Abrikosov flux-lines in two-band superconductors with mixed dimensionality

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Abstract
We study vortex structure in a two-band superconductor, in which one band is ballistic and quasi-two-dimensional (2D), and the other is diffusive and three-dimensional (3D). A circular cell approximation of the vortex lattice within the quasiclassical theory of superconductivity is applied to a recently developed model appropriate for such a two-band system (Tanaka \textit{et al} 2006 \textit{Phys. Rev. B} 73 220501(R); Tanaka \textit{et al} 2007 \textit{Phys. Rev. B} 75 214512). We assume that superconductivity in the 3D diffusive band is ‘weak’, i.e. mostly induced, as is the case in MgB\textsubscript{2}. Hybridization with the ‘weak’ 3D diffusive band has significant and intriguing influence on the electronic structure of the ‘strong’ 2D ballistic band. In particular, the Coulomb repulsion and the diffusivity in the ‘weak’ band enhance suppression of the order parameter and enlargement of the vortex core by magnetic field in the ‘strong’ band, resulting in reduced critical temperature and field. Moreover, increased diffusivity in the ‘weak’ band can result in an upward curvature of the upper critical field near the transition temperature. A particularly interesting feature found in our model is the appearance of additional bound states at the gap edge in the ‘strong’ ballistic band, which are absent in the single-band case. Furthermore, coupling with the ‘weak’ diffusive band leads to reduced bandgaps and van Hove singularities of energy bands of the vortex lattice in the ‘strong’ ballistic band. We find these intriguing features for parameter values appropriate for MgB\textsubscript{2}.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Vortices are complex objects even in conventional type-II superconductors, and vortex structure can reveal the underlying physics of the pairing interaction. The 40 K superconductor MgB\textsubscript{2} [3] is the best material discovered so far for studying multiple-band superconductivity. It can be well described by a two-band model that consists of the ‘strong’ quasi-2D $\sigma$ band (energy gap $\approx 7.2$ meV) and the ‘weak’ 3D $\pi$ band (energy gap $\approx 2.3$ meV), and there is evidence of induced superconductivity [4–8] and strong impurity scattering in the $\pi$ band. By tunnelling along the $c$ axis, Eskildsen \textit{et al} have probed the vortex core structure in the $\pi$ band and have found that the local density of states (LDOS) is completely flat as a function of energy at the vortex centre, with no signature of localized states [5]. Moreover, the core size as measured by a decay length of the zero-bias LDOS was found to be much larger than expected from $H_{c2}$. The existence of two length scales in the vortex lattice has also been suggested by the $\mu$SR measurement [9]. The thermal conductivity measurement [10] has detected a rapid increase of delocalized quasiparticles for fields well below $H_{c2}$. Unusually large vortex core size and the extended nature of quasiparticle motion have also been found in the two-band superconductor NbSe\textsubscript{2} [11–16]. There is the possibility of multiband superconductivity in a number of other materials [17–23], and understanding the electronic structure in the vortex state of multiband superconductors is of great interest.

Theoretically, the vortex state in a two-band superconductor has been studied assuming both bands to be in the clean [24]...
and dirty [25] limit. With superconductivity (mostly) induced in one band, it has been found that there are two different length scales associated with the two bands, and that the averaged zero-bias LDOS increases rapidly as a function of field in the ‘weak’ band. Neither of these models, however, are suitable for describing many MgB2 samples, in which the σ and π bands are in the ballistic and diffusive limit, respectively. We have recently formulated a unique two-band model, in which one band (‘σ band’) is ballistic and the other (‘π band’) is diffusive and there is little interband impurity scattering [1, 2]. This picture is appropriate for describing MgB2, in which two-band superconductivity is retained even in ‘dirty’ samples. (See extensive references in [2].) Having MgB2 in mind, in our model it is assumed that the σ and π bands are quasi-2D and 3D, respectively, and superconductivity is mostly induced in the π band through the pairing interaction with the σ band. We have examined the electronic structure around an isolated vortex and have found that the zero-bias LDOS in the π band can have a decay length much larger than in the σ band. A particularly intriguing feature that emerges in our model is the possible existence of bound states at the gap edge in the ballistic band, in addition to the well-known Caroli–de Gennes Matricon (CdM) bound states [26] in the vortex core.

In this work, we extend our two-band model to describe the vortex lattice and investigate the effects of induced superconductivity and impurities in the ‘weak’ diffusive band on the electronic properties in the mixed state. We have found the presence of highly delocalized quasiparticles for relatively weak fields, in agreement with the experiment on MgB2 [3, 10] and the earlier theoretical works [24, 25]. Furthermore, bandgaps and van Hove singularities of energy bands of the vortex lattice in the ‘strong’ ballistic band can be reduced by coupling with the ‘weak’ diffusive band. There exist gap-edge bound states in the vortex core in the ballistic band—that solely arise from coupling to the diffusive band—also in the vortex lattice.

2. Formulation

We utilize a recently developed model appropriate for a system with coupled ballistic and diffusive bands [1, 2]. Both the ballistic and diffusive limits can be described within the quasiclassical theory of superconductivity, in which all the physical information is contained in the quasiclassical Green function, or propagator. We write the propagator in band α as \( \hat{g}_\alpha(\varepsilon, \tilde{p}_\alpha, \tilde{R}) \), where \( \varepsilon \) is the quasiparticle energy measured from the chemical potential, \( \tilde{p}_\alpha \) the quasimomentum on the Fermi surface corresponding to band α and \( \tilde{R} \) the spatial coordinate. The hat refers to the 2 × 2 matrix structure in the Nambu–Gor’kov particle–hole space. In the clean σ band, \( \hat{g}_\sigma(\varepsilon, \tilde{p}_\sigma, \tilde{R}) \) satisfies the Eilenberger equation [27, 28]:

\[
[\varepsilon \hat{\tau}_3 - \hat{\Delta}_\sigma, \hat{g}_\sigma] + i \hbar \tilde{v}_\sigma \cdot \nabla \hat{g}_\sigma = 0, \tag{1}
\]

where \( \tilde{v}_\sigma \) is the Fermi velocity and \( \hat{\Delta}_\sigma \) the (spatially varying) order parameter. The three Pauli matrices are denoted by \( \hat{\tau}_i \), \( i = 1, 2, 3 \), and \( [ \ldots, \ldots ] \) denotes the commutator. Motivated by the Fermi surface of MgB2, we assume a cylindrical Fermi surface and treat the σ band as quasi-two-dimensional. The σ-band coherence length is defined as \( \xi_\sigma = \hbar v_F / \pi T_c \), where \( T_c \) is the transition temperature, and is used as the length unit.

We assume that the π band is in the diffusive limit. In the presence of strong impurity scattering, the momentum dependence of the quasiclassical Green function is averaged out and the equation of motion for the resulting propagator \( \hat{g}_\pi(\varepsilon, \tilde{R}) \) reduces to the Usadel equation [29]:

\[
[\varepsilon \hat{\tau}_3 - \hat{\Delta}_\pi, \hat{g}_\pi] + \nabla \frac{\hbar D}{\pi} (\hat{g}_\pi \nabla \hat{g}_\pi) = 0, \tag{2}
\]

with the diffusion constant tensor \( D \). Throughout this work, we assume an isotropic tensor \( D_{ij} = D \delta_{ij} \) and define the π-band coherence length \( \xi_\pi = \sqrt{\hbar D / 2 \pi T_c} \). Both ballistic and diffusive propagators are normalized according to \( \hat{g}_\sigma^2 = \hat{g}_\pi^2 = -\pi^2 \mathbf{1} \) [27].

The quasiparticles in different bands are assumed to be coupled only through the pairing interaction. Self-consistency for the spatially varying parameters in both the bands is achieved through the coupled gap equations:

\[
\Delta_\alpha(\tilde{R}) = \sum_\beta V_{\alpha\beta} N_{\pi\beta} \mathcal{F}_\beta(\tilde{R}), \tag{3}
\]

where \( \alpha, \beta \in \{\sigma, \pi\} \) and \( \hat{\Delta}_\alpha = \hat{\tau}_i \text{Re} \Delta_\alpha - \hat{\tau}_3 \text{Im} \Delta_\alpha \). The coupling matrix \( V_{\alpha\beta} \) determines the pairing interaction, \( N_{\pi\beta} \) is the Fermi surface density of states on band \( \beta \) and

\[
\mathcal{F}_\sigma(\tilde{R}) = \int_{-\varepsilon_c}^{\varepsilon_c} \frac{de}{2\pi i} (f_\sigma(\varepsilon, \tilde{p}_\sigma, \tilde{R})) \tilde{p}_\sigma \text{tanh}(\frac{\varepsilon}{2T_c}),
\]

\[
\mathcal{F}_\pi(\tilde{R}) = \int_{-\varepsilon_c}^{\varepsilon_c} \frac{de}{2\pi i} f_\pi(\varepsilon, \tilde{R}) \text{tanh}(\frac{\varepsilon}{2T_c}). \tag{4}
\]

Here \( f_\alpha \) is the upper off-diagonal (1, 2) element of the matrix propagator \( \hat{g}_\alpha \) and \( \varepsilon_c \) is a cutoff energy (that will be ultimately eliminated as discussed below). The Fermi surface average over the σ-band is denoted by \( \langle \cdots \rangle_{\tilde{p}_\sigma} \). In this work, we consider isotropic s-wave coupling as is the case for MgB2.

To study the mixed state, we introduce a circular cell approximation, meaning that we simulate the vortex unit cell by a circle. Other suggestions for circular cell approximations have been introduced in [30] and [31] for the Usadel and Eilenberger equations, respectively. We assume strong type-II superconductivity, in which case the spatial variation of magnetic field within the unit cell can be neglected for fields not too close to \( H_{c1} \). This is the case for MgB2. We assume that the magnetic field is in the −z direction (taking into account that the electron charge \( e < 0 \), this gives a positive phase winding). The vector potential is then given by

\[
\tilde{A}(\tilde{r}) = -\frac{H_0}{2} r \hat{e}_\theta, \tag{5}
\]

with \( \tilde{H}_0 = -H_0 \hat{e}_z = \nabla \times \tilde{A} \) and \( r = \sqrt{x^2 + y^2} \). The radius of the vortex unit cell is determined by the fact that one flux quantum penetrates the unit cell:

\[
H_0 \pi r_0^2 = \Phi_0, \tag{6}
\]
with $\Phi_0 = \hbar c/2|e| = \pi \hbar c/|e|$. Thus

$$\frac{2e}{\hbar c} A_0(r) = \frac{r}{r_c^2}. \quad (7)$$

This can be used directly in both the Eilenberger and the Usadel equation. In both cases, the vector potential can be incorporated by the replacement

$$\nabla_i X \rightarrow \tilde{\partial}_i X \equiv \nabla_i X - i \left[ \frac{e}{\hbar c} \tilde{E}_3 A_i, \tilde{X} \right], \quad (8)$$

where the $\circ$ symbol involves a time convolution if $X$ is time-dependent; otherwise it simply implies matrix multiplication. Note that in the diffusive case this also affects the expression for the current density. This can be obtained by the requirement of local gauge invariance that the local gauge transformation

$$\tilde{g} \rightarrow e^{iX \tilde{g}} \circ \tilde{g} \circ e^{-iX \tilde{g}}, \quad (9)$$

$$\tilde{A} \rightarrow \tilde{A} + \frac{hc}{e} \nabla \tilde{X}, \quad (10)$$

$$\Phi \rightarrow \Phi - \frac{\hbar}{e} \tilde{A} \quad (11)$$

with any $\chi(\tilde{r}, t)$ should leave the basic equations of motion (transport equations) invariant (in our case there is no time dependence, hence no scalar potential $\Phi$). The vector and scalar potentials can be gauged locally away by writing down the equations at any point $R$ with $\nabla \tilde{X} = -\tilde{e}_3 A$ and $\tilde{\partial}_i \tilde{X} = \tilde{\partial}_i \Phi$. Thus, the equations with potentials can be obtained by observing that

$$\nabla(\tilde{e}_3 \tilde{g}) \circ \tilde{g} \circ e^{-iX \tilde{g}} = e^{iX \tilde{g}} \circ \left( \nabla \tilde{g} + i \left[ \nabla X \tilde{g}, \tilde{g} \right] \right) \circ e^{-iX \tilde{g}}. \quad (12)$$

Now, we use the Riccati parametrization of the Green functions for both the Eilenberger [32–35] and Usadel [36] equations:

$$\tilde{g}_0 = -\frac{\hbar e}{1 + \gamma_0 \tilde{y}_0} \left( 1 - \frac{\gamma_0 \tilde{y}_0}{2\gamma_0} \frac{2\gamma_0}{\gamma_0 \gamma_0 - 1} \right), \quad (13)$$

where $\tilde{y}_0(\epsilon, \tilde{p}_F, \tilde{R}) = \gamma_0^*(\epsilon^*, \tilde{p}_F, \tilde{R})$ and $\tilde{y}_0(\epsilon, \tilde{R}) = \gamma_0^*(\epsilon^*, \tilde{R})$.

Because the transport equations for the Riccati amplitudes must also be invariant under any local gauge transformation, we can write them down immediately by noting that the above gauge transformation means

$$\gamma \rightarrow e^{iX} \circ \gamma \circ e^{-iX}, \quad (14)$$

$$\tilde{\gamma} \rightarrow e^{-iX} \circ \tilde{\gamma} \circ e^{iX}, \quad (15)$$

or, if we have no time dependence,

$$\gamma \rightarrow e^{2iX} \gamma, \quad (16)$$

$$\tilde{\gamma} \rightarrow e^{-2iX} \tilde{\gamma}. \quad (17)$$

Similarly, $\Delta \rightarrow e^{2iX} \Delta$ and $\Delta^* \rightarrow e^{-2iX} \Delta^*$. We thus obtain for the clean $\sigma$ band

$$\Delta_{\sigma} + 2\epsilon \gamma_{\epsilon} + \Delta_{\sigma}^* \gamma_{\epsilon}^2 + i\hbar v_{F\sigma} \tilde{\partial}_i \gamma_{\sigma} = 0, \quad (18)$$

with $\tilde{\partial}_i = (\nabla_i + 2i\nabla \chi) = (\nabla_i - i\tilde{E}_3 A_i)$, and

$$\Delta_{\sigma}^* = 2\epsilon \tilde{y}_\sigma + \Delta_{\sigma} \gamma_{\sigma}^2 + i\hbar v_{F\sigma} \tilde{\partial}_i \tilde{y}_\sigma = 0, \quad (19)$$

with $\tilde{\partial}_i = (\nabla_i - 2i\nabla \chi) = (\nabla_i + i\tilde{E}_3 A_i)$. For the dirty $\pi$ band, we have [36]

$$\Delta_{\pi} + 2\epsilon \gamma_{\pi} + \Delta_{\pi}^* \gamma_{\pi}^2 - i\hbar D \left( \tilde{\partial}_i \tilde{\partial}_i \gamma_{\pi} - \frac{2\gamma_{\pi} (\tilde{\partial}_i \gamma_{\pi})^2}{1 + \gamma_{\pi} \gamma_{\pi}} \right) = 0, \quad (20)$$

and

$$\Delta_{\pi}^* - 2\epsilon \tilde{y}_{\pi} + \Delta_{\pi} \gamma_{\pi}^2 - i\hbar D \left( \frac{2\gamma_{\pi} (\tilde{\partial}_i \gamma_{\pi})^2}{1 + \gamma_{\pi} \gamma_{\pi}} \right) = 0. \quad (21)$$

We consider a vortex extending in the $z$ direction, with its centre situated at $x = y = 0$ for each $z$. We write $(x, y) = r(\cos \phi, \sin \phi)$ and $(v_{Fx}, v_{Fx}) = v_F(\cos \theta, \sin \theta)$, and $\Delta = |\Delta(r)|e^{i\phi}, \gamma = \gamma(\theta; \phi, r)e^{i\theta}$, and $\tilde{y} = \tilde{y}(\theta; \phi, r)e^{-i\theta}$. Then we can use the above equations with the quantities $|\Delta|, \gamma(\theta; \phi, r)$, and $\tilde{y}(\theta; \phi, r)$, and with the replacements $\tilde{\partial} \rightarrow (\nabla + i\tilde{e}_3 A_0(r)\tilde{e}_3 + i\tilde{e}_0/r)$ and $\tilde{\partial} \rightarrow (\nabla + i\tilde{e}_3 A_0(r)\tilde{e}_3 - i\tilde{e}_0/r)$. Here we have used $\nabla \phi = \tilde{e}_0/r$.

To obtain the Riccati amplitudes in the 2D ballistic band, we must first solve for the boundary values along the unit cell circle, from which to integrate the Riccati equations along a given trajectory. To simulate the phase change across a unit cell boundary, we impose the boundary condition (here we omit the subscript $\sigma$)

$$\gamma_{\text{in}}(\theta; \phi, r_c) = -\gamma_{\text{out}}(\theta; \phi + \pi, r_c), \quad (22)$$

where in and out refer to incoming and outgoing trajectories, respectively, and similarly for $\tilde{\gamma}$. For each trajectory we solve for the boundary value $\gamma_{\text{in}}$ self-consistently.

For the 3D diffusive band, we use the symmetry

$$\gamma_{\text{in}}(\phi, r) = \gamma_{\text{in}}(0, r)e^{i\phi}, \quad (23)$$

$$\tilde{y}_{\text{in}}(\phi, r) = \tilde{y}_{\text{in}}(0, r)e^{-i\phi}. \quad (24)$$

Then equations (20) and (21) reduce to the following dimensionless equations for $\gamma_\sigma(0, r) = \gamma_\sigma(r) \equiv \gamma_\sigma$ and $\tilde{y}_\sigma(0, r) = \tilde{y}_\sigma(r) \equiv \tilde{y}_\sigma$:

$$|\Delta_{\pi}|(1 + \gamma_{\pi}^2) + 2\epsilon \gamma_{\pi} = i \left( \frac{\xi_{\pi}}{\xi_{\pi}} \right)^2 \times \left( \frac{\gamma_{\pi}^2}{\gamma_{\pi}} + 1 + \gamma_{\pi} \gamma_{\pi} \right) \frac{1}{1 + \gamma_{\pi} \gamma_{\pi}} \gamma_{\pi} \frac{1 - \gamma_{\pi} \gamma_{\pi}}{1 + \gamma_{\pi} \gamma_{\pi}} = 0, \quad (25)$$

$$|\Delta_{\pi}|(1 + \gamma_{\pi}^2) - 2\epsilon \gamma_{\pi} = i \left( \frac{\xi_{\pi}}{\xi_{\pi}} \right)^2 \times \left( \frac{\gamma_{\pi}^2}{\gamma_{\pi}} + 1 + \gamma_{\pi} \gamma_{\pi} \right) \frac{1}{1 + \gamma_{\pi} \gamma_{\pi}} \gamma_{\pi} \frac{1 - \gamma_{\pi} \gamma_{\pi}}{1 + \gamma_{\pi} \gamma_{\pi}} = 0. \quad (26)$$
The boundary condition in the dirty case is that the first derivative of \( \gamma_r(r) \) and \( \gamma_\sigma(r) \) is zero at the cell boundary.

We solve for the order parameters by diagonalizing the (cutoff-dependent) interactions and thus transforming the gap equations (3) into the form

\[
\begin{pmatrix}
\Delta^{(0)}_\pi \\
\Delta^{(1)}_\pi
\end{pmatrix} = \begin{pmatrix}
\lambda^{(0)}_\pi & 0 \\
0 & \lambda^{(1)}_\pi
\end{pmatrix}
\begin{pmatrix}
F^{(0)}_\pi \\
F^{(1)}_\pi
\end{pmatrix},
\]

where \( F^{(0)}_\pi \) and \( F^{(1)}_\pi \) are the anomalous amplitudes in the diagonal basis. The larger eigenvalue, say \( \lambda^{(0)}_\pi \), determines \( T_c \) and can be eliminated together with \( \epsilon_\pi \). The smaller eigenvalue \( \lambda^{(1)}_\pi \) can be parametrized by the cutoff-independent quantity

\[
\Lambda = \frac{\lambda^{(0)}_\pi \lambda^{(1)}_\pi}{\lambda^{(0)}_\pi - \lambda^{(1)}_\pi}.
\]

We solve the set of equations (18), (19), (25), and (26) along with the gap equations for the order parameters self-consistently.

After self-consistency has been achieved, the LDOS in each band can be calculated by

\[
N_\sigma(\epsilon, \vec{R})/N_{\text{FS}} = -\Im(g_\sigma(\epsilon, \vec{p}_\text{FS}, \vec{R}))\tilde{p}_\sigma/\pi,
\]

\[
N_\pi(\epsilon, \vec{R})/N_{\text{FS}} = -\Im(g_\pi(\epsilon, \vec{R}))/\pi,
\]

where \( g_\sigma \) is the upper diagonal (1, 1) element of \( g_\pi \).

The current density around the vortex has contributions from both the \( \sigma \) and the \( \pi \) bands. The corresponding expressions are

\[
\frac{\overline{J}_\pi(\vec{R})}{2\epsilon N_{\text{FS}}} = \int_{-\infty}^{\epsilon} \frac{d\epsilon}{2\pi} \Im(g_\pi(\epsilon, \vec{p}_\text{FS}, \vec{R})) \tilde{p}_\pi \tanh\left(\frac{\epsilon}{2T}\right),
\]

\[
\frac{\overline{J}_\sigma(\vec{R})}{2\epsilon N_{\text{FS}}} = \frac{\partial}{\partial \epsilon} \int_{-\infty}^{\epsilon} \frac{d\epsilon}{2\pi} \Im(f_\sigma \partial f_\pi) \tanh\left(\frac{\epsilon}{2T}\right).
\]

In our model, the bulk behaviour of the system is completely specified by four material parameters, \( \rho_0, n_\sigma/n_\pi, T_c \) and \( \Lambda \). Here \( \rho_0 \) is the zero-temperature bulk gap ratio, \( \rho_0 = \Delta^{(1)}_\pi/\Delta^{(1)}_\pi \), and \( n_\sigma = N_{\text{FS}}/(N_{\text{FS}} + N_{\text{FS}}) \). For MgB2, \( \rho_0 \approx 0.3 \) and \( n_\sigma/n_\pi \approx 1-1.2 \) [5, 10, 37]. The zero-temperature gap equations for a homogeneous system relate \( \Lambda \) with \( \rho_0, n_\sigma/n_\pi \), and the bulk gap ratio near \( T_c \) [2]. From this relation we find that, for MgB2, \( \Lambda \) can be positive or negative [38–41] and can be close to zero [39]. Negative \( \Lambda \) implies that the effective Coulomb interaction dominates over the effective pairing interaction in the subdominant \( \lambda^{(1)}_\pi \) channel, and in this case superconductivity is purely induced in the \( \pi \) band (with \( \Delta_\pi > 0 \), while \( \Delta^{(1)}_\pi < 0 \)).

In the presence of inhomogeneity, there is another material parameter, namely \( \xi_\pi/\xi_{\text{FS}} \), where \( \xi_{\text{FS}} \simeq 6.8 \text{ nm} \) (\( T_c = 39 \text{ K} \)) for MgB2 [2]. As discussed in section 3, to reproduce the experimental data of [5] we find \( \xi_\pi/\xi_{\text{FS}} \approx 2 \), for \( \rho_0 = 0.3 \) and \( n_\pi/n_\pi = 1 \). The condition for the \( \pi \) band to be in the dirty limit so that the Usadel equation is applicable is \( \xi_\pi/\xi_{\text{FS}} < 5 \) for MgB2 [2]. We present results for \( \rho_0 = 0.1, 0.3, 0.5; \xi_\pi/\xi_{\text{FS}} = 1, 3, 5; n_\pi/n_\pi = 1, 1.2 \); and \( \Lambda = -0.1, 0, 0.1 \); and discuss the effects of induced superconductivity and hybridization of the diffusive and ballistic bands. For a given cell radius \( r_c \), the corresponding field strength is given by equation (6) in units of \( hc/|e|\xi_{\text{FS}}^2 \), which is about 13 T for MgB2.

3. Results

3.1. Order parameter

In figure 1 we show the order parameter magnitudes in the two bands ((a), (b)) and their ratio ((c), (d)) as a function of coordinate \( x \) along a path through the vortex centre for \( \xi_\pi/\xi_{\text{FS}} = 1, 3, 5, \rho_0 = 0.3, n_\sigma = n_\pi, T = 0.1T_c, r_c/\xi_{\text{FS}} = 5 \), for \( \Lambda = 0.1 ((a), (c)) \) and -0.1 ((b), (d)). The unit cell radius \( r_c/\xi_{\text{FS}} = 5 \) corresponds roughly to 0.5 T for MgB2. The vortex structure is affected significantly by the Coulomb interaction and the impurity scattering rate in the \( \pi \) band. For \( \Lambda > 0 \), \( |\Delta_{\pi}(x)/\Delta_{\sigma}(x)| \) is smaller than the bulk gap ratio \( \rho_0 \) in the vortex core. While for \( \xi_\pi/\xi_{\text{FS}} = 1 \) the ratio recovers more or less to the bulk value at the cell boundary, as \( \xi_\pi/\xi_{\text{FS}} \) increases, \( |\Delta_{\pi}(x)/\Delta_{\sigma}(x)| \) is suppressed more strongly and \( |\Delta_{\pi}(x)/\Delta_{\sigma}(x)| \) is smaller than \( \rho_0 \) in the entire unit cell (for \( \xi_\pi \sim r_c \)). Furthermore, through coupling with the dirty \( \pi \) band, suppression of the \( s \)-band order parameter by magnetic field is also enhanced for larger \( \xi_\pi/\xi_{\text{FS}} \). This suppression of the order parameter and enlargement of the core area in the \( \sigma \) band with increasing \( \xi_\pi/\xi_{\text{FS}} \) are more drastic when the Coulomb repulsion is dominant in the \( \pi \) band (\( \Lambda < 0 \)). Interestingly, in this case, the depletion of \( |\Delta_{\pi}(x)| \) is relatively small and \( |\Delta_{\pi}(x)/\Delta_{\sigma}(x)| \) is substantially larger than \( \rho_0 \), especially for larger \( \xi_\pi/\xi_{\text{FS}} \).

Changes in the order parameter magnitudes in the two bands and their ratio as the field strength changes are illustrated.
Figure 2. Order parameters $|\Delta_\pi(x)|$ and $|\Delta_\sigma(x)|$ and their ratio as a function of coordinate $x$ along a path through the vortex centre for $\xi_\pi/\xi_\sigma = 5$, $\rho_0 = 0.3$, $n_\pi = n_\sigma$, $T = 0.1T_c$, $r_c/\xi_\sigma = 4, 6, 10$, for $\Lambda = 0.1$ ((a), (c)) and $-0.1$ ((b), (d)). We illustrate the influence of the diffusivity in the $\pi$ band on the critical temperature in figures 3 ($\rho_0 = 0.3$) and 4 ($\rho_0 = 0.5$) for $n_\pi = n_\sigma$ and $r_c/\xi_\pi = 10$, for (a) $\xi_\pi/\xi_\sigma = 3$ and (b) 5. In these figures the order parameter magnitudes at the cell boundary, $|\Delta(x)|$, in the two bands are plotted as a function of temperature $T$ for $\Lambda = -0.1$ and $0.1$, along with that for a single clean band. Points are results obtained by self-consistent calculation and curves are guides to the eye. In a single ballistic band, the critical temperature where $|\Delta(x)|$ vanishes is slightly smaller than the zero field $T_c$. When the ballistic $\sigma$ band is coupled with the diffusive $\pi$ band, the critical temperature is reduced further and superconductivity is more suppressed by magnetic field for $\Lambda = -0.1$ than for $\Lambda = 0.1$. This difference is enhanced for larger $\xi_\pi/\xi_\sigma$, as a result of stronger suppression of the $\sigma$-band order parameter as discussed above. These effects of the diffusivity and the Coulomb interaction in

in figure 2, for $\xi_\pi/\xi_\sigma = 5$, $\rho_0 = 0.3$, $n_\pi = n_\sigma$ and $T = 0.1T_c$ for various values of $r_c$; for $\Lambda = 0.1$ ((a), (c)) and $-0.1$ ((b), (d)). The result for $r_c/\xi_\pi = 10$ is similar to that for an isolated vortex. It can be seen clearly that, for $\Lambda > 0$, the $\pi$-band order parameter is suppressed strongly by magnetic field and the core area is enlarged. In contrast, for $\Lambda < 0$, the depairing effect is more manifest in the $\sigma$ band, with $|\Delta_\pi(x)/\Delta_\sigma(x)|$ reaching about two times $\rho_0$ in the vortex centre. It is clear that, while superconductivity is (mostly) induced in the $\pi$ band, Coulomb interactions can renormalize substantially the length scales and the core sizes in the two bands in different ways. We illustrate the influence of the diffusivity in the $\pi$ band on the critical temperature in figures 3 ($\rho_0 = 0.3$) and 4 ($\rho_0 = 0.5$) for $n_\pi = n_\sigma$ and $r_c/\xi_\sigma = 10$, for (a) $\Lambda = 0.1$ and (b) 5. In these figures the order parameter magnitudes at the cell boundary, $|\Delta(r_c)|$, in the two bands are plotted as a function of $T$ for $\Lambda = 0.1$ and $-0.1$, along with that for a single clean band. Points are results obtained by self-consistent calculation and curves are guides to the eye. In a single ballistic band, the critical temperature where $|\Delta(r_c)|$ vanishes is slightly smaller than the zero field $T_c$. When the ballistic $\sigma$ band is coupled with the diffusive $\pi$ band, the critical temperature is reduced further and superconductivity is more suppressed by magnetic field for $\Lambda = -0.1$ than for $\Lambda = 0.1$. This difference is enhanced for larger $\xi_\pi/\xi_\sigma$, as a result of stronger suppression of the $\sigma$-band order parameter as discussed above. These effects of the diffusivity and the Coulomb interaction in
the $\pi$ band can be drastic when the coupling between the two bands is strong, as demonstrated for $\rho_0 = 0.5$ in figure 4.

A quantity to characterize the vortex core structure is the vortex core size defined by [42, 43]

$$\xi_c^{-1} = \frac{\beta (r = 0)}{\partial r} \frac{1}{\Delta (r = \infty)}, \quad \text{(31)}$$

where $r$ is the radial coordinate measured from the vortex centre and $\Delta (r = \infty) \equiv \Delta (r_c)$ is the ‘bulk’ order parameter in the vortex lattice. Around an isolated vortex in a single clean band, the order parameter exhibits the KP effect [42], i.e. shrinkage of the vortex core size as $T$ is lowered, approaching zero in the zero-temperature limit [43–45]. This is due to depopulation of higher-energy bound states in the vortex core. In an s-wave superconductor with nonmagnetic impurities, however, the core size as defined above saturates as $T$ approaches zero [44, 45]. This stems from broadening of the bound core states that removes the singular behaviour in the spatial variation of the order parameter in the vortex core. The vortex core shrinking ceases when $k_\parallel T$ becomes smaller than the energy width of the zero-energy bound states in the core.

When a ballistic and a diffusive band are coupled, the KP effect is induced in the diffusive band, as found in [2, 45] for an isolated vortex. In the vortex lattice, when vortices are well separated, one finds the KP effect in a single clean band as well as in coupled clean and dirty bands. This is demonstrated in figures 5 ($\Lambda = 0.1$) and 6 ($\Lambda = -0.1$), in which $\xi_c$ in the two bands is plotted as a function of $T$ for $\xi_\pi / \xi_\sigma = 3$, $\rho_0 = 0.3$, and $n_\pi = n_\sigma$, for (a) $r_c / \xi_\pi = 10$ and (b) $r_c / \xi_\pi = 5$. The core size in the case of a single clean and dirty band is also shown. As can be seen in figure 5(a), for $\Lambda > 0$, the core size in the $\pi$ band is larger than that in the $\sigma$ band for all temperatures. The $\pi$-band order parameter exhibits the KP effect also when the Coulomb repulsion dominates (figure 6(a)), and in this case $\xi_c$ as defined above is always smaller in the $\pi$ band than in the $\sigma$ band (except for $T$ very close to the critical temperature). Also note that, with dominating Coulomb interactions, the $T$-linear behaviour of the KP effect is better developed in the $\pi$ band than in the $\sigma$ band.

As magnetic field increases and vortices come closer together, the bound state wavefunctions of neighbouring vortices begin to overlap and form energy bands, and quasiparticles can travel through the periodic array of vortices [11, 46–48] (see also references in [11]). We have performed our calculation for the cell radius $r_c \geq 4$. For this range of $r_c$, we find that, in a single diffusive band, the core size $\xi_c$ becomes smaller as $r_c$ decreases for any given temperature. Such shrinkage of the vortex core as field increases can be understood as due to intervortex transfer of quasiparticles [11], with higher-energy core bound states turning into extended states. This is also a trend for a single clean band as well as coupled ballistic and diffusive bands for relatively high $T$ and relatively large $r_c$. However, as can be seen in figures 5(b) and 6(b), for relatively strong field, $\xi_c$ is finite in the zero-temperature limit; since the derivative of the order parameter at the vortex centre remains finite as temperature approaches zero. Thus for a given (low) temperature, $\xi_c$ can increase as a function of field strength above a certain critical value. This is illustrated in figure 7, where $\xi_c$ is plotted as a function of field strength $H_0$ for $T / T_c = 0.1$, $\xi_\pi / \xi_\sigma = 3$, $\rho_0 = 0.3$ and $n_\pi = n_\sigma$ for (a) $\Lambda = 0.1$ and (b) $\Lambda = -0.1$. In both bands, as field increases, the core size is reduced initially, but at some critical strength it starts increasing. In a single ballistic band, $\xi_c$ behaves similarly as a function of $H_0$: this is consistent with the work by Miranović et al [49], who examined the effects of impurities on the vortex core size by including impurity scattering in the Eilenberger equation (single band). They have also found that, for a very small mean free path, the core size decreases monotonically as a function of field strength, as we find for a single diffusive band. In the case of two bands, $\xi_c$ in the $\pi$ band has nonmonotonic behaviour as in the $\sigma$ band, and the low-temperature value of $\xi_c$ is larger (smaller) in the $\pi$ band than in the $\sigma$ band for $\Lambda > 0 (<0)$. 

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**Figure 5.** Vortex core size as defined by equation (31) in the two bands as a function of temperature $T$ for $\xi_\pi / \xi_\sigma = 3$, $\rho_0 = 0.3$, $n_\pi = n_\sigma$, $\Lambda = 0.1$, for (a) $r_c / \xi_\pi = 10$ and (b) $r_c / \xi_\pi = 5$. The results for a single clean and dirty band are also shown.

**Figure 6.** Same as figure 5 except for $\Lambda = -0.1$. 

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**Table:**

- $\xi_c$ values for various band structures and temperatures.
- Comparison of $\xi_c$ for clean and dirty bands.

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**Equation:**

\[ \xi_c^{-1} = \frac{\beta (r = 0)}{\partial r} \frac{1}{\Delta (r = \infty)}, \quad \text{(31)} \]
3.2. Spectral properties of diffusive band

In the diffusive \( \pi \) band, the LDOS is completely flat as a function of energy at the vortex centre, as found for an isolated vortex [1, 2] and for coupled diffusive bands [25]. This is in agreement with the observation with STM [5]. The vortex core size as measured by a decay length of the zero-bias LDOS has also been probed by STM [5]. When superconductivity is (mostly) induced in a ‘weak’ band in a coupled two-band system, such a decay length can be much larger in the ‘weak’ band than in the ‘strong’ band [1, 2, 24, 25]. We find that, in the vortex state, there is little change in the zero-bias LDOS as the vortex core size as defined by equation (31) in the two bands as a function of field \( H_0 \) for \( \xi_\pi /\xi_\sigma = 3 \), \( \rho_0 = 0.3 \), \( n_\pi = n_\sigma \), \( T/T_c = 0.1 \), for (a) \( \Lambda = 0.1 \) and \( \Lambda = -0.1 \).

Figure 7. Vortex core size as defined by equation (31) in the two bands as a function of field \( H_0 \) for \( \xi_\pi /\xi_\sigma = 3 \), \( \rho_0 = 0.3 \), \( n_\pi = n_\sigma \), \( T/T_c = 0.1 \), for (a) \( \Lambda = 0.1 \) and \( \Lambda = -0.1 \).

The LDOS at the vortex centre for \( n_\pi = n_\sigma \), \( T/T_c = 0.5 \), and \( \Lambda = 0 \) also shows a slight change compared to the isolated vortex in the \( \sigma \) band (negative \( \Lambda \)) can enhance intervortex transfer of \( \pi \)-band quasiparticles. For a fixed \( \rho_0 \), the diffusion in the \( \pi \) band (larger \( \xi_\pi /\xi_\sigma \)) enhances intervortex transfer of \( \pi \)-band quasiparticles. For a given \( \xi_\pi /\xi_\sigma \), the weaker the induced superconductivity, the stronger the extension and overlap of quasiparticle states. The Coulomb repulsion in the \( \pi \) band (negative \( \Lambda \)) can enhance these effects further: e.g. for the parameter set for figure 8(b), the dependence of the LDOS on \( \Lambda \) is significant for \( \rho_0 = 0.1 \).

Figure 8. Zero-bias LDOS in the \( \pi \) band as a function of distance \( r \) from the vortex centre for \( n_\pi = n_\sigma \), \( T/T_c = 0.5 \), \( \Lambda = 0.1 \), 0, -0.1, \( r_c /\xi_\sigma = 20 \), for (a) \( \rho_0 = 0.3 \), \( \xi_\pi /\xi_\sigma = 1, 3, 5 \) and (b) \( \xi_\pi /\xi_\sigma = 3 \), \( \rho_0 = 0.1, 0.3, 0.5 \).

For a fixed \( \rho_0 \), the diffusion in the \( \pi \) band (larger \( \xi_\pi /\xi_\sigma \)) enhances intervortex transfer of \( \pi \)-band quasiparticles. For a given \( \xi_\pi /\xi_\sigma \), the weaker the induced superconductivity, the stronger the extension and overlap of quasiparticle states. The Coulomb repulsion in the \( \pi \) band (negative \( \Lambda \)) can enhance these effects further: e.g. for the parameter set for figure 8(b), the dependence of the LDOS on \( \Lambda \) is significant for \( \rho_0 = 0.1 \).

To characterize the core size, we plot in figure 9 the half-decay length \( \xi_c \) of the zero-bias LDOS in the \( \pi \) band as a function of \( \xi_\pi /\xi_\sigma \) for \( \rho_0 = 0.3 \), \( n_\pi = n_\sigma \), \( T/T_c = 0.1 \), \( r_c /\xi_\sigma = 20 \), \( \Lambda = 0.1 \), 0, -0.1. For MgB\(_2\), \( \xi_\sigma = 10 \) nm and the observed \( \xi_c \approx 30 \) nm corresponds to \( \xi_\pi /\xi_\sigma \approx 2 \) in our model.

Figure 9. Half-decay length \( \xi_c \) of the zero-bias LDOS in the \( \pi \) band as a function of \( \xi_\pi /\xi_\sigma \) for \( \rho_0 = 0.3 \), \( n_\pi = n_\sigma \), \( T/T_c = 0.1 \), \( r_c /\xi_\sigma = 20 \), \( \Lambda = 0.1 \), 0, -0.1. For MgB\(_2\), \( \xi_\sigma = 10 \) nm and the observed \( \xi_c \approx 30 \) nm corresponds to \( \xi_\pi /\xi_\sigma \approx 2 \) in our model.
on \( \Lambda \) becomes noticeable. For MgB\(_2\), the experimental value of \( \xi_v \approx 30 \) nm corresponds to \( \xi_\pi/\xi_\sigma \approx 2 \) in our model. In [25] such a plot of \( \xi_v \) was made for coupled dirty bands for \( \xi_\pi/\xi_\sigma < 2.5 \): overall \( \xi_v \) in this case is slightly smaller than our \( \xi_v \).

### 3.3. Spectral properties of ballistic band

A particularly interesting feature found in our model of coupled ballistic and diffusive bands is that, through coupling with the ‘weak’ diffusive band, there can be additional bound states at the gap edge in the ‘strong’ ballistic band. We find such bound states for an isolated vortex [1, 2] as well as for the vortex lattice. In figure 10 the LDOS at the vortex centre in the \( \sigma \) band is plotted as a function of energy \( \epsilon \) for \( \rho_0 = 0.3, 0.5 \), \( \xi_\pi/\xi_\sigma = 3, \eta_\pi/\eta_\sigma = 1.2 \), \( T/T_c = 0.5 \), \( r_c/\xi_\sigma = 20 \); for (a) \( \Lambda = 0.1 \) and (b) −0.1. The result for a single ballistic band is also shown.

In [25] such a plot of \( \xi_v \) was made for coupled dirty bands for \( \xi_\pi/\xi_\sigma < 2.5 \): overall \( \xi_v \) in this case is slightly smaller than our \( \xi_v \).

In figure 11 the LDOS for \( \xi_\pi/\xi_\sigma = 3, 5 \), \( \eta_\pi/\eta_\sigma = \eta_\pi \), \( \Lambda = -0.1 \), \( T/T_c = 0.5 \), \( r_c/\xi_\sigma = 10 \); for (a) \( \rho_0 = 0.3 \) and (b) 0.5. The result for a single ballistic band is also shown.

### 3.4. Current density

In figure 12 the current densities \( j(r) \) in the two bands as a function of distance \( r \) from the vortex centre are shown for \( \xi_\pi/\xi_\sigma = 3, \rho_0 = 0.5, \eta_\pi = \eta_\pi, \Lambda = -0.1 \) and \( r_c/\xi_\sigma = 10 \) for various temperatures. The current density contribution from the \( \pi \) band can be substantial, and even dominating as demonstrated in this figure, for larger \( \rho_0 \) and \( \xi_\pi/\xi_\sigma \). As temperature is lowered, the \( \sigma \)-band current density exhibits the KP effect and is more confined around the vortex centre.
For stronger coupling of the two bands, the KP effect becomes manifest also in the $\pi$ band. Deviation of the magnetic field distribution from the uniform field, $\delta H(r) = H(r) - H_0$, can be obtained from $j(r)$ by integrating the Maxwell equation, where a parameter $\kappa \equiv \sqrt{8\pi e^2v_F^2N_{\sigma}/c^2}/\xi_\sigma$ comes in. For MgB$_2$, $\kappa \approx 14$. The $\delta H(r)$ as a function of $r$ is illustrated in figure 13 for $\xi_\pi/\xi_\sigma = 3$, $n_\pi = n_\sigma$, $\Lambda = -0.1$, $T/T_c = 0.1$, $r_c/\xi_\pi = 10$ and $\kappa = 10$ for $\rho_0 = 0.3$ and 0.5. In figure 13(a) a partial contribution from each band is shown, while 13(b) presents the total field distribution. It can be seen that, when coupling of the two bands is increased, field fluctuations in the $\pi$ band (hence those in the total field) are enhanced significantly, while the $\sigma$ band contribution hardly changes.

3.5. Phase diagram

We show in figure 14 the upper critical field $H_{c2}(T)$ for $T$ near $T_c$ for $\rho_0 = 0.3$, $n_\pi = n_\sigma$ and $\Lambda = \pm 0.1$ for (a) $\xi_\pi/\xi_\sigma = 3$ and (b) 5, along with the result for a single clean band. Although $H_{c2}$ is sensitive to the amount of impurities in the sample, in MgB$_2$ single crystals, $H_{c2}$ for a field parallel to the $c$ axis has been measured to be $H_{c2}(T = T_c/2) \approx 2$ T in several experiments [50–60]. This value roughly corresponds to $\Lambda$ somewhere between $-0.1$ and 0.1 for $\xi_\pi/\xi_\sigma = 3$, $\rho_0 = 0.3$ and $n_\pi = n_\sigma$ in our model. When the $\sigma$ band is coupled with the $\pi$ band, $H_{c2}$ is substantially reduced from the single-band value, and decreases further when the Coulomb repulsion dominates or the diffusivity increases in the $\pi$ band. This is consistent with stronger suppression of the order parameter and enlargement of the vortex core area in the $\sigma$ band. Furthermore, for relatively large $\xi_\pi/\xi_\sigma$, $H_{c2}(T)$ develops an upward curvature near $T_c$ (figure 14(b)). This is interesting in light of the theoretical work based on the Eliashberg theory by Mansor and Carbotte, who studied the effects of Fermi velocity anisotropy and impurities on $H_{c2}$ [61]. Their prediction for MgB$_2$ is that, for a field in the $c$ direction (where the Fermi velocities in the two bands are assumed to be the same), $H_{c2}(T)$ exhibits an upward curvature near $T_c$ when the $\pi$ band is clean and the $\sigma$ band is dirty, while it has a quasilinear $T$ dependence for the dirty $\pi$ and the clean $\sigma$ band (as observed in several experiments; see references in [61]). Such an upward curvature in $H_{c2} (\parallel c)$ has been observed in some experiments on MgB$_2$ single crystals [62–64].
4. Conclusion

In conclusion, we have studied the effects of induced superconductivity and impurities on the electronic structure in the vortex lattice of a two-band superconductor, in which a ‘weak’ 3D diffusive band and a ‘strong’ 2D ballistic band are hybridized through the pairing interaction. We have found that the Coulomb repulsion and the diffusivity in the ‘weak’ dirty band enhance suppression of the order parameter and enlargement of the vortex core by magnetic field in the ‘strong’ clean band. As a result, critical temperature and field (where the order parameter at the vortex unit cell boundary vanishes) are reduced, and increased diffusivity in the dirty band can result in an upward curvature of the upper critical field near the transition temperature. The Kramer–Pesch effect arising from thermal depopulation of higher-energy bound states tends to disappear as the field becomes stronger and overlap of quasiparticle states of neighbouring vortices increases. The zero-bias LDOS in the diffusive band has a decay length much larger than that in the ballistic band, indicating substantial, or even dominating, and exhibit the Kramer–Pesch and resulting field fluctuations in the diffusive band can be reduced, and increased diffusivity in the dirty band can lead to smearing of energy bands of the vortex lattice and van Hove singularities at the band edges in the vortex–core LDOS in the ‘strong’ ballistic band. Furthermore, bound states tend to disappear at the gap edge in the ballistic band, in addition to the well-known Caroli–de Gennes–Matricon bound states. These effects are enhanced for increased coupling, diffusivity and Coulomb repulsion. Finally, the current density contribution in the vortex core and resulting field fluctuations in the diffusive band can be substantial, or even dominating, and exhibit the Kramer–Pesch effect manifest in the current density when coupling with the ballistic band is strong. We find the above intriguing features in the quasiparticle spectra for parameter values appropriate for MgB$_2$.

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