Local enhancement of spin and orbital antiferromagnetism around a single vortex in high-Tc superconductors

J.An\textsuperscript{1} and Chang-De Gong\textsuperscript{2,1,3}

\textsuperscript{1}National key laboratory of solid state microstructures, Department of Physics, Nanjing University, Nanjing 210093, China

\textsuperscript{2}Chinese Center of Advanced Science and Technology (World Laboratory), P.O. Box 8730, Beijing 100080, China

\textsuperscript{3}Department of Physics, Chinese University of Hong Kong, Hong Kong, China.

(November 16, 2018)

Abstract

In a simple model we investigate three competing orders: d-wave superconductivity, spin and orbital antiferromagnetism (AF) in the vicinity of a single vortex in a cuprate superconductor. We find that when the potential for the orbital AF $V_d$ is comparatively small, the spin-density-wave (SDW) order has an enhancement at the vortex core center, and the ”d-density-wave” (DDW) order exhibits a rather weak behavior around the core and vanishing small away from the core. However, when $V_d$ becomes large, globally, the SDW order decreases and the DDW order increases; locally, not only the peak of the SDW order around the core still exists, though relatively suppressed, but also a local peak for the DDW order finally appears. Similar effects are also revealed for the features when varying doping. Comparisons with experiments are discussed.
The microscopic structure around the field-induced vortices of high-Tc cuprate superconductors (HTCS) is a challenging problem in condensed matter physics. Physically, when an external magnetic field is applied to a HTCS, an Abrikosov vortex lattice will be produced. By destroying the superconducting (SC) order locally, in the small regions centered around the vortex cores, the normal state is formed. Experimentally, muon spin rotation measurements in underdoped \( \text{YBa}_2\text{Cu}_3\text{O}_{6+x} \) [1], nuclear magnetic resonance in optimally doped \( \text{Tl}_2\text{Ba}_2\text{CuO}_{6+\delta} \) [2] have found the evidence for the presence of local AF in the vortex cores. Furthermore, the presence of both local AF and charge order in the vicinity of the field-induced vortices has been revealed recently by neutron scattering experiments in optimally doped and underdoped \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \) [3], scanning tunneling spectroscopy (STS) in \( \text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta} \) [4]. Theoretically, the SO(5) theory [5] has predicted an AF core in the underdoped cuprate superconductors, where a superspin, combining the AF and the d-wave superconductivity, rotate from lying inside the SC plane into AF sphere, when the core is approached. On the other hand, staggered-current correlations were predicted recently in lightly doped \( t-J \) model [6,7]. In addition, based on the SU(2) gauge theory of the \( t-J \) model, a staggered-current state for the vortex core has been proposed [8], where the transition from the SC state to the staggered-current state when approaching the core was interpreted in terms of the rotation of an isospin vector, which has the meaning of the internal quantization axis of the boson condensate. Other theories also predict in the vortex core region the staggered current correlations [9], charge order [10,11], both SDW and charge order [12–15], while a prediction of simultaneous presence of charge, spin and orbital AF in the core region is still absent. The purpose of this letter is to investigate this possibility in a unified framework. We find that both the spin and orbital AF correlations has an enhancement at the vortex core center.

Here we assume the DDW state (or the staggered-current state, or the orbital AF state) [16,17] as the candidate state for the pseudogap, which characterizes the normal state around the vortex cores. In addition, it is well known that the competition between the d-wave superconductivity and antiferromagnetism plays a rather prominent role in the mechanism
of superconductivity. Therefore, in the vortex core regions, at least three ordering tendencies
cOMPete with one another and so are responsible for the mechanism of the microscopic
structure of the vortices. These orderings are d-wave paring, spin AF, and the DDW order.
We model our system as the following effective mean-field Hamiltonian, which is an extension
of the model in reference [18] in an external magnetic field,
\[ H = \{ \sum_{<i,j>\sigma} (-t + (-1)^iW_{ij}) - t' \sum_{<i,j>'\sigma} \exp(i\varphi_{ij})c_{i\sigma}^+c_{j\sigma} \\
\sum_i(U_{i\sigma} - \mu)c_{i\sigma}^+c_{i\sigma} + \sum_{<i,j>} (\Delta_{ij}c_{i\uparrow}^+c_{j\downarrow}^+ + H.c.) \} \]
(1)
where \( t, t' \) are the hopping integrals for the nearest neighbors (n.n) \(<i, j>\) and the next-
nearest neighbors (n.n.n.) \(<i, j>\)', respectively. \( \varphi_{ij} = \frac{\Phi_0}{\Phi_0} \int_{r_i}^{r_j} d\mathbf{r} \cdot \mathbf{A}(\mathbf{r}) \),
where \( \Phi_0 = \frac{hc}{2e} \) is the superconducting flux quantum and the external magnetic field \( \mathbf{H} = \nabla \times \mathbf{A} \)
is directed along \( z \) axis. The DDW order parameter is defined as \( W_{ij} = (-1)^iV_d \sum_\sigma < c_{i\uparrow}^+c_{j\downarrow}^+ - c_{i\downarrow}c_{j\uparrow} > \),
which is proportional to the physical current flowing along the bond \( ij \) and so it is naturally gauge invariant and then keeps the gauge invariance
of the Hamiltonian. \( V_d \) is the potential for the DDW channel, which favors a current-
carrying state. \( U_{i\sigma} = Un_{i,-\sigma} \) is the spin-dependent scattering potential, where \( U \) is the on-site repulsion, favoring an antiferromagnetic SDW order. \( \Delta_{ij} = V_p < c_{i\uparrow}^+c_{j\downarrow}^+ - c_{i\downarrow}c_{j\uparrow} > \) is
the SC spin-singlet pairing order parameter, where \( V_p \) is the attractive pairing interaction. \( \mu \)
is the chemical potential. Note that the above model can be taken as the mean-field version
of a more complicated and correlated model, such as \( t - U - V \) model. By decomposing
the electron annihilating operator into quasiparticles’ creating and annihilating operators:
\( c_{i\sigma} = \sum_\alpha (u_{n\sigma}(i)\gamma_{n\sigma} + v_{n\sigma}\gamma_{n,-\sigma}^+) \), the above Hamiltonian can be diagonalized by solving the
following Bogoliubov-de Gennes (BdG) equations in a self-consistent way [19],
\[ \begin{pmatrix} H_{ij}^\dagger & \Delta_{ij} \\
\Delta_{ij}^* & -H_{ij} \end{pmatrix} \Psi(j) = E\Psi(i) \]
(2)
where the quasiparticle wave function \( \Psi(i) = (u_{\uparrow}(i), v_\downarrow(i))^T \). The single-particle Hamiltonian
reads \( H_{ij}^\sigma = (-t + (-1)^iW_{ij})\delta_{i+s,j} - t'\delta_{i+s',j} + (U_i n_{i,-\sigma} - \mu)\delta_{ij} \) with the subscript \( \delta = (\pm 1, 0) \) or
\( (0, \pm 1), \delta' = (\pm 1, \pm 1) \) or \((\pm 1, \mp 1)\). The self-consistent DDW and SC order parameters read respectively:

\[
W_{ij} = (-1)^i \times iV_d \Im \sum_{n\sigma} \exp(i\phi_{ij})(u_{n\sigma}(i)u_{n\sigma}^*(j) + v_{n\sigma}(i)v_{n\sigma}^*(j))\tanh(\beta E_n/2),
\]

\[
\Delta_{ij} = \frac{\gamma}{2} \sum_n \sigma \{u_{n\sigma}(i)v_{n-\sigma}^*(j) - v_{n\sigma}(i)u_{n-\sigma}(j)\} \tanh(\beta E_n/2).
\]

All the sum over \( n \) is restricted to only positive eigenvalues \( E > 0 \) for an excitation energy should be positive-definite.

For simplicity, here the length and energy are measured in the units of the lattice constant \( a \) and the nearest-neighbor hopping \( t \), respectively. To extract the low-energy physics, we set the temperature to be zero. By using the periodic boundary condition, the BdG equations are solved self-consistently for a square lattice of 40 \times 40 sites. We have chosen a symmetric gauge, where the vector potential can be written as \( A = \frac{1}{2} r \times H \) with \( r \) the radius vector measured from the square center. The gauge phase \( \phi_{ij} \) on the link between sites at two different edges of the boundary can be so chosen that all the boundary effect be removed except at the four corners of the square. In the region we are interested in, the corners’ boundary has a rather small effect on it and the results we have obtained should still be very convincing. The starting state is the uniform d-wave superconducting state with vanishing small staggered magnetization and staggered current. The d-wave symmetries \( \Delta_{i,i+\delta} = \pm \Delta_0 \), \( W_{i,i+\delta} = \pm W_0 \), with + for \( \delta = (\pm 1, 0) \) and − for \( \delta = (0, \pm 1) \), are preserved at the beginning of the iterating.

In the whole article, we take the on-site energy \( U = 3 \), the pairing interaction \( V_p = 1.3 \), the n.n.n hopping integral \( t' = -0.25 \). The magnitude of \( H \) is so chosen that the total flux passing through the square lattice is a flux quantum \( \Phi_0 \). The numerical results shows that when the value of \( V_d \) is relatively small, the DDW order will be absent or be uniformly vanishing small. For \( V_d = 0.5 \), we plot in Fig. 1 the spacial profiles of the vortex structure for the electron occupation number \( n = 0.86 \). The site-dependent DDW order parameter \( W_i \) is defined as \( W_i = \frac{1}{4}(W_{i,i+e_x}+W_{i,i-e_x}-W_{i,i+e_y}-W_{i,i-e_y}) \). Here \( V_d \) is so weak that it can hardly stabilize a staggered current. Actually, the staggered current is found to be nearly uniformly distributed and vanishing small. The d-wave SC order parameter vanishes at the vortex core.
center and tends to be finite when away from the core. The gauge-invariant site-dependent SC order parameter $|\Delta_i|$ defined as $|\Delta_i| = \frac{1}{4} |\tilde{\Delta}_{i,i} + \tilde{\Delta}_{i,i+e_x} - \tilde{\Delta}_{i,i+e_y} - \tilde{\Delta}_{i,i-e_y}|$ with $\tilde{\Delta}_{i,j} = \Delta_{ij} e^{i \phi_{ij}}$ [20], weakly fluctuates and is not homogeneous even when the distance from the core centre is larger than the superconducting coherence length $\xi_0$. The antiferromagnetic SDW order parameter $m = (-1)^i (n_{i\uparrow} - n_{i\downarrow})$ (the staggered magnetization) shows an enhanced peak at the vortex core center, exhibiting strong AF correlation. The presence of another eight symmetric-positioned small peaks around the vortex core implies the possibility of the quasi-periodic magnetic structure with a much longer period $\xi_m$ (peak-peak separation) than $\xi_0$. Here $\xi_m$ is a length scale of order about $8a \sim 10a$, which can be compared to experiment [4]. The electron charge-density-wave (CDW) order parameter exhibits a similar modulation to the SDW. The enhanced peak at the core center means the vortex carries a negative charge. Another eight small peaks in the CDW appear at nearly the same spatial places as the SDW. Note that in the trivial case of $H = 0$, the homogeneous SDW order increases by decreasing doping, or increasing electron density. Surprisingly, this global characteristic seems to be locally correct in this parameter region: the CDW form local peaks just where the SDW have peaks.

In Fig. 2, we plot the same graphs for the same parameters except $V_d = 0.65$. Now the strength of the DDW potential $V_d$ is so large that not only a homogeneous small staggered current is stabilized, but also a great local enhancement is formed at the core center. In another word, the staggered-current correlations become much stronger when approaching the vortex core from the outside. This local enhancement of the staggered current can be interpreted as the effect of the local formation of the normal pseudogap region through destroying the SC order around the vortex core. This current-carrying state apparently breaks the time reversal symmetry. This is consistent with the argument based on the $t-J$ model, where an enhanced staggered current correlation when approaching the vortex center was predicted [8]. The d-wave SC order parameter approaches zero at the vortex core center. Away from the vortex core, the SC order parameter tends quickly to be a finite constant. Here the absence of the weak modulation in the SC order parameter is associated with the
suppression of the modulation in the SDW order parameter. The SDW still shows a strong peak (local maximum) at the core center, whereas the eight small peaks surrounding the core are so suppressed that they are hardly visible. This suppression of the magnetic modulation is due to the competition between the SDW and DDW order parameters. Generally, the presence of the DDW order frustrates the SDW order [21], whereas the presence of the SDW order seems to have a relative weak effect on the DDW order. Therefore the DDW order leads to the suppression of the spin AF correlations outside the vortex core. Inside the core, there exists two competing effects: the DDW still suppresses the SDW, whereas the disappearance of the SC order tends to increase the SDW. Combination of the two competing effects causes the enhanced SDW order to be still present inside the core, whereas the SDW order is strongly suppressed by the DDW order outside the core. The electron charge distribution (or CDW) exhibits a feature similar to that of the SDW, where a local maximum is formed at the vortex core center, causing a negative vortex charge. The electrons are accumulated locally by expelling out the holes at the vortex core, favoring more strong spin AF correlations.

In order to make more clear the characteristic of the vortex structure when the staggered-current correlations are dominant, we show the case \( V_d = 1 \) in Fig. 3. The strength of the DDW order is so strong that a nearly homogeneous DDW order is induced, except that a relatively small local peak appears at the core center. The magnitude of the DDW order is greatly increased, which then cause a great suppression on the SDW order. The SDW order is nearly homogeneous and vanishing small. A relatively small peak is still present for the SDW order at the vortex center due to its characteristic as the local normal state. The electron density is also nearly homogeneous except a small broad local peak at the core center. The inset of Fig. 3 shows the variation of the spatial averaged SDW (solid squares) and DDW (solid circles) order parameters with \( V_d \) for the same other parameters. \( V_d \) has a threshold \( V_d^c \approx 0.55 \), above which the DDW order appears and begin to increase, while the SDW order begin to decrease.

Similar effects were found for the case where the doping level changes. We show in Fig. 
the spatial vortex structure with the electron occupation number \( n = 0.91 \) and \( n = 0.94 \), respectively. Combined with Fig.2, it can be seen that small doping strongly favor a SDW order, both globally, and locally at the vortex core. The local peak of the SDW order is strongly enhanced. This great local enhancement comes from not only the doping effect, but also the normal state characteristic by destroying the SC order locally at the vortex core. The two effects have the same tendencies to increasing the SDW order, so the relatively great local enhancement is well explained. A quasi-periodic magnetic structure also appears in the SDW, indicating that this is not the feature just belonging to the optimal system, which is consistent with the observation by the neutron scattering experiments [3]. The relative local DDW peak at the core center decreases when decreasing doping. This can be explained if we note that (i) zero doping stabilizes a strong SDW order and a much smaller DDW order because of the on-site energy, which depresses the ability of the electrons’ hopping between sites, and then the DDW order can be seen to have a tendency to decrease when decreasing doping; (ii) the vortex core is a hole-poor region, relative to the region outside the core. Due to the same reason that the core has the nature of the normal state, the local peak of the DDW survives, though rather small, when decreasing doping. The CDW order always has an enhanced peak at the core center when doping level changes, and as a consequence, it is always indicating a negative vortex charge in the parameter region considered, in contrast to that of Chen [22], where a change of sign of the vortex may be possible, when vortex cores without AF are formed. This may be due to the large Coulomb on-site energy we have chosen, so that the core without AF is never stabilized.

This work is supported by the Chinese National Natural Science Foundation.
REFERENCES

[1] R. I. Miller et al., Phys. Rev. Letts 88, 137002 (2002).

[2] K. Kakuyanagi, K. Kumagai, Y. Matsuda, and M. Hasegawa, Phys. Rev. Letts 90, 197003 (2003).

[3] B. Lake et al., Science 291, 1759 (2001); B. Lake et al., Nature (London) 415, 299 (2002).

[4] J. E. Hoffman et al., Science 295, 466 (2002).

[5] S. C. Zhang, Science 275, 1089 (1997); D. P. Arovas, A. J. Berlinsky, C. Kallin, S. C. Zhang, Phys. Rev. Lett 79, 2871 (1997).

[6] D. A. Ivanov, P. A. Lee, and X. G. Wen, Phys. Rev. Letts 84, 3958 (2000).

[7] P. W. Leung, Phys. Rev. B 62, 6112 (2000).

[8] P. A. Lee, X. G. Wen, Phys. Rev. B 63, 224517 (2001); J. Kishine, P. A. Lee and X. G. Wen, Phys. Rev. Letts, 86, 5365 (2001).

[9] Q. H. Wang, J. H. Han, D. H. Lee, Phys. Rev. Letts 87, 167004 (2001).

[10] J. E. Hoffman, K. McElroy, D.-H. Lee, K. M. Lang, H. Eisaki, S. Uchida, J. C. Davis, Science 297, 1148 (2002).

[11] Q. H. Wang, D. H. Lee, Phys. Rev. B 67, 020511 (2003).

[12] M. Franz, D. E. Sheehy, and Z. Tešanović, Phys. Rev. Letts 88, 257005 (2002); M. Franz, Z. Tešanović, Phys. Rev. B 63, 064516 (2001).

[13] J. X. Zhu, I. Martin, A. R. Bishop, Phys. Rev. Letts 89, 067003 (2002); J. X. Zhu, C. S. Ting, Phys. Rev. Letts 87, 147002 (2001).

[14] H. D. Chen, J. P. Hu, S. Capponi, E. Arrigoni, S. C. Zhang, Phys. Rev. Letts 89, 137004 (2002).
[15] Y. Zhang, E. Demler, S. Sachdev, Phys. Rev. B 66, 094501 (2002).

[16] S. Chakravarty, R. B. Laughlin, D. K. Morr, C. Nayak, Phys. Rev. B 63, 094503 (2001).

[17] C. Nayak, Phys. Rev. B 62, 4880 (2000); C. Nayak, Phys. Rev. B 62, 6135 (2000).

[18] J. X. Zhu, W. Kim, C. S. Ting, J. P. Carbotte, Phys. Rev. Letts 87, 197001 (2001).

[19] See for example, Y. Wang and A. H. MacDonald, Phys. Rev. B 52, 3876 (1995); P. I. Soininen, C. Kallin, A. J. Berlinsky, Phys. Rev. B 50, 13883 (1994).

[20] In an external magnetic field, the conventional definition $|\Delta_i| = \frac{1}{4} |\Delta_{i,i+e_x} + \Delta_{i,i-e_x} - \Delta_{i,i+e_y} - \Delta_{i,i-e_y}|$ is not invariant in the gauge transformations $c_{i\sigma} \to c_{i\sigma} e^{-i\theta_i}$, $\Delta_{ij} \to \Delta_{ij} e^{-i(\theta_i + \theta_j)}$, $\varphi_{ij} \to \varphi_{ij} - \theta_i + \theta_j$.

[21] J. An and C. D. Gong, Phys. Rev. B 63, 174434 (2001).

[22] Y. Chen, Z. D. Wang, J. X. Zhu, C. S. Ting, Phys. Rev. Letts 89, 217001 (2002).
FIGURES

FIG. 1. The spatial distribution of (a) the d-wave SC order parameter, (b) electron density, (c) the staggered magnetization, (d) the DDW order parameter for a $40 \times 40$ lattice. Only the center $34 \times 34$ lattice is shown to eliminate the corners’ boundary effect. Parameter values: $t' = -0.25$, $U = 3$, $V_p = 1.3$, $V_d = 0.5$ and $n = 0.86$.

FIG. 2. The same as Fig. 1 except $V_d = 0.65$.

FIG. 3. The same as Fig. 1 except $V_d = 1.0$.

FIG. 4. The spatial distribution of (a), (c) electron density; (b), (d) the staggered magnetization; (c), (f) the DDW order parameter. Parameters have the same values as Fig. 2 except $n=0.91$ for (a), (b), (c), whereas $n=0.94$ for (d), (e), (f).
Fig. 1

An & Gong
Fig. 2  An & Gong
Fig. 3  
An & Gong
Fig. 4  An & Gong