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Author(s)	Han, Q; Wang, ZD; Li, XG; Zhang, LY
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Impurity state in the vortex core of d -wave superconductors: Anderson impurity model versus the unitary impurity model

Qiang Han,^{1,2} Z. D. Wang,^{1,2,3,*} X.-G. Li,¹ and Li-yuan Zhang⁴¹Structure Research Laboratory, Department of Material Science and Engineering, University of Science and Technology of China, Hefei Anhui 230026, China²Department of Physics, University of Hong Kong, Pokfulam Road, Hong Kong, China³Texas Center for Superconductivity, University of Houston, Houston, Texas 77204⁴Department of Physics, Peking University, Beijing 100871, China

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Using an extended Anderson/Kondo impurity model to describe the magnetic moments around an impurity doped in high- T_c d -wave cuprates and in the framework of the slave-boson mean-field approach, we study numerically the impurity state in the vortex core by exact diagonalization of the well-established Bogoliubov–de Gennes equations. The low-energy impurity state is found to be in good agreement with scanning-tunneling-microscopy observation. After pinning a vortex on the impurity site, we compare the unitary impurity model with the extended Anderson impurity model by examining the effect of the magnetic field on the impurity state. We find that the impurity resonance in the unitary impurity model is strongly suppressed by the vortex, while it is insensitive to the field in the extended Anderson impurity model.

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Effects of nonmagnetic impurities, such as zinc, doped in the CuO_2 plane of high- T_c materials have attracted much attention in recent years as it may help us to better understand the underlying mechanism of high- T_c superconductivity.¹ The low-energy (near zero) impurity resonant state in d -wave superconductors was first predicted in Refs. 2–4 based on a unitary scattering-potential impurity model and later successfully observed in a series of beautiful atomic-scale scanning-tunneling-microscopy (STM) experiments.^{5–7} in the vicinity of individual Zn ions in $\text{Bi}_2\text{Sr}_2\text{Ca}(\text{Cu}_{1-x}\text{Zn}_x)_2\text{O}_{8+\delta}$. Since Zn^{++} has no spin itself (and is therefore nonmagnetic), it is natural to treat the impurity as a pointlike scalar potential scatterer of conduction electrons. Indeed, both energy position and fourfold-symmetric spatial distribution⁷ of the local density of states (LDOS) of quasiparticles can be explained consistently by theoretical calculations based on the t -matrix scattering-potential theory in the unitary limit.³ Nevertheless, the sign and magnitude of the scattering potential as well as the particle-hole symmetry play a crucial role in determining the exact energy level of impurity resonant state relative to Fermi energy. The scattering potential chosen in various theoretical studies differs largely from -4.4 eV to 18.9 eV.^{8–10} The continuum t -matrix theory, which assumed particle-hole symmetry and *repulsive* potential, predicted impurity states with energy³ consistent with the STM observation⁷ that the resonance lies slightly below the Fermi level; on the other hand, the particle-hole symmetry is not applicable to high- T_c cuprates, and theoretical calculations^{9,10} show that in the absence of such symmetry only strong *attractive* potential can produce or impurity state with negative energy while repulsive potential¹⁰ gives positive energy contrary to experiment results. Furthermore, the unitary impurity model has difficulty in accounting for the spectra distribution pattern of differential conductances at the resonance energy. The experiment shows that the zero-bias peak is strongest on the Zn

ion with a local maximum on its second-nearest-neighbor Cu sites⁷ while the unitary impurity model concluded that the spectral weight on an Zn atom is negligibly small and local maximum peaks are on nearest-neighbor Cu sites of the impurity.^{3,11,10} In order to reconcile the apparent discrepancy, the effect of the interlayer tunneling matrix elements, such as a blocking effect of a BiO layer¹¹ and a fork model,¹⁰ have been employed to reproduce the distribution of spectral weight. At present, whether the spatial pattern of the tunneling conductance of the impurity resonance is intrinsic in the CuO_2 plane or the interlayer tunneling effect must be considered is still an open question for both theoretical investigation and further experimental examination. Recently, several alternative theoretical models^{8,9,12,13} have been suggested, which take the effect of the Kondo screening of the local magnetic moments induced around the zinc atom into account, mostly motivated by the observation of nuclear-magnetic-resonance^{14–16} (NMR) and neutron-scattering experiments^{17,18} that staggered magnetic moments are developed around the Zn ion with a total net spin 1/2. When Kondo spin dynamics of such moments was considered, by including an exchange interaction between the induced spin and the spin of conduction electrons in the model Hamiltonian, Polkovnikov *et al.*⁹ produced an impurity state whose energy dependence and spatial pattern may fit well with STM spectra, without a strong scattering potential and the specific characteristic of interlayer tunneling matrix elements.

Motivated by the above controversy between the unitary impurity model and the model invoking induced magnetic moments, in this work we intend to compare these two models in the case that a single vortex line is pinned by the impurity. To describe the Kondo effect of the magnetic moments and the effect of the vortex, we introduce an extended Anderson impurity model with a phase factor dependent on site and vortex. In the absence of the vortex, both models with appropriate parameters can generate low-lying impurity

states. However, when a vortex is present, for the unitary impurity model, the pronounced LDOS peak generated around the Zn impurity is largely decreased or even destroyed, indicating the vanishing of the impurity resonance by the vortex core, while for the extended Anderson impurity model, the existence of the vortex center has a weak effect on the impurity state. Such a difference may be examined readily by STM experiments on $\text{Bi}_2\text{Sr}_2\text{Ca}(\text{Cu}_{1-x}\text{Zn}_x)_2\text{O}_{8+\delta}$ samples subject to a strong magnetic field.

In this work, we adopt an extended Hubbard model on a two-dimensional (2D) lattice with nearest-neighbor (NN) hopping and NN pairing interaction to model the d -wave high- T_c cuprates and the extended Anderson impurity model to describe the magnetic moments around the impurity (zinc ion) doped in the CuO_2 plane. The model Hamiltonian is expressed as

$$H = H_{\text{dsc}} + H_{\text{imp}}, \quad (1)$$

where

$$H_{\text{dsc}} = - \sum_{\langle i,j \rangle \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \sum_{\langle i,j \rangle \sigma} (\Delta_{ij} c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger + \text{H.c.}) - \sum_{i,\sigma} \mu c_{i\sigma}^\dagger c_{i\sigma}, \quad (2)$$

and

$$H_{\text{imp}} = H_{\text{mag}} + V_I c_{0\sigma}^\dagger c_{0\sigma}. \quad (3)$$

Here H_{dsc} is the BCS-like Hamiltonian of the host d -wave superconductor described on a 2D lattice. $\langle i,j \rangle$ refers to the NN sites and t_{ij} the hopping integral between sites i and j . μ is the chemical potential. $\Delta_{i,j}$ is the bond pairing potential defined as $\Delta_{ij} = -V_d \langle c_{i\downarrow} c_{j\uparrow} \rangle$ with V_d the effective pairing strength between electrons on NN sites. H_{imp} represents the impurity Hamiltonian which includes both an on-site scattering-potential term represented by V_I and the term H_{mag} describing the local moments around the impurity. As suggested by NMR experiments,^{14–16} the induced magnetic moments with net spin 1/2 are mainly located at the four NN Cu sites of the central Zn impurity site $\mathbf{r}_0 = (0,0)$ while negligibly right on the Zn site; therefore, as in Ref. 9, we assume that the magnetic impurity with an effective 1/2 spin may reside only in the NN sites and couples with conduction electrons on the NN sites. Namely, the H_{mag} may be modeled by the extended Anderson impurity model with strong Hubbard repulsion U_d as $H_{\text{mag}} = \sum_{\sigma} \epsilon_d d_{\sigma}^\dagger d_{\sigma} + U_d d_{\uparrow}^\dagger d_{\downarrow}^\dagger d_{\downarrow} d_{\uparrow} + \sum_{\mathbf{r}_i = \tau, \sigma} V_h(i) (e^{i\phi_i} c_{i\sigma}^\dagger d_{\sigma} + \text{H.c.})$ with $\tau = \pm \hat{\mathbf{x}}, \pm \hat{\mathbf{y}}$ unit vectors, where ϵ_d is the d -electron energy level and V_h is the hybridization of the moments with the conduction electrons. As a modification to the coupling term in the ordinary Anderson impurity model, we here introduce a site-dependent phase factor ϕ_i , which is found to be quite crucial in determining the energy level and even the existence of the impurity state if V_I is not so strong. Note that under the mean-field decoupling scheme of Ref. 19, the present model for H_{mag} is essentially equivalent to the magnetic impurity (Kondo) model in Ref. 9, where it is written as $\sum_i K_i \mathbf{S} \cdot \mathbf{s}(i)$

with the summation being over the NN sites of the impurity, and $\mathbf{S} = \sum_{\alpha\beta} d_{\alpha}^\dagger \sigma_{\alpha\beta} d_{\beta} / 2$ and $\mathbf{s} = \sum_{\alpha\beta} c_{\alpha}^\dagger \sigma_{\alpha\beta} c_{\beta} / 2$ representing, respectively, the spin operators of the magnetic impurity and the conduction electrons. This is because this spin-exchange term can be transformed by the mean-field decoupling scheme in Ref. 19: $K \sum_i \mathbf{S} \cdot \mathbf{s}(i) \rightarrow -3K/8 \sum_{\sigma} [\chi_i^* c_{i\sigma}^\dagger d_{\sigma} + \text{H.c.}]$, where a complex Hubbard-Stratonovich field $\chi_i = \langle c_{i\sigma}^\dagger d_{\sigma} \rangle$ is introduced as an effective hopping amplitude between the d -level and conduction electrons. At this stage, one can see clearly that the phase factor ϕ_i introduced in our model and that of the field χ_i are closely related. Assuming the fourfold rotational symmetry with respect to the impurity site, there are four inequivalent arrangements of ϕ_{τ} , that is,

$$\phi_{\tau}^{(m)} = m \times \theta(\tau), \quad (4)$$

with $m = 0, 1, 2$, and 3, $\theta(\pm \hat{\mathbf{x}}) = (\pi/2) \mp (\pi/2)$, and $\theta(\pm \hat{\mathbf{y}}) = \pm (\pi/2)$. In Ref. 9, a nontrivial d -wave pattern of χ_i has been found to have the lowest free-energy saddle point, whose phase corresponds to $m = 2$, matching the underlying symmetry of local bond pairing potential $\Delta_{0,i}$. When the vortex exists, the symmetry of the underlying pairing potential would change from the local d -wave pattern to that responding to the winding of phase. Therefore, it appears reasonable to expect that ϕ might change from $m = 2$ to $m = 1$ as a vortex is pinned at the impurity site. We find that such a response of ϕ to the magnetic field is quite crucial in keeping the impurity state in the vortex core.

In the treatment of the extended Anderson impurity model at low temperatures, U_d is assumed to be infinite as usual, which forbids double occupancy of electrons on the d level. Therefore, the slave-boson mean-field theory^{20,21} can be applied as in Refs. 8 and 22 where the d -electron operator is written as $d_{\sigma}^\dagger = f_{\sigma}^\dagger b$ with f_{σ} the spin-carrying fermion operator and b the holon operator. Furthermore, the single occupancy constraint $\sum_{\sigma} f_{\sigma}^\dagger f_{\sigma} + b^\dagger b = 1$ should be obeyed. At the mean-field level, the holon operators b and b^\dagger are approximated by a c number b_0 and the constraint is enforced on average by introducing a Lagrange multiplier λ_0 . Accordingly, the mean-field H_{imp} becomes

$$H_{\text{imp}} = \sum_{\sigma} \tilde{\epsilon}_d f_{\sigma}^\dagger f_{\sigma} + \sum_{\mathbf{r}_i = \tau, \sigma} \tilde{V}_h(i) (e^{i\phi_i} c_{i\sigma}^\dagger f_{\sigma} + \text{H.c.}) + V_I c_{0\sigma}^\dagger c_{0\sigma} + \lambda_0 (b_0^2 - 1) \quad (5)$$

with renormalized parameters $\tilde{\epsilon}_d = \epsilon_d + \lambda_0$ and $\tilde{V}_h = V_h b_0$. By applying the self-consistent mean-field approximation and performing the Bogoliubov transformation, diagonalization of the Hamiltonian can be achieved by solving the following Bogoliubov–de Gennes (BdG) equations:

$$\sum_j \begin{pmatrix} H_{i,j} & \Delta_{i,j} \\ \Delta_{i,j}^* & -H_{i,j}^* \end{pmatrix} \begin{pmatrix} u_j^n \\ v_j^n \end{pmatrix} = E_n \begin{pmatrix} u_j^n \\ v_j^n \end{pmatrix}, \quad (6)$$

where u^n, v^n are the Bogoliubov quasiparticle amplitudes with a corresponding eigenvalue E_n and $H_{i,j} = -\delta(\mathbf{r}_i + \tau - \mathbf{r}_j) [t_{i,j \neq i_d} - (\delta_{i,i_d} + \delta_{j,i_d}) \tilde{V}_h e^{i\phi_{\tau}}] - \delta_{i \neq i_d, j} [\mu - \delta(\mathbf{r}_i - \mathbf{r}_0) V_I] + \delta_{i,i_d} \tilde{\epsilon}_d$. Here, i, j represent the index of the

2D lattice sites with i_d as the index for the magnetic moment residing on the NN sites of the doped impurity. $\Delta_{i,j}$ is defined between a pair of NN sites on the 2D lattice and is calculated according to the self-consistent conditions

$$\Delta_{i,j} = \frac{V_d}{2} \sum_n (u_i^n v_j^{n*} + u_j^n v_i^{n*}) \tanh\left(\frac{E_n}{2k_B T}\right) \quad (7)$$

and

$$b_0^2 = 1 - 2 \sum_n \{|u_{i_d}^n|^2 f(E_n) + |v_{i_d}^n|^2 [1 - f(E_n)]\}. \quad (8)$$

Once the BdG Eq. (6) is solved self-consistently, the quasi-particle spectrum can be obtained, and the LDOS proportional to the differential tunneling conductance observed in STM experiments is given by

$$\rho(\mathbf{r}_i, E) = - \sum_n [|u_i^n|^2 f'(E_n - E) + |v_i^n|^2 f'(E_n + E)], \quad (9)$$

where $f(E)$ represents the Fermi distribution function.

I. UNITARY IMPURITY MODEL

First, we study the variation of the impurity state when a vortex line is sitting on the impurity site within a unitary impurity model. Exact diagonalization is applied and the BdG equations are solved self-consistently. In studying the electronic structure of the vortex lattice in d -wave superconductors, a magnetic unit cell which accommodates two vortices is usually employed in numerical studies.^{23–27} Such a method has been applied to treat impurity effects in the mixed state of s -wave²⁸ and d -wave²⁹ superconductors. The primitive translation vectors of the magnetic unit cell are $\mathbf{R}_x = aN_x \hat{x}$ and $\mathbf{R}_y = aN_y \hat{y}$, where a is the lattice constant and will be set as unity. The pairing potential winds by 4π around the magnetic unit cell. The quasiparticle amplitudes u^n and v^n are classified by the magnetic Bloch quasimomentum \mathbf{k} .

The parameters we choose are $\mu = -0.2t$, $V_d = 2.2t$ which give rise to $\Delta_d = 0.274t$ (accordingly, $\Delta_{\max} \simeq t$) and $T_c = 0.45t$. We here intentionally take a relatively large amplitude of the energy gap Δ_{\max} with respect to real materials, because a large energy gap can sufficiently lower the LDOS peak corresponding to the vortex core states and in our case a broad structure is achieved near the vortex center,³⁰ which enables us to distinguish the LDOS peak of the unitary impurity from that corresponding to the vortex core states. The on-site attractive scattering potential is chosen as $V_I = -10t$. In Fig. 1 the LDOS at the NN site of Zn site is plotted. In the absence of magnetic field (dashed line), a sharp peak is found at $E_0/\Delta_{\max} = -0.02$ corresponding to the impurity resonance. In the inset, the spatial distribution of the LDOS at resonance energy, $\rho(\mathbf{r}, E_0)$, is shown, indicating that the spectral weight is concentrated at the NN sites of the impurity while it is vanishingly small at the impurity site. These results are qualitatively consistent with previous nu-

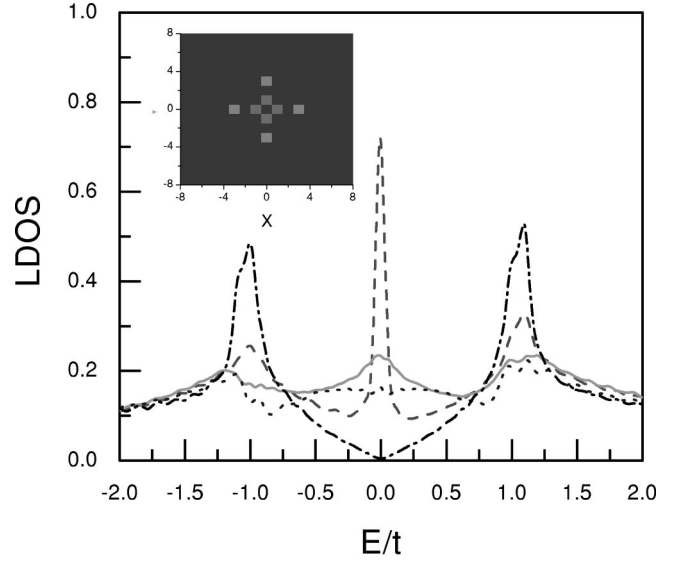


FIG. 1. LDOS versus energy at an NN site within the unitary impurity model for the cases (i) without a vortex (dashed line), (ii) a vortex pinned at the impurity site (solid line), and (iii) a vortex core without impurity (dotted line). The bulk density of states is also plotted for reference (dash-dotted line). Inset shows the spatial distribution of the LDOS at energy $E_0/\Delta_{\max} = -0.02$ in a 16×16 region for case (i).

merical investigations. When a vortex is pinned right on the impurity site, from Fig. 1 (solid line) we can see that the LDOS peak at the NN site of Zn is significantly suppressed and mixes with the vortex core states without identification of the impurity resonance state any more. As a strong scattering potential, the unitary impurity can drive the spectral weight on it mainly to its NN sites no matter if the vortex is present or not. However, in the absence of the vortex, the LDOS at a specific energy is raised, leading to a resonance state, while in the presence of a vortex, the LDOS on NN sites is increased in a wide energy range as seen in Fig. 1 and thus it is more reasonable to state that the vortex core states are strengthened by the impurity scattering. Broadening of the impurity resonance state by the magnetic field exists when the supercurrent of the vortex disturbs the energy spectrum of d -wave superconductors *via* a Doppler shift.³¹ However, in our case the smearing of the impurity resonance state is not induced by the supercurrent because the impurity is on the vortex center where supercurrent is zero. We attribute it to the nature of topological singularity of the vortex center where the phase of pairing potential varies arbitrarily, which makes the vortex center itself a strong scatter of electrons.³² Therefore, it is the vortex that modifies the background electronic structure which is responsible for the impurity resonance and accordingly makes the impurity resonance indiscernible.

II. EXTENDED ANDERSON IMPURITY MODEL

We now address the impurity state in the presence of Kondo screening of the magnetic moments described by the extended Anderson impurity model. First we consider the

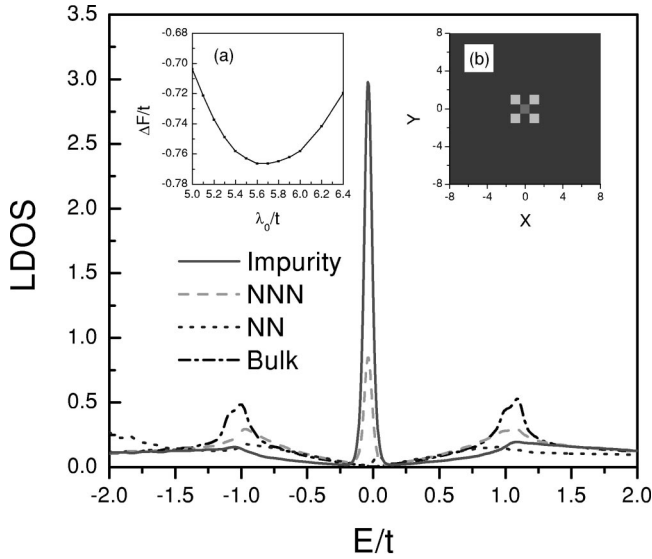


FIG. 2. LDOS versus energy at the impurity site (solid line), next-NN site (dashed line), and NN site (dotted line) under zero field within the extended Anderson impurity model. The bulk density of states is also plotted for reference (dash-dotted line). (a) shows the variation of ΔF as a function of λ_0 and (b) gives the spatial distribution of the LDOS at energy $E_0/\Delta_{\max} = -0.04$.

case in the absence of applied magnetic field. We set $m = 2$ in Eq. (4) in consideration of free-energy minimization.⁹ The exact diagonalization is performed on a 24×24 square lattice, which is seen to be sufficiently large due to the localized feature of the impurity state. The scattering potential V_I is simplified as zero (the role of nonzero V_I will be discussed later). The bare d level is set as $\epsilon_d = -4t$ and the coupling strength $V_h = 2t$ (Kondo screening regime). The value of the Lagrange multiplier λ_0 is determined by minimizing the free energy of the system as indicated in the inset of Fig. 2 and the corresponding value of b_0 is calculated self-consistently according to Eq. (8). In the inset of Fig. 2, ΔF as a function of λ_0 is plotted, where ΔF represents the change of the free energy when the local magnetic moments couple with conduction electrons. We find that for the chosen parameters the lowest free energy occurs when $\lambda_0 \approx 5.6t$ with $b_0 \approx 0.64$. Figure 2 gives LDOS on the Zn site, its NN site, and next-NN (NNN) site. There is a sharp peak at the energy $E_0/\Delta_{\max} = -0.04$, which is well consistent with STM measurement. Right on the Zn site, the peak is strongest and local maximum peaks are on the NNN sites, while on the NN sites peaks are rather weak and also at $-E_0/\Delta_{\max} = 0.04$. The spatial distribution of the LDOS at E_0 is shown in the inset of Fig. 2, also in agreement with STM spectra⁷ and with a theoretical study based on another approach on an essentially equivalent model.⁹ Our analysis shows that the impurity state induced by the magnetic moment is a bound state with a very short attenuation length $\sim \sqrt{2}a$.

Recent STM measurements³³ of impurity states induced by Zn^{++} and Mg^{++} doped in $\text{YBa}_2\text{CuO}_{6.9}$ reported that the

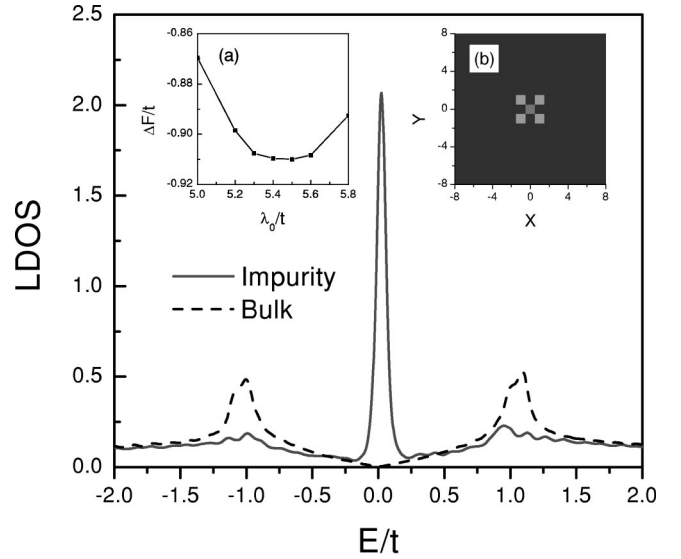


FIG. 3. Same as in Fig. 2 except that a vortex is pinned on the impurity site. (b) gives the spatial distribution of the LDOS at energy $E_0/\Delta_{\max} = 0.02$.

resonance energies are at (-10 ± 2) and (4 ± 2) meV, being not necessarily near zero bias. Based on our model, with the fixed coupling strength, e.g., $V_h = 2t$, both the bare d level ϵ_d and on-site scattering potential V_I could adjust the resonance position of the impurity state. When $V_I = 0$ and ϵ_d ranges from 0 to $-4t$, E_0/Δ_{\max} varies from -0.18 to -0.04 . An attractive (negative) V_I drives the energy position below the Fermi level further (e.g., when $V_I = -1t$, E_0/Δ_{\max} varies from -0.42 to -0.26 as ϵ_d ranges from 0 to $-4t$), while a repulsive one makes the resonance energy approach or even cross the Fermi level and become positive (e.g., when $V_I = t$, $E_0/\Delta_{\max} = 0.25$ with $\epsilon_d = -4t$). However, too large V_I ($\gg t$) can affect the spin-induced impurity state strongly and double-resonance peaks^{13,34} are found in the unitary limit, which disagrees with the STM spectra.

When a vortex is pinned on the impurity site, we expect that there is a rearrangement of $\phi_r^{(m)}$ according to the winding of the phase of the order parameter so that the phases of the Hubbard-Stratonovich field χ_i and the local bond pairing potential between NN sites $\Delta_{0,i}$ have the best match. Therefore, m will vary from 2 to 1 when a vortex is present. This is quite important as other choices of m (0,2,3) are found to result in the disappearing of the impurity state. The numerical results are shown in Fig. 3, which plots the LDOS as a function of energy on the impurity site. A strong single peak is seen near the Fermi level, indicating that the impurity state still survives under the field. Being different from the case without a vortex, the peak is lowered slightly and moved to positive bias $E_0/\Delta_{\max} = 0.02$, while the spatial pattern of the impurity state is not modified (see the inset of Fig. 3).

In summary, we have compared the extended Anderson impurity model with the unitary impurity model by studying numerically the impurity state of a d -wave superconductor as

a vortex is pinned on the impurity site. We find that the impurity resonance governed by the scattering-potential mechanism is sensitive to the presence of a vortex, while the impurity bound state generated from the magnetic-moments mechanism seems rather robust to the field. Therefore, it may be helpful to clarify the dominant mechanism of the impurity state in Zn or Mg impurity-doped cuprates by examining the existence of the impurity resonance, the variation of its energy, and even the STM spatial pattern in the presence of a strong magnetic field.

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*Author to whom correspondence should be addressed. Email address: zwang@hkucc.hku.hk

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