IMPURITY BOUND STATES IN THE PSEUDOGAP PHASE OF HIGH-T_c CUPRATES*

David Parker, Kazumi Maki and Stephan Haas

Department of Physics and Astronomy, University of Southern California
Los Angeles, CA 90089-0484, USA

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We study the impurity bound states in d-wave charge and spin density wave (CDW & SDW) phases, which are candidate models for the pseudogap regime in the high-T_c cuprates. The Bogoliubov–de Gennes equations for a single impurity are solved. When the impurity is nonmagnetic, there is no distinction between CDW and SDW. The bound state wave function exhibits a fourfold symmetry pattern analogous to the d-wave superconducting phase. In addition, the wave function exhibits a checkerboard-like pattern, previously observed around the vortex bound states in the underdoped region of Bi2212. These predictions should be readily accessible to scanning tunneling microscope experiments.

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After a long controversy a new picture of the pseudogap phase in the cuprate superconductors is emerging. It now appears that T^* is not a crossover temperature, but rather indicates the transition temperature T_c to a condensed phase. So far d-wave charge density wave (CDW) [1, 2] and d-wave spin density wave (SDW) [3] have been proposed to describe this regime. The $d_{x^2-y^2}$-wave nature of the energy gap in the pseudogap regime is well known from angle resolved photoemission studies [4]. More recently, the nature of the pseudogap phase has been explored by neutron scattering [5] and optical dichroism [6] measurements. We have recently argued that these two experiments favor SDW over CDW [7].

Here we consider a single nonmagnetic impurity in CDW or SDW. For a nonmagnetic impurity there is no difference between CDW and SDW. The Bogoliubov–de Gennes equations for $d_{x^2-y^2}$-wave CDW are given by [8]

$$Eu(\boldsymbol{r}) = \left(-\frac{\nabla^2}{2m} - \mu - V(\boldsymbol{r})\right) u(\boldsymbol{r}) + \frac{1}{p_F^2}\Delta(\partial_x^2 - \partial_y^2)v(\boldsymbol{r})\,, \qquad (1)$$

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$$Ev(\boldsymbol{r}) \;=\; -\left(-\frac{\nabla^2}{2m}+\mu+V(\boldsymbol{r})\right)v(\boldsymbol{r})+\frac{1}{p_{\mathrm{F}}^2}\Delta(\partial_x^2-\partial_y^2)u(\boldsymbol{r})\,, \qquad (2)$$

where μ is the chemical potential, p_{F} is the Fermi momentum, and $V(\boldsymbol{r}) = V_0\delta^2(\boldsymbol{r}) > 0$ is an isotropic impurity scattering potential, centered at $\boldsymbol{r} = \boldsymbol{0}$.

Compared with the equations for a d-wave superconductor, the sign of the $\mu + V(\boldsymbol{r})$ term in the second equation has changed. But otherwise the BdG equations have the same structure. Also, as in our earlier analysis we consider a strong impurity potential, $V(\boldsymbol{r}) \approx \Delta$, where Δ is the superconducting order parameter for $T = 0\,\mathrm{K}$. As to the actual value of Δ, the available data indicates $\Delta = 2.14\,T_{\mathrm{c}}$ if we identify $T_{\mathrm{c}} = T^*$ [9]. Indeed, we may take this as evidence that the underlying density wave has d-wave symmetry. In the limit $|\mu| \ll \Delta$, Δ should be the same as for d-wave superconductors in the weak-coupling limit [10].

We find a variational solution of the BdG equations by making use of the Ansatz [8]

$$u(\boldsymbol{r}) \;=\; A\exp\left(-\gamma r\right)\left(J_0(p_{\mathrm{F}}r)+\sqrt{2}\beta J_4(p_{\mathrm{F}}r)\cos\left(4\phi\right)\right)\,, \qquad (3)$$

$$v(\boldsymbol{r}) \;=\; \sqrt{2}A\alpha\exp\left(-\gamma r\right)J_2(p_{\mathrm{F}}r)\cos\left(2\phi\right)\,, \qquad (4)$$

where $J_l(p_{\mathrm{F}}r)$ are Bessel functions of the first kind, α, β, and γ are variational parameters, and A is a global normalization factor. Inserting this into Eqs. (1) and (2) we obtain

$$\begin{aligned} E &= K-V-\frac{\Delta\alpha}{\sqrt{2}}\,,\\ (E+2\mu)\alpha &= -K\alpha-\frac{\Delta\left(1+\frac{\beta}{\sqrt{2}}\right)}{\sqrt{2}}\,,\\ E\beta &= K\beta-\frac{\Delta\alpha}{2}\,, \end{aligned} \qquad (5)$$

where $K \simeq \gamma^2/2m$, and $V = \langle V(\boldsymbol{r})\rangle$.

Let us now consider a strong-scattering Zn impurity. In Bi2212 this gives rise to a bound state at $E \to 0$ [11]. Assuming $V \approx \Delta$ as in Ref. [8], we obtain $K = 0.3\Delta$, $\alpha = -0.8$, and $\beta = -1.33$. Then the differential tunneling conductance is given by

$$\frac{\partial I}{\partial V}(\boldsymbol{r},V) \propto \mathrm{sech}^2\left(\frac{eV-E_0}{2T}\right)\times\left|u(\boldsymbol{r})+\cos\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi y}{a}\right)v(\boldsymbol{r})\right|^2. \qquad (6)$$

The conduction at $eV = E_0$ is dominated by the above combination of $u(\boldsymbol{r})$ and $v(\boldsymbol{r})$. Two brief comments on this result are in order:

1. Unlike d-wave superconductors, both $u(\boldsymbol{r})$ and $v(\boldsymbol{r})$ are hole wave functions. Furthermore, $v(\boldsymbol{r})$ has an extra phase factor $\exp(-i\boldsymbol{Q}\cdot r)$ relative to $u(\boldsymbol{r})$, where $\boldsymbol{Q}$ [*e.g.* $(\pi/a,\pi/a)$] is the nesting vector. Since there are four nesting vectors, the sum over these four vectors gives the wave function in Eq. (6).

2. There is another solution with the dominant $v(\boldsymbol{r})$ component at $E = E_0 - 2\mu$. In $d_{x^2-y^2}$-wave superconductors this corresponds to the solution with $E = -E_0$. This solution gives the combination

$$v(\boldsymbol{r}) + \cos\left(\frac{\pi x}{a}\right)\cos\left(\frac{\pi y}{a}\right)u(\boldsymbol{r})\,. \tag{7}$$

In Fig. 1 we show the spatial patterns of these solutions as they should be observed by scanning tunneling microscopy. As one would expect, there is a close similarity to those found in d-wave superconductors, although there is a superstructure which is not present in the superconducting regime. This arises from the interference between $u(\boldsymbol{r})$ and $v(\boldsymbol{r})$. For plotting the above figures we assumed that $\gamma = 0.2p_{\mathrm{F}}$.

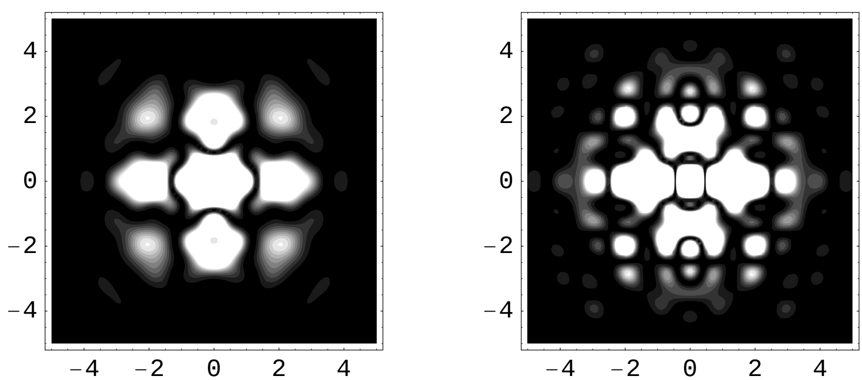

Fig. 1. Spatial variation of the local tunneling conductance, centered at a strong-scattering impurity, such as Zn, in a $d_{x^2-y^2}$-wave CDW system, (a) using Eq. (6), and (b) using the conjugate wave function of Eq. (7).

We may conclude that the impurity bound state in a $d_{x^2-y^2}$-density wave phase produces a picture similar to those in d-wave superconductors. Moreover, there is a checkerboard-like superstructure clearly visible in the 2D spatial pattern. Therefore, the detection of this impurity bound state wave function may provide another test of the notion that the pseudogap phase is d-density wave. Furthermore, a magnetic impurity, such as Ni, can differentiate SDW from CDW. The analysis of such weak-scattering Ni impurities will be reported in a future publication.

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