Nanoscale Zeeman localization of charge carriers in diluted magnetic semiconductor-permalloy hybrids

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We investigate the possibility of charge carrier localization in magnetic semiconductors due to the presence of a highly inhomogeneous external magnetic field. As an example, we study in detail the properties of a magnetic semiconductor-permalloy disk hybrid system. We find that the giant Zeeman response of the magnetic semiconductor in conjunction with the highly non-uniform magnetic field created by the vortex state of a permalloy disk can lead to Zeeman localized states at the interface of the two materials. These trapped states are chiral, with chirality controlled by the orientation of the core magnetization of the permalloy disk. We calculate the energy spectrum and the eigenstates of these Zeeman localized states, and discuss their experimental signatures in spectroscopic probes.

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Diluted magnetic semiconductors (DMS) based on III-V alloys doped with Mn have attracted a lot of interest recently, due to their relatively high Curie temperatures $T_C$ (110 K for Ga$_{0.95}$Mn$_{0.05}$As) [1], below which they exhibit ferromagnetic order. In the ferromagnetic state, the charge carriers are spin-polarized, making these materials ideal sources of spin-polarized currents. To date, most suggested applications involving DMS are based on this property and therefore are restricted to operation in a range of temperatures $T < T_C$. On the other hand, in the paramagnetic phase $T > T_C$ both the III$_{1-x}$Mn$_x$V and the more established II$_{1-x}$Mn$_x$VI DMSs (which have even lower critical temperatures) show giant Zeeman response to external magnetic fields. In our opinion, this can lead to interesting applications in the paramagnetic state, and consequently at rather elevated temperatures.

Convincing experimental evidence for Zeeman splitting in the range of 30 meV for external fields of a few Tesla is provided by photoluminescence spectroscopy studies [2]. Even relatively small external magnetic fields of 0.1 – 0.5 T can easily lead to a 15 meV splitting of electronic energy levels [3]. Comparing this to the vacuum Zeeman splitting of $\sim 0.06$ meV for $B = 0.5T$ suggests that the effective gyromagnetic ratio of charge carriers in diluted magnetic semiconductors is $g > 500$. The origin of this hugely enhanced Zeeman effect is attributed [4] to the strong magnetic coupling $\sum_i J_{sp-d}(\vec{s} - \vec{R}_i) \cdot \vec{S}_i$ between the spin $\vec{s}$ of the charge carrier and the spins $\vec{S}_i$ of the Mn located at $\vec{R}_i$. In the paramagnetic state, a small magnetic field $\vec{B}$ induces a magnetization $\langle \vec{S}_i \rangle \sim \chi \vec{B}$ of the Mn spins, resulting in an effective Zeeman-like $\vec{s} \cdot \vec{B}$ coupling between the charge carrier spin and the magnetic field, in addition to the regular Zeeman coupling $-g_0\mu_B \vec{s} \cdot \vec{B}$ present in non-magnetic semiconductors. The scale of this additional coupling is set by the large exchange energy $J_{sp-d}$ and results in a large effective $g$-value. This also implies that $g(T)$ has a strong $T$-dependence through the magnetic susceptibility, and therefore can be tuned over a large range of values. This scenario is strongly supported by magneto-optical absorption measurements [4] of the Zeeman splitting at the band edge, which clearly exhibits a Brillouin-type dependence on the magnetic field.

The presence of giant Zeeman response in DMS implies that a moderate external magnetic field with a strong spatial variation on nanometer scale can be a very effective confining agent for spin-polarized charge carriers in these systems. Provided that such highly inhomogeneous external fields can be created and controlled adequately in a DMS, Zeeman-induced localization presents a new route for manipulation of spin-polarized charge carriers at relatively high temperatures.

Non-uniform magnetic fields with nanoscale spatial variations are known to appear in a variety of systems, such as the Abrikosov flux lattice [5] and arrays of nanoscale holes in superconducting films [6]. However, one of the most promising possibilities, which we investigate in this Letter, is provided by the magnetic vortex state [7] of nanoscale magnetic disks of ferromagnetic permalloy Ni$_{80}$Fe$_{20}$, Co or Fe. In the remanent state of such nanomagnets, the local magnetization near the perimeter of fairly thin disks has an in-plane vortex-like arrangement. This is energetically more favorable than a single ferromagnetic domain, since the exchange energy lost due to the gradual vortex rotation is more than compensated by the cancellation of the total dipole energy. This pattern is maintained for almost the entire volume of the disk. However, near the center of the disk, exchange interaction wins over dipole-dipole interaction and shape anisotropy, and the local magnetization is forced out of the plane of the disk. What is remarkable about this topological singularity in the magnetization is the extremely short length scales and high fields involved: Very recent experimental investigations indicate that the
radius of the magnetic core is about 30 nm in permalloy disks and 10 nm in Fe disks, with maximum field values at the core in the 0.5-1.0 Tesla range. In this paper we show that such highly inhomogeneous magnetic fields provides a very effective localization agent for charge carriers in a system with large Zeeman effect.

We investigate the properties of magnetic disks for which the height \( d \) is small compared to radius \( R \). In this limit, the disks exhibit vortex magnetization of the following general type

\[
\vec{M}(\vec{r}) = M_0(\rho)\vec{e}_\phi + M_z(\rho)\vec{e}_z
\]

where cylindrical coordinates \( \vec{r} = (\rho, \phi, z) \) are used. [Note that \( r \neq |\vec{r}| \). Using Maxwell’s equations, we find the magnetic field created by a magnetization of the type described in Eq. (1). For the setup shown in Fig. \( \text{11} \) the magnetic field created in the DMS layer \( z > 0 \) is

\[
\vec{B}(\vec{r}) = \vec{b}(\vec{r}) - \vec{b}(\vec{r} + \vec{d}e_z),
\]

where, in cylindrical coordinates \( \vec{r} = (\rho, \phi, z) \):

\[
b_r(\rho, z) = \frac{\mu_0}{2\pi}\int_0^\rho\frac{d\rho M_z(\rho)}{\sqrt{(r + \rho)^2 + z^2}} \{K(f(r, \rho, z))\}
\]

\[
-E(f(r, \rho, z)) \cdot \rho^2 + z^2 - \rho^2 \cdot [(r - \rho)^2 + z^2]^{-1}\}
\]

\[
b_\phi(\rho, z) = 0
\]

and

\[
b_z(\rho, z) = \frac{\mu_0 z}{\pi}\int_0^\rho\frac{d\rho M_z(\rho)}{(r + \rho)^2 + z^2} \cdot \frac{E(f(r, \rho, z))}{\sqrt{(r + \rho)^2 + z^2}}
\]

while the corresponding magnetic vector \( \vec{A}(\vec{r}) = \vec{a}(\vec{r}) - \vec{a}(\vec{r} + \vec{d}e_z) \), in the Coulomb gauge \( \nabla \cdot \vec{A} = 0 \), is given by

\[
a_r(\rho, z) = a_z(\rho, z) = 0
\]

and

\[
a_\phi(\rho, z) = -\frac{\mu_0 z}{2\pi r}\int_0^\rho\frac{d\rho M_z(\rho)}{(r + \rho)\sqrt{(r + \rho)^2 + z^2}} \times
\]

\[
\left[(r - \rho)\Pi \left(\frac{4\rho}{(r^2 + z^2)^2}, f(r, \rho, z)\right) + (r + \rho)K(f(r, \rho, z))\right]
\]

Here, \( f(r, \rho, z) = \sqrt{4\rho^2}/[(r + \rho)^2 + z^2] \) and the elliptic functions \( K(k), E(k) \) and \( \Pi(\nu, k) \) are defined in Ref. 13

The fact that only \( M_z(\rho) \) enters these equations is expected, since the field lines induced by \( M_\phi(\rho) \) are closed, and therefore this component does not contribute to the magnetic field outside the magnetic disk. Recent micromagnetic simulations have shown \( \text{10, 14} \) that the magnetization inside the disk is well fitted by the simple parameterization

\[
|M_z(\rho)|/M_0 = \begin{cases} (\rho^2 - r^2)/(\rho^2 + r^2) & , r \leq \rho_c \\
0 & , r > \rho_c \end{cases}
\]

and \( |M_\phi(\rho)| = \sqrt{M_0^2 - M_z^2(\rho)} \). Such a structure is also known as a meron configuration in quantum Hall systems \( \text{17} \). In permalloy disks, the saturation magnetization is \( \mu_0 M_0 = 1.06 \) T and the core radius \( \rho_c \approx 30 \) nm, if the disk radius \( R \gg \rho_c \). [The core radius \( \rho_c \) decreases with decreasing \( d \). The core magnetization \( M_z \) has been observed experimentally in permalloy disks of typical height \( d = 50 \) nm and radii \( R = 0.1 - 1 \) \( \mu m \) as well as Fe disks with \( d = 9 \) nm and \( R = 200 - 500 \) nm \( \text{10} \).]

Using Eqs. (2) and (3), we find the magnetic field created by the vortex inside the diluted magnetic semiconductor to have a typical profile as shown in Fig. \( \text{14} \). Inside the DMS layer, \( B_z(\rho, z) \) is largest at \( r = z = 0 \), and decreases with increasing \( r \) and \( z \). \( B_r(\rho, z) = 0 \) as expected for a dipole-like field. However, \( B_z(\rho, z) \) reaches a maximum value which is roughly half of the maximum \( B_z(r, z) \) value for the same \( z \), at a distance \( r \) of the order of \( \rho_c \). The giant Zeeman effect present in the DMS systems leads to the possibility of trapping carrier states in the strong magnetic field near the disk surface.

The eigenstates of a charge carrier placed in such a magnetic field are given by the Schrödinger equation:

\[
\left\{ \frac{1}{2m}[\vec{p} + q\vec{A}(\vec{r})]^2 - g\mu_B\vec{B}(\vec{r}) \cdot \vec{p}(\vec{r}) \right\} \phi(\vec{r}) = E\phi(\vec{r})
\]

where, as already mentioned, the large \( g \)-factor effectively accounts for the magnetic exchange of charge carriers with locally magnetized Mn spins. The Hamiltonian given in Eq. (8) neglects electron-electron interactions. To first order, this is justified if the carrier concentration is either large enough that screening is very effective, or for low electron concentrations where only a small num-
ber of electrons might be trapped below each disk. In
the latter case, Eq. 3 should accurately describe the
strongest-bound state; for higher energy bound states,
one should also include the screening provided by elec-
trons occupying inner shells. We omit this complication
here. Eq. 5 also assumes that the Mn spins create a
smooth polarizing field for the electron, ignoring possi-
ble local fluctuations due to the fact that Mn spins are
distributed randomly in the DMS. This so-called virtual
crystal approximation has already been used extensively
to describe DMS systems.

Given the symmetries of the magnetic and vector fields
[Eqs. (2,3)], Eq. 8 has solutions of the following general
form:
\[ \phi_m(r, \phi, z) = \exp(i m \phi) \left( \phi_1^{(m)}(r, z) \phi_2^{(m)}(r, z) \exp[i \phi] \right) \tag{9} \]
where the angular momentum \( m \) is an integer. The ex-
tra phase \( \exp[i \phi] \) in the spin-down component has two
significant consequences: (1) \( \sigma_z \) is not a good quan-
tum number. [Besides the \( \langle \delta \sigma_z \rangle \neq 0 \) part, the ex-
tpectation value of the spin acquires a radial contribution
\( \langle \delta_s \rangle \sim \exp(i \phi) \), for all \( m \). This is clearly due to the
existence of a radial part \( B_r(r, z) \) in the magnetic field],
and (2) the (usually expected) degeneracy between states
with \( \pm m \) is now lifted. The reason is that the presence of
the magnetic field breaks the time-reversal symmetry
responsible for this degeneracy. This has interesting con-
sequences, as described below.

The general form of the wave function given above
allows us to draw immediate conclusions regarding se-
lection rules governing the electromagnetic response of
the electronic states trapped in the DMS by the vortex
magnetic field. Assume that the system is ex-
posed to monochromatic radiation, and let \( \vec{A}_L(\vec{r}) \) and
\( \vec{B}_L(\vec{r}) = \nabla \times \vec{A}_L(\vec{r}) \) be the vector potential, re-
trespectively
sively magnetic field associated with it. Then the Schrödinger
equation 8 acquirethree here, terms, proportional
to \( \vec{A} \cdot \vec{B}_L(\vec{r}) \), \( (\vec{p} + q \vec{A}) \cdot \vec{A}_L(\vec{r}) \) and to \( \vec{A}_L^2(\vec{r}) \), in order of
dercreasing magnitude. Assume that the beam propagates
along the \( z \)-axis and is circularly polarized, \( \vec{B}_L^z(z) \sim
(\vec{e}_x \pm i \vec{e}_y) \exp(ikz) \). Using Eq. 9 it is straightforward
to find the selection rules \( \langle m' \vec{A} \cdot \vec{B}_L \rangle |m \rangle \sim \delta_{m',m\pm1} \).
(The term \( (\vec{p} + q \vec{A}) \cdot \vec{A}_L(\vec{r}) \) obeys the same selection rules,
while the \( \vec{A}_L^2(\vec{r}) \) term induces two-photon processes but
with a vanishingly small probability 13). This selection
rule implies that the absorption of a right (left) circularly
polarized photon excites the electron to a level with an \( m \)
increased (decreased) by one unit. If levels with \( \pm m \) are
no longer degenerate, the system will interact different-
ly with photons of different circular polarizations.

Let us now use a simplified model to demonstrate the
lifting of the \( \pm m \) degeneracy. First, the terms involving
the vector field \( \vec{A}(\vec{r}) \) are removed from Eq. 8. This is
justified since they are vanishingly small compared to the
Zeeman term, due to the supplementary enhancement of
the latter by the interaction with the Mn spins. Second,
since we are interested in the most strongly-bound states,
which are likely to be localized at small \((r, z)\) values, we
use Taylor series for the magnetic fields in this region,
given (up to quadratic terms) by:
\[
B_r(r, z) = \mu_0 M_0 B \left( \frac{z}{\rho_c} \right) \frac{r}{\rho_c} \\
B_z(r, z) = \mu_0 M_0 \left[ A \left( \frac{z}{\rho_c} \right) - b_3 \frac{r^2}{\rho_c^2} \right]
\]
where the functions
\[
A(z) = b_1 - b_2 z + 2 b_3 z^2 \quad \text{and} \quad B(z) = \frac{b_2}{2} - 2 b_3 z
\]
have been introduced for later convenience. These fields
continue to satisfy the condition \( \nabla \cdot \vec{B} = 0 \), as neces-
sary. The coefficients \( b_1, b_2 \) and \( b_3 \) are complica-
ted functions of \( d/\rho_c \). In the limit \( d/\rho_c \to \infty \), we find \( b_1 = 1/2, \)
\( b_2 = (\pi + 2)/4 \) and \( b_3 = 1 \). These asymptotic values turn
out to give reasonable approximations for the typical ex-
perimental parameters \( d = 50 \) nm and \( \rho_c = 10 - 30 \) nm,
with relative errors less than 10% for \( d/\rho_c = 5/3 \) and
decreasing very fast to zero for larger ratios 13. As a re-
result, the asymptotic values will be used in the remain-
der of this paper.

With these simplifications, we look for eigenfunctions
[see Eq. 3] of the following form:
\[ \phi_1^{(m)}(r, z) = a_1 \left( \frac{r}{\rho_c} \right)^{|m|} \exp \left( \frac{-r^2}{2b_2} \right) \]
\[ \phi_2^{(m)}(r, z) = a_2 \left( \frac{r}{\rho_c} \right)^{|m+1|} \exp \left( \frac{-r^2}{2b_2} \right) \]
Both components are regular for \( r \to 0 \). The functions
\( a_1(z/\rho_c) \) and \( a_2(z/\rho_c) \) are determined, in dimensionless
units \( z/\rho_c \to z \), by the set of coupled equations:
\[
\left[ \frac{4(|m|+1)}{b^2} - \frac{d^2}{dz^2} - \alpha A(z) \right] a_1 + \frac{s-1}{2} \alpha B(z) a_2 = e a_1 \tag{10}
\]
\[
\left[ \frac{4}{b^2} - \alpha \right] a_1(z) + \frac{s+1}{2} \alpha B(z) a_2(z) = 0 \tag{11}
\]
\[
\left[ \frac{4(|m|+s+1)}{b^2} - \frac{d^2}{dz^2} + \alpha A(z) \right] a_2 - \frac{s+1}{2} \alpha B(z) a_1 = e a_2 \tag{12}
\]
\[
\left[ \frac{4}{b^2} + \alpha \right] a_2(z) + \frac{s-1}{2} \alpha B(z) a_1(z) = 0 \tag{13}
\]
Here, \( s = 1 \) if \( m \geq 0 \) and \( s = -1 \) if \( m < 0 \). We
define the energy unit \( E_0 = \hbar^2/(2m \rho_c^2) \) and use \( e = E/E_0 \), while \( 2\alpha = \mu_B \mu_0 M_0/E_0 \) is the ratio between
the maximum Zeeman energy and this energy unit. This number is rather large. If we use $\rho_e = 30$ nm and $\mu_0 M_0 = 1.06$ T (typical values for permalloy disks), $m = 0.5 m_0$ (band value for heavy hole mass in GaAs) and use the estimated effective gyromagnetic factor to be $g = 500$, we find $|\alpha| \approx 175$.

If $s = +1$, we see from Eq. (13) that there is a non-trivial solution if and only if $4 b^2 = -\alpha$, which is possible if $\alpha < 0$. This is the case when $M_0 < 0$, i.e., the $z$-axis disk magnetization $M_z$ points away from the DMS surface [20]. With $b^2 = \sqrt{4/|\alpha|}$, Eq. (11) has the solution $a_1(z) = \frac{1}{2} B(z) a_2(z)$. Using this in Eq. (12) we find

$$a_2(z) = \exp(-k z),$$

where $k > 0$ is linked to the eigenenergy through $e_m = 2 \sqrt{|\alpha| (m + 2) + \alpha \frac{(6 - \pi)(10 + \pi)}{128} - k^2}$. Finally, Eq. (10) must be satisfied up to powers of $z^0$ (the magnetic fields, and therefore the functions $a_1$ and $a_2$, are accurate only up to $z^2$, meaning that the second derivative of $a_1$ is accurate only up to $z^0$). This gives

$$k = -0.321 \sqrt{|\alpha| + 1.127 |\alpha|} \text{ (with } k > 0 \text{ satisfied for any } |\alpha| > 1.56).$$

In other words, up to a large negative constant the spectrum $e_m = 2 \sqrt{|\alpha| m}$ is similar to that of a harmonic oscillator ($s = +1$). For typical values for the vortex core radius and effective mass (constants which set the energy scale $E_0$ as given above), the level spacing is in the range of $3 - 6$ meV, which should be accessible by most spectroscopic tools.

To summarize, for $M_z < 0$ we find only solutions with $s = +1$ or $m \geq 0$, proving that the $\pm m$ degeneracy is indeed lifted in this simplified case. For $M_z > 0$, the reverse is true; we find only solutions with $m < 0$. However, these simple solutions only hold for small values of $m$, where the wave-functions are localized at small $r$ and $z$ and the Taylor series for the magnetic fields are valid. To find the true spectrum, one must integrate Eq. (10) numerically for the full expression of the magnetic fields; this work is in progress and the results will be reported elsewhere [10]. We expect that the degeneracy between $\pm m$ eigenstates is lifted in the general case as well. As already discussed, this means that the system will interact differently with photons of different circular polarization, depending also on the orientation (sign of) the magnetic disk core magnetization $M_z$. Such a property may be useful in designing spintronic devices: the memory bit ($M_z$ up or down) controls the properties of the trapped electronic states, and therefore the behavior of the whole device. Other geometries, such as lines of ordered disks, could be used to trap and transport electric currents with similar non-trivial spin properties.

In conclusion, we suggest a different route to creating spintronic devices that can operate at room temperature, by combining the giant Zeeman effect of diluted magnetic semiconductors in the paramagnetic state with the highly inhomogeneous magnetic field created by nanoscale permalloy disks, or other nano-patterned magnetic material structures. In particular, we have shown that electronic states can be trapped near the surface of a magnetic disk. Their properties can be suitably tailored using various diluted magnetic semiconductors and various types of magnetic disks, as well as by varying the temperature (since the effective $g$-factor has significant temperature dependence). Since time-reversal symmetry is broken in the presence of the magnetic field, the system will interact non-trivially with any other system which has a definite chirality, such as circularly polarized light. To our knowledge, this is the first time that Zeeman-induced localization has been suggested and demonstrated theoretically, or that electronic states with such unusual spin-polarization have been derived. Experiments to test these ideas are currently in progress [22].

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[1] H. Ohno et al., Appl. Phys. Lett. 69, 363 (1996).
[2] See, for example, S. Lee et al., Phys. Rev. B 61, 2120 (2000) and references therein.
[3] J. Furdyna, J. Appl. Phys. 64, R29 (1988).
[4] N. Dai et al., Phys. Rev. B 50, 18 153 (1994).
[5] S. J. Bending et al., Phys. Rev. Lett. 65, 1060 (1990).
[6] V. Metlushko et al., Phys. Rev. B 59, 603-607 (1999).
[7] R. P. Cowburn et al., Phys. Rev. Lett. 83, 1042 (1999).
[8] T. Shinjo et al., Science 289, 930 (2000).
[9] J. Raabe et al., J. Appl. Phys. 88, 4437 (2000).
[10] A. Wachowiak et al., Science 298, 577 (2002).
[11] A. Hubert and R. Schäfer, Magnetic Domains (Springer, Berlin, 1998).
[12] J. D. Jackson, Classical Electrodynamics, (John Wiley & Sons, 3rd edition, 1998).
[13] $E(k) = \int_0^\pi d\theta \sqrt{1 - k^2 \sin^2 \theta}$, $K(k) = \int_0^\pi d\theta \sqrt{1 - k^2 \sin^2 \theta}$, $\Pi(\nu, k) = \int_0^\pi d\theta \sqrt{(1 - k^2 \sin^2 \theta)(1 - \nu^2 \sin^2 \theta)}^{-1}$.
[14] Gyorgy Csaba, (unpublished).
[15] A. Aharoni, J. Appl. Phys. 68, 2892 (1990).
[16] N. A. Usos and S. E. Peschany, J. Magn. Magn. Mater. 118, L290 (1993).
[17] D. J. Gross, Nucl. Phys. B 132, 439 (1978).
[18] If the beam is shined along the DMS surface (propagation in the xOy plane) transitions are allowed between any two states $m$ and $m'$, i.e. there are no selection rules.
[19] M. A. Berciu and Boldizsár Jankó, (unpublished).
[20] $\alpha < 0$ is also realized if $M_z > 0$, but $g < 0$, i.e. charge carriers are antiferromagnetically coupled to Mn spins. In the following we use the convention that $g > 0$.
[21] Proper boundary conditions must be imposed before the exact eigenstates can be found. These depend on the nature of the DMS-permalloy interface.
[22] J. Furdyna et al., (unpublished).