Why the critical temperature of high-$T_c$ cuprate superconductors is so low: 
The importance of the dynamical vertex structure

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To fathom the mechanism of high-temperature ($T_c$) superconductivity, the dynamical vertex approximation (DΓA) is evoked for the two-dimensional repulsive Hubbard model. After showing that our results well reproduce the cuprate phase diagram with a reasonable $T_c$ and dome structure, we keep track of the scattering processes that primarily affect $T_c$. We find that local particle-particle diagrams significantly screen the bare interaction at low frequencies, which in turn suppresses antiferromagnetic spin fluctuations and hence the pairing interaction. Thus we identify dynamical vertex corrections as one of the main oppressors of $T_c$, which may provide a hint toward higher $T_c$’s.

Introduction. More than three decades after the discovery of the high-$T_c$ cuprate superconductors [1], the quest for higher (or even room-temperature) $T_c$ superconductors remains one of the biggest challenges in solid-state physics. Despite intensive efforts, we are still stuck with $T_c \lesssim 130$ K [2]. Nonetheless the cuprates do remain the arguably most promising material class, at least at ambient pressure [3].

In this arena, theoretical estimations of $T_c$, specifically identifying the reason why it is so low (as compared with the starting electronic energy scales of $\sim$ eV), should be imperative if one wants to possibly enhance $T_c$. Through many theories proposed and intensively debated, it has become clear that superconductivity in the cuprates is interlinked with electronic correlations, which are considered to mediate the pairing through spin fluctuations [4]. The simplest and most widely used model for cuprates is the repulsive Hubbard model on a square lattice, where a formidable problem is that the scale of $T_c$ is orders of magnitude smaller than the Hubbard interaction $U$ and the hopping amplitude $t$, which has been a key question from the early stage of high-$T_c$ studies [5]. Various approaches have been employed to attack the problem, see e.g. Refs. [6–14]. Thus, while the conventional phonon-mediated superconductors can now be accurately captured by density functional theory for superconductors (SCDFT) [15,16], a full understanding of $T_c$ in the Hubbard model has yet to come. One inherent reason for the low $T_c$ is the $d$-wave symmetry of the gap function arising from the local repulsion.

A possibly essential mechanism that reduces $T_c$ comes from vertex corrections. Migdal’s theorem [17], which works so nicely for phonon-mediated pairing, is no longer applicable to unconventional superconductivity due to the electron correlation. For strongly correlated systems, we should in fact expect vertex corrections to be a major player, affecting $T_c$ and changing it with respect to simpler (e.g., mean-field-like) treatments [18, 19].

Thanks to recent extensions of the dynamical mean-field theory (DMFT) [20–22], specifically the dynamical vertex approximation (DΓA) [23–26], the dual-fermion [27] and other related approaches [14, 28–33], such vertex corrections can now be studied for strong correlations; see [34] for a review. Owing to this development we now understand the (local) vertex structures much better [34–37], e.g., how they affect the spectral function and lead to pseudogaps in the normal phase [26, 29, 30, 38–43]. This now puts us in a position to shed light on the impact of dynamical vertex corrections on superconductivity.

In this paper, we analyze how vertex corrections affect $T_c$. We find that the dynamical structure (frequency dependence) of the vertex, $\Gamma(\nu, \nu', \omega)$, is actually essential for estimating $T_c$. Note that $\Gamma$ is non-perturbative; it sums up the local contribution of all Feynman diagrams (to all orders in the interaction) connecting two incoming and two outgoing particles. Physics of strongly correlated electrons such as the quasiparticle renormalization and the formation of Hubbard bands are hence encoded in $\Gamma$. On top of such correlations already included in DMFT, the DΓA further incorporates non-local correlations, in particular spin and superconducting fluctuations, see Fig. 1 and [34]. The present results show that the dynamics of $\Gamma$, which turns out to reduce the pairing interaction in a low-frequency regime, suppresses $T_c$ by one order of magnitude. We unravel the physical origin in the relevant dynamical vertex structure, as it is passed from the local vertex to the magnetic vertex describing antiferromagnetic spin fluctuations and, eventually, to the pairing interaction.

Model and methods. We consider the two-dimensional
single-orbital Hubbard model,
\[ \mathcal{H} = \sum_{\mathbf{k}, \sigma} \epsilon(\mathbf{k}) c_{\mathbf{k}, \sigma}^\dagger c_{\mathbf{k}, \sigma} + U \sum_{i} \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}, \]
where \( c_{\mathbf{k}, \sigma}^\dagger (c_{\mathbf{k}, \sigma}) \) creates (annihilates) an electron with spin \( \sigma = \uparrow, \downarrow \) and wave-vector \( \mathbf{k} \), \( U \) is the on-site Coulomb repulsion, and \( \hat{n}_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma} \). The two-dimensional band dispersion is given by \( \epsilon(\mathbf{k}) = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - 2t''(\cos 2k_x + \cos 2k_y) \) with \( t, t' \), and \( t'' \) being the nearest, second, and third neighbor hoppings, respectively. We consider two sets of hopping parameters: (a) \( t' = t'' = 0 \), and (b) \( t'/t = -0.20, t''/t = 0.16 \) which corresponds to the band-structure of \( \text{HgBa}_2\text{CuO}_{4+\delta} \) [44, 45].

We adopt the DΓA as a method that incorporates non-local correlations beyond the local correlations treated in DMFT. In the DΓA [23, 26, 34], the local two-particle vertex \( \Gamma \) that is irreducible in the particle-hole channel is calculated from a DMFT impurity problem. We employ the exact diagonalization as an impurity solver to this end, but also checked against quantum Monte Carlo simulations [46–49], see Supplemental Material [50].

From \( \Gamma_{\sigma'\sigma}(\nu, \nu', \omega) \), the non-local vertex \( F_{\sigma'\sigma}(k, k', q) \), which describes, among others, longitudinal and transversal spin-fluctuations, is obtained via the Bethe-Salpeter equation in the vertical particle-hole channel [as visualized in Fig. 1 (b)] and transversal particle-hole channel [not shown]. \( F_{\sigma'\sigma}(k, k', q) \) depends on the spin \( (\sigma, \sigma') \), two fermionic \( (k, k') \) and one bosonic \( (q) \) four-vectors consisting of momentum and Matsubara frequency, i.e. \( k = (k, \nu) \). From \( F \), the DΓA self-energy \( \Sigma(k) \) is in turn computed via the Schwinger-Dyson equation [34]; spin fluctuations included in \( \Sigma(k) \) give rise to a pseudogap in the non-local Green’s function \( G(k) \) [26, 40, 50].

For studying superconductivity, we extend here the existing DΓA treatment. That is, we extract, from \( F \), the particle-particle irreducible vertex \( \Gamma_{pp}(k, k', q = 0) = F(k', -k - k') - \Phi_{pp}(\nu, \nu', \omega = 0) \) (with four-vector in particle-particle convention). Here \( \Phi_{pp} \) is defined as the local reducible vertex diagrams in the particle-particle channel, which are included in \( F \) but need to be subtracted to obtain the \( \Gamma_{pp,Q=\mathbf{k}-\mathbf{k}'}(\nu, \nu') \), see [50] for details. The vertex \( \Gamma_{pp} \) contains spin fluctuations as a pairing glue, and we can now insert it into the particle-particle ladder [as illustrated in Fig. 1 (c) for selected diagrams]. For evaluating this ladder, we use the linearized gap (Eliashberg) equation [51]:
\[ \lambda \Delta(k) = -\frac{1}{\beta N_k} \sum_{k'\neq k} \Gamma_{pp}(k, k', q = 0) G(k') G(-k') \Delta(k'). \]

Here, \( \Delta(k) \) is the anomalous self-energy, \( \lambda \) the superconducting eigenvalue with \( \lambda \rightarrow 1 \) signaling an instability toward superconductivity [52], \( \beta = 1/T \) the inverse temperature, and \( N_k \) the number of \( \mathbf{k} \) points.

Size and dome shape of \( T_c \). We first show the superconducting eigenvalue \( \lambda \) for the two sets of hopping parameters in Fig. 2 (a) and (b), respectively. In the doping region in Fig. 2, the \( d \)-wave has the largest \( \lambda \), while antiferromagnetic fluctuations become dominant close to half-filling, c.f. Refs. [26, 53]. A superconducting insta-
The latter eventually leads to a reduced $T_c$. Thus we have traced that the local vertex corrections are responsible for the reduction of $T_c$, where an important message is that their dynamical structures from the local $\delta \Gamma_{pp}$ the pairing vertex $\Gamma_m$ in which we take the dynamical vertex is widened, $\lambda$ is seen to dramatically decrease, already when a few frequencies are taken into account. This signifies that the low-frequency part of the dynamical $\Gamma_m$ is quite important.

The results well reproduce the phase diagram of the cuprates with a dome structure and peaks that amount to $T_c \approx 50 - 80$ K around $n = 0.80 - 0.95$ if we take a typical $t \approx 0.45$ eV [54]. We can explain the physical origin of the $T_c$ dome as follows: antiferromagnetic spin fluctuations that mediate the pairing become stronger [i.e., $\Gamma_{pp}$ in Fig. 2 (d)] toward half-filling, while close to half-filling the self-energy blows up and damps $G(k)$ in Fig. 2 (c). The latter eventually leads to a pseudogap at smaller dopings within the central peak in a three-peak spectrum, see Supplemental Material [50]. Thus the dome appears as a consequence of two opposing factors: $\Gamma_{pp}$ and $G(k)$ in the gap equation (2). We can see in Fig. 2 (d) that $\Gamma_{pp}$ is sharply peaked at around $Q = (\pm \pi, \pm \pi)$ (with some offset and splitting because of incommensurability), leading to a $d$-wave $\Delta(k)$ in Eq. (2). Let us note that a superconducting dome has also been reported in e.g. [6, 7, 13, 14], but not in the dual-fermion approach [10, 12].

**Importance of the dynamical vertex structure.** Let us now look into the structure of the vertex $\Gamma(\nu, \nu', \omega = 0)$ against frequencies $\nu, \nu'$. As we shall see below, if we start from a mean-field or random phase approximation (RPA)-like treatment, where $\Gamma_m(\nu, \nu', \omega) = \Gamma_{\nu \nu'} - \Gamma_{\nu' \nu}$, is replaced with the bare $-U$ in the Bethe-Salpeter ladder [55], this would yield stronger spin fluctuations and over-estimate $T_c$ by an order of magnitude.

We can elucidate this point in an energy-resolved fashion by taking the local irreducible vertex in the magnetic channel $\Gamma_m(\nu, \nu', \omega)$ only up to a frequency $n_{vertex}$, with the bare $(-U)$ adopted outside this range [56] (pictorially this means taking Fig. 1 (a) instead of Fig. 1 (b) for large frequencies). In Fig. 3 (a), we plot the eigenvalue $\lambda$ against $n_{vertex}$ [57]. As the region $n_{vertex}$ in which we take the dynamical vertex is widened, $\lambda$ is seen to dramatically decrease, already when a few frequencies are taken into account. This signifies that the low-frequency part of the dynamical $\Gamma_m$ is quite important.

Figure 3 (b) displays the deviation, $\delta \Gamma_m(\nu_n, \nu_{n'}; \omega = 0) \equiv \Gamma_m(\nu_n, \nu_{n'}; \omega = 0) - (-U)$, for a (a) second-order, or (b) third-order perturbation theory for $U = 6t, t' = t'' = 0, n = 0.825$, and $T/t = 0.067$. In each panel, the inset shows a typical diagram taken into account, and the corresponding eigenvalue $\lambda$ is indicated.
the suppression of the local $\Gamma_m$ as the key ingredient for low $T_c$’s, we can now pin-point which physical processes are at its origin. In Fig. 4 we show the contributions to $\delta \Gamma_m$ in (a) second-order and (b) third-order perturbation theory, where we show a typical diagram along with the eigenvalue $\lambda$ estimated in DGA when $\Gamma_m$ is replaced by the displayed local vertex [57]. When the bare value $(-U; \delta \Gamma_m = 0)$ is used instead of the full $\Gamma_m$, $\lambda$ is enhanced dramatically from the correct value $0.45$ to $2.49$ for $T/t = 0.067$ ($T_c$ increases accordingly from $0.01t$ to $0.13t$). We can see that most of the dynamical effect is already included in the second-order particle-particle diagram in Fig. 4(a), which compensates the bare contribution $(-U)$ for $\nu_m \approx -\nu \nu'$, and strongly reduces $\lambda$ back to $0.40$. Third-order diagrams in Fig. 4(b) slightly enhance $\lambda$, and already resemble the full vertex qualitatively. Thus the second-order particle-particle diagrams in Fig. 4(a) constitute by far the major process for the suppression of the $\lambda$.

Hence it is worthwhile to look into this second-order contribution in more detail. The local irreducible vertex $\Gamma_m$ is the building block for the non-local particle-hole ladder that leads to magnetic fluctuations as visualized in Fig. 1(b). If we take $\Gamma_m(\nu, \nu', \omega) = - U$ as in Fig. 1(a) or the left part of Fig. 5, we obtain the standard RPA with a Stoner-enhanced spin susceptibility,

$$\chi = \chi_0/(1 - U \chi_0) = \chi_0 + \chi_0 U \chi_0 + \chi_0 U \chi_0 U \chi_0 \ldots \quad (3)$$

While all the terms enhance the susceptibility in this geometric series in $U$, local vertex corrections do need to be included in the particle-hole ladder with $\Gamma_m(\nu, \nu', \omega) = - U + \delta \Gamma_m(\nu, \nu', \omega)$ as a building block. In Fig. 4(a) we have identified the second-order particle-particle contribution to $\delta \Gamma_m > 0$ to be most important for suppressing antiferromagnetic spin fluctuations, and the inclusion of such a contribution $\delta \Gamma_m$ in the ladder series for $\Gamma_m$ is visualized in the right part of Fig. 5.

The difference from the RPA ladder comprising $-U$ and particle-hole bubbles (left block in Fig. 5) is that $\delta \Gamma_m > 0$ has (in the second order) two $-U$’s and a local particle-particle bubble (right block in Fig. 5). This bubble, being a particle-particle bubble, depends on the frequency combination $\nu + \nu' + \omega$ rather than on $\omega$ alone as in particle-hole bubbles. This, first of all, gives the pronounced frequency structure of $\delta \Gamma_m$ in Fig. 4(a). Since Fig. 5 shows typical diagrams that contribute to $\Gamma_m$, we can also see that, with a $\delta \Gamma_m$ located at an end of the ladder, $\Gamma_m$ and $\Gamma_{pp} = F - \Phi_{pp}$ inherits a similar frequency structure as in Figs. 3(c,d); see Supplemental Material [50] for a general explanation.

Second, at its maximum ($\omega = 0, \nu = -\nu$), the particle-particle bubble $\sum_{\nu''} G(\nu') G(-\nu'') = \sum_{\nu''} G(\nu'') G^*(\nu'')$, has a sign opposite to the particle-hole bubble $\sum_{\nu', \nu''} G(\nu'') G(\nu'')$, because the biggest contribution comes from $\text{Im} G(\nu)$. Hence $\delta \Gamma_m$ partially compensates the second-order RPA contribution, $U \chi_0 U$ in Eq. (3).

This is the reason why $\delta \Gamma_m$ reduces the bare $U$, whereas the RPA ladders Eq. (3) enhances it.

Now we are in a position to finally grasp a physical picture: while a repulsive interaction can give rise to a spin-fluctuation mediated attraction through the particle-hole channel, a local repulsive interaction $U$ always leads to a repulsion between two particles in the particle-particle channel, too. As we have seen in Fig. 5, this repulsion in the particle-particle channel reduces the antiferromagnetic spin fluctuations, albeit only for certain frequency combinations. With reduced antiferromagnetic spin fluctuations, superconductivity is suppressed.

**Conclusion and outlook.** We have extended the DGA formalism for studying superconductivity in the repulsive Hubbard model on a square lattice. Our results well reproduce the superconducting dome and typical values of $T_c \approx 50 - 80$ K for the cuprates. We have pinpointed the importance of dynamical vertex corrections. That is, $T_c$ would be around room temperature if the pairing interaction was built from a ladder with the bare interaction $U$. However, local vertex corrections give rise to a pronounced frequency structure accompanied with a suppression (screening) of the irreducible magnetic vertex $\Gamma_m$ (i.e., the effective interaction in the magnetic channel). This in turn suppresses antiferromagnetic spin fluctuations and the pairing glue ($\Gamma_{pp}$) for superconductivity in the particle-particle channel.

Thus local particle-particle fluctuations are at the origin of the suppression of $\Gamma_m$, so that it is intriguing to ask: can one possibly evade this oppressor of $T_c$? This is not simple: As the leading correction that reduces the bare interaction $U$ is $\sim U^2$, the suppression becomes smaller for weaker Coulomb interactions, but so do the antiferromagnetic spin fluctuations. Local particle-particle fluctuations can be suppressed by disorder or a magnetic field [58], but this would degrade the non-local particle-particle (superconducting) fluctuations, too. One way-
out might be to exploit the characteristic frequency structure of $\Gamma_m$, possibly in combination with a frequency-dependent (local) interaction, which may originate from off-site (extended Hubbard) interactions as described in dual-boson [59] and extended-DMFT [60–64] approaches, or from phonons. A further route may be a proper design of the band structure, including multi-orbital models. Another, completely different outcome of the frequency structure in the vertex is that it may possibly realize exotic gap functions on the frequency axis.

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Supplemental materials to

“Why the critical temperature of high-$T_c$ cuprate superconductors is so low: The importance of the dynamical vertex structure”

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I. CALCULATION OF THE PAIRING VERTEX $\Gamma_{pp}$

In this section, we explain how to calculate the pairing interaction $\Gamma_{pp}$ within the ladder DΓA formalism. We can fix one bosonic frequency ($\omega$) to treat a two-particle quantity as a matrix that depends on two fermionic frequencies ($\nu, \nu'$). The nonlocal two-particle vertex $F_r$ is then calculated in the ladder expansion through the matrix equation based on local irreducible matrix $\Gamma_r$,

\[
F_r = \Gamma_r - \Gamma_r \chi_0 F_r,
\]

with $r = d, m$ denoting the density (d) or magnetic (m) channel, and $\chi_0$ is the bare bubble susceptibility. The density and magnetic vertex $\Gamma_{d/m}$ are obtained by $\Gamma_{d/m} = \Gamma_{\uparrow \uparrow} \pm \Gamma_{\downarrow \downarrow}$, whose particle-hole convention is displayed in Fig. S.1(a). Let us express $\Gamma_r$ as $\Gamma_r = \mathcal{U}_r + \delta \Gamma_r$ as in the main text, where $\mathcal{U}_r$ is the matrix with all the elements being $U_{dd} = U$ and $U_{dm} = -U$ for $r = d$ and $m$, respectively [1]. Then the Bethe Salpeter equation reads

\[
F_r = (\mathcal{U}_r + \delta \Gamma_r) \sum_{n=0}^{\infty} [(-\chi_0(\mathcal{U}_r + \delta \Gamma_r))^n]
\]

\[
+ \delta \Gamma_r \sum_{n=0}^{\infty} [(-\chi_0\delta \Gamma_r)^n]\mathcal{U}_r \left[1 - \mathcal{U}_r \xi_r \right] \sum_{n=0}^{\infty} [(-\chi_0\delta \Gamma_r)^n]
\]

\[
= \sum_{n=0}^{\infty} [(-\delta \Gamma_r \chi_0)^n] \mathcal{U}_r \left[1 - \frac{\mathcal{U}_r \xi_r}{1 + \mathcal{U}_r \xi_r} \right] \sum_{n=0}^{\infty} [(-\chi_0\delta \Gamma_r)^n]
\]

where $\chi_r = \tilde{\chi}_r/(1 + U_r \tilde{\chi}_r)$ is the physical susceptibility, and we have used that $1 + \delta \Gamma_r \sum_{n=0}^{\infty} [(-\chi_0\delta \Gamma_r)^n] (-\chi_0) = \sum_{n=0}^{\infty} [(-\delta \Gamma_r \chi_0)^n]$. The above equation is a generalization of the discussion in the main text; it explicitly shows that
$F_\tau$ reduces to RPA in the limit $\delta \Gamma_\tau \to 0$. If we introduce a finite $\delta \Gamma_\tau$, the physical susceptibility is modified through Eq. (S.3). We can see that the vertex correction $\delta \Gamma$ affects not only the physical susceptibility (that depends only on $\omega$) but also the vertex structure itself (which depends on $\nu, \nu', \omega$). While we now employ $\delta \Gamma$, following the main text, we can alternatively express $F_\tau$ without infinite summation as

$$F^{\nu \nu'}_\tau = (\chi^{\nu}_0)^{-1} \left[ \delta_{\nu, \nu'} - \chi^{\nu \nu'}_r (\chi^0_0)^{-1} \right] + U_r (1 - U_r \chi_r) \gamma^{\nu \nu'}_r,$$

where $(\chi^{-1})^{-1} = \chi^{-1} + \delta \Gamma_r$ and $\gamma^{\nu \nu'}_r \equiv (\chi^{\nu}_0)^{-1} \sum \nu' \chi^{\nu \nu'}_r$. This is the same expression as previously employed in ladder DΓA (for details see [2]), and we have used this formulation in the actual calculations. As in the self-energy calculation, we consider a Moriya-esque $\lambda$-correction for $F$ by replacing the physical $\chi_r$ as [1–3]

$$\chi^{\nu}_r \equiv (\chi^{-1}_r + \lambda_r)^{-1}.$$  

In the ladder DΓA, the two-particle vertex $F_{\tau \uparrow \downarrow}$ is related to the ladder-expanded vertex $F_\tau$ through

$$F_{\text{ladder,}\uparrow \downarrow}(k, k', q) = \frac{1}{2} \left[ F_{d,q}(\nu, \nu', \omega) - F_{m,q}(\nu, \nu', \omega) \right] - F_{m,k'-k}(\nu, \nu + \omega, \nu' - \nu) - F_{\text{loc,}\uparrow \downarrow}(\nu, \nu', \omega).$$

Here, both the particle-hole and the transversal particle-hole channels are considered with the local double-counting terms subtracted [1, 2], and the pairing vertex is calculated as

$$\Gamma_{pp}(k, k', q = 0) = F_{\text{ladder}}(k', -k, k - k') - \Phi_{\text{loc,pp}}(k, k', q = 0)$$

for which the particle-particle convention as displayed in Fig. S.1(b) is employed. For singlet pairing, for which $\Delta(k) = \Delta(-k)$, we can use $\Gamma^s_{pp}$ defined as

$$\Gamma^s_{pp}(k, k', q = 0) \equiv \Gamma^s_{pp,Q=k-k'}(\nu, \nu') = \frac{1}{2} F_{d,k-k'}(\nu', -\nu, (\nu - \nu')) - \frac{3}{2} F_{m,k-k'}(\nu', -\nu, (\nu - \nu')) - F_{\text{loc,}\uparrow \downarrow}(\nu', -\nu, (\nu - \nu')) - \Phi_{\text{loc,pp}}(\nu', \nu', \omega = 0),$$

which is the same as $\Gamma_{pp}$ for singlet eigenvectors if we take the symmetric component under the sign change of $k$ ($k \leftrightarrow -k$). For triplet pairing, for which $\Delta(k) = -\Delta(-k)$, we can similarly use $\Gamma^t_{pp}$ defined as

$$\Gamma^t_{pp}(k, k', q = 0) \equiv \Gamma^t_{pp,Q=k-k'}(\nu, \nu') = \frac{1}{2} F_{d,k-k'}(\nu', -\nu, (\nu - \nu')) + \frac{1}{2} F_{m,k-k'}(\nu', -\nu, (\nu - \nu')) - F_{\text{loc,}\uparrow \downarrow}(\nu', -\nu, (\nu - \nu')) - \Phi_{\text{loc,pp}}(\nu', \nu', \omega = 0).$$

II. CONVERGENCE AGAINST FREQUENCY RANGE OF THE VERTEX

Due to the heavy computational cost, we can only consider a limited range of frequency ($n_{\text{core}} \approx 160$ positive frequencies) for the vertex, while superconductivity occurs at quite low temperatures which corresponds to a fine frequency grid. Therefore, it is a challenge to obtain well-converged results against the frequency range of the local
FIG. S.2: Dependence of the \(d\)-wave superconductivity eigenvalue on \(1/n_{\text{core}}\) for a fixed \(n_{\text{outer}}\), or \(1/n_{\text{outer}}\) for a fixed \(n_{\text{core}}\) for (a) \(n = 0.825, t'/t'' = 0\), and (b) \(n = 0.90, t'/t = -0.20, t''/t = 0.16\) with \(U/t = 6.0, T = 0.01t\). These parameters correspond approximately to the optimal doping region in Fig. 1(a),(b) in the main text. Horizontal lines are guides to the eye for the (converged) \(\lambda\) value at \(n_{\text{core}} = 159\) for \(n_{\text{outer}} = 1024\) (left) and \(n_{\text{outer}} = 2048\) (right).

two-particle quantities in DMFT. Here, instead of simply solving the Bethe-Salpeter equation for such a limited frequency range, we consider a wide frequency range (\(n_{\text{outer}}\) points on the positive side). For the outer frequencies, we use the bare \(U_r = \pm U\) instead of \(\Gamma_{\text{ph}}\) (which is restricted to \(n_{\text{core}}\) positive frequencies). This supplementation of \(\Gamma_{\text{ph}}\) by \(U_r\) is done twice: once for calculating \(\Gamma_{\text{ph}}\) from the impurity susceptibility and again when solving the Bethe-Salpeter equation. Figure S.2 shows the dependence of the result on the inner range \(n_{\text{core}}\) (the range for the two-particle data in DMFT) and on the outer range \(n_{\text{outer}}\) (the range for the bare \(U\) contribution). We can see that the \(n_{\text{core}}\) dependence quickly converges if we take into account a wide range of the bare \(U\) contribution. While convergence with respect to \(n_{\text{outer}}\) is not fast, we can treat a large frequency range for the bare \(U\) contribution without much computational costs (note the computational bottleneck is the exact diagonalization (ED) calculation of the local vertex). In the calculation shown in Fig. 1 in the main text, we take \(n_{\text{outer}} = 1024\) and up to \(n_{\text{core}} = 100\) for the lowest temperature \((T = 0.01t)\), and for Figs. 2 and 3 we take \(n_{\text{outer}} = 1024\) and \(n_{\text{core}} = 120\).

III. COMPARISON WITH CT-QMC RESULTS

Here, we show the comparison with the eigenvalues \(\lambda\) that are obtained with continuous-time quantum Monte Carlo (CT-QMC) \([4–7]\) as an impurity solver. The result in Fig. S.3 demonstrates that the ED discretization error hardly affects the \(\lambda\) values presented in the present paper. Note that the error which comes from using different \((n_{\text{core}}, n_{\text{outer}})\) for ED and CT-QMC is smaller than the size of symbols. We have also checked the calculated \(\Sigma(k)\) agrees with CT-QMC result.

IV. MOMENTUM DEPENDENCE OF THE SPECTRAL WEIGHT

In this section, we discuss spectra in the DΓA calculations in more detail, to specifically look at how a pseudogap develops. First in Fig. S.4, instead of showing the spectral weight obtained with analytical continuation, we present Green’s function \(G\) at imaginary time \(\tau = \beta/2\)

\[
-\beta G(k, \tau = \beta/2) = \pi \int A(k, \omega) \left[ \frac{\beta}{2\pi \cosh(\frac{\beta\omega}{2})} \right] d\omega, \quad (S.11)
\]

which reflects the spectral weight \(A(k, \omega = 0)\) with a finite temperature blurring and has the advantage that no analytical continuation is needed. We can see, in Fig. S.4 for various fillings, a strong reduction of the spectral weight around the anti-nodal directions along \(k = (\pm \pi, 0), (0, \pm \pi)\). Accordingly, the Fermi surface shrinks into Fermi arcs as we approach the half filling, as observed in experiments for cuprates. In Fig. S.5 we note that in this region,
FIG. S.3: Comparison of results for the $d$-wave superconductivity eigenvalue $\lambda$ between two impurity solvers: CT-QMC (with $n_{\text{outer}} = 400$ and $n_{\text{core}} = 50$ for $T \leq 0.013t$, and $n_{\text{core}} = 80$ for $T = 0.010t$) and ED (with $n_{\text{outer}} = 1024$ and $n_{\text{core}} = 50$ for $T \leq 0.02t$, $n_{\text{core}} = 80$ for $T = 0.013t$, and $n_{\text{core}} = 100$ for $T = 0.010t$). Here we take $U/t = 6.0, t' = t'' = 0$, and $n = 0.825$ which correspond approximately to the optimal doping region in Fig. 1(a) in the main text.

FIG. S.4: Momentum dependence of $G(k, \tau = \beta/2)$ for the fillings indicated at $U = 6t, t' = t'' = 0, T/t = 0.02$.

$|G(k, \omega_n = \pi/\beta)|$ has quite a different structure from the spectral weight Eq.(S.10), while $\text{Im}G(k, \omega_n = \pi/\beta)$ is similar to $\beta G(k, \tau = \beta/2)$ but with larger temperature blurring.

Let us next show in Fig. S.6 the analytically continued density of states $\rho(\omega) = \sum_k A(k, \omega)$ as obtained from a Padé fit, at a higher temperature ($T = 0.1t$) where the Padé fit works more reliably. Here, we can see a salient pseudogap structure toward half-filling ($n \geq 0.90$) as well as the lower and upper Hubbard band structure.

These demonstrate that the DFA approach describes a pseudogap structure along with Hubbard bands for the parameter region studied here. The method also describes that antiferromagnetic correlations (and ordering) fade away when doping puts the system away from half filling, see Fig. 2 (d) in the main text and Ref. [8].
FIG. S.5: Green’s function \(|G(\mathbf{k}, \omega_n = \pi/\beta)|\) and \(-\text{Im} G(\mathbf{k}, \omega_n = \pi/\beta)\) plotted against momentum for a filling \(n = 0.925\). Other parameters and color codes are the same as in Fig. S.4. Note a difference in the color code from Fig. 2 (c) in the main text.

FIG. S.6: Densities of states for the fillings indicated at \(U = 6t, t' = t'' = 0, T/t = 0.1\).

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