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# Vortex core states in the presence of a staggered flux phase

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We investigate the vortex properties of a system where superconductivity competes with a staggered flux state. Such a competition has been proposed to be at the origin of the pseudogap phenomenon observed in the cuprates. We show that the presence of a staggered flux state is responsible for a substantial modification of the vortex structure and reversion of the vortex charge. We demonstrate that this scenario may explain some experimental results obtained with the help of scanning tunneling microscopy.

*Keywords:* Mixed state; High–temperature superconductivity; Pseudogap

## 1. Introduction

The understanding of the experimentally found normal state pseudogap is considered as one of the crucial problems of high–$T_c$ superconductivity. This phenomenon is related to the observed reduction of the density of states at the Fermi level which occurs at a temperature $T^*$ being much higher than the superconducting transition temperature $T_c$. Many experimental results suggest that at $T_c$ the pseudogap smoothly merges into the superconducting gap. However, there exist also contradictory data that support the presence of two gaps below $T_c$. Although, the existence of the pseudogap has been confirmed by various experiments, the underlying mechanism has remained unclear so far.

Two main hypotheses have been proposed. According to the first one, the pseudogap appears to be the precursor to the superconducting state which originates from the presence of incoherent Cooper pairs, the latter undergoing a Bose–Einstein condensation at the superconducting phase transition. This hypothesis explains a smooth merging of the pseudogap into the superconducting gap. This explanation seems to be supported by the recent observation of a vortex–like Nernst signal above $T_c$ [18] which also merges smoothly into the analogous signal at the superconducting phase transition [17].

According to the second hypothesis there is an additional, hidden order that coexists and/or competes with superconductivity [3]. This is a tempting concept

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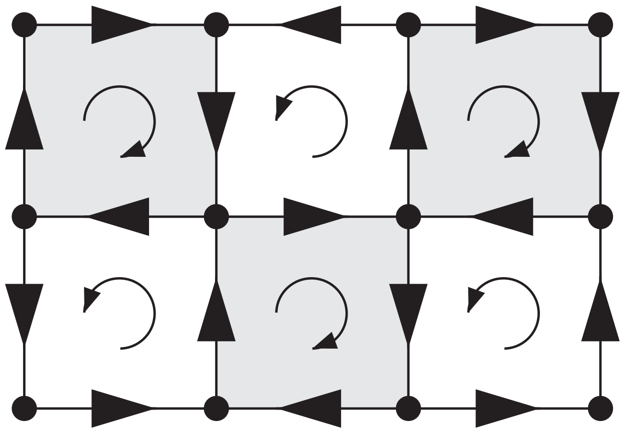

Figure 1. Schematic plot of orbital currents in the staggered flux phase.

since it would naturally explain the nonmonotonic doping dependence of $T_c$. Also the fact that, for example, Zn substitution destroys superconductivity whereas the pseudogap remains unaffected by the impurities [7], suggests different origins of both gaps. In present paper we investigate some aspects of the second hypothesis. The staggered flux state is one of the commonly assumed candidates for the hidden order [12]. This state is also refereed to as a *d*–density wave (DDW). According to this idea the pseudogap opens due to the condensation of particle–hole pairs with an angular momentum $l = 2$. Then, there are orbital currents, which alter from one plaquette to the neighboring one, as can be inferred from figure 1. It has been discussed that, in contradistinction to superconductivity, the DDW appears to be robust against an external magnetic field [13]. Therefore, the investigation of the vortex structure can provide a unique possibility to test this hypothesis. Since superconductivity is locally suppressed in the vortex core, one can expect a strong enhancement of the competing order, i.e., the formation of a staggered flux phase. Moreover, this would allow to compare the theoretical results with recent experimental data obtained with the help of scanning tunneling microscopy (STM).

In this context we would like to mention that it was predicted forty years ago that bound states should occur in the vortex core of *s*–wave superconductors [2]. It was then experimentally confirmed that such states exist in $NbSe_2$ [5]. In the case of *d*–wave superconductors, instead of truly bound states, one would expect the presence of extended states with a continuous energy spectrum [4]. Although a recent STM experiment allowed to identify the bound states in some of the high–temperature superconductors (HTSCs), which are usually considered as *d*–wave superconductors [10], none of the existing explanations has fully been accepted. On the other hand, the core states have not been observed in other STM experiments so far. Instead, a gap–like structure has been found to exist in the center of the vortex core. This has been identified as the pseudogap which smoothly merges into the superconducting gap outside the the vortex core [15]. Another interesting feature is related to the vortex charge. According to BCS theory the vortex charge originates from the difference between the chemical potentials of the normal and superconducting states and should be relatively small [1]. However, in HTSCs the effective vortex charge is a few orders of magnitude as large. Moreover, change of doping can revert its sign [8].

In the present paper we show that the existence of a hidden order can help to understand and to explain experimental data concerning the vortex structure, in particular the vortex charge.

## 2. Model

We investigate a two–dimensional square lattice immersed in a perpendicular magnetic field. We assume the magnetic field to be uniform, which is justified for extreme type–II superconductors. We start with a mean–field Hamiltonian which describes a system with coexisting DDW and DSC orders

$$H = -t \sum_{\langle ij \rangle \sigma} e^{i\theta_{ij}} a^{\dagger}_{i\sigma} a_{j\sigma} - \mu \sum_{i\sigma} a^{\dagger}_{i\sigma} a_{i\sigma} + H', \tag{1}$$

where

$$H' = \sum_{\langle ij \rangle} \left( a^{\dagger}_{i\uparrow} a^{\dagger}_{j\downarrow} \Delta_{ij} + a_{i\downarrow} a_{j\uparrow} \Delta^{*}_{ij} \right) + \sum_{\langle ij \rangle \sigma} (-1)^{i} D_{ij}\, e^{i\theta_{ij}} a^{\dagger}_{i\sigma} a_{j\sigma}. \tag{2}$$

Here $a^{\dagger}_{i\sigma}$ creates an electron with spin $\sigma$ at site $i$; $\mu$ is the chemical potential; $t$ is the nearest–neighbor hoping integral in the absence of magnetic field and $\exp i\theta_{ij}$ is the Peierls phase factor, responsible for the diamagnetic response of the system:

$$\theta_{ij} = \frac{e}{\hbar c} \int_{R_j}^{R_i} \mathrm{A} \cdot d\mathrm{l}.$$

The first term in equation (2) is the nearest–neighbor pairing that leads to anisotropic superconductivity of $d$–wave symmetry (DSC)

$$\Delta_{ij} = -\frac{1}{2} V_{\mathrm{DSC}} \langle a_{i\downarrow} a_{j\uparrow} - a_{i\uparrow} a_{j\downarrow} \rangle. \tag{3}$$

The second term is responsible for the onset of the staggered flux phase with the order parameter given by:

$$D_{ij} = (-1)^{i} \frac{1}{2} V_{\mathrm{DDW}} \langle e^{i\theta_{ij}} a^{\dagger}_{i\sigma} a_{j\sigma} - e^{i\theta_{ji}} a^{\dagger}_{j\sigma} a_{i\sigma} \rangle. \tag{4}$$

In order to obtain a diagonal form of the mean–field Hamiltonian one introduces a set of new Fermionic operators $\gamma_{n\sigma}$,

$$a_{i\uparrow} = \sum_{l} u_{il} \gamma_{l\uparrow} - v^{*}_{il} \gamma^{\dagger}_{l\downarrow}, \quad a_{i\downarrow} = \sum_{l} u_{il} \gamma_{l\downarrow} + v^{*}_{il} \gamma^{\dagger}_{l\uparrow}, \tag{5}$$

where $u_{il}$ and $v_{il}$ are determined by the Bogoliubov–de Gennes equations

$$\sum_{j} \begin{pmatrix} \mathcal{H}_{ij} & \Delta_{ij} \\ \Delta^{*}_{ij} & -\mathcal{H}^{*}_{ij} \end{pmatrix} \begin{pmatrix} u_{jl} \\ v_{jl} \end{pmatrix} = E_{l} \begin{pmatrix} u_{il} \\ v_{il} \end{pmatrix}, \tag{6}$$

and the single particle Hamiltonian is given by

$$\mathcal{H}_{ij} = \left[ -t\delta_{i+\delta,j} + (-1)^{i} D_{ij} \right] e^{i\theta_{ij}} - \mu \delta_{ij}. \tag{7}$$

Then, the Hamiltonian expressed in terms of the new operators takes the form:

$$H = \sum_{l\sigma} E_{l} \gamma^{\dagger}_{l\sigma} \gamma_{l\sigma} + \mathrm{const.} \tag{8}$$

Both order parameters, $\Delta_{ij}$ and $D_{ij}$, can be determined from the iterative solutions of the equation (3–7). In order to compare the numerical results with the STM data we have calculated the local density of states (LDOS), $\rho_i(\omega) = -(1/\pi)\mathrm{Im}\,\langle\langle a_{i\sigma} \mid a^{\dagger}_{i\sigma}\rangle\rangle_{\omega+i\epsilon}$. We have also calculated the local concentration of carriers $n_i = \int d\omega f(\omega)\rho_i(\omega)$, where $f(\omega)$ is the Fermi function. This quantity allows one to estimate the effective vortex charge.

## 3. The vortex structure

We have solved the Bogoliubov–de Gennes equations for an isolated vortex for the case of a $35 \times 35$ lattice with one superconducting flux quantum piercing this area. For a typical lattice constant of 0.4 nm this choice corresponds to a magnetic field of the order of 10 T. We use the nearest–neighbor hopping integral as unit of energy and assume that the interactions strength is $V_{\mathrm{DDW}} = 1.6$ and $V_{\mathrm{DSC}} = 1.4$. This specific choice of the potentials allows one to reproduce the phase diagram of HTSCs. However, the most qualitative results presented in this paper remain valid also for other values of $V$'s.

We have found that the vortex structure depends on the occupation number $n$ and that it reflects the presence of various phases in the phase diagram: (i) for $n \to 1$ the DDW order dominates and superconductivity does not occur; (ii) for larger doping superconductivity sets in and both types of ordering coexist in the bulk material; (iii) for sufficiently large doping the DSC dominates while the DDW is absent. In the presence of a magnetic field an additional phase can occur which is an intermediate one with respect to the phases of (ii) and (iii). In the latter phase the staggered fluxes appear in the vicinity of the vortex core and vanish away from the core, as can be inferred from figure 2. In the present paper we predominantly investigate this phase. Investigations of the cases (ii) and (iii) can be found in [11] and [16], respectively. Figure 2 shows the behavior and magnitudes of the order parameters defined by

$$\Phi_i^{\mathrm{DSC}} = \frac{1}{4}\left(\Delta_{i,i+\hat{\mathbf{x}}} + \Delta_{i,i-\hat{\mathbf{x}}} - \Delta_{i,i+\hat{\mathbf{y}}} - \Delta_{i,i-\hat{\mathbf{y}}}\right), \tag{9}$$

$$\Phi_i^{\mathrm{DDW}} = \frac{1}{4}\left(D_{i,i+\hat{\mathbf{x}}} + D_{i,i-\hat{\mathbf{x}}} - D_{i,i+\hat{\mathbf{y}}} - D_{i,i-\hat{\mathbf{y}}}.\right) \tag{10}$$

Since the staggered flux phase hardly depends on the magnetic field its enhancement in the vortex core mainly originates from the competition between the two types of ordering. It order to verify this hypothesis we have calculated

$$\langle\Phi\rangle \equiv \sqrt{\left(\Phi_i^{\mathrm{DDW}}\right)^2 + \left(\Phi_i^{\mathrm{DSC}}\right)^2}.$$

This quantity allows to obtain a rough estimate of the total gap in LDOS. As can be seen in figure 3, $(\Phi^{\mathrm{DDW}})^2$ increases in the vortex core approximately by the same amount by which $(\Phi^{\mathrm{DSC}})^2$ decreases.

Apart from the case of half–filling, the DDW and DSC gaps open at different energies: While superconducting gap opens at the Fermi level, the DDW gap opens in the middle of the band. This feature is responsible for another interesting physical fact related to the vortex charge. In order to show this, we consider a homogeneous system in the absence of a magnetic field. Opening of the superconducting gap leads then to only a small change of the chemical potential. In contrast to this, the opening

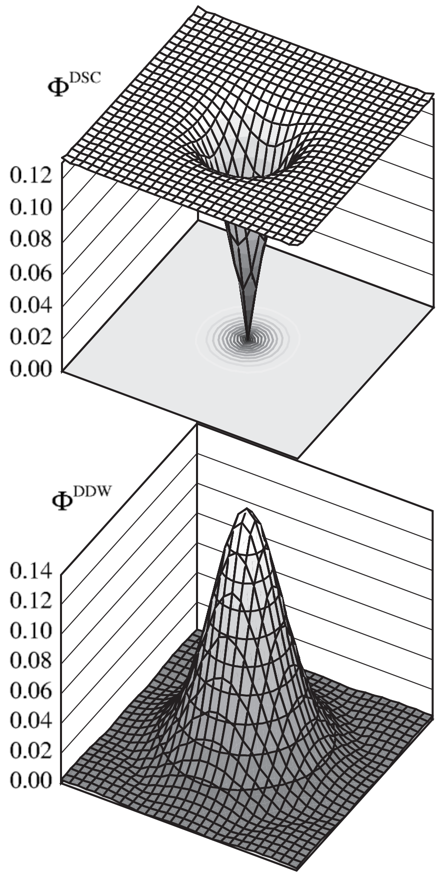


Figure 2. Vortex structure calculated for the occupation number $n = 0.9$ at temperature $k_B T = 0.05$. The upper panel shows the superconducting order parameter whereas the lower one shows the DDW order parameter, see equations (9) and (10).

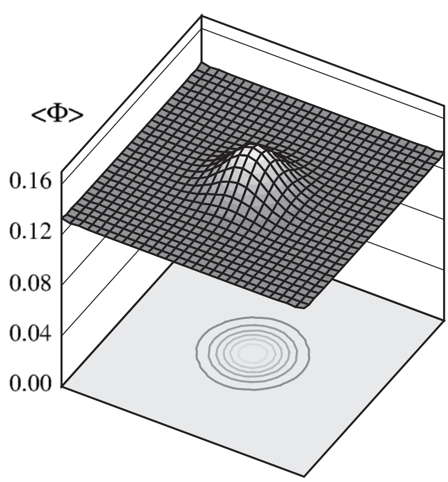


Figure 3. Behavior of the quantitiy $\langle\Phi\rangle \equiv [(\Phi_i^{\mathrm{DDW}})^2 + (\Phi_i^{\mathrm{DSC}})^2]^{1/2}$ in the vicinity of the vortex. The model parameters are the same as used in figure 2.

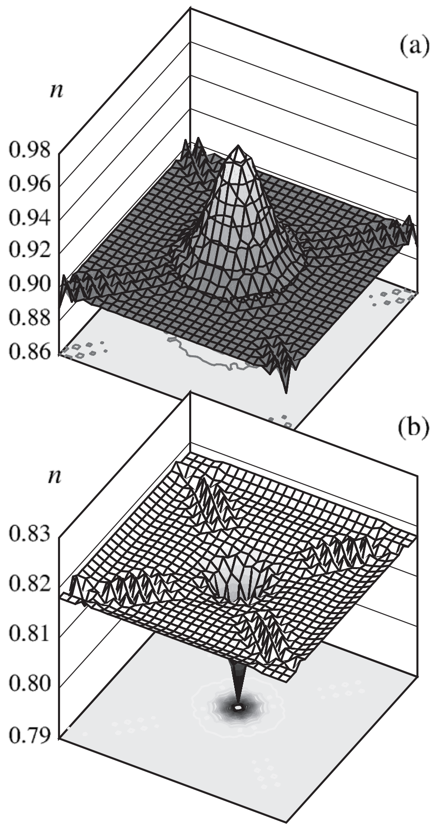


Figure 4. The electron concentration $n_i$ in the vicinity of vortex calculated at $k_B T = 0.05$ for $n = 0.9$ (upper panel) and $n = 0.81$ (lower panel). The DDW gap opens in the vortex core only in the first case, i.e., for $n = 0.9$.

of the DDW gap results in a significant shift of the quasiparticle poles. In particular, for $n < 1$ the states in the vicinity of the Fermi level are shifted toward lower energies. This feature is of crucial importance for the vortex charge. At small dopings, opening of the DDW gap in the vortex core is accomplished by a strong enhancement of the carrier concentration, as can be inferred from figure 4a. For larger doping, there is no gap in the vortex core and the local concentration of electrons is less than in the bulk material, see figure 4b. The doping–induced inversion of the vortex charge remains in agreement with the recent experimental result obtained for YBCO [8]. It has been found that the vortex charge is negative (positive) for overdoped (underdoped) compounds. Moreover, its magnitude is much larger than predicted by the BCS theory.

Coexistence of DSC and DDW orders also leads to a substantial modification of the LDOS in the vicinity of the vortex core. We briefly summarize the experimental data before we analyse the numerical results. STM measurements on $YBa_2Cu_3O_{7-x}$ clearly reveal the existence of bound states [10]. Close to the Fermi level there are two peaks separated by about 11 meV. However, in the case of BSCCO there exist contradictory data, and the presence of the bound states is still unclear. Small peaks at $\pm 7$ meV have been reported [14]. On the other hand, the core states have not been observed in other STM experiments [15]. Instead, the pseudogap has been

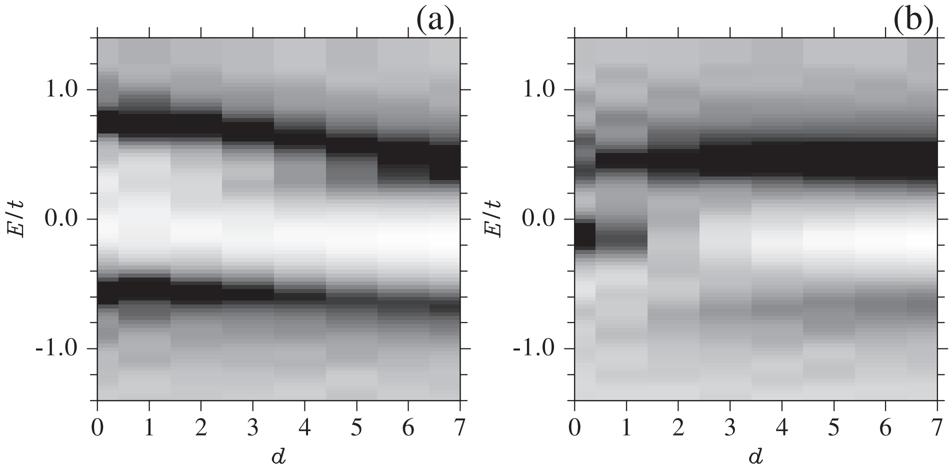


Figure 5. LDOS calculated at various distances $d$ from the vortex center. The dark/light areas correspond to large/small values of LDOS. Panels (a) and (b) show the results obtained for $n = 0.9$ and $n = 0.81$, respectively. The DDW gap opens in the vortex core only in the first case, i.e., for $n = 0.9$.

found to exist in the vortex core. When approaching the vortex center the superconducting gap evolves smoothly into the pseudogap. Additionally, the coherent peak at positive bias shifts towards higher energy, whereas the peak at negative bias does not move. These experimental results can be explained by the DDW scenario. Figure 5 shows the LDOS at various distances from the vortex core. figure 5a has been obtained for moderate doping, when DSC and DDW orders coexist in the vicinity of the vortex. For comparison, we present also data obtained for large doping, when the DDW order does not occur, see figure 5b. We notice that the onset of the staggered flux state is responsible for the absence of the zero bias conductance peak and the asymmetry of the LDOS. The latter feature originates from the fact the DDW gap opens at higher frequency than the superconducting one. One should keep in mind that the DDW and DSC order parameters have nodes at the same regions of the Fermi surface and, therefore, the bound states do not occur. In order to account for the presence of these states one should include components with other symmetries either in the superconducting or in the density wave channel (the total gap should be nodeless).

Finally, we discuss the decay of the DDW order when moving away from the vortex center. We have found that for moderate doping the decay is of oscillating character. There exist lines where the DDW order changes sign which corresponds to reversion of the staggered fluxes. Such a case is shown in figure 6, where we have marked the regions of reversed current circulation. The resulting pattern shows a checkerboard–like modulation. A similar pattern has recently been observed in overdoped BSCCO [6]. In the present approach, the magnitude of the staggered fluxes is too small to explain the observed antiferromagnetic order [9]. However, the DDW state should stabilize the antiferromagnetic ordering of spins, because it locally enhances the concentration of electrons towards half–filling. A direct coupling between staggered fluxes and spins may contribute to this ordering as well.

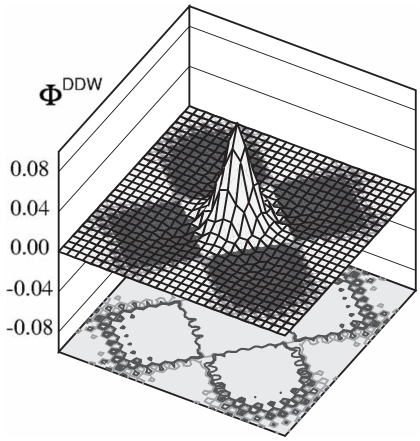


Figure 6. DDW order parameter calculated for $n = 0.84$ and $k_B T = 0.01$. The shaded areas correspond to reverted circulation of the orbital currents.

## 4. Summary and concluding remarks

We have investigated a few properties of the superconducting vortex in the presence of a staggered flux phase like the scenario of competing DSC and DDW orders which has been recently proposed for the description of the pseudogap phenomenon. Our investigation has been carried out on a mean–field level based on the Bogoliubov–de Gennes equations. The model parameters used for $V_{\mathrm{DSC}}$ and $V_{\mathrm{DDW}}$ have been adjusted such that the phase diagram of HTSCs is reproduced. Besides the phases being present in the diagram, an external magnetic field leads to appearance of additional phase. In this phase the staggered fluxes exist only in the vicinity of the vortex core which leads to a substantial modification of the vortex. We have found that opening of a DDW gap in the vortex core leads to a reversion of the vortex charge and is responsible for the asymmetry of the local density of states. Therefore, the DDW scenario may straightforwardly explain some of the recent experimental results. However, in the present approach both gaps vanish at the same points of the Fermi surface and, therefore, bound states are not formed in the vortex core. In order to remove this drawback one must extend the presented analysis, for example, by allowing for nodeless gaps either in the superconducting or in the charge density channel. In addition, inclusion of next–nearest neighbor interactions will give rise to further components of the order parameters, changing the original nodes. This problem is presently under investigation.

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