Magnetic templating by superconducting films, disks and rings

A Amthong and S Crampin
Department of Physics, University of Bath, Bath BA2 7AY, UK
E-mail: aa281@bath.ac.uk

Abstract. Dilute magnetic semiconductors (DMSs), exhibiting both semiconducting and magnetic properties, are interesting materials for novel spintronic devices. Because of the giant Zeeman effect in the paramagnetic state, non-uniform magnetic fields can manipulate the spin texture of carriers in the DMS. A tight-binding model is developed to describe the energy bands formed due to the magnetic field associated with a type-II superconducting film above a DMS layer. Magnetic flux concentrated at the edges of superconducting disks and rings above DMS layers is shown to result in edge-confined states.

1. Introduction
Following the discovery of the giant Zeeman effect in dilute magnetic semiconductors (DMSs) [1], there has been much interest in DMSs in nonuniform magnetic fields [2, 3] because the giant Zeeman splitting can play an important role not only in confining charge carriers, but also in manipulating their spin degrees of freedom, with applications in spintronics. It has been first predicted by Berciu and Jankó [4] that the inhomogeneous magnetic field created by nanoscale permalloy disks can trap spin polarised carriers in DMSs, leading to Zeeman bound states. Another possibility for obtaining non-uniform fields on the nanoscale is to use fields associated with superconductors (SCs). A sufficiently strong uniform external magnetic field can penetrate into type-II SC films in the form of periodic lattices of Abrikosov vortices. A hybrid system consisting of a SC film above a DMS layer illustrated in Fig. 1 has been explored by Rappoport et al [5], who found the nearly spin polarised localised states induced by the magnetic field due to a single vortex can interact to form a band structure. Because each vortex carries a fixed unit of magnetic flux, $\phi_0/2 = h/2e$, the distance between vortices depends on the magnitude of the external field. Hence the applied field can control the band structure by moving vortices, illustrating one benefit of such a hybrid device.

As part of a joint theoretical and experimental research programme in Bath we have revisited this heterostructure, as well as beginning an exploration of magnetic templating due to other SC nanostructures. Below we present a tight-binding theory of the energy spectrum induced by the magnetic fields associated with a periodic lattice of SC vortices, developed to validate a “brute-force” diagonalisation of the Hamiltonian using a Landau-level basis, and which will form the basis of future modelling of low-dimensional vortex structures and spin-charge pumps. We also present preliminary results illustrating localised states associated with SC disks and rings.

Published under licence by IOP Publishing Ltd
2. Energy spectrum due to a vortex lattice using a Landau level basis

An ideal type-II SC film will allow a magnetic field $B_0$ between the lower and upper critical field strengths to penetrate through the formation of the triangular Abrikosov vortex phase. With each vortex carrying a magnetic flux quantum, the distance between vortices $a$ is fixed by $B_0 = \phi_0/\sqrt{3}a^2$. Assuming that the magnetic field $\vec{B}_0$, within the thin DMS a distance $z$ beneath the SC film is the summation of the fields for periodically distributed single vortices [6], $\vec{B}_v$, one can write $\vec{B}_L(\vec{r}; z) = \sum_R \vec{B}_v(\vec{r} - \vec{R}; z) = B_0 \hat{z} + \sum_{\vec{G} \neq 0} e^{i\vec{G} \cdot \vec{r}} \vec{G}(z)$, where $\vec{R}$ and $\vec{G}$ are direct and reciprocal lattice vectors, with an analogous Fourier decomposition of the associated vector potential $\vec{A}_L(\vec{r}; z) = \vec{A}_0(\vec{r}) + \sum_{\vec{G} \neq 0} e^{i\vec{G} \cdot \vec{r}} \vec{A}_G(z)$, where $\vec{A}_0(\vec{r}) = (0, B_0x, 0)$ in the Landau gauge. Electrons (charge $-e$) within the DMS may then be described by the Hamiltonian

$$\hat{H} = \frac{1}{2m^*} [\hat{p} + e\vec{A}_L(\vec{r}; z)]^2 - \frac{1}{2} g_{\text{eff}} \mu_B \vec{B} \cdot \vec{B}(\vec{r}; z),$$

and because $g_{\text{eff}}$ is typically extremely large in DMSs, $\vec{A}_L$ can be replaced by $\vec{A}_0$ without significant loss of accuracy. Eigenstates of (1) may be found by numerical diagonalisation [5], using a basis of spin-polarised Landau level (LL) eigenstates corresponding to the solution of (1) for a homogeneous field $\vec{B}_L = B_0 \hat{z}$. A magnetic unit cell is adopted containing two vortices, corresponding to the lattice $\vec{R} = n\vec{a} + \ell\vec{b}$ with $\vec{a} = (a, 0)$ and $\vec{b} = (0, b)$, $b = \sqrt{3}a$. This ensures that $\hat{H}$ commutes with magnetic translation operators [7, 8, 9] $\hat{T}_M(\vec{R}) = e^{ie\vec{B}_0 \vec{R} \times \vec{y}/\hbar\vec{T}(\vec{R})}$ that satisfy $\hat{T}_M(\vec{R})^2 \hat{T}_M(s\vec{R}) = \hat{T}_M(\vec{R} + s\vec{R})$, and so its eigenstates may be labelled by a wavevector $\vec{k}$ within the associated magnetic Brillouin zone (inset, Fig 2a). Basis functions [10]

$$\Psi_{n, \vec{k}, \sigma}(\vec{r}) = \sum_\lambda e^{-ik_x r^2/(2\lambda)} \phi_{n, k_y + \lambda 2\pi},$$

where $\lambda = \sqrt{ab}/2\pi$ is the magnetic length and $\phi_{n, k_y, \sigma}(\vec{r})$ are LL eigenstates in the Landau gauge with energies $E_{n, \sigma} = (n + 1/2)\hbar\omega_C - (1/2)g_{\text{eff}} \mu_B B_0 \sigma$, represent suitable eigenstates of the magnetic translation operators. Using these to expand the eigenfunctions $\psi_{\vec{k}}(\vec{r})$ of (1) containing the non-uniform field as

$$\psi_{\vec{k}}(\vec{r}) = \sum_{n, \sigma} d_{n, \sigma}(\vec{k}) \Psi_{n, \vec{k}, \sigma}(\vec{r}),$$

substituting into $\hat{H}\psi_{\vec{k}}(\vec{r}) = E_{\vec{k}}\psi_{\vec{k}}(\vec{r})$, multiplying by $\Psi_{n, \vec{k}, \sigma}^\dagger$ and using orthonormality gives the matrix equation

$$-\frac{1}{2} g_{\text{eff}} \mu_B \sum_{n', \sigma'} \vec{\sigma}_{\sigma\sigma'} \cdot \vec{b}_{n, n'} d_{n', \sigma'}(\vec{k}) = (E_{\vec{k}} - E_{n, \sigma}) d_{n, \sigma}(\vec{k}),$$

where $\vec{\sigma}_{\sigma\sigma'} = \chi_{\sigma} \sigma \chi_{\sigma'}$, and

$$\vec{b}_{n, n'} = \delta_{\vec{r}, \vec{r}'} \sqrt{\frac{T^1}{S^1}} \sum_{\vec{G} \neq 0} \vec{B}_G(z)(i\sqrt{g}) S - T \left( L_T S - T_G(g) e^{-g/2} e^{i\phi g} e^{i(k_x G_y - k_y G_x) 2} \left( \frac{G_x - iG_y}{G} \right)^{n-n'} \right)$$

Figure 1. Schematic illustration of the periodic lattice of vortices, spacing $a$, in a type-II superconducting film above a DMS (blue layer).
Figure 2. Band structure of electrons in the DMS for applied fields $B_0$ of (a) 0.06 T, (b) 0.07 T, (c) 0.10 T, (d) 0.15 T, (e) 0.19 T, and (f) 0.26 T, corresponding to vortex spacings $a/\lambda$ of (a) 5.0, (b) 4.6, (c) 3.8, (d) 3.2, (e) 2.8, and (f) 2.4. The inset in (a) shows the Brillouin zone.

with $G = (p\hat{\mathbf{R}}, q\hat{\mathbf{A}})$, $g = l^2 G^2 / 2$, $S (T)$ the greatest (smallest) of $n$ and $n'$, and $L_n^m (x)$ an associated Laguerre polynomial.

Fig. 2 shows results obtained with $\lambda = 40$ nm, $\xi = 35$ nm (corresponding to Nb), $z = 4$ nm, and typical DMS parameters $m^* = 0.5 m_e$, $g_{eff} = 500$. At high fields the spectrum approaches Landau levels as the corrugation in $B_L$ becomes insignificant. At low fields, flat bands correspond to the energy levels of Zeeman bound states associated with isolated vortices, because the separation $a$ is large. At intermediate fields, the behaviour is more complex. Band energies shown in the figure are converged to 6 d.p. using basis set dimensions ranging from 170 for the lowest fields, down to 50 for the highest.

Although these results appear sensible, they differ from those in Ref. [5]. Expressions for the basis functions and our matrix elements are also different. Partly to confirm our analysis, and to develop an alternative framework for the weakly interacting vortex limit, we have considered a tight-binding description presented in the following section.

3. Energy bands using a tight-binding model

When the distance between vortices is large, the band structure tends to the energy levels of states trapped by isolated vortices. We therefore expect that a tight-binding (TB) model can be developed to describe the spectrum in the low field limit. To do so we express the wavefunction in the presence of the vortex lattice as a superposition of isolated vortex states [5] which we labelled by an angular momentum index $m$, unit cell $\mathbf{R} = (na, \ell b)$ which is a magnetic translation vector, and location within the unit cell through $\tau \in \{0, 1\}$, with $\mathbf{r}_\tau = \tau (a/2, b/2)$:

$$|\psi\rangle = \sum_{\mathbf{R}, \tau, m} a_{m, \mathbf{R}} |m, \tau, \mathbf{R}\rangle. \quad (6)$$

The influence of the vector potential on the Hamiltonian matrix elements is included as [11]

$$\langle \mathbf{R}' | \hat{H}^A (\mathbf{r}', \hat{\mathbf{p}} + e\mathbf{A}) | \mathbf{R} \rangle = \exp \left[ -ie \hbar \int_{\mathbf{R}}^{\mathbf{R}'} A(\mathbf{r}) \cdot d\mathbf{r}' \right] \langle \mathbf{R}' | \hat{H}^0 (\mathbf{r}', \hat{\mathbf{p}}) | \mathbf{R} \rangle, \quad (7)$$

where $\hat{H}^A$ and $\hat{H}^0$ are the Hamiltonian with and without the vector potential respectively. Using $\hat{A}_0 (\mathbf{r}) = B_0 x \hat{x}$ for $\hat{A}$ gives

$$\hat{H}^A = \sum_{\mathbf{R}, \tau', m'} \sum_{\mathbf{R}, \tau, m} |m, \tau, \mathbf{R}\rangle e^{\pm ie(\mathbf{r}_\tau - \mathbf{r}_{\tau'}) \cdot (\hat{A}_0(\mathbf{R}_\tau) + \hat{A}_0(\mathbf{R}_{\tau'}))} \langle m', \tau', \mathbf{R}'| \hat{H}^0 | m', \tau', \mathbf{R}' \rangle |m, \tau, \mathbf{R}\rangle \langle m, \tau, \mathbf{R}\rangle. \quad (8)$$
where $\vec{R} - \vec{R}_r$ and $\hat{H}^0 = \frac{1}{2m} \vec{p}^2 - \frac{1}{2} g_{eff} \mu_B \vec{B} \cdot \vec{L}$. A magnetic translation operator for magnetic translation vector $\vec{L}$ may be written as

$$\hat{T}_M(\vec{L}) = \sum_{\vec{R},\tau,m} |m,\tau,\vec{R} \rangle e^{\vec{R} \cdot \vec{L}} \langle m,\tau,\vec{R} - \vec{L}|,$$

which commutes with (8) and satisfies $\hat{T}_M(\vec{L}) \hat{T}_M(\vec{L}') = \hat{T}_M(\vec{L} + \vec{L}')$, so its eigenvalues can be implied to be $e^{i \vec{k} \cdot \vec{L}}$. Hence we propose wavefunctions of electrons in the presence of the field due to a vortex lattice of the form, 

$$|\psi_k\rangle = \sum_{\tau,m} a_{m,\tau,k}|m, \tau, \vec{k} \rangle,$$

where $|m, \tau, \vec{k}\rangle = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{-i \vec{k} \cdot \vec{R}'} e^{i \vec{R}' - \vec{R} \cdot \vec{A}_0(\vec{R})} |m, \tau, \vec{R} \rangle$ is an orthonormal eigenstate of $\hat{T}_M(\vec{L})$ in the nearest neighbour TB approximation, $\langle m', \tau', \vec{R}' | m, \tau, \vec{R} \rangle = \delta_{m'm} \delta_{\tau'\tau} \delta_{\vec{R}' \vec{R}}$, and $N$ is the number of unit cells. The Schrödinger equation can be derived straightforwardly,

$$\sum_{\tau',m'} \langle m, \tau, \vec{k} | \hat{H}^A | m', \tau', \vec{k}' \rangle a_{m',\tau',\vec{k}'} = E_k a_{m,\tau,k},$$

where analysis gives

$$\langle m, \tau, \vec{k} | \hat{H}^A | m', \tau', \vec{k}' \rangle = \delta_{\vec{k},\vec{k}'} \sum_{\vec{R}} e^{i (\vec{k} \cdot \vec{R} - \vec{k}' \cdot \vec{R}') + i \vec{R} \cdot \vec{A}_0(\vec{R}) - i \vec{R}' \cdot \vec{A}_0(\vec{R})} \cdot \langle \vec{R} + \vec{A}_0(\vec{R}), \vec{R}' + \vec{A}_0(\vec{R}') | \hat{H}^0 | m, \tau, \vec{R} \rangle \langle \vec{R} - \vec{A}_0(\vec{R}), \vec{R}' - \vec{A}_0(\vec{R}') | m', \tau', \vec{R}' \rangle \delta_{\vec{k},\vec{k}'} \delta_{\vec{k}',\vec{k}} \delta_{\vec{k}',\vec{k}'} \delta_{\vec{k}',\vec{k}'} \delta_{\vec{k}',\vec{k}'}$$

$$\times \langle m, \tau - \tau', \vec{R} | \hat{H}^0 | m', 0, 0 \rangle.$$  

In the spirit of the nearest neighbour TB approximation, we assume that the hopping term in (12) vanishes except when $\vec{R} - \vec{R}'$ is zero ("on-site", $\langle m, 0, 0 | \hat{H}^0 | m', 0, 0 \rangle = E_m \delta_{m'm}$) or points to a vortex nearest neighbour to the origin, when we have $\langle m, \tau - \tau', \vec{R} | \hat{H}^0 | m', 0, 0 \rangle = e^{i \phi (m' - m)} t_{mm'}$ where $\vec{R} - \vec{R}' = a (\cos \phi, \sin \phi)$.

If we only include $m = 0$ states, then $\hat{H}^A$ can be represented by a 2-by-2 matrix which reduces at $\vec{k} = 0$

$$\hat{H}^A = \begin{pmatrix} E_0 + 2t_{00} & 0 \\ 0 & E_0 - 2t_{00} \end{pmatrix}.$$  

from which the TB parameters $E_0$, $t_{00}$ may be determined by fitting to the eigenvalues at $\Gamma$ found with the LL basis. Fig. 3 compares the resulting TB bands along high symmetry directions with those found using the LL basis, for various vortex lattice spacings, and the variation in the associated TB parameters. Similarly modelling the $m = \pm 1$-derived bands ignoring couplings to other isolated-vortex states gives a 4-by-4 Hamiltonian which involves 5 unique parameters, $E_{-1}$, $E_1$, $t_{-1,-1}$, $t_{-1,+1}$, and $t_{+1,+1}$, which we fix by requiring that the 4 eigenvalues at $\vec{k} = \Gamma$ and the lowest eigenvalue at $\vec{k} = X$ agree with those obtained using the LL basis expansion. Fig. 4 shows the subsequent agreement between the TB bands and the LL-basis bands along high symmetry directions, and the TB parameters obtained.

As $a$ increases the magnitudes of the hopping parameters $t_{mm'}$ decreases, as it becomes increasingly difficult for electrons to jump between Zeeman potential wells. The on-site energies also saturate with increasing vortex spacing at the energy level of the associated bound state for an isolated vortex, the deviation for smaller $a$ being due to the influence of stray fields from neighbouring vortices. Both Fig. 3 and Fig. 4 show that the TB description becomes
Figure 3. Comparison between the lowest energy bands obtained using tight-binding with isolated-vortex $m = 0$ states only and those found using the Landau-level basis for $a/\lambda = (a) 3.4$, (b) 3.8, (c) 4.2, and (d) 4.6. Also shown in (e) is the dependence of the tight-binding parameters on the vortex spacing.

Figure 4. Comparison between the bands derived from $m = \pm 1$ states using the tight-binding method, and those found with the Landau-level basis for $a/\lambda = (a) 4.2$, (b) 4.4, (c) 4.6, and (d) 5.0. In (e) we show the variation of the tight-binding parameters on the vortex spacing.

Increasingly good as the vortex spacing increases, with the bands derived from the more tightly bound $m = 0$ states being described generally better than the $|m| = 1$-derived bands. Even better agreement can be achieved by including hopping between states with different $|m|$, at the expense of additional parameters. However, the results shown here are sufficient to demonstrate the success of the TB description, and the agreement between the two sets of energy band calculations using the LL basis and the TB method confirm that our results with the former are correct.

4. Confined states due to superconducting nanostructures
Screening currents induced in SC disks and rings above a DMS when placed in a uniform applied field can also result in inhomogeneous total magnetic fields that can influence electrons in the DMS. As illustrated in Fig. 5a, flux focussing results in typical $\sim |r - r_0|^{-1/2}$ variations in magnetic field components near an edge at $r_0$. Due to the giant Zeeman interaction in the DMS, these field profiles induce a series of bound states, in which spin-$\uparrow$ and spin-$\downarrow$ components exhibit different spatial distributions, Fig. 5b,c. In the absence of an applied field, flux trapped within the ring can also cause bound states, with energies that depend upon the number of flux quanta that are trapped. Investigations into these and related systems are currently underway.
5. Summary
We have developed and validated a tight-binding model to describe the electronic structure of states in a DAMS beneath a type-II superconducting film. This will form the basis of studies of other low-dimensional systems. We have also identified states localised by the concentration in magnetic flux that occurs at the edges of superconducting disks and rings.

References
[1] Furdyna J K 1988 J. Appl. Phys. 64 R29
[2] Berciu M, Rappoport T G and Jankó B 2005 Nature 435 71
[3] Redliński P, Wojtowicz T, Rappoport T G, Libál A, Furdyna J K and Jankó B 2005 Phys. Rev. B 72 085209
[4] Berciu M and Jankó B 2003 Phys. Rev. Lett. 90 246804
[5] Rappoport T G, Berciu M, and Jankó B 2006 Phys. Rev. B 74 094502
[6] Carneiro G and Brandt E H 2000 Phys. Rev. B 61 6370
[7] Brown E 1964 Phys. Rev. 133 A1038
[8] Opechowski W and Tam W G 1969 Physica 42 529
[9] Wal A 2008 Physica B 404 1040
[10] Pfannkuche D and Gerhardt R 1992 Phys. Rev. B 46 12606
[11] Graf M and Vogl P 1994 Phys. Rev. B 51 4940

Figure 5. (a) Radial and normal component magnetic field profiles in a DMS beneath a superconducting ring with ratio of inner to outer radius $a/b=0.4$. (b) Radial dependence of the spin-$\uparrow$ component of the lowest 3 states confined at each of the inner and outer edges. (c) As (b), but spin-$\downarrow$. 