Mechanism of pseudogap probed by a local impurity

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The response to a local strong non-magnetic 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, two distinctly different scenarios are proposed for the pseudogap in cuprates, depending on whether the pseudogap phase is independent of the pairing gap. In the phase-fluctuation (PF) scenario, 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 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. 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. It creates four hole-like 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.) 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, 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 tunnelling microscopy, 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. 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. 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. but with only limited success for PF. Recently the extended impurity was discussed in the PF scenario, and a numerical study was performed for a local impurity in the DDW scenario. 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

\[
H = \sum_{(ij)} (\psi_i^\dagger h_{ij} \psi_j + \text{h.c.}) - \mu \sum_i \psi_i^\dagger \sigma_3 \psi_i, \quad \text{where} \quad \psi_i = (f_{i\uparrow}, f_{i\downarrow})^T \quad \text{is the Nambu spinor,} \quad \mu \text{is the chemical potential,} \quad \sigma_3 \text{is the third Pauli matrix, and}
\]

\[
h_{ij} = -i\sigma_3 + \begin{pmatrix}
0 & \Delta_{ij} \\
\Delta_{ij}^* & 0
\end{pmatrix},
\]

with \(\Delta_{ij} = \Delta_0 \eta_{ij} \exp(i\varphi_{ij})\), where \(\Delta_0\) is the pairing amplitude, \(\eta_{ij} = 1 (-1)\) for \(x\)-direction (\(y\)-direction) bonds, and \(\varphi_{ij}\) 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 \( \Psi \rightarrow e^{-i\phi/s}\sqrt{2}\Psi \) so that \( \Delta_{ij} \rightarrow \Delta_0 \eta_{ij} \) no longer carries the phase, whose effect migrates to the hopping part in \( h_{ij} : -\sigma_3 \rightarrow -\sigma_3 e^{i(\phi_i - \phi_j)} s/2 \). In the continuum limit, the phase difference between neighboring sites translates to the phase gradient \( 2\eta = e^{-i\phi/s} \sum_0 \), and corresponds to the superfluid velocity. It varies at the length scale of the London penetration depth, being much larger than the Fermi wave-length. Thus it is valid to adopt the quasi-classical approximation, in which Fermions see a microscopically constant \( q \), while \( q \) itself varies macroscopically. In this sense, the (matrix) Greens function \( G_0 \) for the \( \Psi \) Fermions influenced by \( q \), is determined by, in momentum space,

\[
G_0^{-1}(k, \omega_n; q) = \left( i\omega_n - \varepsilon_{k+q, i} + \Delta_k \over \Delta_k \right)
\sim (i\omega_n - q \cdot v_k)\sigma_0 - q \cdot \sigma_3 + \Delta_k \sigma_1 \tag{1}
\]

Here \( \varepsilon_k = -2t (\cos k_x + \cos k_y) - \mu \), \( \Delta_k = 2\Delta_0 (\cos k_x - \cos k_y) \), \( v_k = v_0 k \). As is well known, the low energy excitations in this system are located around the four nodes \( k = 0, \pm K, \pm K \) in the momentum space, with \(-4t \cos K = \mu \). The second line in Eq. \ref{H} is the usual Doppler approximation. At low energies, \( q \cdot v_k \) can be well approximated by its value at the four nodes \( D_n = q \cdot v_{k_n} \). We shall use the first (second) line of Eq. \ref{H} for numerical (qualitative and analytical) discussion. \[1\]

The real space Greens function is obtained by the Fourier transform, \( G_0(i, j, \omega_n; q) = \sum_k G_0(k, \omega_n; q) \exp[i(k \cdot (r_i - r_j))] \). Of special interest is the local Greens function \( g(\omega_n; q) = G_0(i = j, \omega_n; q) \).

Due to the d-wave pairing symmetry, \( g_{12} = g_{21} = 0 \). (We suppress the arguments if applicable.) On the other hand,

\[
g_{11}(\omega_n; q) = -g_{22} = \int dE N_0(E; q) / (\omega_n - E), \tag{2}
\]

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

with \( \Lambda = 4[\pi\Delta_0^2 / (t^2 + \Delta_0^2)]^{1/4} \). A cutoff at \( |E| > E_c = \min (4t, 4\Delta_0) \) is necessary in applying Eq. \ref{H}. Anticipating its effect in the impurity scattering, we point out briefly the behavior of \( N_0 \): 1) It exhibits a four-fold symmetry in the direction of \( q \). 2) At \( |E| \ll E_c \), the leading contribution comes from the first term in \( \Gamma_0 \). It is particle-hole symmetric around \( E = 0 \) at any \( \mu \) and \( q \). 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 \( \mu \), this is included in the second term in \( \Gamma_0 \). Clearly, \( N_0(E = 0; q) \propto q_s \), as first pointed out by Volovik. \[2\]

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),

\[
G(i, j, \omega_n; q) = G_0(i, j, \omega_n; q) + G_0(i, 0, \omega_n; q) T(\omega_n; q) G_0(0, j, \omega_n; q), \tag{4}
\]

\[
T^{-1}(\omega_n; q) = 1 / (V\sigma_3 + V_n\sigma_0) - g(\omega_n; q), \tag{5}
\]

where \( V \) (or \( V_n \)) 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

\[
N(i, \omega; q) = -(1/\pi) \text{Im} G_{11}(i, i, \omega + i0^+; q). \tag{6}
\]

We emphasize that the off-diagonal elements of \( G_0 \) in Eq. \ref{H} contribute to the density of states. Conceptually, neglecting such contributions, as in Ref. \[1\], 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 \( \omega_n \rightarrow \omega + i0^+ \), the resonance in LDOS is determined by \( \text{Re}(T^{11}_{11}) = 0 \) or \( \text{Re}(T^{22}_{12}) = 0 \). This is equivalent to \( \text{Re}[g_{11}(\pm \omega + i0^+; q)] = V^{-1} \), and immediately implies two resonance peaks in a general situation, an essential feature of pairing. For a strong scatter, \( V^{-1} \rightarrow 0 \). In the case of \( q_s = 0 \), a sharp resonance exists in the LDOS at the sites nearest to the impurity. \[1\] 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 \( \text{Re}[g_{11}(i0^+; q_s)] = 0 \) from Eq. \ref{H}. The resonance is at \( \omega = 0 \). However, it is not sharp, and its width scales with \( N(0; q_s) \) \( \propto q_s \) in accordance with the Fermi golden rule. 2) The effect of a finite \( \mu \) 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 \( \Gamma_0 \). 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 four-fold symmetric in the direction of the relevant super-current, so is the broadening phenomenon.

Thermal phase fluctuations are governed by the Kosterlitz-Thouless (KT) theory. \[3\] In the quasi-classical approximation, this just amounts to an average over \( q_s \). For illustrative purpose, one can assume a Gaussian distribution \( \exp(-q^2_{\perp}/2n_{v})/(2\pi n_{v}) \) for \( q_s \), with \( n_{v} \) scaling with the density of free vortices (anti-vortices). \[4\] The average LDOS is thus \( \langle N(i, \omega; q_s) \rangle \). 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.

**DDW scenario**: We assume that the effective Hamiltonian for the uniform DDW metal is

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

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

\[
\begin{pmatrix}
G_{AA}^{(0)} \\
G_{BA}^{(0)} \\
G_{BB}^{(0)}
\end{pmatrix} = \frac{1}{2} \sum_{k,\nu=\pm} \frac{A_{k,\nu} \exp(\text{i}k \cdot \textbf{r}_{ij})}{\omega_{\nu} + \mu - \nu E_k}, \tag{8}
\]

where \( A_{k,\nu} = \sigma_0 + \nu\sigma_1X_k/E_k + \nu\sigma_2D_k/E_k \), \( E_k = \sqrt{X_k^2 + D_k^2} \), \( X_k = 2t(\cos k_x + \cos k_y) \), and \( D_k = 2D_0(\cos k_x - \cos k_y) \). 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 \( G^{(0)}_{ij}(i, j, \omega_n) \) in terms of the original \( c \)-electrons. This is related to the above as

\[
G^{(0)}_{ij}(i \in \alpha, j \in \beta, \omega_n) = G^{(ij)}_{\alpha\beta}(i, j, \omega_n), \tag{9}
\]

where \( \alpha, \beta = A, B \).

The unperturbed on-site Greens function is independent of sublattices, \( g_{i}(\omega_n) = G^{(0)}_{i}(0, 0, \omega_n) = \int dE N_0(E)/(\omega_n - E) \) with \( N_0(E) = \sum_{k,\nu} \delta(E - E_k + \nu\mu) = |E + \mu|/(4\pi DT) \) 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.

**FIG. 1.** Results with \( \Delta_0 = 0.17t \), \( \mu = -0.3t \) and \( V = 100t \). (a) \( N(r_{nn}, \omega) \) versus \( \omega \). Solid lines: \( n_v = 0 \sim 10^{-6}, 10^{-4}, 10^{-3}, \) and \( 5 \times 10^{-3} \) with decreasing peaks. The dotted line is the LDOS at \( n_v = 0 \) and \( V = 0 \) for comparison. (b) \( N(r, 0.05\omega) \) 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).
The resonance state is defined by $\text{Re} [g_c(\omega + i0^+)] = 0$ or equivalently $\text{Re} [g_c(\omega + i0^+)] = V^{-1}$. Using the approximate $N_0$, $g_c(\omega + i0^+)$ is given by

$$-\text{sgn}(\omega + \mu)N_0(\omega)\ln\left(\frac{E^2}{(\omega + \mu)^2} - 1\right) - i\pi N_0(\omega).$$

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 $V^{-1} \rightarrow 0$, the resonance energy is $\omega = -\mu$ from the above expression of $g_c$ and $N_0(-\mu) = 0$. In fact, this result is exact since the exact symmetry in $N_0$ mentioned above guarantees $\text{Re} [g_c(\omega + i0^+)] = 0$. This resonance energy is exactly at the mid-point of the two symmetric bands, in much the same way as the mid-gap 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.

![Fig. 2](image_url) Results with $D_0 = 0.17t$ and $\mu = -0.3t$. (a) $N(\mathbf{r}_n, \omega)$ versus $\omega$. (b) $N(\mathbf{r}, \omega = -\mu)$ versus $\mathbf{r}$.

The LDOS $N(i, \omega)$ can be easily calculated from Eq. (10). In Fig. 2(a) we present the LDOS at $\mathbf{r}_n$ 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 four-fold symmetric, similar to the case of a d-wave superconductor except that the resonance here is at $-\mu$ instead of at zero energy.

After the submission of this paper, we become aware of a related but independent work. [3]

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