Density of states in a split superconducting vortex

L. Komendová and R. Hlubina
Department of Experimental Physics, Comenius University, Mlynská Dolina F2, 842 48 Bratislava, Slovakia
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Based on an analysis of a generalized xy spin model, it has been suggested recently that vortices with split cores may be realized in the cuprates. In the present work we solve the Gor'kov equations for a *d*-wave BCS superconductor in the presence of an isolated vortex with a split core and thereby we determine the local tunneling density of states in the vicinity of such a vortex. We find only marginal differences between the densities of states in the core regions of usual and split vortices. Therefore the experimental observation of unusual vortex core shapes cannot be interpreted as a straightforward consequence of vortex splitting.

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Scanning tunneling spectroscopy of the vortices in $Bi_2Sr_2CaCu_2O_{8+\delta}$ has shown[1] that vortex cores may split into several subcomponents with a spacing in the range 10–100 Å. In Refs. 1 and 2, the complex core shapes were interpreted as a result of the vortex hopping between different pinning sites which is sufficiently fast on the time scale of the experiment.[1,2] Recently, in Ref. 3 an alternative interpretation of the tunneling experiments has been proposed, according to which the splitting of the vortices into subcomponents is of static origin.

The basic idea of Ref. 3 is quite simple. Namely, it is well known that on length scales smaller than the penetration depth, the superconducting condensate can be modeled by an xy spin model. In Ref. 3 it has been suggested that a single CuO_2 plane can be described by a modified xy spin model,

$$H_{\mathrm{xy}} = \sum_{\langle\alpha\beta\rangle} [J_1 \cos(\theta_\alpha - \theta_\beta) - J_2 \cos(2\theta_\alpha - 2\theta_\beta)], \qquad (1)$$

where the indices α,β label the links of the CuO_2 lattice and θ_α is the phase of a Cooper pair at link α; the sum runs over all nearest-neighbor pairs of links $\langle\alpha\beta\rangle$. The cases $J_1>0$ and $J_1<0$ describe the *d*-wave and *s*-wave superconductors, respectively. It was observed that, provided that $J_2>0$, in the vicinity of the critical point $J_1=0$ the vortices spontaneously split into two half vortices separated by a domain wall, suggesting a possible connection with the experimental results.[1]

It is worth pointing out that at the critical point $J_1=0$ the half vortices are deconfined, i.e., the superconducting state supports elementary excitations carrying flux $\frac{h}{4e}$. Such a state might be called charge $4e$ superconductor. In the context of classical spin models, charge $4e$ superconductivity corresponds to a nematic phase. It has been shown[4,5] that at finite temperatures the nematic phase of the model Eq. (1) is stabilized also for nonvanishing values of J_1. Thus, if the picture advanced in Ref. 3 is valid, the cuprates might be located close, along the J_1 axis, to an exotic charge $4e$ superconductor. Interestingly, several other theoretical studies of strongly correlated electron models also suggest the possibility of charge $4e$ superconductivity in certain regions of their phase diagrams.[6,7]

It should be pointed out, however, that the experiment reported in Ref. 1 measures the local tunneling density of states (DOS), which is not directly accessible within the bosonic theory based on Eq. (1). In order to check the applicability of Ref. 3 to the tunneling experiments more directly, we need to construct a fermionic theory.

In this paper we study the simplest fermionic model. Namely, we describe the CuO_2 plane by the standard one-band tight-binding (grand-canonical) Hamiltonian with BCS pairing treated in the mean-field approximation,

$$H = -\sum_{ij}\left[t_{ij}\sum_{\sigma} c_{i\sigma}^\dagger c_{j\sigma} + \Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + \Delta_{ij}^* c_{j\downarrow} c_{i\uparrow}\right], \qquad (2)$$

where the indices i and j label the lattice sites of the square lattice, t_{ij} are the matrix elements for tunneling between i and j, the field Δ_{ij} describes the pairing, and $t_{ii}=\mu$, where μ is the chemical potential. We assume that $t_{ij}=t$ if i and j are nearest-neighbor sites and $t_{ij}=t'=-0.3t$ if i and j are next-nearest-neighbor sites; all remaining tunneling amplitudes t_{ij} are assumed to be vanishing. With these values of t_{ij}, the model is known to reasonably reproduce the experimental spectrum of the cuprates. The pairing field Δ_{ij} is assumed to be nonvanishing only for nearest-neighbor sites i and j. We require that the pairing field is symmetric, $\Delta_{ij}=\Delta_{ji}$, as appropriate for a singlet superconductor. In the presence of a vortex, Δ_{ij} is necessarily not translationally invariant. In order to minimize the number of input parameters, we neglect the suppression of the pairing amplitude in the vicinity of the vortex core. This can be justified by the work of Berthod, who has shown that the core states are determined primarily by the phase field of the order parameter.[8] Therefore we consider a pairing field Δ_{ij} given by the following ansatz:

$$\Delta_{ij} = \Delta e^{i\psi_{ij}} e^{i\theta_{ij}}. \qquad (3)$$

In other words, we consider a pairing field with a homogeneous amplitude and two sources of phase modulation. The phase field ψ_{ij} describes the *d*-wave symmetry of the pairing and therefore $\psi_{ij}=0$ and $\psi_{ij}=\pi$ for horizontal and vertical links, respectively. On the other hand, the phase field θ_{ij} describes the phase modulation due to the presence of a superconducting vortex.[10] Note that we have neglected the Peierls phases of t_{ij} and Δ_{ij} due to the magnetic field. This is justified at our length scales of interest around the vortex core, which are much smaller than the penetration depth.[8]

The main goal of the present work is to determine the DOS in the core region of a split vortex. For definiteness we take for θ_{ij} the optimal phase field determined in Ref. 3 for the model Eq. (1) with $J_1/J_2=0.21$ which is shown in Fig.

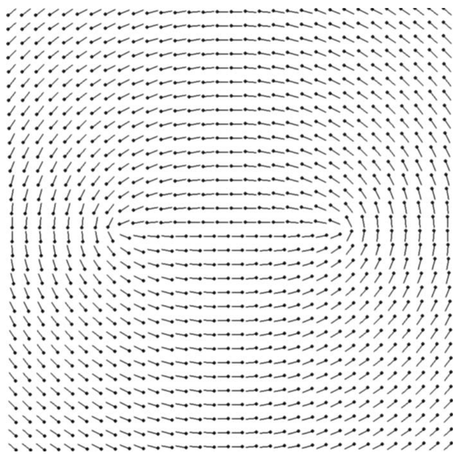

FIG. 1. Phase field in a split vortex with $J_1/J_2=0.21$. Every arrow represents the phase θ_α of the link α. The center of the arrow is located in the middle of the link. Two half vortices are visible, in each of them phase winds by π. The half vortices are connected by a domain wall along which the phase jumps by $\approx\pi$. The vortex looks conventional at length scales much larger than the separation between the half vortices.

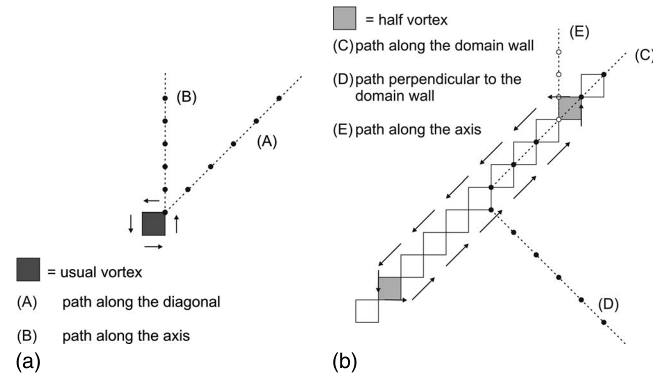

FIG. 2. The bullets show those sites of the Cu lattice at which we present the results for the DOS. Left panel: usual vortex with $J_2=0$. The vortex core is located at the black plaquette. Right panel: split vortex with $J_1/J_2=0.21$. The two half vortices are located at the shaded plaquettes. In both panels, the arrows show (schematically) the circulating phase field θ_{ij}. Note (Ref. 3) that the Cu lattice is rotated by 45° with respect to the lattice of links α shown in Fig. 1.

1.[9] For comparison, we have studied the DOS also in a conventional vortex with the phase field θ_{ij} determined for $J_2=0$.

In what follows we determine the DOS by the same method which was applied by Berthod to a conventional vortex.[8] Let us start by defining the retarded diagonal and off-diagonal Green's functions,

$$G_{ij\sigma}(t) = -\frac{i}{\hbar}\langle\{c_{i\sigma}(t), c^\dagger_{j\sigma}\}\rangle\theta(t),$$

$$F_{ij\sigma}(t) = -\frac{i}{\hbar}\langle\{c^\dagger_{i-\sigma}(t), c^\dagger_{j\sigma}\}\rangle\theta(t).$$

Making use of the equations-of-motion method and observing that the spin index is irrelevant, we find the explicit form of the Gor'kov equations for $G_{ij}(t)$ and $F_{ij}(t)$,

$$i\hbar\,\partial G_{kl}(t)/\partial t = \delta_{kl}\delta(t) - \sum_j [t_{kj}G_{jl}(t) + \Delta_{kj}F_{jl}(t)],$$

$$i\hbar\,\partial F_{kl}(t)/\partial t = \sum_j [t_{kj}F_{jl}(t) - \Delta^*_{kj}G_{jl}(t)].$$

In order to ensure the convergence of the integrals that follow, instead of the functions $X(t)$, where $X=G_{ij}, F_{ij}$, let us consider the functions $X(t)e^{-\Gamma t}$ damped by an inverse lifetime $\Gamma>0$. More physically, finite values of Γ may be thought of as a result of the scattering processes not taken into account in Hamiltonian (2). Let us define the Fourier transforms as follows:

$$X(\omega) = \int dt e^{i(\omega+i\Gamma)t}X(t),$$

$$X(t) = \int \frac{d\omega}{2\pi}e^{-i(\omega+i\Gamma)t}X(\omega).$$

With these definitions the Gor'kov equations can be written as a set of algebraic equations,

$$[\hbar(\omega+i\Gamma)\mathbf{1} + t]G(\omega) + \Delta F(\omega) = \mathbf{1},$$

$$[\hbar(\omega+i\Gamma)\mathbf{1} - t]F(\omega) + \Delta^* G(\omega) = 0.$$

Note that from now on, we do not write down the spatial indices of the matrices t, Δ, $G(\omega)$, and $F(\omega)$. Introducing the normal-state Green's-function matrix $G^0(\omega)=[\hbar(\omega+i\Gamma)\mathbf{1}+t]^{-1}$, the Gor'kov equations can be explicitly solved for the diagonal Green's function,

$$G(\omega) = [\mathbf{1} - G^0(\omega)\Sigma(\omega)]^{-1}G^0(\omega), \tag{4}$$

$$\Sigma(\omega) = -\Delta[G^0(-\omega)]^*\Delta^*. \tag{5}$$

Since we assume that in the normal state the problem is translationally invariant, the normal-state Green's function $G^0(\omega)$ can be determined easily by Fourier transformation. On the other hand, in the presence of a vortex, i.e., of a nontranslationally invariant phase field θ_{ij}, the self-energy matrix $\Sigma_{ij}(\omega)$ is not translationally invariant. Therefore $G(\omega)$ has to be calculated for a finite lattice containing a vortex, first by determining $\Sigma(\omega)$, then by calculating the inverse of the matrix $\mathbf{1}-G^0(\omega)\Sigma(\omega)$, and finally by matrix multiplication. In this work we present the results for our largest lattices with 96×96 sites. In order to arrive at spectral functions without unphysical spikes, the inverse lifetime Γ has to be chosen at least comparable to the level spacing of our problem. In order to be able to work with reasonably small Γ, following Berthod,[8] we have determined $G^0_{ij}(\omega)$ on much larger lattices; typically we have performed a fast Fourier transformation on lattices with 1024×1024 sites.

Once we have determined the diagonal Green's function $G_{ij}(\omega)$ for various ω in the vicinity of the chemical potential

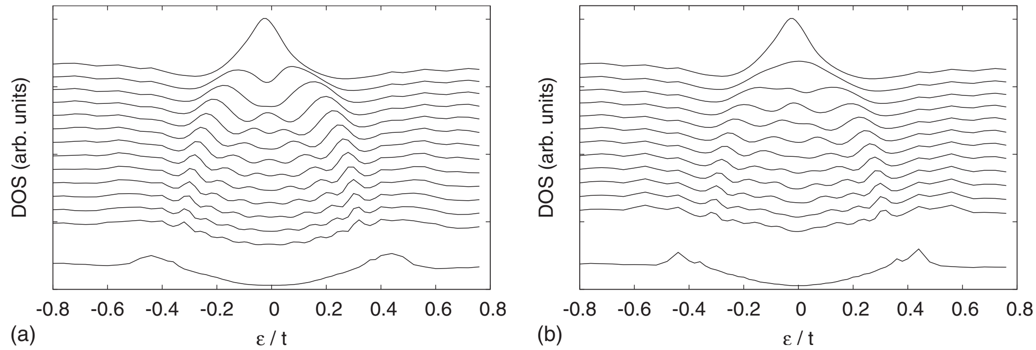

FIG. 3. DOS in a usual vortex. The left and right panels show the data along the paths A and B in Fig. 2, respectively. In both panels, the topmost curves correspond to the core site and the lowest curves correspond to remote sites; the DOS at the latter sites is essentially equal to the bulk value. Except for the lowest curves, the data have been shifted vertically for clarity.

at $\omega=0$, we can calculate the tunneling density of states $A(i,\varepsilon)$ at energy ε in the lattice point i using $A(i,\varepsilon)=-\pi^{-1}\,\mathrm{Im}\,G_{ii}(\varepsilon/\hbar)$.

In the rest of this paper we present numerical results for $A(i,\varepsilon)$. All data have been obtained for $t'=-0.3t$, $\Delta=0.2t$, and $\mu=2t$. With this choice of parameters, the maximum gap at the Fermi surface is $\Delta_{\max}\approx 0.4t$. If we take $t\approx 0.3$ eV, our $\Delta_{\max}$ is about four times larger than the experimental value of $\Delta_{\max}$ in the cuprates. We have deliberately chosen a larger gap since our energy resolution is $\hbar\Gamma=0.01t\approx 3$ meV. We have taken a larger value of μ than required by the actual electron count of the cuprates because for a realistic μ combined with our choice of Δ, the Van Hove singularity of the noninteracting density of states would lie within the superconducting gap and this does not seem to agree with experiments.

We have studied the spatial pattern of $A(i,\varepsilon)$ for two phase fields θ_{ij}: for a usual vortex determined for the spin model with $J_2=0$ and for a split vortex with $J_1/J_2=0.21$. In Fig. 2 we show for both phase fields the paths on the square Cu lattice along which we present our results for $A(i,\varepsilon)$.

In Fig. 3 we present the results for the DOS in a conventional vortex. The vortex center coincides with the center of an elementary plaquette of the CuO_2 plane. Therefore there are four core sites; low-energy bound states have a large weight at these core sites. As one moves away from the vortex center, bound states appear at higher energy and far away from the vortex the density of states approaches its

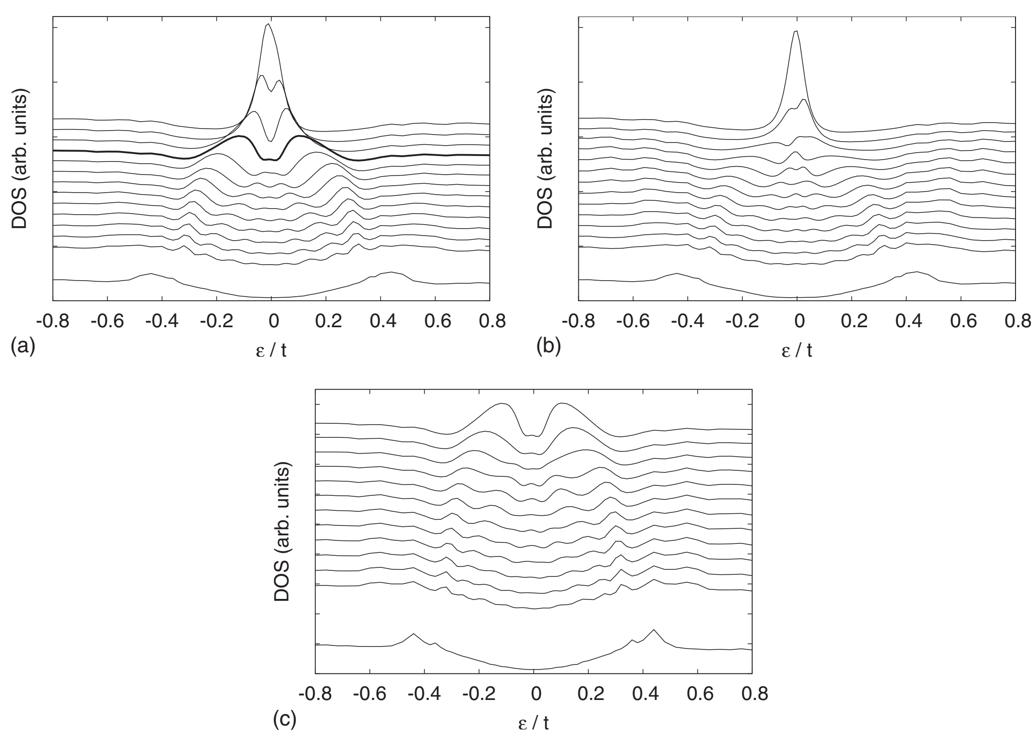

FIG. 4. DOS in a split vortex with $J_1/J_2=0.21$. The upper left, upper right, and bottom panels show the data along the paths C, D, and E in Fig. 2, respectively. In all panels, the topmost curves correspond to sites at the domain wall and the lowest curves correspond to remote sites. The thick line in the upper left panel corresponds to the half-vortex site (the only open bullet along path C). Except for the lowest curves, the data have been shifted vertically for clarity.

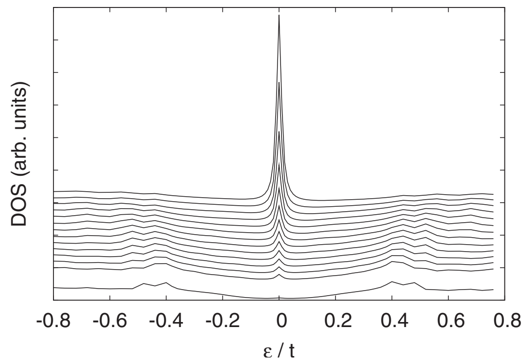

FIG. 5. DOS in the vicinity of a diagonal grain boundary with a phase shift of π between the grains. The various curves display the density of states at increasing distance from the grain boundary. The topmost (lowest) curve corresponds to the grain-boundary (remote) site. Except for the lowest curve, the data have been shifted vertically for clarity.

bulk value. These results are consistent with previous studies, see Ref. 8, and references therein.

In Fig. 4 we show the spatial evolution of the DOS in the core region of a split vortex. The qualitative similarity to the results for the usual vortex presented in Fig. 3 is evident; at the midpoint between the half vortices, which plays the role of the center of a usual vortex, there is a large peak at the chemical potential. With increasing distance from the midpoint, the zero-bias peak splits into two peaks, which finally merge with the bulk coherence peaks. The only qualitative difference between Fig. 4 and the results for the usual vortex is the presence of an asymmetry between the two diagonal directions in Fig. 4 whereas the spectra are the same along both diagonals in the usual vortex. This is because in a split vortex, the core states are preferentially located along the domain wall joining the half vortices. One can observe from Fig. 4 that, surprisingly, the most singular density of states is realized at the midpoint site between the half vortices and not at the half-vortex sites, as originally expected in Ref. 3. The expectations of Ref. 3 were based on the fact that the largest currents and magnetic fields were found in the vicinity of the half-vortex sites, i.e., at the end points of the domain wall. The singular behavior at the midpoint site has to do with the phase jump by π along the domain wall joining the half vortices, see Fig. 1. In order to prove this, we have calculated the DOS in the vicinity of a diagonal grain boundary, with an overall phase shift of π between the two grains. The DOS for this system is plotted in Fig. 5. Bound states at zero energy are seen to form at the boundary, in agreement with earlier studies.[11–13] This confirms that it is the π shift which is at the origin of the zero-energy states in the vicinity of the midpoint site. Consistent with this interpretation is also the comparison of Figs. 3 and 4 which shows that the zero-bias peak is broader in the usual vortex than in the split vortex, although both data sets were calculated with the same parameters, except for the phase field θ_{ij}.

Before concluding, it is worth pointing out that the experimental DOS in unsplit vortices looks very different from the *d*-wave prediction, Fig. 3. Surprisingly, the DOS in the core region resembles that found in the pseudogap state; the coherence peaks at $\pm\Delta_{\max}$ are suppressed and there are only weak features due to in-gap states at finite energy. This has been attributed, e.g., to an in-core admixture of a different pairing component to the pure *d*-wave superconducting state, to an unconventional normal state in the vortex core, or to phase fluctuations, see Ref. 2 for a review. It seems fair to say, however, that consensus has not been reached yet on this issue.

As regards the experiments on split vortices, they have found spatially separated islands in which the coherence peaks were suppressed.[1] These corelike islands were immersed in the sea with a bulklike DOS. While our BCS-like approach cannot explain the absence of the zero-bias peaks in the core, it might have the potential to find regions with the most singular DOS inside the vortex; we did hope that these regions would turn out to be spatially separated for a split vortex. The present work shows that this is not the case.

So should the idea of static vortex splitting be abandoned? In absence of an accepted theory of the cuprate core states we cannot tell for sure. The reason is that a more sophisticated microscopic theory of an unsplit vortex, which has to go beyond the model Eq. (2), may be also consistent with the hypothesis about static splitting of the vortices.

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