Mechanism of Pseudogap Probed by a Local Impurity

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The response to a local strong nonmagnetic impurity in the pseudogap phase is examined in two distinctly different scenarios: phase fluctuation (PF) of pairing field and d-density-wave (DDW) order. In the PF scenario, the resonance state is generally double peaked near the Fermi level, and is abruptly broadened by vortex fluctuations slightly above the transition temperature. In the DDW scenario, the resonance is single peaked and remains sharp up to gradual intrinsic thermal broadening, and the resonance energy is analytically determined to be at minus of the chemical potential.

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Aside from others [1], two distinctly different scenarios are proposed for the pseudogap in cuprates [2], depending on whether the pseudogap phase is independent of the pairing gap. In the phase-fluctuation (PF) scenario [3], it is speculated that the normal state contains preformed Cooper pairs, and the phase fluctuation of the pairing field destroys superconductivity. As the pairing gap has a d-wave symmetry in the internal momentum space, the d-wave-like dispersion of the pseudogap [4] follows immediately. An advantage of this scenario is that it involves no symmetry breaking, and is adiabatically connected to the paramagnetic Mott insulator. Such a normal state is not a Fermi liquid. In the second scenario, the normal state is free of pairing instability, but is in a symmetry-breaking d-density-wave (DDW) state [5]. The latter is an ordered state of staggered orbital current, and was discussed in other contexts already in the early stage of high-T_c physics [6]. It creates four holelike Fermi pockets in the nodal directions. The volume enclosed by the Fermi pockets scales exactly as the doping level x. Thus the pseudogap is from the band structure effect. The normal state is a Fermi liquid, namely, a DDW metal.

In this Letter, we discuss the resonance state due to a strong nonmagnetic local impurity in the pseudogap phase, which turns out to be markedly different in these scenarios. In the PF scenario, it is two peaked near the Fermi level, broadened by the vortex fluctuations (in addition to the intrinsic thermal broadening), and is thus strongly temperature dependent near the superconducting transition temperature T_c. (This is a complementary result to the extended impurity one [7].) In contrast, we analytically verify that the resonance state is single peaked, remaining sharp and pinned at minus of the chemical potential in the DDW metal [8], and identify the underlying mechanism for the pinning effect. We propose to measure the temperature and doping dependence of the impurity state by, e.g., scanning tunneling microscopy [9], in order to tell the mechanism of the pseudogap (or whether the normal state is a Fermi liquid).

In a d-wave superconductor, a local strong impurity is known to give rise to a resonant state near the Fermi level [10]. The state is almost real as the scattering rate into the continuum is limited by the vanishing density of states near the Fermi level (in an unperturbed system) because of the d-wave pairing symmetry. Qualitatively similar resonant states are found numerically in a d-wave superconductor with DDW order [8]. This is because (1) the resonant impurity state *near* the Fermi level is a generic feature of d-wave pairing, and (2) the only significant effect of DDW is to generate a specific band structure, on top of which d-wave pairing occurs.

Returning to the normal state, it is natural to expect *qualitatively different* responses to local impurities in the PF and DDW scenarios, since in the DDW normal state no pairing occurs. An earlier attempt to address the resonance in the pseudogap phase was made in Ref. [11], but with only limited success for PF. Recently the *extended* impurity was discussed in the PF scenario [7], and a numerical study was performed for a *local* impurity in the DDW scenario [8]. In this Letter, we compare the behaviors of the same local impurity in both PF and DDW scenarios.

Phase-fluctuation scenario.—The effective mean field Hamiltonian in a square lattice for a d-wave superconductor may be written as $H = \sum_{\langle ij\rangle}(\Psi_i^\dagger h_{ij}\Psi_j + \text{H.c.}) - \mu\sum_i \Psi_i^\dagger\sigma_3\Psi_i$, where $\Psi_i = (f_{i\uparrow}, f_{i\downarrow}^\dagger)^{\mathrm{T}}$ is the Nambu spinor, μ is the chemical potential, σ_3 is the third Pauli matrix, and

$$h_{ij} = -t\sigma_3 + \begin{bmatrix} 0 & \Delta_{ij} \\ \Delta_{ij}^* & 0 \end{bmatrix},$$

with $\Delta_{ij} = \Delta_0\eta_{ij}\exp(i\varphi_{ij})$, where Δ_0 is the pairing amplitude, $\eta_{ij} = 1$ (-1) for x direction (y direction) bonds, and φ_{ij} is the phase. In the PF scenario, the pairing field is disordered by thermal and/or quantum fluctuations of vortices at zero applied magnetic field. In the following discussion we assume that the vortex fluctuations are thermal.

It is possible to make a singular gauge transform $\Psi_i \to e^{-i\phi_i\sigma_3/2}\Psi_i$ so that $\Delta_{ij} \to \Delta_0\eta_{ij}$ no longer carries the phase, whose effect migrates to the hopping part in h_{ij}: $-t\sigma_3 \to -t\sigma_3 e^{i(\phi_i-\phi_j)\sigma_3/2}$. In the continuum limit, the phase difference between neighboring sites translates to the phase gradient $2\mathbf{q}_s \equiv e^{-i\phi}\frac{\nabla}{i}e^{i\phi}$, and corresponds to the superfluid velocity. It varies at the length scale of the London penetration depth, being much larger than the Fermi wavelength. Thus it is valid to adopt the quasiclassical approximation, in which Fermions see *a microscopically* constant $\mathbf{q}_s$, while $\mathbf{q}_s$ itself varies *macroscopically*. In this sense, the (matrix) Greens function G_0 for the Ψ Fermions influenced by $\mathbf{q}_s$ is determined by, in momentum space,

$$G_0^{-1}(\mathbf{k}, i\omega_n; \mathbf{q}_s) = \begin{bmatrix} i\omega_n - \varepsilon_{\mathbf{k}+\mathbf{q}_s} & \Delta_{\mathbf{k}} \\ \Delta_{\mathbf{k}} & i\omega_n + \varepsilon_{\mathbf{k}-\mathbf{q}_s} \end{bmatrix} \sim (i\omega_n - \mathbf{q}_s\cdot\mathbf{v}_{\mathbf{k}})\sigma_0 - \varepsilon_{\mathbf{k}}\sigma_3 + \Delta_{\mathbf{k}}\sigma_1 . \quad (1)$$

Here $\varepsilon_{\mathbf{k}} = -2t(\cos k_x + \cos k_y) - \mu$, $\Delta_{\mathbf{k}} = 2\Delta_0(\cos k_x - \cos k_y)$, $\mathbf{v}_{\mathbf{k}} = \nabla_{\mathbf{k}}\varepsilon_{\mathbf{k}}$. As is well known, the low energy excitations in this system are located around the four nodes $\mathbf{k}_{n=1,2,3,4} = (\pm K, \pm K)$ in the momentum space, with $-4t\cos K = \mu$. The second line in Eq. (1) is the usual Doppler approximation [12]. At low energies, the Doppler shift $\mathbf{q}_s\cdot\mathbf{v}_k$ can be well approximated by its value at the four nodes $D_n = \mathbf{q}_s\cdot\mathbf{v}_{\mathbf{k}_n}$. We shall use the first (second) line of Eq. (1) for numerical (qualitative and analytical) discussion [13].

The real space Greens function is obtained by the Fourier transform, $G_0(i, j, i\omega_n; \mathbf{q}_s) = \sum_{\mathbf{k}} G_0(\mathbf{k}, i\omega_n; \mathbf{q}_s)\exp[i\mathbf{k}\cdot(\mathbf{r}_i - \mathbf{r}_j)]$. Of special interest is the local Greens function $g(i\omega_n; \mathbf{q}_s) \equiv G_0(i = j, i\omega_n; \mathbf{q}_s)$. Because of the d-wave pairing symmetry, $g_{12} = g_{21} = 0$. (We suppress the arguments if applicable). On the other hand,

$$g_{11}(i\omega_n; \mathbf{q}_s) = -g_{22}^* = \int dE\, N_0(E; \mathbf{q}_s)/(i\omega_n - E) , \quad (2)$$

$$N_0(E; \mathbf{q}_s) \sim (1/8)\sum_{n=1}^{4}\sum_{\nu=\pm}[|E - \nu D_n|/(8\pi t\Delta_0) - \mu(E - \nu D_n)^2\,\mathrm{sgn}(E - \nu D_n)/\Lambda^4], \quad (3)$$

with $\Lambda = 4[\pi t^3\Delta_0^3/(t^2 + \Delta_0^2)]^{1/4}$. A cutoff at $|E| > E_c = \min(4t, 4\Delta_0)$ is necessary in applying Eq. (3). Anticipating its effect in the impurity scattering, we point out briefly the behavior of N_0: (1) It exhibits a fourfold symmetry in the direction of $\mathbf{q}_s$. (2) At $|E| \ll E_c$ and $|D_n| \ll E_c$, the leading contribution comes from the first term in N_0. It is particle-hole symmetric around $E = 0$ at any μ and q_s. This is the fundamental property of d-wave pairing between time-reversed particles. (3) Away from half filling ($\mu \neq 0$), there is a slight asymmetry. To the first order in μ, this is included in the second term in N_0. Clearly, $N_0(E = 0; \mathbf{q}_s) \propto q_s$, as first pointed out by Volovik [12].

In the presence of a local scattering potential at site $i = 0$, the corresponding Greens function G can be obtained within the T-matrix approximation (which is exact if the impurity does not spoil the pairing field),

$$G(i, j, i\omega_n; \mathbf{q}_s) = G_0(i, j, i\omega_n; \mathbf{q}_s) + G_0(i, 0, i\omega_n; \mathbf{q}_s)T(i\omega_n; \mathbf{q}_s) \times G_0(0, j, i\omega_n; \mathbf{q}_s) , \quad (4)$$

$$T^{-1}(i\omega_n; \mathbf{q}_s) = 1/(V\sigma_3 + V_m\sigma_0) - g(i\omega_n; \mathbf{q}_s) , \quad (5)$$

where V (V_m) is the nonmagnetic (magnetic) scattering strength. To simplify our discussion, we shall consider nonmagnetic scattering only. With the impurity, the local density of states (LDOS) is site dependent. At site i it is given by

$$N(i, \omega; \mathbf{q}_s) = -(1/\pi)\,\mathrm{Im}G_{11}(i, i, \omega + i0^+; \mathbf{q}_s) . \quad (6)$$

We emphasize that the off-diagonal elements of G_0 in Eq. (4) contribute to the density of states. Conceptually, neglecting such contributions, as in Ref. [11], the theory would be hardly related to pairing.

Let us discuss the qualitative behavior of the LDOS in our case. Since g is diagonal, so is the T matrix. After analytical continuation $i\omega_n \to \omega + i0^+$, the resonance in LDOS is determined by $\mathrm{Re}(T_{11}^{-1}) = 0$ or $\mathrm{Re}(T_{22}^{-1}) = 0$. This is equivalent to $\mathrm{Re}[g_{11}(\pm\omega + i0^+; \mathbf{q}_s)] = V^{-1}$, and immediately implies two resonance peaks in a general situation, an essential feature of pairing. For a strong scatter, $V^{-1} \to 0$. In the case of $q_s = 0$, a sharp resonance exists in the LDOS at the sites nearest to the impurity [10]. The behavior at $q_s \neq 0$ is as follows: (1) For $\mu = 0$ and $V^{-1} = 0$, we have perfect particle-hole symmetry, so that $\mathrm{Re}[g_{11}(i0^+; \mathbf{q}_s)] = 0$ from Eq. (2). The resonance is at $\omega = 0$. However, *it is not sharp, and its width scales with* $N(0; \mathbf{q}_s)$ ($\propto q_s$) in accordance with the Fermi golden rule. (2) The effect of a finite μ and/or V^{-1} is to generate a slight asymmetry, and thus splits the resonance into two peaks, situated on either side of the Fermi level. Their widths are identical (different) if $\mu = 0$ ($\mu \neq 0$) because of the behavior of N_0. Moreover, at large enough q_s the splitting will be smeared due to the broadening of both peaks.

Before we proceed, we predict from the above results that even below T_c the resonance may be broadened by an in-plane transport current and/or a nearby static vortex. Since N_0 is fourfold symmetric in the direction of the relevant supercurrent, so is the broadening phenomenon.

Thermal phase fluctuations are governed by the Kosterlitz-Thouless (KT) theory [14]. In the quasiclassical approximation, this just amounts to an average over $\mathbf{q}_s$. For illustrative purposes, one can assume a Gaussian distribution $\exp(-\mathbf{q}_s^2/2n_v)/2\pi n_v$ for $\mathbf{q}_s$, with

n_v scaling with the density of free vortices (antivortices) [7]. The average LDOS is thus $N(i,\omega) = \langle N(i,\omega;\mathbf{q}_s)\rangle$. The averaging makes it inconvenient to determine the resonance exactly, since it is the Greens function that should be averaged instead of the T matrix alone. However, qualitative features of the resonance in the LDOS are roughly the same as discussed above, but with a characteristic scale of q_s given by $\sqrt{n_v}$, the inverse vortex spacing.

All of the above predictions are indeed seen in our numerical results. We use Eqs. (1) (the first line) and Eqs. (4)–(6), and average over $\mathbf{q}_s$. In Figs. 1 we present results for $\Delta_0 = 0.17t$, $\mu = -0.3t$, and $V = 100t$. (The results do not change much in the unitary limit $V \gg t$.) Figure 1(a) plots the LDOS at $\mathbf{r}_{nn}$ nearest to the impurity as a function of energy. For $n_v \leq 10^{-6}$ (or vortex spacing $d_v \geq 10^3$ in units of crystal lattice constant a_0), the resonance is sharp and indistinguishable from that with no vortices at all. However, it begins to degrade at $n_v \geq 10^{-4}$ ($d_v \leq 10^2 a_0$), and becomes almost featureless at $n_v = 5 \times 10^{-3}$ ($d_v = 14a_0$). Translating to the temperature dependence using the KT expression $n_v \sim \exp[-\sqrt{aT_c/(T - T_c)}]$ (with $a = 5$ for estimation) one expects no significant change of the resonance at $T - T_c < 0.07T_c$, but it is suddenly degraded as soon as $T - T_c > 0.1T_c$. For $T_c = 40$ K as in a typical underdoped cuprate, the temperature window for this phenomenon to happen is within 4 K. While the exact number should not be taken seriously, *the sudden degrading of the resonant impurity state is a robust and peculiar feature of the PF scenario*. A similar case was found for an extended impurity elsewhere [7]. The dotted line in Fig. 1(a) is the DOS at $n_v = 0$ and $V = 0$ for comparison. It also shows the slight doping-induced particle-hole asymmetry. Figure 1(b) shows the spatial distribution of LDOS at $\omega = 0.05t$ ($\ll |\mu|$), one of the resonance energies, when $n_v = 0$ [10], which should be compared to Fig. 1(c) at $n_v = 5 \times 10^{-3}$, upon which the contrast for the fourfold structure is much weaker.

DDW scenario.—We assume that the effective Hamiltonian for the uniform DDW metal is [5]

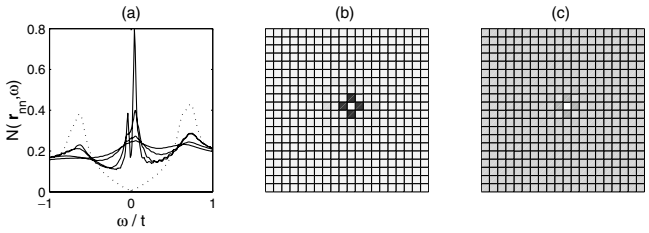

FIG. 1. Results with $\Delta_0 = 0.17t$, $\mu = -0.3t$, and $V = 100t$. (a) $N(\mathbf{r}_{nn},\omega)$ versus ω. Solid lines: $n_v = 0 \sim 10^{-6}$, 10^{-4}, 10^{-3}, and 5×10^{-3} with decreasing peaks. The dotted line is the LDOS at $n_v = 0$ and $V = 0$ for comparison. (b) $N(\mathbf{r}, 0.05t)$ at $n_v = 0$. The impurity is at the center. (c) The same as (b) for $n_v = 5 \times 10^{-3}$. The gray scale is the same in (b) and (c).

$$H = -\sum_{\langle ij\rangle}[(t + iD_{ij})c_i^\dagger c_j + \text{H.c.}] - \sum_i \mu c_i^\dagger c_i\,, \quad (7)$$

where spin index is suppressed, $D_{ij} = D_0\eta_{ij}(-1)^i$, with D_0 being the DDW order parameter.

It proves useful to introduce two sublattices A and B, and denote $c_{i\in A} = A_i$ and $c_{i\in B} = B_i$. The real-space sublattice Greens function is

$$\begin{bmatrix} G_{AA}^{(0)} & G_{AB}^{(0)} \\ G_{BA}^{(0)} & G_{BB}^{(0)} \end{bmatrix} = \frac{1}{2}\sum_{\mathbf{k},\nu=\pm}\frac{A_{\mathbf{k}\nu}\exp(i\mathbf{k}\cdot\mathbf{r}_{ij})}{i\omega_n + \mu - \nu E_{\mathbf{k}}}\,, \quad (8)$$

where $A_{\mathbf{k}\nu} = \sigma_0 + \nu\sigma_1 X_{\mathbf{k}}/E_{\mathbf{k}} + \nu\sigma_2 D_{\mathbf{k}}/E_{\mathbf{k}}$, $E_{\mathbf{k}} = \sqrt{X_{\mathbf{k}}^2 + D_{\mathbf{k}}^2}$, $X_{\mathbf{k}} = 2t(\cos k_x + \cos k_y)$, and $D_{\mathbf{k}} = 2D_0(\cos k_x - \cos k_y)$. Note that the summation over the momentum space is limited to the reduced Brillouin zone. In order to study the impurity problem, we need the real-space Greens function $G_c^{(0)}(i,j,i\omega_n)$ in terms of the original c electrons. This is related to the above as

$$G_c^{(0)}(i\in\alpha, j\in\beta, i\omega_n) = G_{\alpha\beta}^{(0)}(i,j,i\omega_n)\,, \quad (9)$$

where $\alpha,\beta = A,B$.

The unperturbed on-site Greens function is independent of sublattices, $g_c(i\omega_n) \equiv G_c^{(0)}(0,0,i\omega_n) = \int dE\, N_0(E)/(i\omega_n - E)$ with $N_0(E) = \sum_{\mathbf{k}\nu=\pm}\delta(E - \nu E_k + \mu) \sim |E + \mu|/(8\pi Dt)$ being the unperturbed DOS. The second equality in N_0 requires a cutoff at $|E + \mu| > E_c = \min(4D, 4t)$. The symmetry around $E = -\mu$ in N_0, instead of at $E = 0$ in the case of pairing, is exact in our model. This is because doping the system does not change the two *symmetric* bands generated by DDW, but just shift the Fermi level.

Now, the Greens function in the presence of the impurity can again be obtained within the T-matrix formulation,

$$G_c(i,j,i\omega_n) = G_c^{(0)}(i,j,i\omega_n) + G_c^{(0)}(i,0,i\omega_n)T(i\omega_n)G_c^{(0)}(0,j,i\omega_n)\,, \quad (10)$$

$$T^{-1}(i\omega_n) = V^{-1} - g_c(i\omega_n)\,. \quad (11)$$

The resonance state is defined by $\text{Re}[T^{-1}(\omega + i0^+)] = 0$, or equivalently $\text{Re}[g_c(\omega + i0^+)] = V^{-1}$. Using the approximate N_0, $g_c(\omega + i0^+)$ is given by

$$-\text{sgn}(\omega + \mu)N_0(\omega)\ln\left[\frac{E_c^2}{(\omega + \mu)^2} - 1\right] - i\pi N_0(\omega)\,. \quad (12)$$

Thus the resonance occurs below (above) $-\mu$ for a *finite* positive (negative) potential V. For a nonmagnetic impurity, it is single peaked because of the unique condition for the resonance to occur. Again the energy width of the resonance scales with N_0. In the unitary limit $V^{-1} \to 0$, the resonance energy is $\omega = -\mu$ from the above expression of g_c and $N_0(-\mu) = 0$. In fact, this result is *exact*

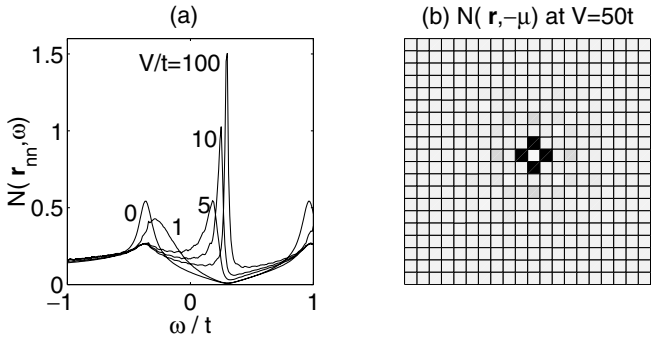

FIG. 2. Results with $D_0 = 0.17t$ and $\mu = -0.3t$. (a) $N(\mathbf{r}_{nn}, \omega)$ versus ω. (b) $N(\mathbf{r}, \omega = -\mu)$ versus $\mathbf{r}$.

since the exact symmetry in N_0 mentioned above guarantees $\mathrm{Re}[g_c(-\mu + i0^+)] = 0$. This resonance energy is exactly at the midpoint of the two symmetric bands, in much the same way as the midgap state exists in a semiconductor. Furthermore it would be infinitely sharp since $N_0(-\mu) = 0$.

The DDW order should not fluctuate significantly once it is well developed, because it is an Ising-like order parameter so that no Goldstone mode exists. Therefore the thermal rounding of the resonance is gradual, with no abrupt change just above T_c, in contrast to the case in the PF scenario.

The LDOS $N(i, \omega)$ can be easily calculated from Eq. (10). In Fig. 2(a) we present the LDOS at $\mathbf{r}_{nn}$ nearest to the impurity. The resonance is single peaked and robust as long as $V \gg t, D$. In Fig. 2(b) we present the spatial dependence of the LDOS at the resonance energy. The pattern is also fourfold symmetric, similar to the case of a d-wave superconductor except that the resonance here is at $-\mu$ instead of at zero energy.

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Note added.—After the submission of this Letter, we became aware of a related but independent work [15].

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[13] In principle, one needs to perform an inverse gauge transform in using Eq. (1) to describe the original (charged) fermions. Fortunately, for any quantity that is gauge invariant, such as the *local* DOS we are considering, the results are the same in both systems.

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