The Density of States in High-\(T_c\) Superconductors Vortices

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We calculated the electronic structure of a vortex in a pseudogapped superconductor within a model featuring strong correlations. With increasing strength of the correlations, the BCS core states are suppressed and the spectra in and outside the core become similar. If the correlations are short-range, we find new core states in agreement with the observations in YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) and Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\). Our results point to a common phenomenology for these two systems and indicate that normal-state correlations survive below \(T_c\) without taking part in the overall phase coherence.

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Among the anomalous properties of high-temperature superconductors (HTS), one of the most intriguing is the pseudogap phenomenon observed in the normal state of underdoped systems. The pseudogap state is marked by a substantial decrease of the one-particle density of states near the Fermi energy, and can be observed in several spectroscopic, thermodynamic, and transport experiments (see Ref. 1 for a review). Its elucidation is widely thought of as one of the keys to the understanding of high-temperature superconductivity. Unfortunately, detailed studies of the low-lying excitations in the pseudogap state are impossible due to the emergence of the superconducting state at low temperature. Vortex-core spectroscopy is perhaps one way into this problem: it has indeed been stated, on the basis of experimental findings, that the local density of states (LDOS) in vortex cores below \(T_c\) reflects the properties of the (pseudogapped) normal state above \(T_c\). More precisely one can argue that the physical state inside vortices should reflect the properties of the normal state at low temperature in the boundary conditions set by a gradual vanishing of the superconducting order in the core. A detailed analysis of this density of states may therefore lead to useful insights into the nature of the pseudogap state itself.

Some characteristics of the vortex cores seem to be now well established in YBa\(_2\)Cu\(_3\)O\(_{7-\delta}\) (YBCO) and Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_{8+\delta}\) (BSCCO), the two systems for which experimental results are available: the LDOS in the core does not display a central peak as predicted by the BCS theory, but particle-hole symmetric low-energy states; noticeably, the amplitude of the core states is much larger in YBCO than in BSCCO. In BSCCO, moreover, the core LDOS shows remarkable similarity (when properly thermally broadened) to the density of states observed above \(T_c\) in the pseudogap regime.

Theoretically, a number of calculations have been done in the past years and competing models of HTS lead to increasingly detailed predictions. The first calculations were undertaken within the Bogoliubov–de Gennes formulation of the BCS theory. For a \(d_{x^2-y^2}\) vortex the LDOS shows a broad zero-bias conductance peak (ZBCP) and a four-fold symmetric shape. This picture is not consistent with the experimental observations in YBCO and BSCCO. In another BCS-type scenario, a secondary order parameter component of a different symmetry is generated locally by the magnetic field and the resultant pair potential no longer has nodes: the central peak would thus be suppressed or split. The absence of ZBCP has also been tentatively explained by the properties of the \(c\)-axis tunneling matrix elements. Many workers in the field believe however that the absence of central peak cannot be explained in the BCS framework, and needs some kind of fundamental extension of the BCS theory that would take into account strong correlations. The first attempts were made within the SO(5) theory and predicted an insulating core, but the detailed predictions of this model seem not to agree with experiment. Some t-J model calculations have predicted a ZBCP split by an induced s-wave order parameter at low doping. Very recently, calculations based on the SU(2) slave-boson theory were reported. The authors make detailed predictions for the LDOS in vortex cores, which do not seem to correspond to the experimental data available today and which should allow to test in a significant way the slave-boson theory of HTS.

In this Letter we present calculations based on the Cooperon-propagator description of HTS. We show that this approach can explain several characteristics of the vortex-core spectra in YBCO and BSCCO. In addition, it allows us to give a tentative explanation for one of the (many) puzzles of HTS, namely whether the gap and pseudogap are of similar (superconducting) origin or whether they correspond to completely different physical processes. This point will be commented upon in the discussion below. First, we briefly review the Cooperon-propagator description of superconductivity, which is entirely based on correlation functions, the electronic self-energy takes the form.
\[ \Sigma(r, s, \tau) = -\int d\bar{\bar{r}} d\bar{s} \left\{ T_r \{ \Delta(r, \bar{r}, \tau) \Delta^\dagger(s, 0) \} \right\} \times G_0(\bar{s} - \bar{r}, -\tau), \]  

where \( \Delta(r, s, \tau) = V(r - s)\psi_\uparrow(r, \tau)\psi_\downarrow(s, \tau), \) \( V(r) \) is the pairing interaction, and \( G_0(r, \tau) \) is the free propagator. In this formalism the superconducting order is characterized by the long-range properties of the pair correlation function. Eq. (1) is valid both above and below \( T_c \) provided higher order correlation effects are not important, and we will assume that it remains valid regardless of the model or approximations involved in calculating \( \langle \Delta \Delta \rangle \). In particular, the BCS theory is recovered by setting \( \langle \Delta \Delta \rangle = \langle \Delta \rangle \langle \Delta \rangle \) where \( \langle \Delta \rangle \) is the BCS order parameter. Following recent studies,\[18\] we model the correlation function (Cooperon propagator) through:

\[ \langle T_r \{ \Delta \Delta \} \rangle = \Delta_p(r - \bar{r})R(\ell/\varrho)\Delta_s(\bar{s} - s) + \left\{ \Delta_s(r - \bar{r})F(\ell/\xi)\Delta_s(\bar{s} - s) \right\} \quad T > T_c^\text{(2)} \]

\[ + \left\{ \Delta_s(r, \bar{r})\Delta_s^\star(\bar{s}, s) \right\} \quad T \leq T_c^\text{(2)}. \]

The first term characterizes the strength and symmetry \( (\Delta_p) \) and the range \( (\varrho) \) of the normal-state correlations leading to the pseudogap below the temperature \( T^* \), with \( \ell = \frac{\varrho}{\xi} \) \( [r + \bar{r} - \bar{s} - s] \) and \( R(x) = e^{-x} \). The second term accounts for the phase-coherence properties of the superconductor and the phase fluctuations responsible for destroying superconductivity. Above \( T_c \), \( \Delta_s \) must be understood as the modulus of a local BCS-like order parameter. The phase physics is contained in the function \( F(x) \sim e^{-x} \) which is the phase-phase correlation function. \( F \) thus reduces to a function of the distance \( \ell \) with a correlation length \( \xi(T) \) diverging at \( T_c \) in the Kosterlitz-Thouless fashion. Below \( T_c \), \( F \) is assumed to factorize, as in the BCS theory, into the product of two local phases. These phases are embodied in the amplitude \( \Delta_s \) which becomes position dependent and complex. A more elaborate model should include dynamic correlations. We showed, however, that Eq. (2) leads to reasonable agreement with some aspects of the experimental density of states as a function of \( T \) in homogeneous systems.\[19\] Eq. (3) may be viewed as a non-local generalization of the Ansatz \( \Delta^2 = \Delta_p^2 + \Delta_s^2 \) introduced in Ref. [19].

In what follows we concentrate on the vortex state at \( T = 0 \), then \( \Delta_s \) plays the role of a BCS gap and vanishes in the vortex cores while its phase winds by \( 2\pi \) in response to the applied field. Eq. (3) basically means that the Cooperon propagator has a short-range part in addition to the long-range part described by \( \Delta_s \). Our central assumption is that these short-range normal-state correlations are not involved in the phase coherence and remain finite in the cores. This view is supported by recent NMR experiments showing that the pseudogap is not affected by a strong magnetic field.\[20\] We also note that similar considerations apply to the spinon and holon fields in theories based on spin-charge separation.\[21, 22\].

Using Eqs. (1) and (2) we calculate the Green’s function for an isolated \( d_{x^2-y^2} \) vortex on a two-dimensional lattice. We neglect Landau-level quantization, as appropriate for low magnetic fields. The modulus of \( \Delta_s \) is proportional to \( \tanh(r/\varrho) \), with \( \varrho \) the lattice parameter. The pseudogap \( \Delta_p \) has \( d_{x^2-y^2} \) symmetry in agreement with photoemission data\[23\] and is assumed uniform in space for simplicity. The self-energy is rewritten as \( \Sigma(\omega) = \Sigma_u(\omega) + \Sigma_i(\omega) \) where \( \Sigma_u \) is uniform and \( \Sigma_i \) contains the inhomogeneous term. The uniform part of the Green’s function is evaluated as \( G_0 = (G_0^{-1} - \Sigma_i)^{-1} \) in reciprocal space, using a 1024 \times 1024 k-point mesh. The band structure is taken from Ref. [24] with the Fermi level located 10 meV above the van-Hove singularity. This yields zero-field DOS’s in qualitative agreement with experiment. The Green’s function is finally evaluated as \( G = (G_0^{-1} - \Sigma_i)^{-1} \) on a \( M \times M \) real-space mesh with the vortex at the center. This step necessitates the inversion of two large matrices \( (M^2 \times M^2) \) for every energy \( \omega \). We have checked that the calculations are well converged with \( M = 41 \) and reproduce the published results of the BCS theory when \( \Delta_p = 0 \) [see Fig. 1(c)].

Our main results are presented in Fig. 1. Fig. 1(a) shows the vortex-core LDOS \( N(r = 0, \omega) \) and the zero-field DOS \( N_0(\omega) \) for a pseudogapped superconductor. Instead of a ZBCP, we find two core states in the vortex spectrum. Our numerical analysis shows that the subgap peaks appear only for moderate values of \( \Delta_p/\Delta_s \) and low values of \( \varrho \). These peaks grow as \( \Delta_p/\Delta_s \) and/or \( \varrho \) decrease, and eventually merge to form the broad BCS peak as \( \Delta_p \to 0 \). An intermediate example is displayed in Fig. 1(b). In fact, weak subgap structures exist also in

FIG. 1: Vortex-core and zero-field DOS for the parameters \( \varrho = 5a \) and (a) \( \Delta = \sqrt{\Delta_p^2 + \Delta_s^2} = 40 \text{ meV}, \Delta_p = 4\Delta_s \); (b) \( \Delta = 20 \text{ meV}, \Delta_p = 2\Delta_s \); (c) BCS limit: \( \Delta_p = 0 \) and \( \Delta_s = 40 \text{ meV} \). Inset: Halved core-level separation as a function of \( \Delta \) for \( \varrho = 5a \) (filled symbols) and \( \varrho = 10a \) (empty symbols). Circles are for \( \Delta_p = 2\Delta_s \) and triangles for \( \Delta_p = 4\Delta_s \). No core states are found for \( \varrho = 10a \) and \( \Delta_p = 4\Delta_s \).
the zero-field DOS: the vortex seems to induce a localization of preexisting low-energy states. We therefore expect those pseudogap-induced core states to be independent of magnetic field as observed in recent experiments[26]. On the contrary the BCS core states were shown to split at high vortex density[14]; a field-dependent splitting is also expected in scenarios based on a secondary idxy order parameter[3].

It was found experimentally that the coherence peaks are suppressed in the core[2,3,4,5], unlike in our results, Fig. 1(a) and (b). In our calculations the spectral weight is the nodal direction). In the BCS gapped case is similar, although reduced by a factor approximately because this part does not vanish in the center of the core. Whether the pseudogap part of the self-energy survives unchanged in the superconducting state or whether it reappears gradually only in the vortex cores should be considered an open problem, although our calculations in the homogeneous system and in the vortex, as well as some experimental evidence[2,28] seem to favor the first term of the alternative. Moreover, the short-range part of the Cooperon propagator only reproduces the experimental results if it is incoherent, i.e., not participating in the overall phase coherence below $T_c$. This belongs today to the conventional wisdom, essentially because this part does not vanish in the center of vortices, and also because of the weak magnetic-field dependence of the pseudogap[2]. Finally, our model involves two different length scales, the superconducting coherence length and the range of the incoherent correlations. We note here that recent experiments by Pan et al.[29] have shown the possible existence of two correlation lengths in BSCCO, although in their interpretation the shortest one is associated with the presence of the oxygen dopants in the BiO plane and is therefore not translationally invariant as in our approach.

The energy $\Delta E$ of the core states is plotted in the inset of Fig. 1 as a function of the gap scale $(\Delta_p^2 + \Delta_s^2)^{\frac{1}{2}}$. The calculated core-state energies increase with the gap width and the correlation length $\xi$ but depend little on $\Delta_p/\Delta_s$. They are in good general agreement with the experimental observations, i.e., 5.5 meV in a YBCO sample with a gap of 20 meV[3], 7 meV for a 32 meV-gap BSCCO[3], and 14 meV for a 45 meV-gap BSCCO[3]. A recent thorough investigation of the BSCCO system indicates a roughly linear relationship between $\Delta E$ and the energy gap[23]. Moreover, the fact that the observed peaks are sharper in YBCO than in BSCCO can be well explained by assuming a smaller value of $\Delta_p/\Delta_s$ in YBCO [see Fig. 1(b)]. This assumption is consistent with the observation that optimally-doped YBCO, unlike optimally-doped BSCCO, seems to have no pseudogap phase above $T_c$.\[20\]

We now discuss the behavior of the LDOS in the vicinity of the core. $N(r, \omega)$ is displayed in Fig. 2(a) as a function of $\omega$ for $r$ along $\hat{x}$, illustrating the weak localization of the core states. The angular average $\bar{N}(r, \omega)$ plotted in Fig. 2(b) at the core-state energy shows the exponential decay of the LDOS, as observed experimentally[2] and in contrast to the algebraic decay of BCS core states. The calculated decay length depends on energy and is $\lambda/a = 6.7$ for the state above $E_F$ and 4.4 for the state below $E_F$. The average 5.6 compares well with the value of $5.7 \pm 0.8$ quoted in Ref. [2] (using $a = 3.83$ A for the BSCCO lattice parameter). Fig. 2(b) also shows the absence of a significant four-fold anisotropy in $N(r, \omega)$ around the core. It is known from semiclassical approaches that a finite lifetime reduces the anisotropy[27]. The pseudogap correlations have the same effect in our calculations. As an illustration we plot in the inset the ratio $\alpha(r) = \int_0^\Delta d\omega \frac{|N(r\hat{n}, \omega) - N(r\hat{x}, \omega)|}{\int_0^\Delta d\omega N(r, \omega)}$ which measures the relative anisotropy of the LDOS at subgap energies ($\hat{n}$ is the nodal direction). In the BCS limit $\alpha(r)$ is maximum around $r/a = 3$, consistently with previous results[3]. The behavior of $\alpha(r)$ in the pseudogapped case is similar, although reduced by a factor $\sim 25$, making the maximum anisotropy smaller than 1%.

Our model Cooperon propagator has deliberately few parameters. The good agreement between numerical results and experimental data gives us confidence that it may contain the relevant input for interpreting vortex-core measurements in HTS. Our calculations show clearly that the same model and parameters used in the pseudogap regime also explain the properties of the core states in vortices. Whether the pseudogap part of the self-energy survives unchanged in the superconducting state or whether it reappears gradually only in the vortex cores should be considered an open problem, although our calculations in the homogeneous system and in the vortex, as well as some experimental evidence[2,28] seem to favor the first term of the alternative. Moreover, the short-range part of the Cooperon propagator only reproduces the experimental results if it is incoherent, i.e., not participating in the overall phase coherence below $T_c$. This belongs today to the conventional wisdom, essentially because this part does not vanish in the center of vortices, and also because of the weak magnetic-field dependence of the pseudogap[2]. Finally, our model involves two different length scales, the superconducting coherence length and the range of the incoherent correlations. We note here that recent experiments by Pan et al.[29] have shown the possible existence of two correlation lengths in BSCCO, although in their interpretation the shortest one is associated with the presence of the oxygen dopants in the BiO plane and is therefore not translationally invariant as in our approach.
According to our picture the pseudogap and superconducting gap may have very different properties, and this seems to be supported by thermodynamic and reflectivity experiments. The apparent contradiction with tunneling and photoemission data, which seem to show that the superconducting gap merges smoothly with the pseudogap at $T_c$, can be resolved if the one-electron energy gap below $T_c$ turns out to be composed of both superconducting gap and pseudogap. This in fact happens in our model, which interestingly produces a single gap structure in the DOS with a smooth evolution across $T_c$, regardless of the relative values of $\Delta_p$ and $\Delta_s$.\(^{[18]}\)

Our theory being semi-phenomenological, it does not provide a deep understanding of the underlying microscopic phenomena. It is compatible, in principle, with any microscopic theory that would predict two energy scales — like the spin-charge separation scenario (which has the spinon gap and the superconducting gap as separate entities) or the theory of stripe-induced superconductivity (where, in one version, one-dimensional spinon field can exist above $T_c$, the superconducting order being created by Josephson coupling between the stripes) or the phase fluctuation picture, as emphasized below — and two length scales associated with these energy scales and appearing in the calculation of the Cooperon propagator. The picture that emerges for the pseudogap state in our model is analogous to a plane rotator model, where the two-dimensional spins would be formed at some temperature $T^*$, but where the phase coherence only concerns the interaction between these spins (or preformed pairs), not the internal structure of the spins themselves. In the model, however, the two-dimensional spins appear only in the correlation function, not as entities located at definite sites. This picture, when proper temperature dependence is included in $\Delta_s(T)$, could lead to a second cross-over temperature within the pseudogap state, perhaps seen in Nernst effect, conductivity, and Hall effect measurements, temperature at which local phase coherence is established between neighboring spins, thus allowing the formation of fluctuating vortices.

In conclusion, we display in this work a reasonably good agreement between a phenomenological theory of the pseudogap state and the experimental data for the vortex-core tunneling spectra in YBCO and BSCCO. Our results argue in favor of a common, pseudogap related, mechanism at the origin of the core states in these materials. The incoherence and short-rangeness of the pseudogap correlations turn out to be the clue to the formation of these states, and endow them with properties (energy, amplitude, spatial decay) which are drastically different from the properties of conventional BCS core states.

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