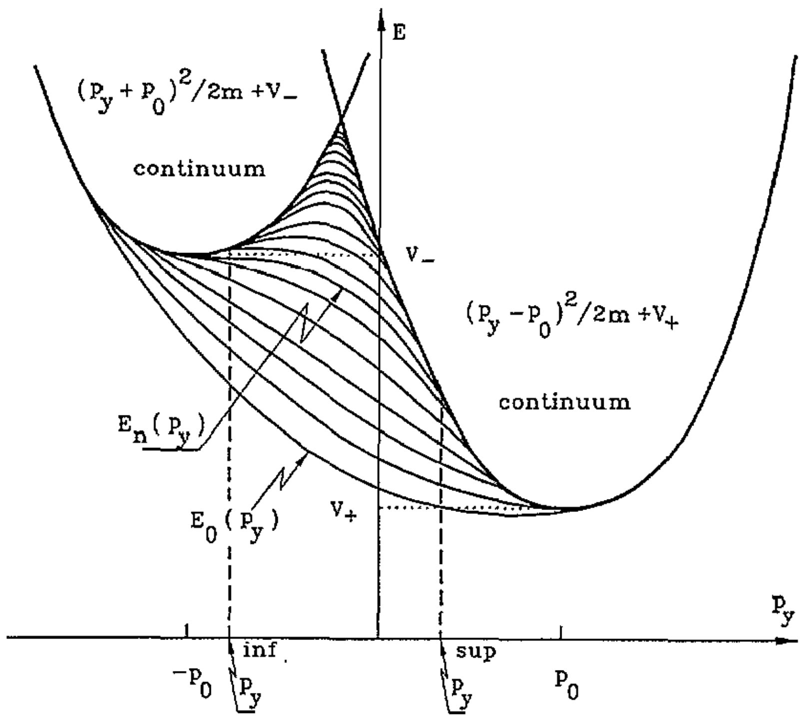

Figure 2. The discrete spectrum $E_n(p_y)$ plotted as a function of n and p_y. For each n, the curve $E_n(p_y)$ approaches the parabolae $(p_y \pm p_0)^2/2m + V_\mp$ at the limits of the stability range, equation (8). The arrows indicate the points of instability for $E_n(p_y)$. Extended states at each side of the film correspond to the continuum levels contained inside the parabolae centred at $\pm p_0$.

Thus we find that the relative strength of α^2 and β determines the sign of m_n^*. In addition, for fixed α^2 and β, m_n^* increases monotonically with n and diverges at $b_n = \alpha$. Thereafter it becomes negative and keeps increasing until $n_{\max}(p_y)$ is reached. The physical origin for this behaviour results from an interplay between the electrostatic interaction, which increases in the proximity of the film boundaries (or p_y approaching the stability limits, equation (8)), and the magnetic interaction, which decreases in the same limits. For small n, the potential term dominates and the energy increases. For larger n, the magnetic interaction is enhanced (by the Lorentz force) and it becomes the dominant term. An immediate consequence of this fact is that the drift velocity along the y axis

$$v_y^n = \partial E_n(p_y)/\partial p_y = [p_y + p_0\beta\Delta/4(b_n^2 - \alpha^2)]/m_n^* \tag{11}$$

may be positive or negative depending on the index n. There are two limiting cases worth noting. If $\alpha = 0$, the p_y dependence of E_n becomes $p_y^2/2m$. In this case the motion in the xy plane is decoupled, being a free particle in the y axis. For $\beta = 0$ and $\alpha \neq 0$, we can easily derive [6]

$$E_n = [\hbar e B_0(1 - \tanh^2 z_0)/mc](n + \tfrac{1}{2}) + \cdots \tag{12}$$

where $\tanh z_0$ is given in equation (6). This result represents the usual Landau formula where the magnetic field is evaluated at the position of the guiding centre $-z_0$. Deleted terms are readily calculated and represent deviations produced by the inhomogeneity of the magnetic field. An unusual property of the spectrum is the coexistence of bound and extended states of equal energy. This fact is a consequence of the gauge field, and is akin to the Bohm–Aharonov effect. For simplicity we consider the $\beta = 0$ case. Then there will be no electrostatic forces and, moreover, the magnetic field vanishes identically outside the film. However, the vector potential does not. This pure gauge term produces an asymptotic 'potential' that confines electrons to the film and prevents them from tunnelling to the degenerate extended states on the outside. This condition will obviously prevail under gauge transformations. Another interesting property of the spectrum is the confining–deconfining effect of the magnetic field. Imagine that $\alpha = 0$ and $\Delta = 0$. There will be an energy range for which states are confined to the film ($E < V_0$). This occurs if $(\beta + \frac{1}{4})^{1/2} - n - \frac{1}{2} > 0$. As α is increased, the condition for boundedness becomes

$$[(\alpha^2 + \beta + \tfrac{1}{4})^{1/2} - n - \tfrac{1}{2}]^2 > \alpha^2 p_y/p_0 = \alpha p_y d/\hbar. \tag{13}$$

We conclude that for $p_y > \bar{p}_y$, where $(\bar{p}_y d/2\hbar)^{2/3} = \frac{4}{3}(\beta - n - \frac{1}{2})$, there will be a range of α for which this condition is violated and the state n unbounded. If α is further increased, equation (13) is again satisfied and the state becomes bounded again. This effect can be understood classically by noting that the Lorentz force transfers kinetic energy, $p_y^2/2m$, into kinetic energy along the x direction. If this transfer is large enough, the electron overcomes the potential barrier and escapes. However, if the magnetic field is too strong, so that the cyclotron radius is smaller than the potential range, the electron remains confined.

We will now consider the ground state of N electrons. Let E_F be the Fermi energy. For a given n, $E_n(p_y) + p_z^2/2m = E_F$ defines an ellipse or a hyperbola depending on the sign of m_n^*. The physical state corresponds to the intersection of the stability strip in p_y, equation (8), and the conics. Clearly the Fermi surface of the extended states are spheres centred at $p_y = \pm p_0$. These states may be either one-sided or fully extended. It is very simple to determine the conditions for which there are no fully extended states. This will happen if $\beta\Delta/4\alpha^2 < 1$ and

$$\frac{p_0^2}{2m}\left[1+\frac{\beta}{\alpha^2}\left(1+\frac{\Delta^2}{16}\right)+\left(\frac{\beta\Delta}{4\alpha^2}\right)^2\right] > E_{\mathrm{F}}. \tag{14}$$

Let us evaluate the Hall current along the y axis, in the case $\Delta \neq 0$. We assume that the system is enclosed inside a cube of side L, with the film located at the midplane and $L \gg d$. By imposing periodic boundary conditions p_y and p_z become discretized. Let n denote the number of nodes that an eigenfunction has along the x axis. This labelling coincides with that of our bound states and will also include extended states. For a given n and p_z, the contribution to the current is

$$I_n(p_z) = -e\frac{L}{2\pi\hbar}\int_{p_y^{\min}}^{p_y^{\max}} \frac{\partial E_n}{\partial p_y}\,\mathrm{d}p_y = 0 \tag{15}$$

since $E_n(p_y^{\max}) = E_n(p_y^{\min}) = E_{\mathrm{F}}$. Let us note, though, that the current carried by the full set of bound states in the range of equation (8) is not zero.

We will next consider an interesting effect that results as a response of the system to an electric field applied in the y direction. Let us assume that equation (14) is satisfied. The momentum will change according to

$$\mathrm{d}p_y/\mathrm{d}t = -eE_y. \tag{16}$$

For the extended states this field will produce a current in the y direction, but for bounded ones, along the x direction. For any given bound state n, p_y will decrease ($E_y > 0$) until the state reaches the lower end of the stability range $p_y^{\inf}$, and is ejected into the continuum at the right of the film. If the direction of the field is reversed ($E_y < 0$), the effect is also reversed. Let us assume that $\Delta > 0$ so that $E_n(p_y^{\inf}) > E_n(p_y^{\sup})$. If for given $E_{\mathrm{F}} - p_z^2/2m$ a band of bounded levels $E_n(p_y)$ is completely full or empty, it will not contribute to the current. On the other hand, a partially filled band will produce a current towards the right of the film. In this case, electrons are captured from the filled extended states at $E_n(p_y^{\sup})$, transported across the film, and ejected into the extended vacant states at $E_n(p_y^{\inf})$. If the electric field is reversed, no transport will take place because recipient states at $E_n(p_y^{\sup})$ are occupied. An idealized arrangement for displaying this effect consists of two concentric cylinders of different materials, so $\Delta \neq 0$, in which the magnetic layer is inserted in between. The inner cylinder has a concentric hole through which an alternating magnetic flux is passed. The induced electric field will be parallel to the film, and if $V_{\mathrm{out}} - V_{\mathrm{in}} = V_0\Delta < 0$, a continuous current will flow radially outwards. It is not difficult to derive an expression for this current. However, such a result would not be very meaningful because the effect of impurities and surface imperfections is being left out of the analysis. In the case of bulk impurities and for films of thickness in the range 10^{-4} cm, a sufficient degree of purity may be achieved so that $\Omega\tau_{\mathrm{b}} \gg 1$ is satisfied, where τ_{b} is the bulk mean free time, $\Omega = (\hbar A/md^2)(1-\tanh^2 z_0)$ and $|z_0| < 1$. In addition, an eigenstate n centred at $-z_0$ will have a width

$$l(z_0) \simeq d/[A(1-\tanh^2 z_0)]^{1/2} \ll d \tag{17}$$

provided $n \ll A$. If we assume that the surface impurity potential is localized at, say, about $x = 1.5d$, and confined to a small fraction of d, it will only affect states at a distance $l(1.5)$ from it, by inducing transitions to nearby overlapping bound or extended states on the same side of the interface. As a result of this, the levels in the neighbourhood of this region will be distorted and the picture of level instability modified. However, we expect that levels inside the film will be little affected and that their transport properties will remain, at least qualitatively, the same.

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