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Superconductivity above a quantum critical point in a metal – gap closing vs gap filling, Fermi arcs, and pseudogap behavior.

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We consider a metal with interaction mediated by fluctuations of an order parameter, which condenses at a quantum-critical point (QCP). This interaction gives rise to fermionic incoherence in the normal state and also mediates pairing. Away from a QCP, the pairing restores fermionic coherence almost immediately below T_c . We show that near a QCP, fermions regain coherence only below a certain T_{cross} , which is smaller than the onset temperature for the pairing, T_p . At $T < T_{cross}$ the system behavior is conventional in the sense that both the density of states (DOS) and the spectral function (SF) have sharp gaps, which *closes in* as T increases. At higher $T_{cross} < T < T_p$, the DOS has a dip, which *fills in* with increasing T , while the SF shows either the same behavior as the DOS, or has a peak at $\omega = 0$, depending on the position on the Fermi surface, leading to a Fermi arc. We argue that phase fluctuations are strong at $T > T_{cross}$, and the actual $T_c \geq T_{cross}$, while at larger $T_c < T < T_p$ the system displays a pseudogap behavior. We argue that our theory explains the crossover from gap closing to gap filling, observed in cuprate superconductors at $T \leq T_c$, and the persistence of the dip in the DOS and the Fermi arc above T_c .

Introduction. Pairing near a quantum-critical point (QCP) in a metal and its intriguing interplay with the non-Fermi liquid (NFL) physics continue to attract high interest in the physics community^{1–8}. Fermionic incoherence, associated with the NFL form of the self-energy in the normal state, acts against pairing, while pairing acts against incoherence by gapping out low-energy states. The competition between the pairing and the NFL has been analyzed analytically, using field-theoretical methods for effective low-energy models^{1,2,6,9–24}, and numerically, by, e.g., FRG, QMC and DMFT techniques^{4,25–28}. Earlier studies have found^{2,9,16,17,20,24} that the tendency to pairing prevails, and a QCP in a metal is surrounded by a superconducting dome.

The issue we discuss here is the feedback from the pairing on the fermions below the onset temperature of the pairing T_p , specifically the behavior of the density of states (DOS) $N(\omega)$ and the spectral function (SF) on the Fermi surface (FS) $A_{\mathbf{k}_F}(\omega)$. Away from a QCP, fermions with energies comparable to the pairing gap become coherent almost immediately below T_p , and this gives rise to sharp peaks in the DOS and the SF, whose frequencies are set by the gap $\Delta_k(T)$ and get smaller as T increases. We show that in the vicinity of a QCP, fermionic coherence is restored only below a certain $T_{cross} < T_p$ (region I in Fig. 3), while at $T_{cross} < T < T_p$ (region II) the system behavior is *qualitatively* different: $N(\omega)$ has a dip at $\omega = 0$ and a hump at a frequency, which scales with T rather than $\Delta(T)$, and remains finite at $T = T_p$, i.e., the DOS fills in with increasing T . The SF either displays the same behavior as the DOS, or shows a single peak at $\omega = 0$, depending on the location on the FS. This gives rise to a Fermi arc. We argue below that the existence of the two regions with qualitatively different behavior of observables is the consequence of the spe-

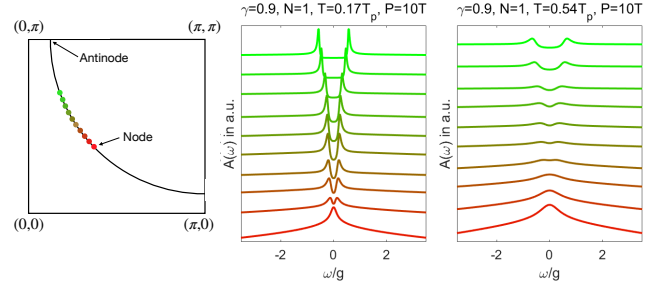


FIG. 1. The spectral function $A_{\mathbf{k}_F}(\omega)$ along the Fermi surface (Red- nodal regions, green – antinodal regions). At $T < T_{cross}$ (the middle panel) $A_{\mathbf{k}_F}(\omega)$ has sharp peaks, which merge at the node. At $T > T_{cross}$ (the right panel), $A_{\mathbf{k}_F}(\omega)$ in nodal region has a single peak at $\omega = 0$ (the Fermi arc), while in the antinodal region it has a dip at $\omega = 0$ and the hump at a finite frequency. At T approaches T_p , the dip fills in and the hump position remains at a finite frequency.

cial role played by fermions with the smallest Matsubara frequencies $\pm\pi T$ for the pairing near a QCP.

We show representatives of our results for the SF for the d -wave form of the gap in Fig. 1. A very similar behavior has been detected ARPES measurements of $A_{\mathbf{k}_F}(\omega)$ along the FS^{29–33}.

We further analyze the role of fluctuations of the phase of $\Delta e^{i\phi(r)}$. We argue that in region II, $\rho_s(T)$ in the action $S = \rho_s(T) \int dr (\nabla\phi(r))^2$ is strongly reduced from its value of order E_F at $T = 0$, to $\phi_s \leq T$. In this situation, phase fluctuations are strong, $\langle\phi^2\rangle \geq 1$, long range superconducting order likely get destroyed³⁴. Then the actual $T_c \geq T_{cross}$, and between T_c and T_p the system displays the pseudogap behavior. This also agrees with the experiments on the cuprates, which found that

the crossover from gap closing to gap filling occurs at $T \leq T_c$ (Ref.²⁹), while the dip in $N(\omega)$ and anti-nodal $A_{\mathbf{k}_F}(\omega)$, and the Fermi arc, disappear at a higher T . We caution that we do not associate the entire pseudogap region in the cuprates with a paired state with no phase coherence. There are other features, like FS reconstruction^{35,36}, charge and nematic orders^{37,38}, and time-reversal symmetry breaking^{39,40}, which we do not address in this study. In this respect our work presents microscopic understanding of “weak” pseudogap behavior — gap filling with increasing T in the DOS and the SF in the anti-nodal regions of the FS, and the development of Fermi arcs in the SF in near-nodal region.

We emphasize that the issue we consider here is different from peak-dip-hump phenomena, which has been associated with the emergence of quasiparticle scattering in a superconductor at frequencies above $\omega \geq (2-3)\Delta$ (Refs. ⁴¹⁻⁴³). The phenomenon we discuss here is the destruction of the peak at $\omega = \Delta$ in region II due to strong quasiparticle scattering even at the lowest energies. This physics has been described phenomenologically⁴⁴⁻⁴⁶, by introducing temperature-dependent fermionic damping $\gamma(T)$, comparable to the gap $\Delta(T)$. Our work presents the microscopic theory of the existence of $\text{Im}\Sigma(\omega \rightarrow 0, T)$ at $T > T_{\text{cross}}$, despite that the gap function is non-zero.

The model. We consider the model of itinerant fermions minimally coupled to fluctuations of the order parameter field, which condenses at a QCP. Within Eliashberg-type approximation, which we adopt, the effective 4-fermion interaction is proportional to the susceptibility of an order parameter integrated along the FS, $\chi(\Omega_m)$. At a QCP, $\chi(\Omega_m) = (g/|\Omega_m|)^\gamma$ is a singular function of frequency (the exponent γ is small near 3D, and in 2D equals 1/3 at a nematic QCP and 1/2 at QCP towards a density-wave order^{2,10,16,17,20}). This $\chi(\Omega_m)$ gives rise to an attraction in at least one pairing channel and also gives rise to NFL behavior in the normal state, setting the competition between the pairing and the NFL behavior. We consider spin-singlet pairing and solve the set of non-linear equations for the pairing vertex and fermionic self-energy on the Matsubara axis, and then convert the results to real frequencies⁹ and obtain the DOS and the SF. We present the details of the calculations in⁴⁷ and here list and discuss the results. For compactness of the equations, we will not label momentum dependence of the gap. We discuss d -wave case later in the text.

Along the Matsubara axis, the coupled equations for the pairing vertex $\Phi(\omega_m)$ and fermionic self-energy $\Sigma(\omega_m)$ are²⁰ ($\tilde{\Sigma}(\omega_m) = \omega_m + \Sigma(\omega_m)$)

$$\begin{aligned}\Phi(\omega_m) &= \pi T \sum_{m'} \frac{\Phi(\omega_{m'}) \chi(\omega_m - \omega_{m'})}{\sqrt{\tilde{\Sigma}^2(\omega_{m'}) + \Phi^2(\omega_{m'})}} \\ \tilde{\Sigma}(\omega_m) &= \omega_m + g^\gamma \pi T \sum_{m'} \frac{\tilde{\Sigma}(\omega_{m'}) \chi(\omega_m - \omega_{m'})}{\sqrt{\tilde{\Sigma}^2(\omega_{m'}) + \Phi^2(\omega_{m'})}},\end{aligned}\quad (1)$$

In principle, one should also include the equation for bosonic self-energy, which describes the feedback from

$\Phi(\omega_m)$ on $\chi(\Omega_m)$ (Refs.⁴³). This feedback effectively makes the exponent γ larger below T_p . However, because regions I and II exist for all γ (see below), this will only affect the location of T_{cross} . Below we neglect this complication and treat the exponent γ as temperature independent.

The thermal contributions to $\Phi(\omega_m)$ and $\tilde{\Sigma}(\omega_m)$ come from $m' = m$ terms in the sums. These contributions can be excluded from the Eliashberg set by analogy with non-magnetic impurities⁴⁸⁻⁵⁰, by re-expressing $\Phi(\omega_m) = \Phi^*(\omega_m) (1 + Q^*(\omega_m))$, $\tilde{\Sigma}(\omega_m) = \tilde{\Sigma}^*(\omega_m) (1 + Q^*(\omega_m))$, where $Q^*(\omega_m) = \pi T \chi(0) / \sqrt{(\tilde{\Sigma}^*(\omega_m))^2 + (\Phi^*(\omega_m))^2}$. The equations for Φ^* and $\tilde{\Sigma}^*$ are the same as in (1) but without $m = m'$ term in the sums. We solve these two equations and then obtain $\Phi^*(\omega)$ and $\tilde{\Sigma}^*(\omega)$ for real ω using spectral decomposition and analytical continuation. In the normal state (at $\Phi^* = 0$) the self-energy has a NFL form $\Sigma^*(\omega) \propto \omega^{1-\gamma}$.

The onset temperature for the pairing $T_p = T_p(\gamma)$ has been obtained in^{2,6,10-16} for specific γ and in^{17,20} as a function of γ . $T_p(\gamma)$ is finite, of order g , and scales as $\gamma^{-1/\gamma}$ at small γ . The pairing gap $\Delta(\omega)$ is defined as $\Delta(\omega) = \Phi(\omega)/\tilde{\Sigma}(\omega)$ and is equally expressed as $\Delta(\omega) = \Phi^*(\omega)/\tilde{\Sigma}^*(\omega)$. The DOS $N(\omega)$ is expressed only via $\Delta(\omega)$: $N(\omega) = N_0 \text{Im} \left[\omega / \sqrt{\Delta^2(\omega) - \omega^2} \right]$ and has no contribution from thermal fluctuations. The SF $A(\omega)$ does depend on the thermal contribution $P = \pi T \chi(0)$: $A(\omega) = (-1/\pi) \text{Im} \left[S(\omega) \omega / \sqrt{\Delta^2(\omega) - \omega^2} \right]$, where $S^{-1}(\omega) = P \text{sgn} \text{Im} \tilde{\Sigma}^*(\omega) + \sqrt{(\Phi^*(\omega))^2 - (\omega + \Sigma^*(\omega))^2}$.

The two regions below T_p . We argue that the existence of the regions I and II is associated with the special role of fermions with Matsubara frequencies $\omega_m = \pm\pi T$ for the pairing. Namely, fermionic self-energy $\Sigma^*(\omega_m)$, which acts against the pairing, is strong for a generic ω_m , but vanishes at $\omega_m = \pm\pi T$, i.e. fermions with these two frequencies can be treated as free particles^{20,51}. Meanwhile, the pairing interaction between fermions with $\omega_m = \pm\pi T$, $\chi(2\pi T) = (g/(2\pi T))^\gamma$ is strong and diverges at $T = 0$. As the consequence, the fermions with $\omega_m = \pi T$ and $-\pi T$ form a bound pair at a larger temperature, T_p , than other fermions, for which strong self-energy acts against pairing. In some range below T_p (region II in Fig. 3) fermions with $\omega_m = \pm\pi T$ act as the source for the pairing for fermions with other ω_m . At a smaller $T < T_{\text{cross}}$ (region I in Fig. 3) fermions with other Matsubara frequencies pair on their own, and fermions with $\omega_m = \pm\pi T$ are no longer special. We verified this by solving the gap equation with and without fermions with $\omega_m = \pm\pi T$. We find (see the inset to Fig. 3) that in the first case the critical temperature is T_p , and in the second it is of order T_{cross} .

The special role of fermions with $\omega_m = \pm\pi T$ can be understood analytically, if we modify the original model such that T_{cross} becomes parametrically smaller than T_p and even vanishes. This can be achieved by

extending the model^{17,20,52} such that the pairing interaction is reduced by $1/N$, but the interaction in the particle-hole channel, leading to NFL behavior in the normal state, remains intact. The ratio T_{cross}/T_p decreases with increasing N , and T_{cross} vanishes for $N > N_{cr}(\gamma) \equiv (1 - \gamma)\Gamma(\gamma/2) \left(\frac{\Gamma(\gamma/2)}{2\Gamma(\gamma)} + \frac{\Gamma(1-\gamma)}{\Gamma(1-\gamma/2)} \right) > 1$. (The line $T_{cross}(N)$ terminates at $N = N_{cr}$, see Fig. 3.) For these N , region II extends down to $T = 0$. We emphasize that the extension to $N > 1$ is just the computational tool to make region II parametrically larger – our ultimate goal is to understand the existence of two regions below T_p for $N = 1$.

The limit $N \gg 1$ can be studied analytically. On the Matsubara axis, we found that the self-energy nearly retains its NFL normal state form, and the pairing gap $\Delta(\pm\pi T)$ is larger by N than $\Delta(\omega_m \neq \pm\pi T)$ (see the inset in panel (a) in Fig.2). The gap $\Delta(\pm\pi T) = \pi T(2/N)^{1/2} (1 - (T/T_p)^\gamma)^{1/2}$ is smaller than T for all temperatures. It emerges at T_p and vanishes at $T = 0$ (panel (a) in Fig.2). This is consistent with the fact that the pairing is fully induced by fermions with $\omega_m = \pm\pi T$ and wouldn't exist without them. On the real axis, we obtained

$$\begin{aligned} \Phi^*(\omega) &= \left(\frac{2}{N}\right)^{3/2} \pi T \left(\frac{g}{\pi T}\right)^\gamma \left[1 - \left(\frac{T}{T_p}\right)^\gamma\right]^{1/2} F_\Phi\left(\frac{\omega}{\pi T}\right) \\ \tilde{\Sigma}^*(\omega) &= \pi T \left(\frac{g}{\pi T}\right)^\gamma F_\Sigma\left(\frac{\omega}{\pi T}\right), \end{aligned} \quad (2)$$

where F_Φ and F_Σ are two scaling functions (Ref.⁴⁷). As the consequence, the frequency dependence of $\Delta(\omega)$ is set by T rather than by the gap. At the smallest frequencies, $\Sigma^*(\omega) \approx i \text{Im} \Sigma^*(0)$ and $\Delta(\omega) \propto i\omega$, as in a gapless superconductor. For such $\Delta(\omega)$, DOS $N(\omega)$ is non-zero down to the lowest frequencies (Fig. 2(c)), and the position of the maximum in $N(\omega)$ scales with T and remains finite at T_p (dots in Fig. 2(c)). As $T \rightarrow T_p$, the dip in the DOS at small ω fills in. The SF (Fig. 2(e),(f)), either shows the same behavior as the DOS, or has a single peak at $\omega = 0$, depending on the strength of the thermal contribution P (and, in, e.g., d -wave case, on the magnitude of $\Delta_{\mathbf{k}_F}(\omega)$).

At smaller $N < N_{cr}$, including physical $N = 1$, fermions with $|\omega_m| \neq \pi T$ can pair on their own at $T < T_{cross}$, without a push from fermions with $|\omega_m| = \pi T$. At these T , the system recovers the expected behavior of a superconductor – $\Delta(\pi T)$ tends to a finite value Δ at $T = 0$ (Fig. 2(b)), $\Delta(\omega)$ along the real axis becomes purely real at $\omega \leq \Delta$, the DOS and the SF have sharp peaks at $\omega = \Delta$ (see the lowest T data in panels (d), (e), (f)). This is region I in our notations. As temperature increases, but remains smaller than T_{cross} , peak positions follow $\Delta(T)$ and shift to smaller ω (the gap "closes"). However, at $T > T_{cross}$, the system crosses over to region II, where the pairing would not be possible without fermions with $\omega_m = \pm\pi T$, and the position of the maxima in the DOS and the SF are set by T rather than $\Delta(T)$, and the dip in the DOS fills in with increasing T .

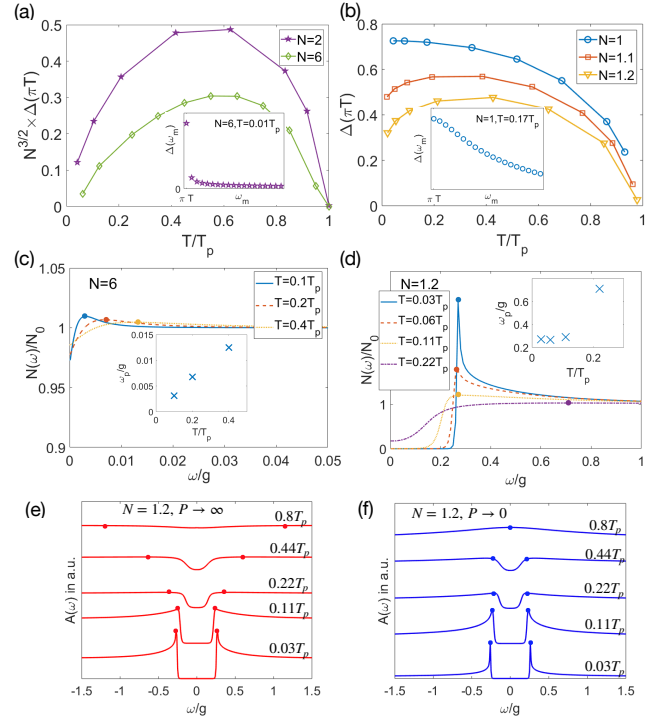


FIG. 2. (a) The gap at the first Matsubara frequency $\Delta(\pi T)$ as a function of temperature for several $N > N_{cr}$. The gap is non-monotonic and vanishes at $T = T_p$ and $T = 0$. Inset – the gap $\Delta(\omega_m)$ vs ω_m at a given T ; (b) Same at $N < N_{cr}$; (c) and (d): The DOS $N(\omega)$ for various T for $N > N_{cr}$ and $N < N_{cr}$. Insets: the position of the maximum in the DOS vs T . (e), (f) – the SF $A(\omega)$ for stronger (e) and weaker (f) thermal contribution to the self-energy.

Role of phase fluctuations. We next verify whether in region II superconducting order is destroyed by phase fluctuations. Our earlier results do not rely on phase coherence and are applicable even in the absence of long-range superconducting order. Moreover, the feedback effect from the pairing on fermionic self-energy is weak in region II already in the absence of phase fluctuations, and phase decoherence only reduces the feedback even further. Still, it is important to understand whether the region II corresponds to superconducting or pseudogap phase.

To analyze the strength of phase fluctuations, we set $\Delta(\omega_m, r) = \Delta(\omega_m) e^{i\phi(r)}$ and compute superfluid stiffness $\rho_s(T)$ as the prefactor for the $\int dr (\nabla\phi(r))^2$ term in the effective action. For a BCS superconductor $\rho_s(T < T_p) \approx E_F/(4\pi)$. Because E_F is assumed to be much larger than T_p , phase fluctuations are weak and $T_c \approx T_p$. In our case, we found in region II

$$\rho_s(T) \approx \frac{T}{N} \left(1 - \left(\frac{T}{T_p}\right)^\gamma\right) \frac{E_F}{\pi T \chi(0)} \left(1 + O\left(\frac{1}{N}\right)\right), \quad (3)$$

where, we remind, $\chi(0)$ is a static susceptibility of a

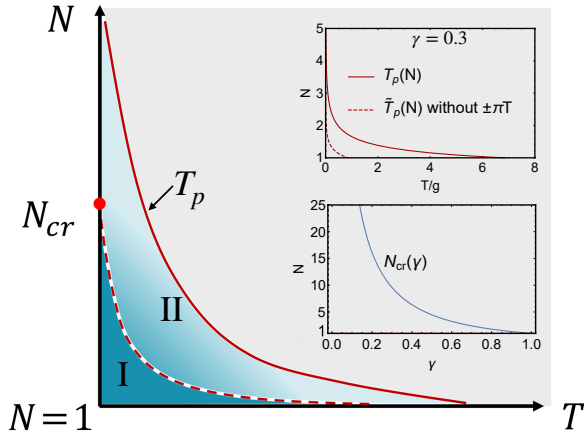


FIG. 3. The phase diagram of our QC model, extended to $N > 1$ (see text). The solid line is the onset temperature for the pairing, $T_p(N)$. The dashed line marks the crossover between BCS-type behavior at $T < T_{cross}$ (region I) and the novel behavior at a higher T (region II), when the fermionic self-energy remains approximately the same as in the normal state. Phase fluctuations likely destroy long-range phase coherence in phase II, in which case the actual $T_c \sim T_{cross}$ and the region II is the pseudogap phase. Insets: T_p obtained with and without fermions with the first Matsubara frequency $\omega_m = \pm\pi T$ for $N = 1$, $N_{cr}(\gamma)$.

critical bosonic field. It diverges at a QCP, so formally $\rho_s(T) \rightarrow 0$. However, Eliashberg theory is only valid when $E_F \geq \pi T \chi(0)$ because the integration over fermionic dispersion only holds up to E_F . This restricts $\chi(0)$ to $\pi T \chi_0 \leq E_F$ and $\rho_s(T)$ to $(T/N)(1 - (T/T_p)^\gamma)$. We see that $\rho_s(T)$ is of order T (even smaller at large N). In this situation, phase fluctuations are strong, $\langle \phi^2 \rangle \geq 1$, and likely destroy long range phase coherence^{34,53} at $T \geq T_{cross}$. Then, a portion of region II becomes the pseudogap phase. In region I the same calculation yields, at a small but finite T , $\rho_s \geq \Delta(T \rightarrow 0) \geq T_{cross}$, i.e., phase fluctuations are weak at $T < T_{cross}$, and phase coherence survives.

Application to d-wave case. To quantitatively apply our results to the cuprates, we (i) assumed that the critical boson is a (π, π) spin fluctuation, (ii) modeled the d -wave symmetry of the gap function by adding $\cos 2\theta$ factor to $\Phi^*(\omega)$, and (iii) used as an input the fact that spin fluctuations become nearly propagating modes be-

low T_p due to the feedback from the pair formation on bosonic self-energy⁵⁴, in which case the exponent $\gamma \leq 1$. We show the results⁵⁵ for the SF $A_{\mathbf{k}_F}(\omega)$ in Fig. 1 for \mathbf{k}_F in near-nodal and anti-nodal regions. The difference between the two is partly due to d -wave gap symmetry and partly due to the difference in the contribution from thermal fluctuations, which are much stronger in the antinodal region. We see that at $T < T_{cross}$, $A_{\mathbf{k}_F}(\omega)$ has two peaks, more strongly separated in the antinodal region. This is an expected result for a d -wave superconductor at $T \ll T_c$. At high $T > T_{cross}$, $A_{\mathbf{k}_F}(\omega)$ near the nodes has a single maximum at $\omega = 0$, while in the antinodal region $A_{\mathbf{k}_F}(\omega)$ has a dip at $\omega = 0$ and a shallow maximum, whose frequency scales with T . This behavior reproduces the key features of ARPES data in Refs.^{29–31,33,55–57}. The behavior of $N(\omega)$ is quite similar to that of $A(\omega)$ in the antinodal region. This is fully consistent with STM data^{56,58}.

Summary. In this paper we analyzed the feedback on the fermions from the pairing near a QCP in a metal, specifically the behavior of the DOS $N(\omega)$ and the SF $A_{\mathbf{k}_F}(\omega)$ on the FS. We considered a system of itinerant fermions with a singular interaction, mediated by the dynamical susceptibility of a critical boson $\chi(\Omega_m) = (g/|\Omega_m|)^\gamma$. We found two distinct regions below the onset temperature for the pairing T_p , which differ in the strength of the feedback from superconductivity on the electrons. At low $T < T_{cross} < T_p$ (region I in Fig. 3) the feedback is strong, and both $N(\omega)$ and $A_{\mathbf{k}_F}(\omega)$ have sharp quasiparticle peaks at $\omega = \Delta(T)$. At higher $T_{cross} < T < T_p$ (region II) the feedback is weak, and $N(\omega)$ has a dip at $\omega = 0$ and a hump at a frequency, which scales with T rather than $\Delta(T)$ and remains finite at $T = T_p$; near T_p the DOS just fills in. The SF either has the same structure as the DOS or a peak at $\omega = 0$ (the Fermi arc), depending on the location on the FS. We associated the physics in region II with the special role of fermions with Matsubara frequencies $\pm\pi T$. We argued that phase fluctuations are strong in region II and destroy phase coherence. Then the actual $T_c \geq T_{cross}$, while in between T_c and T_p the system is in a phase-disordered pseudogap state. A very similar behavior has been detected in tunneling and ARPES studies of the cuprates near optimal doping, and we view our theory as a microscopic explanation of the observed behavior.

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