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Structure of a vortex line in a $d_{x^2-y^2}$ superconductor

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The structure of a vortex line in a $d_{x^2-y^2}$ superconductor is calculated self-consistently in the framework of the Bogoliubov–de Gennes theory. The inner core of the vortex containing localized quasiparticle excitations is found to be separated from the asymptotic pure d-wave state by a region where low-lying fermionic excitations are absent. A domain structure of the relative phase of the s-wave and d-wave components is identified. The results are interpreted in terms of a Ginzburg-Landau theory.

Several theoretical models predict $d_{x^2-y^2}$ symmetry for the energy gap in high-T_c superconducting oxides.[1,2] However, the experimental situation is still unclear. Although there is strong evidence for the existence of a linear density of states in optimally doped Y-Ba-Cu-O,[3] there is evidence both for[4] and against[5] a gap with d-wave symmetry. Nevertheless, in spite of the experimental uncertainty, it is timely to consider the new physics which might arise in a superconductor with a $d_{x^2-y^2}$ order parameter. In particular, it is of interest to consider the order parameter field in the core of a vortex for such a superconductor. This problem was considered by Volovik[6] who studied the modifications of the density of states due to the presence of a vortex line in a superconductor of $d_{x^2-y^2}$ symmetry. In this paper we report a self-consistent solution for the vortex core in a superconductor with $d_{x^2-y^2}$ symmetry, and we interpret our results in terms of the appropriate Ginzburg-Landau free-energy functional.

Symmetry allows the core of a d-wave vortex with the asymptotic gap function $\hat{\Delta}(\vec{k},\vec{r})=\Delta_d(\cos k_x a-\cos k_y a)e^{i\varphi}$ to contain an s-wave-like component with opposite winding of the phase.[6] This somewhat surprising result is due to the interplay of the phase with the nontrivial momentum dependence of the order parameter. The presence of a localized s-wave component can radically alter the properties of the vortex core. In particular, the total gap function is nodeless in the region where s- and d-wave components coexist with nonzero relative phase.[2,6] This leads to a picture in which different kinds of fermionic excitations are found in three different regions of the vortex (see Fig. 1). At the center of the vortex core, where both the s-wave and d-wave components vanish, localized fermionic core excitations[7] will exist. These bound states can have a strong effect on the structure of the vortex core at the low temperatures.[8–10] We call this the inner core of the vortex. It is surrounded by a region where d- and s-wave pairing coexist, mainly with nonzero relative phase, and hence the fermionic excitations in this region are gapped. (However, the gap is suppressed along directions where s- and d-wave components interfere destructively.) We call this the outer core of a d-wave vortex. Outside the outer core, the superconductor is in a pure d-wave state.

In order to study the structure of a d-wave vortex in more detail, we have carried out calculations within Bogoliubov–de Gennes (BdG) theory. This approach was pioneered by Caroli, de Gennes, and Matricon.[8] However, the first self-consistent solution of these equations for the case of a conventional s-wave vortex was obtained only recently.[9]

Here, we consider superconductivity on a square lattice with interatomic spacing a. The pairing interactions are modeled with an attractive interaction between electrons of opposite spin at nearest-neighbor sites and an onsite repulsive term.[11] We consider only the case of spin singlet pairing.

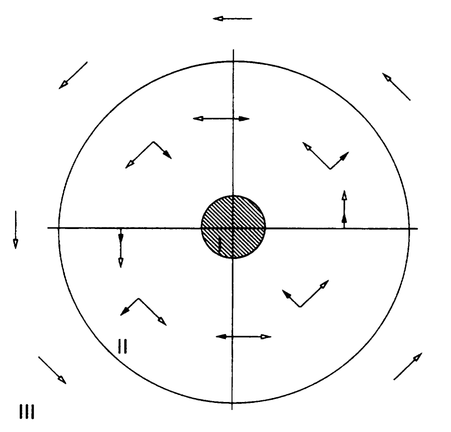

FIG. 1. Three regions of the vortex. The complex s-wave order parameter is represented with a black arrow and the d-wave one with a white arrow. Both the s-wave and d-wave pairing are suppressed in the inner core (labeled I). Localized core excitations are found in this region. This is surrounded by an outer core (labeled II) where d-wave and s-wave pairing coexist. In this region low-energy fermionic excitations are absent (except possibly along those directions for which the relative phase between the s- and d-wave components vanishes). Outside the core (region III) the superconductor is in a pure d-wave state. As the opposite winding of the s- and d-wave components (Ref. 6) is incompatible with the relative phase $\pm\pi/2$ (Ref. 2), four domains are formed. The regions of relative phase $\pi/2$ and $-\pi/2$ are separated by domain walls (indicated by vertical and horizontal lines) where the relative phase varies rapidly.

A small, nonzero interlayer coupling is assumed to stabilize the quasi-two-dimensional situation.

The Bogoliubov–de Gennes equations[12] for this model Hamiltonian are

$$\begin{pmatrix} \hat{\xi} & \hat{\Delta} \\ \hat{\Delta}^* & -\hat{\xi} \end{pmatrix} \begin{pmatrix} u_n(\vec{r}) \\ v_n(\vec{r}) \end{pmatrix} = E_n \begin{pmatrix} u_n(\vec{r}) \\ v_n(\vec{r}) \end{pmatrix}, \tag{1}$$

where

$$\hat{\xi} u_n(\vec{r}) = -t \sum_{\vec{\delta}} u_n(\vec{r}+\vec{\delta}) - \mu u_n(\vec{r}) \tag{2}$$

and

$$\hat{\Delta} v_n(\vec{r}) = \sum_{\vec{\delta}} \Delta_{\vec{\delta}}(\vec{r}) v_n(\vec{r}+\vec{\delta}) + \Delta_0(\vec{r}) v_n(\vec{r}). \tag{3}$$

Here $\vec{\delta}$ denotes a nearest-neighbor vector. The normal-state bandwidth is $8t$, and μ is the chemical potential. We have ignored the coupling to the vector potential in Eq. (2) and are thus assuming the limit of an extreme type-II superconductor.

The gap equation for the nearest-neighbor pairing is

$$\Delta_{\vec{\delta}}(\vec{r}) = \frac{g}{2} \sum_n [u_n(\vec{r}+\vec{\delta}) v_n^*(\vec{r}) + u_n(\vec{r}) v_n^*(\vec{r}+\vec{\delta})] \times \tanh(E_n/2T) \tag{4}$$

and for onsite pairing

$$\Delta_0(\vec{r}) = g_0 \sum_n u_n(\vec{r}) v_n^*(\vec{r}) \tanh(E_n/2T). \tag{5}$$

Positive values for the coupling constants g and g_0 correspond to attraction and negative values to repulsion. Note that the components of the gap operator have the symmetry

$$\Delta_{\vec{\delta}}(\vec{r}) = \Delta_{-\vec{\delta}}(\vec{r}+\vec{\delta}), \tag{6}$$

and therefore it is convenient to consider it to be a property of the nearest-neighbor bonds.

It is known that there are two spatially homogeneous spin singlet solutions to Eqs. (1)–(5) with $g_0=0$. Namely, $\hat{\Delta}(\vec{k}) = 2d(\cos k_x a - \cos k_y a)$ and $\hat{\Delta}(\vec{k}) = 2s(\cos k_x a + \cos k_y a)$ (called d-wave state and extended s-wave state from now on).[11] It is also known that the presence of onsite repulsion $g_0<0$ favors the d-wave state over the extended s-state pairing.[11]

We have solved Eqs. (1)–(5) via exact diagonalization of the BdG Hamiltonian [Eq. (1)] and iteration of the gap equations [Eqs. (4) and (5)]. Given a gap function we obtain the eigenvalues E_n and the Bogoliubov amplitudes u_n and v_n from Eq. (1). These were then used to calculate a new gap function. These steps were repeated until the desired accuracy was obtained.

In order to be able to compare with earlier work[9] and to test the accuracy and feasibility of the numerical method, we studied the problem of a conventional s-wave vortex first. Both smooth boundary conditions[13] and modified periodic boundary conditions, where we compensated for the effect of

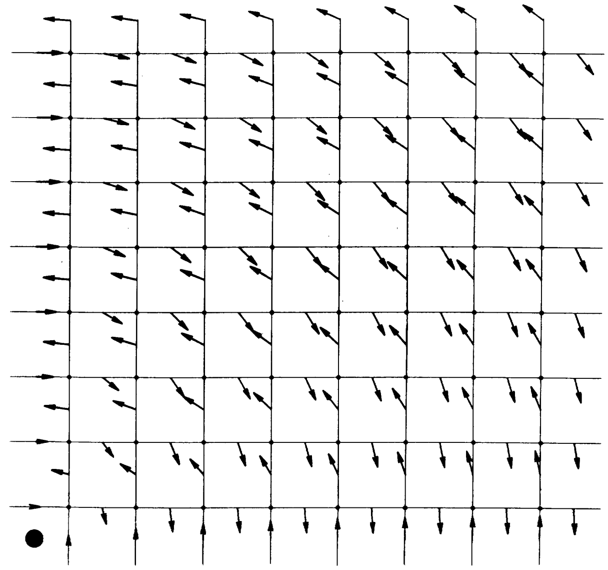

FIG. 2. The first quadrant of the core of a d-wave vortex. The arrows on the nearest-neighbor bonds indicate the magnitude and the phase of the order parameter. The black dot denotes the center of the vortex. Far away from the vortex core the horizontal and vertical bonds have π phase difference indicating a pure d-wave state. The parameters used in the numerical solution of Eqs. (1)–(5) were $T=0.05t$, $\mu=-2t$, $g=3.195t$, $g_0=-3t$. Only the central 8×8 region of the full 16×16 quadrant which was studied is shown.

phase winding, were tried. The structure of the vortex core did not depend on the choice of the boundary condition. The results agreed qualitatively with the results obtained in Ref. 9. However, for the large values of the coupling constant which we employed (typically $g_0=3.2$) there were only a few bound states at the vortex core.

Because of the considerable computational complexity of the problem, we studied only a limited part of the four-dimensional parameter space in the case of the d-wave vortex. We used modified periodic boundary conditions, because they were simpler, and studied bonds in a 16×16 quadrant. Boundary effects where localized within $2-3$ lattice spaces of the boundary. Typical values of the parameters were $T=0.05t$, $\mu=-2t$, $g=3.195$, $g_0=-3$. This choice of parameters corresponds to $d=0.2t$. Temperature was varied in the neighborhood of this point. However, we have not yet studied the temperature dependence in any detail. There were no qualitative changes in the nature of the solution. The same is true for small variations in the chemical potential. All the calculations are in the limit where the coherence length ξ is of the order of a few interatomic spacings a.

In Fig. 2 the first quadrant of the core region of a d-wave vortex is displayed. One sees that close to the center of the vortex, denoted by a black dot, the pairing amplitude of the horizontal and vertical bonds is suppressed. The further suppression along the x and y axis is caused by the destructive interference of the extended s wave

$$s(\vec{r}) = (\Delta_{\hat{x}} + \Delta_{-\hat{x}} + \Delta_{\hat{y}} + \Delta_{-\hat{y}})/4, \tag{7}$$

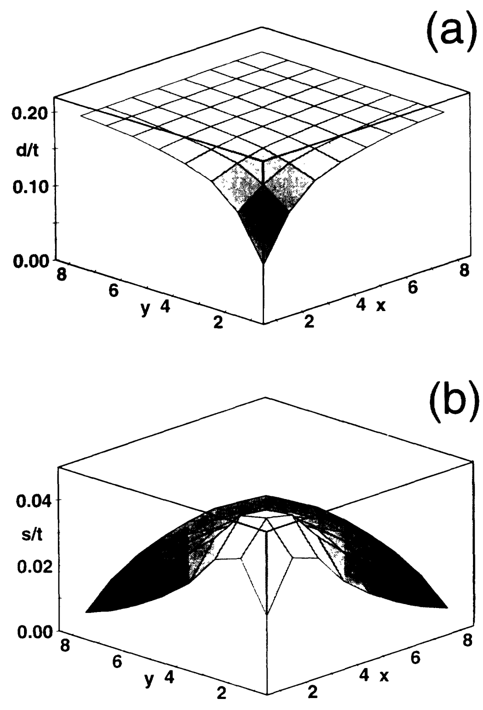

FIG. 3. Same as Fig. 2 but presented in terms of the amplitudes of s- and d-wave pairing denoted with s and d, respectively. The center of vortex is situated at the point (0.5,0.5). The relative phase (not presented here) was found to have the domain structure as indicated in Fig. 1. In particular, the domain walls were found to be oriented along the x and y axes.

where $\hat{x}$ and $\hat{y}$ denote the nearest-neighbor vectors along the x and y axes, and d-wave-like components

$$d(\vec{r}) = (\Delta_{\hat{x}} + \Delta_{-\hat{x}} - \Delta_{\hat{y}}\hat{y} - \Delta_{-\hat{y}})/4 \tag{8}$$

with the opposite winding of the phase. It is also interesting to note that a relative phase close to $\pi/2$, between extended s-wave-like and d-wave-like components, is preferred in a large part of the soft core. This is in agreement with Ref. 2 where it was argued that, if both s-wave and d-wave pairing are present simultaneously, then the relative phase $\pi/2$ is favored.

Since the requirement of maintaining a constant relative phase everywhere is incompatible with the opposite winding of the phase of the d-wave and extended s-wave components, regions of rapid variation of the relative phase arise. The general behavior of the solutions was such that the d-wave-like solution winds uniformly. The s-wave-like solution adjusts to a relative phase close to $\pi/2$ everywhere but in the domain wall regions along the x and y axis (see Fig. 1).

The effect of on-site repulsion on the structure of the vortex core was also studied. For the values considered, $T=0.05t$, $\mu=-2t$, $g=3.195$, $g_0/t=-2.5,-2.75,-3.0,-3.25$, the extended s-wave component is suppressed as the magnitude of the on-site repulsion is increased. For concreteness, the maximum of the extended s-wave-like component (see Fig. 3) decreases from $0.05t$ to $0.045t$ as the on-site repulsion was increased from the $g_0=-2.5$ to $g_0=-3.25$. This can be understood to be due to an increase of the cost in energy of the extended s-wave component as the repulsion is increased.

We can understand the qualitative features of Figs. 1–3 in terms of the Ginzburg-Landau free-energy functional which is appropriate for coexisting s- and d-wave order parameters. For simplicity we ignore other possible order parameters. This is motivated by the fact that Eqs. (1)–(5) with nearest-neighbor attraction and on-site repulsion have only solutions with s- and d-wave symmetry. The free-energy density is sum of the bulk-[2] and gradient-energy terms:[14]

$$f=\alpha_s|s|^2+\alpha_d|d|^2+\beta_1|s|^4+\beta_2|d|^4+\beta_3|s|^2|d|^2 + \beta_4(s^{*2}d^2+\text{c.c.})+\gamma_s|\vec{\nabla}s|^2+\gamma_d|\vec{\nabla}d|^2 + \gamma_v\left(\frac{\partial s}{\partial y}\frac{\partial d^*}{\partial y}-\frac{\partial s}{\partial x}\frac{\partial d^*}{\partial x}+\text{c.c.}\right), \tag{9}$$

where $\alpha_d<0$ and $[\alpha_s-(\beta_3-2|\beta_4|)\alpha_d/(2\beta_2)]>0$ in order for the pure d-wave state to be stable at infinity. Our results correspond to $\beta_4>0$ which leads to a relative phase of $\pm\pi/2$ between s and d in most of the outer core. We interpret the mixed gradient term, in our lattice model, as arising from the different interaction between nearest-neighboring parallel bonds in the same and different rows or columns, i.e., the difference between the terms $\Delta_{\hat{x}}(\vec{r})\Delta_{\hat{x}}(\vec{r}+\hat{x})$ and $\Delta_{\hat{x}}(\vec{r})\Delta_{\hat{x}}(\vec{r}+\hat{y})$ in the free-energy expansion when expressed in terms of bond variables [see Eqs. (7) and (8)]. This term is responsible for the angular anisotropy of the magnitude of the s-wave order parameter shown in Fig. 3(b). The coefficients γ_v and β_4 determine the orientation and shape of the domain walls for the relative phase of s and d.

The mixed gradient term would be expected to give rise to a number of other observable features. For example the vortex-vortex interaction will have an angular-dependent term that could modify the structure of the vortex lattice, the temperature dependence of the upper critical fields, H_{c_2}, will be affected and finite s- and d-wave components will exist in the interface between normal and superconducting regions. Unfortunately, space does not allow us to address these questions further here.

In conclusion we have solved, for the first time, the Bogoliubov–de Gennes equations for the core structure of a $d_{x^2-y^2}$-wave vortex. Three regions of the vortex were identified. In the classical limit this leads to a clear division of the vortex core into three regions with different kinds of fermionic excitations. The inner core region supports localized fermionic excitations resembling those found in the core of a conventional s-wave vortex. This region is surrounded by an outer core where fermionic excitations are gapped because of the coexistence of both d- and s-wave pairing. Interesting domain structure in the relative phase of the d-wave state and extended s-wave state was identified. The size of the outer core was found to decrease as the magnitude of on-site repulsion was increased. Outside the outer core, the superconductor is in a pure d-wave state. The structure and shape of the domains of the vortex core were interpreted in terms of the relevant Ginzburg-Landau free energy. If this kind of structure were observed in a scanning-tunneling-microscopy experiment similar to one performed by Hess *et al.*[15] it would be indicative of d-wave superconductivity.

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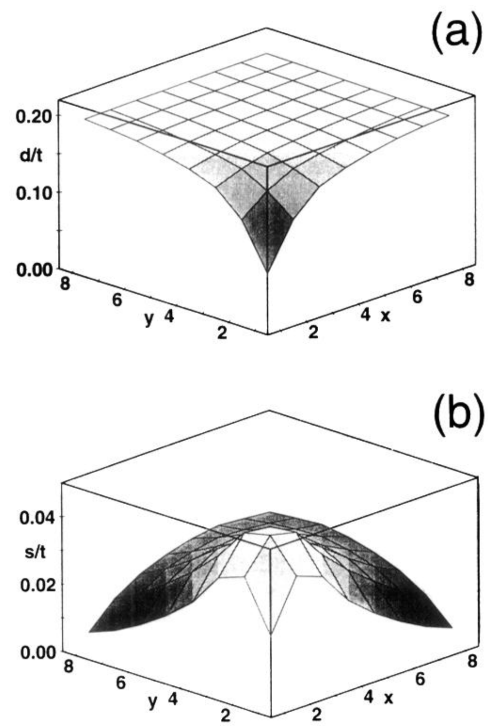

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