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Effects of ballistic and diffusive motion of quasiparticles on spectral properties around a vortex in a two-band superconductor

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Motivated by the recent results on impurity effects in MgB_2, we present a theoretical model for a two-band superconductor in which the character of quasiparticle motion is ballistic in one band and diffusive in the other. We apply our model to calculate the electronic structure in the vicinity of an isolated vortex. We assume that superconductivity in the diffusive (π) band is induced by that in the clean (σ) band, as suggested by experimental evidence for MgB_2. We focus our attention to the spatial variation of the order parameter, the current density, and the vortex core spectrum in the two bands. Our results indicate that the coupling to the π band can lead to the appearance of additional bound states near the gap edge in the σ band that are absent in the single-band case.

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It is now well established that MgB_2 is a two-gap superconductor, and its essential superconducting properties are well described by an isotropic *s*-wave two-band model.[1–8] The two "bands" in MgB_2 are the "strong" σ band that arises from the boron σ orbitals (with the energy gap $\Delta_\sigma \approx 7.2$ meV), and the "weak" π band that derives from the boron π orbitals ($\Delta_\pi \approx 2.3$ meV). Despite the fact that each band consists of a pair of bands, the variation of the gap within each pair of Fermi surfaces can be neglected.[9,10] The two energy gaps are observed to vanish at a common transition temperature T_c: no second transition has been observed, and there is evidence of induced superconductivity in the π band.[5,11,12]

There have been considerable efforts to understand impurity effects in MgB_2 (Refs. 7 and 8). Besides the potential applications of MgB_2 as magnetic devices,[13] these studies have aimed at testing a prediction of the two-band model: the reduction of T_c and the gap ratio by nonmagnetic impurities. However, Mazin *et al.*[14,15] have shown that this does not apply to MgB_2, i.e., for Mg-site impurities or defects, which are more favorable energetically than those at B sites. While the π band is strongly affected, the σ band is more robust, and there is little mixing of the two bands because of negligible interband scattering.[14,15] This is consistent with accumulating experimental evidence that the σ and π bands are essentially in the ballistic and diffusive limit, respectively[16] (see, also, references in Refs. 14 and 15). Nevertheless, so far in theoretical studies both bands have been assumed to be either in the clean[17] or in the dirty[18] limit.

In this Communication, we examine theoretically the effects of induced superconductivity and impurities on the vortex core structure in a two-band superconductor. Our work is motivated by the experiment on the vortex state in MgB_2 using scanning tunneling spectroscopy.[11] We present a unique formulation of coupled quasiclassical Eilenberger and Usadel equations to describe a multiband superconductor with both a ballistic and a diffusive band with negligible interband scattering by impurities: the two bands are assumed to be coupled only by the pairing interaction.

We apply our model to calculate numerically the local density of states (LDOS) and supercurrent density around an isolated vortex. We examine in detail the intriguing spatial variation of these quantities and the order parameter in the two bands. A particularly interesting result emerging from our studies is the possibility of additional bound states near the gap edge in the σ band.

Our model is based on the equilibrium quasiclassical theory of superconductivity, where the physical information is contained in the Green's function, or propagator, $\hat{g}(\epsilon, \mathbf{p}_{F\alpha}, \mathbf{R})$. Here ϵ is the quasiparticle energy measured from the chemical potential, $\mathbf{p}_{F\alpha}$ the quasiparticle momentum on the Fermi surface of band α, and $\mathbf{R}$ is the spatial coordinate (the hat refers to the 2×2 matrix structure of the propagator in the particle-hole space). Although our model is general for any two-band superconductor with a clean and a dirty band, having MgB_2 in mind, we call the two bands σ and π bands, respectively. In the clean σ band, $\hat{g}_\sigma(\epsilon, \mathbf{p}_{F\sigma}, \mathbf{R})$ satisfies the Eilenberger equation[19]

$$[\epsilon\hat{\tau}_3 - \hat{\Delta}_\sigma, \hat{g}_\sigma] + i\mathbf{v}_{F\sigma} \cdot \nabla \hat{g}_\sigma = \hat{0}, \tag{1}$$

where $\mathbf{v}_{F\sigma}$ is the Fermi velocity and $\hat{\Delta}_\sigma$ the (spatially varying) order parameter. Throughout this work, we ignore the external magnetic field (this is justified as MgB_2 is a strongly type-II superconductor). The coherence length in the σ band is defined as $\xi_\sigma = v_{F\sigma}/2\pi T_c$.

In the presence of strong impurity scattering, the Green's function has no momentum dependence and the Eilenberger equation reduces to the Usadel equation.[20] We assume this to be the proper description of the dirty π band, and take the propagator $\hat{g}_\pi(\epsilon, \mathbf{R})$ to satisfy

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

The diffusion constant D defines the π-band coherence length as $\xi_\pi = \sqrt{D/2\pi T_c}$. Both propagators are normalized according to $\hat{g}_\sigma^2 = \hat{g}_\pi^2 = -\pi^2 \hat{1}$.

The quasiparticles in different bands are assumed to be coupled only through the pairing interaction, neglecting interband scattering by impurities. The gap equations for the multiband system are given as

$$\Delta_\alpha(\mathbf{R}) = \sum_\beta V_{\alpha\beta} N_{F\beta} \mathcal{F}_\beta(\mathbf{R}), \tag{3}$$

where $\alpha, \beta \in \{\sigma, \pi\}$, $\hat{\Delta}_\alpha = \hat{\tau}_1 \,\mathrm{Re}\, \Delta_\alpha - \hat{\tau}_2 \,\mathrm{Im}\, \Delta_\alpha$, the coupling matrix $V_{\alpha\beta}$ determines the pairing interaction, $N_{F\beta}$ is the Fermi-surface density of states on band β, and

$$\mathcal{F}_\sigma(\mathbf{R}) \equiv \int_{-\epsilon_c}^{\epsilon_c} \frac{d\epsilon}{2\pi i} \langle f_\sigma(\epsilon, \mathbf{p}_{F\sigma}, \mathbf{R}) \rangle_{\mathbf{p}_{F\sigma}} \tanh\left(\frac{\epsilon}{2T}\right),$$

$$\mathcal{F}_\pi(\mathbf{R}) \equiv \int_{-\epsilon_c}^{\epsilon_c} \frac{d\epsilon}{2\pi i} f_\pi(\epsilon, \mathbf{R}) \tanh\left(\frac{\epsilon}{2T}\right). \tag{4}$$

Here f_α is the upper off-diagonal (1,2) element of the matrix propagator $\hat{g}_\alpha$, $\langle \cdots \rangle_{\mathbf{p}_{F\sigma}}$ denotes averaging over the σ band Fermi surface, and ϵ_c is a cutoff energy.

We solve the system of Eqs. (1)–(4) numerically. The normalization condition is taken into account with the Riccati parametrization for the Green's functions.[21,22] After self-consistency has been achieved for the order parameter, the (for the σ band, angle-resolved) LDOS in each band can be calculated by

$$N_\sigma(\epsilon, \mathbf{p}_{F\sigma}, \mathbf{R})/N_{F\sigma} = -\mathrm{Im}\, g_\sigma(\epsilon, \mathbf{p}_{F\sigma}, \mathbf{R})/\pi,$$

$$N_\pi(\epsilon, \mathbf{R})/N_{F\pi} = -\mathrm{Im}\, g_\pi(\epsilon, \mathbf{R})/\pi, \tag{5}$$

where g_α is the upper diagonal (1,1) element of $\hat{g}_\alpha$.

The current density around the vortex has contributions from both the π band and the σ band. The corresponding expressions are ($e=-|e|$ is the electron charge)

$$\frac{\mathbf{j}_\sigma(\mathbf{R})}{2eN_{F\sigma}} = \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \langle \mathbf{v}_{F\sigma} \,\mathrm{Im}\, g_\sigma \rangle_{\mathbf{p}_{F\sigma}} \tanh\left(\frac{\epsilon}{2T}\right),$$

$$\frac{\mathbf{j}_\pi(\mathbf{R})}{2eN_{F\pi}} = \frac{D}{\pi} \int_{-\infty}^{\infty} \frac{d\epsilon}{2\pi} \,\mathrm{Im}[f_\pi^* \nabla f_\pi] \tanh\left(\frac{\epsilon}{2T}\right). \tag{6}$$

Throughout this work, we focus on the effects of purely induced superconductivity in the π band. Diagonalization of the coupling matrix in Eq. (3) decouples the gap equations. The larger of the two eigenvalues of the matrix, denoted by $\lambda^{(0)}$, determines T_c and can be eliminated together with ϵ_c. The smaller eigenvalue $\lambda^{(1)}$ is parametrized by the cutoff-independent combination $\Lambda = \lambda^{(0)}\lambda^{(1)}/(\lambda^{(0)} - \lambda^{(1)})$. The pairing interactions for MgB_2 have been calculated by *ab initio* methods, employing an electron-phonon coupling model.[3,9] From these studies, taking the Coulomb repulsion[23] into account, we estimate $\Lambda < 0.1$ for MgB_2. We present results for $\Lambda = -0.1$ [implying weak repulsion in the subdominant $\lambda^{(1)}$ channel].[24] In this case, the order parameter in the subdominant channel is negative, while Δ_π is positive. The ratio of the bulk gaps $\rho = \Delta_\pi^{\mathrm{bulk}}/\Delta_\sigma^{\mathrm{bulk}}$ near T_c parametrizes the strength of the induced superconductivity in the π band; experimentally $\rho \approx 0.3$ in MgB_2. For simplicity, we set $N_{F\sigma} = N_{F\pi}$ in our calculations: the densities of states of the two bands in MgB_2 are indeed comparable.[3,11] As to the ratio of the coherence lengths in the two bands, we present results for $\xi_\pi/\xi_\sigma = 1$, 3, and 5. An estimate from experiments[11,25] gives for MgB_2 a value between 1 and 3. The condition for the π band to be in the dirty limit so that the Usadel equation is suitable is $\xi_\pi/\xi_\sigma < (v_{F\pi}/v_{F\sigma})\sqrt{2\pi T_c/3\Delta_\pi}$ (for MgB_2 we estimate $\xi_\pi/\xi_\sigma < 5$). We assume cylindrical symmetry for the σ band.

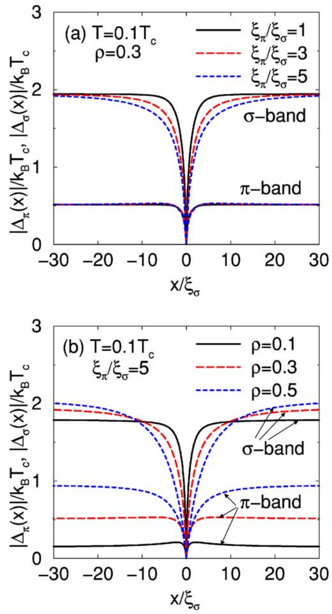

FIG. 1. (Color online) Magnitude of the order parameter, $|\Delta_{\sigma,\pi}(x)|$, in the σ and π bands, as a function of coordinate x on a path through the vortex center, at $T=0.1T_c$: (a) for different ratios ξ_π/ξ_σ and fixed strength of the induced π-band gap, parametrized by the mixing ratio (see text), $\rho=0.3$; (b) for different ρ and fixed $\xi_\pi/\xi_\sigma=5$. Weak effective repulsion due to the Coulomb interaction is assumed in the subdominant $\lambda^{(1)}$ pairing channel, parametrized by $\Lambda=-0.1$ (see text).

In Fig. 1 we present the order-parameter magnitudes for each band as a function of coordinate x along a path through the vortex center. In Fig. 1(a) we show the order parameter variation at $T=0.1T_c$ for several coherence-length ratios ξ_π/ξ_σ and gap ratio $\rho=0.3$. Surprisingly, an increase of ξ_π results in an increase of the recovery length of the order parameter (the characteristic length scale over which the order parameter recovers to the bulk value) in the σ band, while the recovery length in the π band is barely affected. Thus, the recovery lengths in the two bands can differ considerably, even though the superconductivity in the π band is induced by the σ band. In Fig. 1(b), the gap ratio ρ is varied for fixed $\xi_\pi/\xi_\sigma=5$. One can see that, apart from the well-known increase of the bulk Δ_σ/T_c ratio with increasing bulk Δ_π, the recovery length in the σ band increases considerably with increasing ρ. The π-band recovery length is also enhanced together with that of the σ band if $\rho > 0.3$, as can be seen clearly for $\rho=0.5$. For $\rho=0.1$, Δ_π near the vortex core is enhanced from its bulk value.

To understand these effects we have performed calculations for different values of Λ that characterize the Coulomb

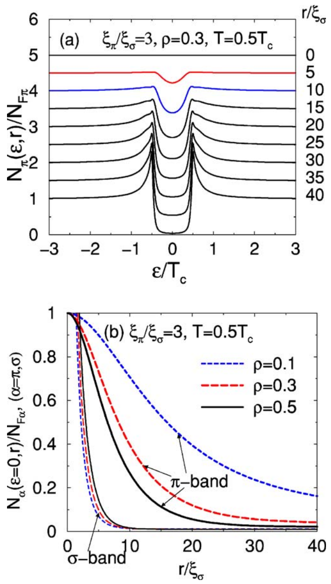

FIG. 2. (Color online) (a) Local density of states (LDOS) for the π band, as a function of energy ϵ for different distances r from the vortex center. The spectra are shifted in a vertical direction for convenience. (b) LDOS at the chemical potential, $\epsilon=0$, as a function of r for different ρ and fixed $T=0.5T_c$, $\xi_\pi/\xi_\sigma=3$.

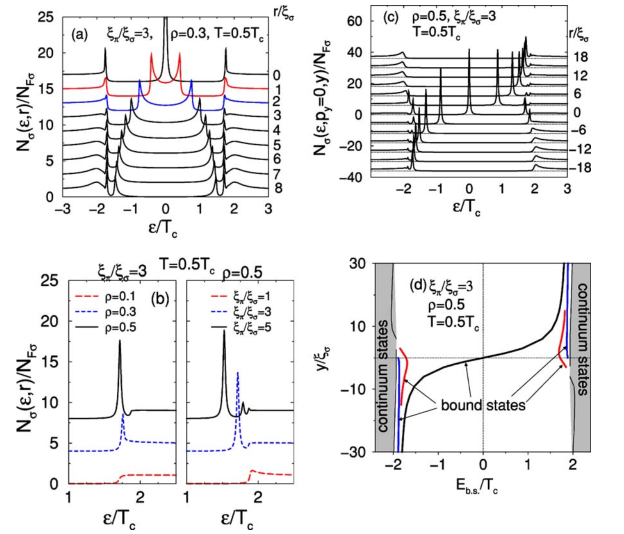

FIG. 3. (Color online) (a) LDOS for the σ band as a function of energy ϵ for different distances r from the vortex center. (b) The development of extra bound states near the gap edge in the σ band for different parameter combinations. The bound states develop for sufficiently large mixing ratio ρ and coherence length ratio ξ_π/ξ_σ. (c) Angle-resolved LDOS for quasiparticles with momentum along the x axis at positions along the y axis in the σ band, showing the bound states as a function of y. The dispersion of the bound states as a function of y is also shown in (d) for $\rho=0.5$, $\xi_\pi/\xi_\sigma=3$, and $T=0.5T_c$. Spectra in (a)–(c) are shifted in a vertical direction for convenience.

repulsion in the π band. We have found that for $\Lambda>0$ the ratio $|\Delta_\pi|/|\Delta_\sigma|$ is reduced in the core region with respect to its bulk value; however, it is enhanced for $\Lambda<0$. This leads to a renormalization of the recovery lengths of the order parameters in both bands.

In Fig. 2 we show the spectral properties of the π band. The LDOS, shown in Fig. 2(a), is flat at the vortex center ($r=0$), in agreement with the experiment of Ref. 11 for MgB_2. Outside the vortex core the BCS density of states is recovered. The decay of the zero-bias LDOS as a function of radial coordinate r is shown in Fig. 2(b), together with that of the σ band [obtained from the data in Fig. 3(a)]. The decay length of the zero-bias DOS is clearly different for the two bands. For the π band it is given by $\xi_\pi\sqrt{\Delta_\sigma/\Delta_\pi}$, and thus dominated by the parameter ρ. In the σ band the length scale of the decay is ξ_σ and thus shorter than that in the π band. The existence of two apparent length scales in the LDOS was also reported in the case of two clean bands[17] and two dirty bands.[18]

In Fig. 3 we show the vortex core spectra in the σ band. The LDOS, $N_\sigma(\epsilon,\mathbf{R})=\langle N_\sigma(\epsilon,\mathbf{p}_{F\sigma},\mathbf{R})\rangle_{\mathbf{p}_{F\sigma}}$, as a function of energy for different values of r is plotted in Fig. 3(a), which shows the well-known Caroli-de Gennes-Matricon bound-state bands at low energies. The unique feature of our model is the additional bound states in the vortex core region near the gap edge, that are clearly visible in Fig. 3(a). This is in strong contrast with the case of a single-band superconductor, where the spectrum near the vortex center is suppressed at the gap edge, showing neither a coherence peak nor additional bound states. The self-consistency of the order-parameter profile is essential for the presence of the bound states. In Fig. 3(b) we illustrate the development of these additional bound states in terms of the spectrum at the vortex center. It can be seen that for a given ξ_π/ξ_σ, the bound states exist for ρ larger than a certain critical value (left panel). For a given ρ, on the other hand, the bound states develop if ξ_π/ξ_σ exceeds a critical value, which is between 1 and 3 for $\rho=0.5$ (right panel). The bound states are, e.g., clearly resolved for $\rho=0.3$ and $\xi_\pi/\xi_\sigma=3$, values appropriate for MgB_2. The bound states move with the gap edge as a function of temperature.

The bound-state spectrum can be most clearly described in terms of the angle-resolved spectra, shown in Fig. 3(c). Here the spectrum of quasiparticles moving in the x direction is shown as a function of position along the y axis. The position of the bound states as a function of y is shown in Fig. 3(d). The main bound-state branch crosses the chemical potential in the vortex center. The additional bound states exist near the gap edge and show a weak dispersion. In fact, a close inspection reveals that there are two branches at the gap edge; however, only one of them is present at the vortex center.

Finally, in Fig. 4 we show contributions from the two bands to the supercurrent density around the vortex. We show the results for $\rho=0.3$, and (a) $\xi_\pi/\xi_\sigma=1$, (b) $\xi_\pi/\xi_\sigma=3$, and (c) $\xi_\pi/\xi_\sigma=5$, at $T/T_c=0.1$, 0.3, and 0.5. The current density from the σ band is enhanced at low temperatures near the vortex center, and the maximum approaches the center as $T\to0$. This is due to the well-known Kramer-Pesch effect for the clean σ band. The current density due to the induced superconductivity in the π band is also enhanced by decreasing temperature, but the maximum does not approach the vortex center as in the σ band. With increasing r, the contribution of the σ band is reduced, and the contribution of

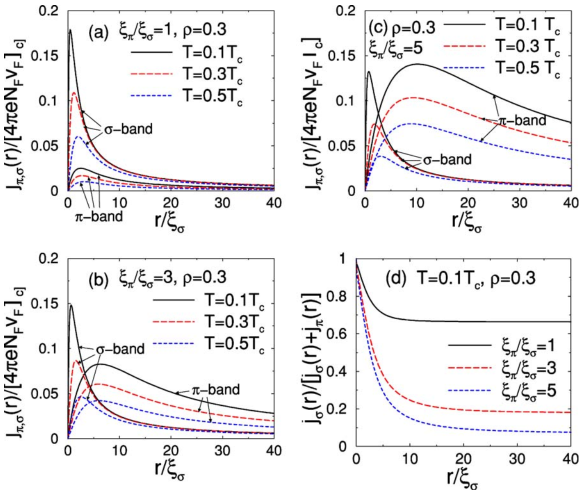

FIG. 4. (Color online) Contribution to the current density as a function of distance from the vortex center, shown separately for the π band and the σ band for fixed mixing ratio $\rho=0.3$ and different temperatures T; for (a) $\xi_\pi/\xi_\sigma=1$, (b) $\xi_\pi/\xi_\sigma=3$, and (c) $\xi_\pi/\xi_\sigma=5$. In (d) the σ-band contribution to the total current density is shown as a function of radial coordinate, for $T=0.1T_c$, $\rho=0.3$, and for different values of ξ_π/ξ_σ.

the π band becomes considerable for $\xi_\pi/\xi_\sigma \gtrsim 3$. The $\mathbf{j}_\sigma$ shows temperature dependence only in the core area, whereas $\mathbf{j}_\pi$ is temperature dependent also far outside the core. To understand this effect, we note that at large r (but small compared to the London penetration depth), the current-density magnitudes are given approximately by $j_\sigma(r) \sim eN_{F\sigma}v_{F\sigma}^2/2r$ and $j_\pi(r) \sim eN_{F\pi}\pi D|\Delta_\pi|/r$. The temperature dependence of j_π is thus dominated by that of $|\Delta_\pi|$.

Another important observation is that, for parameter values appropriate for MgB_2, j_π is considerably large outside the vortex core. In fact, already for $\xi_\pi/\xi_\sigma=3$, j_σ is restricted to the region very close to the vortex center and is negligible outside the core for $\rho \gtrsim 0.3$, as can be seen in Fig. 4(d). The current-density ratio far away from the vortex center is given by

$$\lim_{r \gg \xi_{\pi,\sigma}} \frac{j_\pi(r)}{j_\sigma(r)} = \frac{2N_{F\pi}D\pi|\Delta_\pi|}{N_{F\sigma}v_{F\sigma}^2} = \frac{|\Delta_\pi|}{T_c}\frac{N_{F\pi}}{N_{F\sigma}}\left(\frac{\xi_\pi}{\xi_\sigma}\right)^2. \quad (7)$$

Clearly, the π-band contribution to the current density dominates when $N_{F\pi}\xi_\pi^2/N_{F\sigma}\xi_\sigma^2 > (|\Delta_\pi|/T_c)^{-1}$, which is a case relevant for MgB_2.

In conclusion, we have formulated a model for coupled ballistic and diffusive bands in terms of coupled Eilenberger and Usadel equations. We have studied the effects of induced superconductivity in the "weak" diffusive band on the order parameter, the current density, and the spectral properties of the "strong" ballistic band. We have found that: (a) the recovery lengths of the order parameters in the two bands are renormalized by the Coulomb interaction; (b) the vortex core spectrum in the σ band shows additional bound states at the gap edge; and (c) the current density is dominated in the vortex core by the σ-band contribution, and outside the vortex core the π-band contribution is substantial, or even dominating, for parameters appropriate for MgB_2. Our predictions concerning the vortex core spectrum of the σ band can be tested by tunneling electrons onto the *ab* plane.[6,26] The bound states at the gap edge should be affected only weakly by impurities in the σ band, due to the weak dispersion,[22,27] and by strong electron-phonon coupling, as the relevant phonons have much higher energies.[12]

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