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Vortex Charges in High-Temperature Superconductors

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Based on a model Hamiltonian with competing antiferromagnetic (AF) and *d*-wave superconductivity interactions, the vortex charge is investigated by solving the Bogoliubov–de Gennes equations. We found that the vortex charge is negative when a sufficient strength of AF order is induced inside the vortex core; otherwise, it is positive. By tuning the on-site Coulomb repulsion U or the doping parameter δ, a transition between the positive and negative vortex charges may occur. The vortex charge at optimal doping has also been studied as a function of magnetic field. Recent NMR and Hall effect experiments may be understood in terms of the present results.

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The vortex structure in high temperature superconductors (HTS) has attracted significant interest for many years. Since the parent compounds are antiferromagnetic (AF) Mott insulators, novel physical properties of HTS including those in the vortex state would be expected due to the competition between spin magnetism and superconductivity in these systems. It has been shown theoretically [1–8] that the AF order may appear and coexist with the underlying vortices. In a neutron scattering experiment by Lake *et al.* [9], a remarkable AF-like spin density wave (SDW) was observed in the optimally doped $La_{2-x}Sr_xCuO_4$ in the presence of a strong magnetic field. A muon spin rotation measurement by Miller *et al.* [10] studied the internal magnetic field distribution in the vortex cores of underdoped $YBa_2Cu_3O_{6+x}$, and it revealed a feature in the high-field tail which fits well to a model with static alternating magnetic field. A very recent nuclear magnetic resonance (NMR) experiment by Mitrovic *et al.* [11] showed that the presence of AF order is markedly enhanced in the vortex cores of near-optimally doped $YBa_2Cu_3O_{7-\delta}$. These experiments have provided a strong support for the existence of AF order inside the vortex core in appropriately doped HTS.

On the other hand, the vortex charge in superconductors has also been paid considerable attention both theoretically [12–16] and experimentally [17,18]. In the framework of the BCS theory, Blatter *et al.* [13] pointed out that for an *s*-wave superconductor the vortex charge is proportional to the slope of the density of states at the Fermi level. Hayashi *et al.* [14] proposed that the vortex charge is always holelike and is determined by the quasiparticle structure which is independent of the slope of the density of states. However, the NMR and nuclear quadrupole resonance measurements on $YBa_2Cu_3O_7$ and $YBa_2Cu_4O_8$ [18] seemed to obtain results for the vortex charge, contradictory to that predicted from the existing BCS theory regarding both sign and order of magnitude. In view of this significant deviation, together with the fact that the strong electron correlation with the *d*-wave superconducting (DSC) pairing has not been considered in the existing theories for the vortex charge, we believe that the vortex charge in HTS should be strongly influenced by the competition effect from the AF and DSC orders, of which the former will play a crucial role in determining the charge nature. Also interestingly, Hall effect experiments [17] for HTS seemed to indicate that the Hall signal is electronlike in the underdoped up to slightly overdoped regime but holelike in the overdoped regime, which could be related to the sign of vortex charge [12]. Therefore, it is important to develop a sound theory for the vortex charge with the strong electron correlation and the *d*-wave feature of HTS being taken into account.

In this Letter, we shall answer the following two crucial questions in detail: (i) What is mainly responsible for the vortex charge in the HTS? (ii) How is the sign of vortex charge affected by the doping and the on-site Coulomb repulsion U? Based on a widely adopted effective model Hamiltonian with competing SDW and DSC orders and using a well-developed numerical method [19], we study the vortex charge in the mixed state of *d*-wave HTS subjected to a strong magnetic field. It is found that the vortex charge is mainly determined by the competition of the AF order and the DSC order at the vortex core, and the electronic structure of the vortex core can contain either AF order or normal state, corresponding to a negative (electronlike) or positive (holelike) charge. By tuning U or the doping parameter, the transition between these two kinds of vortices occurs.

Let us begin with an effective model Hamiltonian in a two-dimensional (2D) lattice, in which both the DSC and SDW orders are taken into account:

$$H = -\sum_{i,j,\sigma} t_{ij} c^{\dagger}_{i\sigma} c_{j\sigma} + \sum_{i,\sigma} (U n_{i\bar{\sigma}} - \mu) c^{\dagger}_{i\sigma} c_{i\sigma} + \sum_{i,j} (\Delta_{ij} c^{\dagger}_{i\uparrow} c^{\dagger}_{j\downarrow} + \text{H.c.}) , \quad (1)$$

where $c^{\dagger}_{i\sigma}$ is the electron creation operator, μ is the

chemical potential, and the summation is over the nearest neighboring sites. In the presence of magnetic field B perpendicular to the plane, the hopping integral can be expressed as $t_{ij} = t_0 \exp[i\frac{\pi}{\Phi_0}\int_{\mathbf{r}_j}^{\mathbf{r}_i}\mathbf{A}(\mathbf{r})\cdot d\mathbf{r}]$ for the nearest neighboring sites (i, j), with $\Phi_0 = h/2e$ as the superconducting flux quantum. In the presence of a strong magnetic field, we assume the applied magnetic field to be uniform and choose a Landau gauge $\mathbf{A} = (-By, 0, 0)$. Since the internal magnetic field induced by the supercurrent around the vortex core is so small compared with the external magnetic field that the above assumption is justified. The two possible SDW and DSC orders in cuprates are defined as $\Delta_i^{\mathrm{SDW}} = U\langle c_{i\uparrow}^{\dagger}c_{i\uparrow} - c_{i\downarrow}^{\dagger}c_{i\downarrow}\rangle$ and $\Delta_{ij} = V_{\mathrm{DSC}}\langle c_{i\uparrow}c_{j\downarrow} - c_{i\downarrow}c_{j\uparrow}\rangle/2$, where U and V_{DSC} represent, respectively, the interaction strengths for two orders. The mean-field Hamiltonian (1) can be diagonalized by solving the resulting Bogoliubov–de Gennes equations self-consistently,

$$\sum_j \begin{pmatrix} \mathcal{H}_{ij,\sigma} & \Delta_{ij} \\ \Delta_{ij}^{*} & -\mathcal{H}_{ij,\bar{\sigma}}^{*} \end{pmatrix} \begin{pmatrix} u_{j,\sigma}^{n} \\ v_{j,\bar{\sigma}}^{n} \end{pmatrix} = E_n \begin{pmatrix} u_{i,\sigma}^{n} \\ v_{i,\bar{\sigma}}^{n} \end{pmatrix}, \qquad (2)$$

where the single particle Hamiltonian $\mathcal{H}_{ij,\sigma} = -t_{ij} + (Un_{i\bar{\sigma}} - \mu)\delta_{ij}$, and $n_{i\uparrow} = \sum_n |u_{i\uparrow}^n|^2 f(E_n)$, $n_{i\downarrow} = \sum_n |v_{i\downarrow}^n|^2[1 - f(E_n)]$, $\Delta_{ij} = \frac{V_{\mathrm{DSC}}}{4}\sum_n (u_{i\uparrow}^n v_{j\downarrow}^{n*} + v_{i\downarrow}^{*} u_{j\uparrow}^n) \times \tanh(\frac{E_n}{2k_BT})$, with $f(E)$ as the Fermi distribution function and the electron density $n_i = n_{i\uparrow} + n_{i\downarrow}$. The DSC order parameter at the ith site is $\Delta_i^D = (\Delta_{i+e_x,i}^D + \Delta_{i-e_x,i}^D - \Delta_{i,i+e_y}^D - \Delta_{i,i-e_y}^D)/4$ where $\Delta_{ij}^D = \Delta_{ij} \times \exp[i\frac{\pi}{\Phi_0}\int_{\mathbf{r}_i}^{(\mathbf{r}_i+\mathbf{r}_j)/2}\mathbf{A}(\mathbf{r})\cdot d\mathbf{r}]$ and $\mathbf{e}_{x,y}$ denotes the unit vector along the (x, y) direction. The main procedure of self-consistent calculation is summarized as follows. For a given initial set of parameters $n_{i\sigma}$ and Δ_{ij}, the Hamiltonian is numerically diagonalized and the electron wave functions obtained are used to calculate the new parameters for the next iteration step. The calculation is repeated until the relative difference of order parameter between two consecutive iteration steps is less than 10^{-4}. The solutions corresponding to various doping concentrations can be obtained by varying the chemical potential.

In our calculation, the length and energy are measured in units of the lattice constant a and the hopping integral t_0, respectively. Magnetic unit cells are introduced where each unit cell accommodates two superconducting flux quanta. The related parameters are chosen as follows: the DSC coupling strength is $V_{\mathrm{DSC}} = 1.2$, and the linear dimension of the unit cell of the vortex lattice is $N_x \times N_y = 40 \times 20$. This choice corresponds to the magnetic field $B \simeq 37$ T. The calculation is performed in a very low temperature regime.

Our numerical results indeed show that the AF order is absent inside the vortex core for small U and is induced when U becomes larger. In Fig. 1, we plot typically the spatial profiles of the vortex structure for two types of vortices: a normal d-wave vortex core for small $U(= 2.0)$, where the AF order is absent, and an AF core for larger $U(= 2.4)$, where the AF order is nucleated and spreads out from the core center. They are obtained at the optimal doping $\delta = 0.15$. Figures 1(a)–1(c) correspond to the normal core while 1(d)–1(f) for the AF core. Figures 1(a) and 1(d) illustrate the DSC order parameter pattern, which vanishes at the vortex core center. The center of the vortex core is situated at site (10, 10). Figures 1(b) and 1(e) display the spatial distribution of the staggered magnetization of the induced AF-like SDW order defined as $M_i^s = (-1)^i\Delta_i^{\mathrm{SDW}}/U$. No AF order is seen in the normal core (for $U = 2.0$) while the AF order exists both inside and outside the core (for $U = 2.4$) and behaves like a two-dimensional SDW with the same wavelength in the x and y directions. The size of the AF core here is slightly enlarged from that of the normal core. The induced SDW order reaches its maximum value at the vortex core center and its spatial profile retains the same fourfold symmetry as that of the pure DSC case. The orders of DSC and SDW coexist throughout the whole sample. The appearance of the SDW order around the vortex cores strongly enhances the net electron density (or depletion of the hole density) at the vortex core as shown in Fig. 1(f).

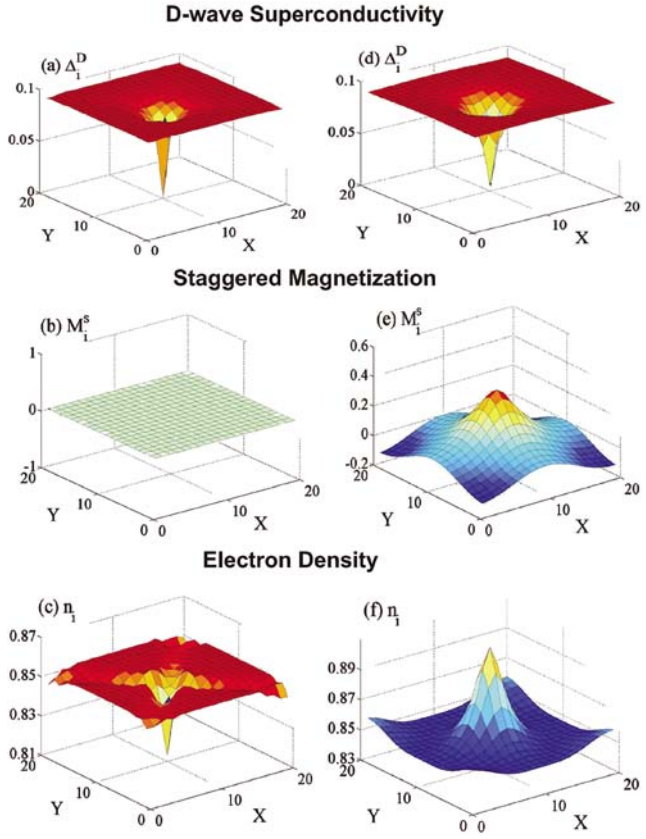

FIG. 1 (color online). Spatial variations of the DSC order parameter Δ_i^D [(a) and (d)], staggered magnetization M_i^s [(b) and (e)], and net electron density n_i [(c) and (f)] in a 20×20 lattice. The left panels [(a), (b), and (c)] and the right panels [(d), (e), and (f)] are for $U = 2.0$ and $U = 2.4$, respectively. The averaged electron density is fixed at $\bar{n} = 0.85$.

An intuitive physical understanding of positive charge for the normal vortex core can be given as follows: for a particle-hole asymmetric system like doped cuprates, the chemical potential for electrons in DSC state would be slightly lower than that of the normal state, when a normal core is imbedded into the DSC background and in order to reach equilibrium, electrons have to flow from the inside to the outside of the core which leads to the electron depletion inside the vortex core, as shown in panel 1(c); while in the case of AF core, the hole number is suppressed and as a result, the vortex carries negative charge. The enhancement of electron number inside the AF vortex core has also been numerically obtained by other calculations [5–8].

To examine the vortex charge Q_v as functions of both δ and U, the upper right inset in Fig. 2 plots the phase diagram of δ versus U for positively (hole-rich) and negatively (electron-rich) charged vortices. It is obvious that the AF vortex core can easily show up in the underdoped regime or with stronger AF interaction, while normal core tends to exist in the overdoped regime or with weaker AF interaction. The electron density inside the core is higher than the average density in the underdoped region, while the electron density becomes lower than the average in the overdoped region. There exists a clear boundary between these two phases. The AF order is generated in the region where the DSC order parameter is suppressed. To estimate the core charge of a single vortex, we first determine the vortex size by examining the spatial profile of DSC order parameter. Next we make a summation of the net electron density inside the vortex core. As shown in Fig. 2, the δ dependence of Q_v/e (the electron number) for $U = 2.4$ exhibits a first-order-like transition at $\delta = \delta_c$ (~ 0.18). The magnitude of the discontinuity reduces to one-third when $U = 2.2$. The critical value of the doping level δ_c is U-value dependent or sample dependent. The larger U case corresponds to larger δ_c. Recent NMR experiments [11] indicated that the AF order exists in the vortex core at the optimal doping level in cuprates, which may imply that the critical doping level δ_c could be extended to a slightly overdoped region. Therefore, it is clear that the related phenomena in the slightly overdoped sample may be qualitatively the same as those in the underdoped sample; e.g., the slightly overdoped sample has the electron-rich vortex core as well. This result agrees well with the experiment for slightly overdoped $YBa_2Cu_3O_7$ [18], in sharp contrast to the hole-rich vortex core predicted by the BCS theory. Also interestingly, even though the origin of Hall sign anomaly is still debatable [20], the vortex charge could make an additional contribution to the sign change in the mixed state Hall conductivity [12]. Our calculations, which are schematically shown in the lower left inset of Fig. 2, would favor that the Hall signal is electronlike from the underdoped to slightly overdoped regime but holelike in the appreciable overdoped regime. This result is consistent with the phase diagram obtained by the Hall effect measurements [17].

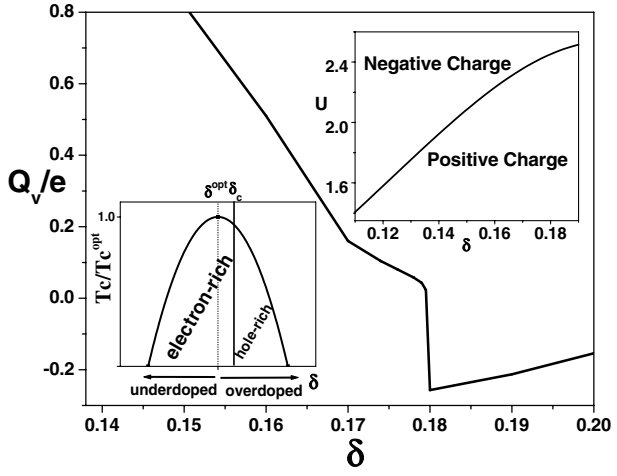

FIG. 2. Doping dependence of the number of vortex charge Q_v/e for $U = 2.4$ where the electron charge $e < 0$. The left inset shows the doping dependence of the sign of the vortex charge (positive for hole rich and negative for electron rich). δ^{opt} and δ_c denote, respectively, the optimal doping and critical doping. The right inset represents the phase diagram of doping level versus interaction strength U for a positive and negative charged vortex.

In addition, the charge magnitude estimated from the BCS theory [13] is two orders smaller than that of experimental observation for HTS. The magnitude of vortex charge estimated from our calculation is about $0.06e$ at 22 tesla, which seems much larger than the experimental estimation $0.005e$-$0.02e$ at 9.4 T for $YBa_2Cu_3O_7$ [18]. The reason appears to be mainly due to a much higher magnetic field used in our calculation, which will lead to a larger AF order. The inset of Fig. 3 represents the approximate extrapolation of the vortex charge magnitude versus the magnetic field. The estimated vortex charge at 9.4 tesla is indeed in the same order of magnitude as reported in the experiment. From Fig. 3, one can clearly see an abrupt jump for the number of vortex charge Q_v/e and staggered magnetization at the vortex core center M_c^s as U varies around 2.11, and this positively or negatively charged vortex transition appears also to be first-order-like. It is now quite clear that the vortex charge is strongly influenced by two competing effects—the suppression of the DSC order at the core center which leads to the depletion of the electrons and the induction of the AF order which favors the accumulation of electrons. Whether the negative vortex charge appears depends solely on whether there is a sufficient AF order inside the vortex core, as is clearly seen in Fig. 3. Although our calculation is based upon the phenomenological Hamiltonian, our results are robust despite different band parameters and should give a qualitative description on the vortex physics in HTS.

We now turn to discuss the experimental results for strongly underdoped $YBa_2Cu_4O_8$ [18] where a positively charged vortex is reported. This seems to be inconsistent

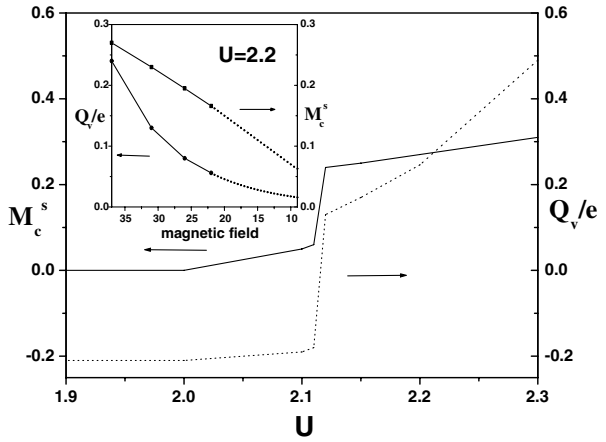

FIG. 3. The interaction strength dependence of the staggered magnetization M_c^s (solid line) at the vortex center and the number of vortex charge Q_v/e (dotted line). The averaged electron density is fixed at $\bar{n} = 0.85$. The inset shows the extrapolation of Q_v/e and M_c^s with magnetic field strength in units of tesla.

with our prediction. We believe that the vortex charge in the above experiment was deduced from an oversimplified assumption that the electron density is uniform either in the absence of magnetic field or far away from the vortex core in this strongly underdoped HTS. In fact, experiments showed clearly the remarkable inhomogeneities in the underdoped sample [21,22]. Many theoretical studies including the present one also show the presence of stripelike charge density structures in the strongly underdoped sample [5,7,23,24]. Upon the application of a magnetic field, the spatial charge distribution could become more inhomogeneous even away from the vortex core. Therefore, their estimation of the vortex charge for the underdoped $YBa_2Cu_4O_8$ might be invalid. For the slightly overdoped HTS, the sample is less inhomogeneous, and their estimation may be qualitatively correct.

With respect to the complexity of the underdoped case, we suggest to use the spatially resolved high magnetic field NMR [11] to probe the vortex charge. In this way, a clear resolution of the vortex core region can be reached since the fraction of the spectrum inside the core grows with the increase of the magnetic field. It seems better to probe the vortex charge in slightly underdoped samples to test our results because the strongly underdoped samples have the complications mentioned above. We would also like to pinpoint that the high resolution STM may be a good candidate to probe the vortex charge by integrating the local density of states up to the chemical potential. The spatial electron density distribution can also be directly imaged by the electrostatic force microscope, which detects the force gradient acting on the tip, and the scanning surface potential microscopy, which measures the first harmonic of the force. If the vortex indeed possesses the charge as we find here, these direct imaging techniques can be utilized as powerful tools to study the vortex dynamics in HTS.

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