Spin scattering turns complex at strong coupling: the key to pseudogap and Fermi arcs in the Hubbard model

Friedrich Krien,¹ Paul Worm,¹ Patrick Chalupa,¹ Alessandro Toschi,¹ and Karsten Held¹

¹Institute for Solid State Physics, TU Wien, 1040 Vienna, Austria

We analyze the pseudogap phenomenon of hole-doped cuprates via a Feynman-diagrammatic inspection of the Hubbard model. Our approach captures the pivotal interplay between Mott localization and Fermi surface topology beyond weak-coupling spin fluctuations, which open a spectral gap near hot spots. We show that strong coupling and particle-hole asymmetry give rise to another mechanism: the spin-fermion vertex develops a large imaginary part. While its real part always suppresses the electronic lifetime, the imaginary part has a twofold effect. For antinodal fermions a gap opening is boosted; conversely, around the node Fermi arcs are protected.

Introduction — The single-band Hubbard model is believed to capture key physics of the cuprates [1, 2] and nickelates [3–5]. Various numerical and theoretical approaches show that this model exhibits the so-called pseudogap phase [6–28], an extreme nodal/antinodal dichotomy of the Fermi surface (FS), where spectral weight is concentrated on Fermi arcs [29, 30].

The important role played by spin fluctuations [6–8, 18, 31, 32] is naturally suggested by the proximity to an antiferromagnetic phase. In the weak-coupling picture a spectral gap opens near hot spots [22, 31, 32], which is observed in electron-doped cuprates [33, 34]. In the hole-doped case the gap instead opens near the antinodes [30] and a reconstruction of the FS [22, 23, 35, 36] is evidenced by quantum oscillations [37]. Other features not easily explained by weak-coupling spin fluctuations are the good Fermi liquid properties of underdoped cuprates [38] and indications of broken time-reversal symmetry [39–41]. Alternative origins of the pseudogap [42–47] are hence under consideration.

Spin fluctuations are collective excitations which affect the propagation of the same (quasi)fermions they originate from. This effect can be described diagrammatically in terms of an effective interaction, the spin-fermion vertex Γ. Often Γ is interpreted as the scattering of a particle (hole) with the spin fluctuations, see Fig. 1 (a,b). However, it also describes creation/annihilation of particle-hole pairs, see Fig. 1 (c,d).

Let us consider the propagation of holes, the dominant charge carriers in underdoped cuprates. They couple to spin fluctuations via particle-hole pair creation/annihilation [diagram (e)] or hole scattering [diagram (f)]; the intermediate state is either a particle or a hole, respectively. As spin fluctuations extend over a correlation length ξ, the transferred momentum can deviate from the antiferromagnetic wave vector Q = (π, π) in a circle ∼ 1/ξ, for example, areas ‘arc, pg, hs’ in panel (g). Because of the warped FS, Q connects the nodal (ARC) region with mostly particle-like intermediate states in area ‘arc’. The antinodal (PG) region is connected to hole-like states in area ‘pg’. As the result, at ARC most of the available intermediate states correspond to diagram (e), whereas at PG diagram (f) dominates.

At weak coupling, where the spin-fermion vertex is purely real, this dichotomy is irrelevant. Both processes enhance the damping (imaginary part of the self-energy). The intermediate states ‘on shell’, i.e., on the FS, prevail, which is ideally suited for hot spots (HS). Hence, for large ξ a gap opens at the HS. This weak-coupling mechanism is at odds with numerical data at strong coupling [49], where the pseudogap opens at the antinode (PG).

In this Letter, based on parquet dual fermion [50–52] calculations for the Hubbard model and analytic considerations, we identify the precise strong-coupling mechanism responsible for the pseudogap dichotomy. At strong coupling, and if particle-hole symmetry is broken [53, 54], the spin-fermion vertex acquires a large imaginary part [55–57]. As a result, the processes Fig. 1

FIG. 1. (a) Particle and (b) hole scattering, (c) creation and (d) annihilation of an electron-hole pair at the spin-fermion vertex. Filled and open arrowheads denote particles and holes. Hole self-energy diagrams show (e) particle-hole creation and (f) hole scattering. (g) Noninteracting Green’s function. Red (blue) indicates G′ < 0 (G′ > 0) above (below) the FS. The intermediate state in (e,f) is offset by Q = (π, π) from the initial state within a circle ∼ 1/ξ; dashed lines show the AZB [48]. The pseudogap results from asymmetry of diagrams (e,f): Fermi arcs (ARC) are cooled down by electron-hole creation (e), while the pseudogap (PG) region is damped by hole scattering (f). Hot spots (HS) are roughly balanced.
(e) and (f), but now with off-shell (virtual) intermediate states, lengthen and shorten the lifetime, respectively. Parts of the FS inside (outside) the antiferromagnetic zone boundary (AZB) are cooled (heated). This explains why the ARC is more Fermi-liquid-like than previously expected and why the antinodal PG is actually hotter than the eponymous HS.

**Method and model** — Diagrammatic extensions [24] of dynamical mean-field theory (DMFT) [58] have proven useful to study spin fluctuations in strongly correlated systems. To reduce bias [59] we employ the method of Ref. [52], corresponding to the parquet approximation [60] for dual fermions [50, 51]. Through the boson-exchange formalism [61, 62] we establish a relationship to the spin-fermion model. We apply this machinery to the hole-doped Hubbard model, \( H = - \sum_{\langle ij \rangle} t_{ij} c_{i \sigma} \hat{c}_{j \sigma} + U \sum_i n_i \hat{n}_i \). Here, \( c_{i \sigma}^{\dagger} (c_{i \sigma}) \) create (annihilate) an electron with spin \( \sigma \) at site \( i \); \( n_{\sigma} = c_{i \sigma}^{\dagger} c_{i \sigma} \). The hopping parameters \( t = 1 \), \( t' = -0.2t \), \( t'' = 0.1t \), and interaction \( U = 8t \) correspond to \( \text{Bi}_2\text{Sr}_2\text{La}_x\text{CuO}_6 \) [63].

**Imaginary part of the spin-fermion vertex** — To illustrate the mechanism in the spirit of fluctuation diagnostics [18, 19], we consider the following ansatz for the contribution of spin fluctuations with an energy \( \omega \) and momentum \( \mathbf{q} \) to the self-energy, \( \Sigma_{\text{sp}}(k, q) \propto -G_{k+q} W_q \Gamma_{kq} \). Here, \( k = (k, \nu), q = (q, \omega) \) are momentum-energy four-vectors, \( W_q = -U - \frac{i}{\hbar} \chi_q U \) denotes the (real-valued) screened interaction, \( \chi_q \) the spin susceptibility. To obtain the full self-energy \( \Sigma_{\text{sp}}(k) \) due to spin fluctuations we still have to sum over momenta \( q \) and frequencies \( \omega \). In addition, the full self-energy contains also a momentum-independent contribution \( \Sigma_{\text{loc}}(\nu) \) due to strong local correlations [64], i.e., \( \Sigma(k) = \Sigma_{\text{loc}}(\nu) + \Sigma_{\text{sp}}(k) \). In the following we consider only the dominant static \( q_0 = (q, \omega = 0) \) contribution to the imaginary part of the self-energy,

\[
\Sigma_{\text{sp}}''(k, q_0) \propto -[G''_{k+q_0} \Gamma_{kq_0} + G''_{k+q_0} \Gamma_{kq_0}] W_{q_0}. \tag{1}
\]

Crucially, \( \Gamma \) has a real \( (\Gamma') \) and an imaginary part \( (\Gamma'') \). We note that an imaginary vertex was recently considered in Yukawa-SYK models [65, 66]. However, to the best of our knowledge, the importance of \( \Gamma'' \) for the pseudogap dichotomy has not been realized before.

Let us start by considering the conditions for a sizeable \( \Gamma'' \) in the simpler case of the Anderson impurity model (AIM). We denote its local spin-fermion vertex as \( \Gamma_{\text{loc}}(\nu, \omega) \). The leading vertex correction due to local spin exchange has the imaginary part [59, 67],

\[
\Gamma_{\text{loc}}''(\nu, \omega = 0) \approx -\frac{\text{TU}^2}{2} \chi_{\text{sp}}(0, \nu) g''(\nu), \tag{2}
\]

where \( \chi_{\text{sp}} \) is the spin susceptibility, \( T \) the temperature, \( g' \) and \( g'' \) denote real and imaginary part of the impurity Green’s function. Sufficient for a large \( \Gamma_{\text{loc}}''(0^+, \omega = 0) \) are the following conditions: (i) strong particle-hole asymmetry (\( g' \) vanishes at symmetry), (ii) large enough spectral weight \( -g''(0^+) / \pi \), (iii) large \( \chi_{\text{sp}}(0, 0) \) (preformed local moment). All of these conditions are satisfied by the DMFT solution of the Hubbard model in the relevant parameter regime for hole-doped cuprates. In general the vertex \( \Gamma \) in the Hubbard model depends on momenta, however, as our numerical calculations below show, the here outlined conditions remain relevant for a large \( \Gamma'' \).

**Effect on lifetime** — We analyze Eq. (1) and put the qualitative considerations regarding Fig. 1 on mathematical grounds. The spin-fermion self-energy for holes [68] is given either by diagram (e) or (f). The respective particle- or hole-like intermediate state carries the momentum \( \mathbf{k} + \mathbf{q} \).

The real part of the vertex makes no difference between (e) and (f). The corresponding term in Eq. (1) is always negative: \( -G'\Gamma'W < 0 \) since \( G'' < 0 \), \( \Gamma' \approx 1 > 0 \), and \( W < 0 \). Therefore, \( \Gamma' \) universally enhances the magnitude of the imaginary part of the self energy (the scattering rate) [7, 20, 22, 31, 69].

On the contrary, the sign of \(-G'\Gamma'W \) in Eq. (1) depends on the intermediate state. We find in our calculations that \( \Gamma''(\mathbf{k}, \nu, \mathbf{q}, \omega = 0) \) is an odd function of \( \nu \) and in the parameter regime for hole-doped cuprates \( \Gamma'' \approx 0 \) for Matsubara frequency \( \nu > 0 \). However, the sign of the real part of the Green’s function differs:

\[
G'(k + q, 0^+) = \frac{\mu - \varepsilon_{k + q} - \Sigma'(k + q, 0^+) - \Sigma''(k + q, 0^+)^2}{\left(\mu - \varepsilon_{k + q} - \Sigma'(k + q, 0^+)ight)^2 + \Sigma''(k, 0^+)^2} \tag{3}
\]

for particle-like (hole-like) intermediate virtual states in Fig. 1 (e) and (f), respectively. We set \( \nu > 0 \), hence

\[
-G'_{k + q_0} \Gamma''_{kq_0} W_{q_0} \left\{ \begin{array}{ll}
< 0 & \text{if } k + q \text{ is hole-like,} \\
> 0 & \text{if } k + q \text{ is particle-like.}
\end{array} \right. \tag{3}
\]

The former enhances the electronic scattering at the Fermi level, the latter diminishes it. This dichotomy resembles a chemical bonding, where the hybridization with a virtual state at higher (lower) energy reduces (enhances) the energy of the initial state [70]. The difference is that, due to the complex vertex, this now becomes a dichotomy for the state’s lifetime (not its energy).

**Relevance to hole-doped cuprates** — By applying this reasoning to underdoped cuprates, we gain the key insight of our work: the pseudogap originates in the asymmetry of diagrams (e) and (f) of Fig. 1, introduced by the imaginary part of the spin-fermion vertex.

Colors in panel (g) indicate the sign of \( G'(k, \nu = \pi/5) \), where we use the noninteracting Green’s function \( G^0 \) at a suitable filling. Let us consider the points ARC, PG, and HS marked with filled square, circle, and diamond, respectively. Through the vector \( \mathbf{Q} = (\pi, \pi) \) and circles \( \sim 1/\xi \) we identify the available intermediate states in areas arc, pg, and hs. Red color of the intermediate state (particle, \( G' < 0 \)) indicates a contribution to the self-energy like diagram (e). Blue color (hole, \( G' > 0 \)) corresponds to diagram (f). Hence, according to Eq. (3), Fermi arcs inside the AZB are cooled, while correlation
effects are enhanced on the outside [48]. At HS positive and negative contributions roughly cancel.

**Semi-analytical model self-energy** — The mechanism for the pseudogap due to $\Gamma''$ is superimposed with the conventional one based on $\Gamma'$ and the outcome depends qualitatively on the ratio $\Gamma''/\Gamma'$. To describe this interplay in a minimal model we define the ansatz

$$\Sigma_{sp}(k, \nu = \pi T) \propto \Gamma_e T \sum_q \frac{G^0(k + q, \nu = \pi T)}{(Q - q)^2 + \xi^{-2}},$$

where $G^0$ is the noninteracting Green’s function shown in Fig. 1, $\Gamma_e = e^{i\phi}$, a complex number with phase 0 $\geq \xi \geq -\pi/2$ and of unit length, $T/t = 1/5$, and $N$ the number of lattice sites. We restrict the discussion to $\nu = 0$ as before [71], and assume the Ornstein-Zernike form for $\chi_q$ peaked around $Q = (\pi, \pi)$ with correlation length $\xi$. For simplicity we consider only $\Gamma_e \equiv \Gamma_e(\nu = \pi T)$, but in general the $\nu$-dependence must ensure odd parity, $\Gamma''(-\nu) = -\Gamma''(\nu)$. Here we rotate $\Gamma_e = e^{i\phi}$ in the complex plane by an angle $\phi$ away from $\Gamma_e = 1$ ($\phi = 0$) which corresponds to weak coupling [22].

Fig. 2 shows $\Sigma_{sp}^T(k, \phi) \propto \rho/\pi T$ along the FS parameterized by $\phi = \arctan(k_y/k_x)$ from the nodal direction to the antinodal direction, with increasing correlation length. Brown lines show the result for $\phi = 0$ ($\Gamma = 1$), which is always negative and for large enough $\xi$ develops a minimum near the hot spot ($\phi_{HS} \approx 1.31$), as expected. Dark blue lines show the result for $\phi = -\pi/2$ ($\Gamma_e = -i$) where real and imaginary part of the weak-coupling self-energy are essentially interchanged. Evidently, for suitable $\phi$ and $\phi$ the minimum of $\Sigma_{sp}^T$ lies at $\phi = \pi/2$, i.e., a gap first opens in the antinodal direction instead of the hot spot. At the same time a finite $\Gamma''_c = \sin(\kappa) < 0$ can lead to positive values of $\Sigma_{sp}^T$ for angles $\phi < \phi_{HS}$: clearly, for large $\Gamma''_c$ the ansatz (4) is meaningful only as a correction to a negative $\Sigma_{loc}(\nu)$, representing local correlations.

That is, non-local spin fluctuations enhance the lifetime of Fermi arcs.

**Numerical results** — We apply the parquet solver for dual fermions presented in Ref. [52] and evaluate the self-energy $\Sigma_k$ and the (dual) spin-fermion vertex $\Gamma_{k\phi}$. The dual formulation implies some more specific features addressed in the supplemental material [59], but the physical interpretation of $\Gamma$ is consistent with the discussion above. We fix the lattice size to $N = 16 \times 16$, the temperature is $T = 0.15t$.

Fig. 3 (a,b) show the Green’s function in the pseudogap phase at doping $\delta = 0.01$. Black symbols mark Fermi arc (ARC), pseudogap (PG), and hot spot (HS) momentum on the FS. (c) Self-energy and (d) spin-fermion vertex $G(k, \nu = \pi T)$ at these and further momenta as a function of $\nu$. Triangles show local DMFT quantities.
Γ for ν = πT as a function of q for various dopings. The real part is overall reduced by vertex corrections (Γ′ < 1) and it is suppressed in particular near Q. This is a precursor to the decoupling of Goldstone excitations from fermions in the antiferromagnet, known as Adler principle [55, 56, 72–75]; in the extreme case ξ → ∞ it requires that the vertex vanishes at the ordering vector [73]. For larger dopings the suppression moves to incommensurate momenta [59]. At PG, the Adler principle does not apply for small doping because of the gap.

Figs. 3 and 4 show that Γ'' is large and, hence, the scattering mechanism sketched in Fig. 1 needs to be taken into consideration. To reveal its quantitative effect we analyze the contribution Σ''sp(k, q) of nonlocal spin fluctuations to the dual self-energy, it has a form similar to Eq. (1) [59]. First, we integrate Σ''sp(k, ν = πT, q, ω = 0) with respect to q over a circle with radius r_q, centered at Q. This corresponds to circles as in Fig. 1, beginning with Q and ending with the entire Brillouin zone [76]. The result is shown as full lines in Fig. 5. A patch of momenta q ≈ Q contributes to the integral, whose final result is negative for PG and HS, but positive for ARC.

This dichotomy can be traced back to Γ'''. To show this, we split the fluctuation diagnostic into contributions from the real and imaginary part, G' and G'', of the dual Green’s function. We remind that for Γ'' = 0 the real part G' contributes nothing to the integral for Σ''sp [cf. Eq. (1)]. Dashed lines in Fig. 5 show the contribution of G'', which is negative, and absolutely smaller at ARC than at HS and PG. This corresponds to the conventional mechanism which opens a gap near hot spots for ξ → ∞ [22, 31, 32]. Dotted lines in Fig. 5 show the contribution of G', which is positive at ARC, negative at PG, and vanishingly small at HS, corresponding to the mechanism sketched in Fig. 1. The pseudogap opens at PG as the combined effect of both mechanisms. Their contributions are comparable at PG, but it is G' (Γ''') which differentiates the PG from the HS (opens the gap at PG first). With only G'' (Γ′) PG and HS would have similar lifetimes. As already seen in the semi-analytical model, due to Γ'' non-local spin fluctuations even protect (cool) the ARC (Σ'' > 0). We have thus shown that nonlocal spin fluctuations at strong coupling enhance (weaken) correlation effects outside (inside) the AZB.

Finally, we explicitly differentiate between scattering rate and quasiparticle weight by fitting the Matsubara self-energy with a fourth-order polynomial. The left panel of Fig. 6 shows ∫ Σ''sp(k, ν = πT, q, ω = 0)/(βN) as a function of doping. As expected, for small dopings the scattering rate is very large at PG, a gap opens and Z_k, defined through the slope of Σ, loses its meaning as a quasiparticle weight [69]. At ARC the scattering rate is significantly suppressed compared to DMFT, while Z_k remains similar. Hence, the suppression of the self-energy inside the AZB corresponds primarily to a reduction of the scattering rate (enhancement of the lifetime). The protection of the ARC is so effective that down to δ = 0.01 we do not observe the opening of a gap inside the AZB.

Conclusions — We identified a mechanism for spin-fermion scattering that arises from a combination of strong correlations and particle-hole asymmetry. It dampens quasiparticle excitations on those parts of the Fermi surface that lie outside of the antiferromagnetic zone boundary, whereas lifetimes on the inside are actually enhanced by spin fluctuations. This may explain why the Fermi arcs observed in underdoped cuprates are cut off at the antiferromagnetic zone boundary [77] and exhibit remarkably good Fermi-liquid properties [38].

This strong-coupling mechanism opens the pseudogap even though the correlation length is smaller than the thermal de Broglie wavelength (for δ = 0.01 we estimate ξ ≈ 1.6 [59], while ξω ≥ 2.1 [31]). Nevertheless, only classical spin fluctuations (ω = 0) are relevant for the self-energy [71].

As a more speculative remark, we note that an imaginary part of the fermion-boson vertices is associated, in...
high-energy physics, to a violation of the time-reversal symmetry [78]. How this might be related to similar symmetry violations in the cuprates suggested by specific experiments [39–41] outlines an intriguing question for future theoretical investigations.

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Supplemental material – Spin scattering turns complex at strong coupling: the key to pseudogap and Fermi arcs in the Hubbard model

Friedrich Krien,1 Paul Worm,1 Patrick Chalupa,1 Alessandro Toschi,1 and Karsten Held1

1Institute for Solid State Physics, TU Wien, 1040 Vienna, Austria

These notes provide additional information on theoretical and method aspects in Section S.1, and additional results supporting the statements of the main text in Section S.2. In Sec. S.1A, basics of the dual fermion formalism are recounted. In Sec. S.1B, we motivate our choice of the parquet approximation. In Sec. S.1C, key aspects of the parquet solver are explained. In Sec. S.1D, the fluctuation diagnostic is defined. In Sec. S.1E we show how the parquet solutions can be converged in the pseudogap regime. In Sec. S.1D, calculation details are listed. In Sec. S.2A, additional observables and the doping dependence are presented. In Sec. S.2B, we demonstrate that in a wide doping and interaction range the spin-fermion vertex has a large imaginary part. Finally, in Sec. S.2C, we show that the diagrammatic approximation Eq. (4) of the main text holds for the relevant frequencies.

S.1. METHOD

Note: We reserve some freedom in the notation, for example, $\Gamma_{kq}$, $\Gamma(k,q)$, and $\Gamma(k,\nu,\mathbf{q},\omega)$ are all equivalent.

A. Dual formalism and definitions

We employ the method introduced in Ref. [1], which is based on the dual fermion formalism [2], one of several diagrammatic extensions [3–7] of the dynamical mean-field theory (DMFT, [8]). We reiterate here only the definitions needed in relation with the main text. In DMFT one solves the effective Anderson impurity model (AIM),

$$S_{\text{AIM}} = - \sum_{\nu\sigma} c^{\dagger}_{\nu\sigma}(\nu + \mu - h_{\nu})c_{\nu\sigma} + U \sum_{\omega} n_{\uparrow,\omega} n_{\downarrow,\omega}.$$  \hfill (S.1)

Here $c, c'$ are Grassmann variables, $\mu$ the chemical potential, and $\nu$, $\omega$ the fermionic and bosonic Matsubara frequencies, respectively. Here and in the following, summations over $\nu, \omega$ imply multiplication with the temperature $T = \beta^{-1}$, summations over momenta imply division by the number of lattice sites $N$. The hybridization function $h_{\nu}$ is fixed according to the prescription $\sum_{\nu} G_{\nu}^{\text{DMFT}} = g_{\nu}$, where $G_{\nu}^{\text{DMFT}}$ is the Green’s function in DMFT approximation and $g$ is the local Green’s function of the AIM. We keep $h_{\nu} \equiv h_{\nu}^{\text{DMFT}}$ of DMFT also in our parquet dual fermion calculations.

Our approach requires several higher correlation functions of the AIM:

$$f^\alpha(\nu, \nu'; \omega) = \frac{-1}{2} \sum_{\sigma_1} \delta^{\alpha}_{\sigma_1} \delta^{\sigma_2}_{\sigma_2} \langle c^{\dagger}_{\nu\sigma_1} c^{\dagger}_{\nu'\sigma_2} c^{\dagger}_{\nu'\uparrow,\sigma_2} c_{\uparrow,\sigma_1} \rangle - \beta g_{\nu} g_{\nu'} \delta_{\nu \nu'} + 2 \beta g_{\nu} g_{\nu'} \delta_{\omega} \delta_{\alpha, \text{ch}},$$ \hfill (S.2)

$$\chi^\alpha(\omega) = (\rho_{-\omega}^\alpha \rho_{\omega}^\alpha) - \beta \langle n \rangle \langle n \rangle \delta_{\omega} \delta_{\alpha, \text{ch}}, \quad w^\alpha(\omega) = U^\alpha - \frac{1}{2} U^\alpha \chi^\alpha(\omega) U^\alpha,$$ \hfill (S.3)

$$\Gamma^{\alpha}_{\text{loc}}(\nu, \omega) = \frac{1}{2} \sum_{\sigma_1} \delta^{\alpha}_{\sigma_1} \delta^{\sigma_2}_{\sigma_2} \langle c^{\dagger}_{\nu\sigma_1} c^{\dagger}_{\nu'\sigma_2} \rho_{\omega}^\alpha \rangle + \beta g_{\nu} \langle n \rangle \delta_{\omega} \delta_{\alpha, \text{ch}}.$$ \hfill (S.4)

The label $\alpha = \text{ch, sp}$ denotes charge or spin flavor, $\rho_{\text{ch}} = n_{\uparrow} + n_{\downarrow} = n$ and $\rho_{\text{sp}} = n_{\uparrow} - n_{\downarrow}$ the charge and spin density, $U_{\text{ch}} = U$ and $U_{\text{sp}} = -U$ the bare Hubbard interaction for the respective channel. We refer to the various correlation functions as vertex ($f$), susceptibility ($\chi$), screened interaction ($w$), and boson-fermion vertex ($\Gamma_{\text{loc}}$). We focus on its spin part, i.e., the spin-fermion vertex and the corresponding screened interaction; we denote them for simplicity as

$$\Gamma_{\text{loc}}^{\text{sp}} = \Gamma_{\text{loc}}, \quad w^{\text{sp}} = w.$$ \hfill (S.5)

In practice we use a continuous-time quantum Monte Carlo solver [9] with improved estimators [10] for calculating the particle-hole correlation functions defined above. Our method also requires singlet particle-particle correlation functions [1], which are measured instead using the worm-sampling [11] of w2dynamics [12].
In the dual formalism the Hubbard model is mapped to the action
\[ S[d^*, d] = -\sum_{k, \sigma} \tilde{G}_0^{-1}(k) d^*_k \sigma d_k \sigma + \frac{1}{4} \sum_{k, q, \omega, \sigma_i} \tilde{g}_{\nu, \sigma_1 \sigma_2 \sigma_3 \sigma_4} d^*_k d^*_{k+q+\nu, \sigma_2} d_{k+q, \sigma_3} d_{k+q, \sigma_4}, \]  
(S.6)

Grassmann numbers \( d^*, d \) represent the dual fermions, \( \tilde{G}_0 = G^{\text{DMFT}} - g \) is the nonlocal DMFT Green’s function. Higher than quartic interactions between dual fermions are neglected, as usual done with few exceptions[13, 14]. The dual self-energy is given as,
\[ \Sigma_k = \sum_{k'} \tilde{G}_{k'} f^{\text{ch}}_{\nu, \omega, \nu, \omega = 0} - \frac{1}{4} \sum_{k, q} \tilde{G}_{k+q} \left[ F^{\text{ch}}_{k, q} X^{0, \sigma} \tilde{G}_{k, \nu, \omega = 0} f^{\text{ch}}_{\nu, \omega} + 3 F^{\text{sp}}_{k, q} X^{0, \sigma} \tilde{G}_{k, \nu, \omega = 0} f^{\text{sp}}_{\nu, \omega} \right], \]  
(S.7)

where \( X^{0, \sigma}_{k, q} = \tilde{G}_{k} \tilde{G}_{k+q} \) denotes a bubble of dual Green’s functions \( \tilde{G} = [(\tilde{G}_0)^{-1} - \tilde{\Sigma}]^{-1} \) and \( F \) is the full vertex of the dual fermions. Both \( F \) and \( \tilde{G} \) still need to be calculated self-consistently as explained in the next Section.

### B. Choice of approximation

The dual formalism corresponds only to the mapping of the problem of the Hubbard model to the action (S.6), with the purpose of reaching the strong-coupling regime [15, 16] and improving the convergence of diagrams with the frequency cutoff [17]. The question which diagrams are taken into account for the full vertex \( F \) in Eq. (S.7) should be kept separate, in particular, no choice of diagrams corresponds to ‘the dual fermion approach/approximation’. Sets of diagrams for the dual vertex \( F \) discussed in the literature are the second-order approximation [18, 19], the ladder approximation [7, 13], the parquet approximation [1, 20], and stochastic sampling [21, 22], in ascending order of ‘completeness’. Also contributions of higher-order vertices to the dual self-energy have been discussed [14] (which we do not consider here because it undercuts the computational efficiency). The question which diagrams are taken into account is one of physical setting, computational feasibility, convergence, and the need to avoid bias.

In the context of the doped Hubbard model and the pseudogap one often encounters the notion of ‘competing orders’. To be unbiased in this respect one needs to include the feedback between the different channels without making an a priori choice, i.e., take the parquet diagrams into account. At the outset of this work we expected that competing or exotic orders may play a role in the formation of the pseudogap, but the explanation for the pseudogap given in the main text does not require competing orders. It may therefore seem that the ladder approximation [3, 13] is sufficient, which takes the feedback of magnetic fluctuations on the self-energy into account. In fact, the ladder approximation does capture key aspects of the physics described in the main text (see Fig. S.4 below). However, it would not be convincing to base the arguments in the main text only on the ladder approximation for the following reasons:

First, of central importance for our explanation of the pseudogap is the spin-fermion vertex \( \Gamma \). In the ladder approximation this quantity is given as [17]
\[ \Gamma(\nu, q) = \Gamma_{\text{loc}}(\nu, \omega) + \sum_{\nu'} f^{\text{sp}}(\nu, \nu', \omega) - \Gamma_{\text{loc}}(\nu, \omega) \omega(\nu') \Gamma_{\text{loc}}(\nu', \omega) \tilde{X}^{0}(\nu', q) \Gamma(\nu', q), \]  
(S.8)

where \( \tilde{X}^{0}(\nu', q) = \sum_k \tilde{X}^0_{k q} \). Since in the ladder approximation vertex corrections are local, \( \Gamma \) does not depend on the fermionic momentum \( k \). Physically this means that the coupling to paramagnons is the same for all fermions, which is an atavism that can be traced back to the DMFT approximation. However, in the pseudogap regime an extreme nodal/antinodal dichotomy develops and we have to expect that fermions near the nodes are coupled differently to paramagnons than those near the antinodes. This is indeed the case, as in the pseudogap regime the Adler principle is an atavism that can be traced back to the DMFT approximation. However, in the pseudogap regime an extreme nodal/antinodal dichotomy develops and we have to expect that fermions near the nodes are coupled differently to paramagnons than those near the antinodes. This is indeed the case, as in the pseudogap regime the Adler principle applies to the Fermi arcs, but not to momenta where the pseudogap opens (see main text). We discuss the ladder approximation for \( \Gamma \) again further below in Sec. S.2B.

Second, the presence of strong local correlations introduces a large eigenvalue in the charge channel (see also Fig. S.2). This is plausible due to the Ward identity which implies that
\[ \lim_{\omega \to 0} \lim_{q \to 0} \Gamma^{\text{ch}}(\nu, q, 0, q, \omega) \propto \left( 1 - \frac{d \Sigma(k, \nu)}{d \nu} \right) \bigg|_{\nu = 0}, \]  
(S.9)

where \( \nu, \omega \) are real frequencies in this equation. For a Fermi liquid the right-hand-side corresponds to the inverse quasiparticle weight \( Z_{q}^{-1} \) (this underlines again that the \( k \)-dependence of \( \Gamma \) is important when \( Z_{q} \) is strongly anisotropic). The vertex is thus enhanced in the strongly correlated regime where \( Z \) is small. On Matsubara frequencies this is
FIG. S.1. Double decomposition of the vertex function according to Ref. [1]. Top: Single-boson exchange decomposition of the full vertex [36]. The momentum dependence of the fermion-boson vertices is fully retained. Bottom: Parquet equation for the multi-boson exchange. The momentum dependence of the four-point vertices is parameterized using the truncated unity [37].

connected to a large eigenvalue of the Bethe-Salpeter equation for finite frequencies \( \omega \) (because \( q \) must go to zero first), in particular for \( \omega_1 = 2\pi T \) (see Fig. S.2).

This effect is already present in DMFT, leading to a divergence of the boson-fermion vertex at the zero-temperature Mott transition [23]. Interestingly, Eq. (S.9) is valid both in the charge and in the spin channel but in practical calculations using Matsubara frequencies the corresponding eigenvalue is much larger in the charge channel [23], presumably because the Mott gap is a charge gap. A large eigenvalue at finite frequency has been observed also in fRG studies [24, 25]. Strong local correlations (‘Mottness’) are a sufficient, but not a necessary condition for this eigenvalue to be large. (It should not be confused with the eigenvalue associated to \( \alpha = ch, q = 0, \omega = 0 \), which corresponds to the phase separation instability, even though phase separation and the Mott transition often go hand in hand [23, 26].)

However, in DMFT and also in the ladder dual fermion approximation the large eigenvalue has no feedback on other channels; including this feedback requires at least the parquet diagrams. Although the Ward identity is violated by the parquet approximation [27] we do find the corresponding large eigenvalue, which for strong coupling is in fact the leading instability for all considered dopings (see panel (b) of Fig. S.3). Hence, to avoid a potential source of bias we allow the mutual renormalization of the different channels via the parquet diagrams.

Third, even in absence of competition, a strong fluctuation can interact with itself in the sense of an effective \( \phi^4 \)-theory [28–30]. It was shown by Bickers and Scalapino [31] that this ‘self-renormalization’ is included in the parquet diagrams; in terms of the \( 1/N \) expansion the parquet is comparable to the so-called self-consistent screening approximation [32]. In the Bethe-Salpeter equation this feedback corresponds to the renormalization of the irreducible vertex. However, in the ladder approximation the latter is fixed and local, cf. Eq. (S.8), and hence the self-renormalization of bosonic fluctuations is neglected in the ladder approximation [33]. It is indeed the case that the accuracy of the ladder approximation worsens at the onset of the pseudogap regime [34], where spin fluctuations are strong, while it is improved by the parquet diagrams [35].

C. Parquet solver

We explain aspects of the parquet solver for dual fermions presented in Ref. [1] relevant for the main text.

For a long time, since the introduction of the parquet approach, the full solution of the parquet equations on a large lattice was considered to be computationally unfeasible. Applications to impurity models and small clusters were pioneered in Refs. [38–42], see Ref. [43] for a review. The computational bottleneck is the memory required to store the various vertex functions [44]. Very recently, based on concepts used in the fRG [45–47], progress was made to compress the information encoded in the parquet vertices, which depend on three momenta and three frequencies. The expansion and truncation of vertices in a form-factor basis allows to treat much larger lattice sizes [37, 48], for example, a vertex quantity \( \Phi \) is transformed as,

\[
\Phi(k, \nu, k', \nu'; q, \omega) \rightarrow \Phi(\ell, \nu, \ell', \nu'; q, \omega),
\]

where \( \ell, \ell' \) denote form-factor indices (corresponding in our case to the form factors of the square lattice). The change of basis is exact, but only a small number of form factors is kept (truncated unity). This corresponds to cutting off the respective momentum argument in real space (cf. Fig. 7 of Ref. [37]). That is, discarding form factors with index
$\ell > \ell_{\text{max}}$ implies to cut off $\Phi(r, \nu, r', \nu', q, \omega)$ with respect to $r, r'$, the Fourier conjugate variables of $k, k'$, respectively. The truncated-unity approximation is therefore suitable when the vertex quantity $\Phi$ is short-ranged in real space.

However, in the pseudogap regime spin fluctuations are longer-ranged, in particular at weak coupling [34, 35], but also at strong coupling a number of nearest neighbor shells should be taken into account. To remedy this, the parquet diagrams were regrouped in Refs. [1, 49] in terms of single- and multi-boson exchange [36], as shown in Fig. S.1. The regrouping of diagrams is exact and therefore has no effect on the parquet approximation itself. But the convergence with the number of form factors can be improved drastically, as we explain in the following.

The single-boson exchange (SBE) diagrams carry the bare momentum argument of the fluctuation and hence should not be truncated in real space. For example, for spin fluctuations the SBE diagram reads,

$$
\Delta(k, \nu, k', \nu', q, \omega) = \Gamma(k, \nu, q, \omega) W(q, \omega) \Gamma(k', \nu', q, \omega),
$$

where $W$ is the screened interaction. In the method of Ref. [1] the full momentum dependence of $\Gamma$ and $W$ is retained. The diagrams $\Delta$ of SBE type are constructed in the horizontal [cf. Eq. (S.11)] and vertical particle-hole channels, and in the particle-particle channel, see top of Fig. S.1 and Ref. [36].

On the other hand, the residual vertex $\Lambda^\text{Uirr}$ in Fig. S.1 corresponds to multi-boson exchange (notice that $\lambda^\text{Uirr}$ is a local residual vertex [36] and vertices $M$ represent multi-boson exchange in the horizontal and vertical particle-hole channels and in the particle-particle channel [1]). This vertex is much more short-ranged compared to the full vertex $F$ because the momentum argument of spin fluctuations appears only under integrals. This makes the multi-boson exchange amenable for the truncated-unity approximation [1, 49]. As a result, the form-factor expansion for $\Lambda^\text{Uirr}$ converges quickly, even in the presence of very long-ranged spin-density wave fluctuations. In principle, the convergence with the form factors could worsen if $\Lambda^\text{Uirr}$ develops a strong momentum dependence. In the pseudogap regime at weak coupling [35] this is not observed.

For the strong-coupling regime the effect of higher form factors will be investigated elsewhere. In the main text we show the self-energy computed with only one form factor. This allows us to reach small dopings efficiently (cf. Sec. S.1E); tests for larger dopings (not shown) did not reveal a major effect if further form factors are included. The reason for this is that the particle-particle channel is not yet important; if $d$-wave superconducting fluctuations develop alongside antiferromagnetic spin fluctuations further form factors are required to capture their competition. Nevertheless, even in this case a single form factor may still describe qualitatively the correct physics [48].

As Eq. (S.11) shows, the spin-fermion vertex is not only a passive output that we can compute using the parquet vertices but a central quantity which is stored and updated over the iterations. It is obtained from the full vertex as,

$$
\Gamma(k, q) = \Gamma^\text{loc}(\nu, \omega) + \sum_{k'} [F^\text{sp}(k, k', q) - \Delta(k, k', q)] \tilde{X}^0(k', q) \Gamma^\text{loc}(\nu', \omega).
$$

In contrast to the ladder approximation in Eq. (S.8), $\Gamma$ inherits the complete momentum dependence from the full vertex function $F$. We can hence capture the nodal/antinodal dichotomy of $\Gamma$ in the pseudogap regime. The dual screened interaction $W$ is obtained from $\Gamma$ through

$$
W(q) = \frac{w(\omega)}{1 - w(\omega) \Pi(q)}, \quad \Pi(q) = \sum_k \Gamma^\text{loc}(\nu, \omega) \tilde{X}^0(k, q) \Gamma(k, q),
$$

where $\Pi$ is the dual polarization.

**D. Fluctuation diagnostic**

In the main text we are interested in the contribution of spin fluctuations to the (dual) self-energy. This idea has been coined a ‘fluctuation diagnostic’ [50-54] which we adopt here, but with two modifications [35, 55].

First, we are not interested in a fluctuation diagnostic of local correlations. They instead are our baseline against which we compare the contribution of nonlocal correlations. Fortunately, this separation of local and nonlocal correlations is already intrinsic to the dual formalism where the approximation for the self-energy of the real fermions is given as,

$$
\Sigma(k) = \Sigma^{\text{DMFT}}(\nu) + \frac{\tilde{\Sigma}(k)}{1 + g(\nu) \hat{\Sigma}(k)}.
$$

Here, $\Sigma^{\text{DMFT}}$ is the local self-energy of the self-consistent AIM (S.1) of DMFT. Notice that while local and nonlocal correlations are separated, there remains some ambiguity in the choice of the hybridization function $h_\nu$ of the AIM.
While this may lead to quantitative differences and shifts between $\Sigma^{\text{DMFT}}$ and $\sum k \tilde{\Sigma}(k) / [1 + g(\nu)\tilde{\Sigma}(k)]$, the mechanism that opens the pseudogap is intrinsically nonlocal and does not depend on this choice. In the literature good results have been obtained using $h^{\text{DMFT}}$ or by fixing $h$ using the prescription $\tilde{G}_{\text{loc}} = 0$ [18, 22, 35, 56].

Second, the original fluctuation diagram is based on the Fierz ambiguity and one adopts one of three equivalent reference frames (charge, spin, or particle-particle [50, 53]). In the dual formalism the Fierz ambiguity is however reduced due to the fact that the bare interaction $f^{\text{ch/sp}}$ has a flavor. Instead, we make use of the decomposition into SBE diagrams intrinsic to our method (cf. Fig. S.1). We obtain the contribution of single spin fluctuations to the self-energy according to Ref. [35],

$$
\tilde{\Sigma}_{\text{sp}}(k) = -\frac{3}{2} \sum_{k',q} \tilde{G}(k + q) \Delta(k, k', q) \tilde{X}^0(k', q) f^{\text{sp}}(\nu', \nu, \omega).
$$

(S.15)

In the main text we are interested in the contribution of nonlocal spin fluctuations to the imaginary part $\Sigma''$ of the lattice self-energy (S.14). The denominator $1 + g(\nu)\tilde{\Sigma}(k)$ in Eq. (S.14) is complex but its real part is leading and we can hence focus our attention on $\tilde{\Sigma}''_{\text{sp}}$. Using (S.11) we write Eq. (S.15) as

$$
\tilde{\Sigma}_{\text{sp}}(k) = -\frac{3}{2} \sum_{q} \tilde{G}(k + q) \Gamma(k, q) W(q) \tilde{\Gamma}(\nu, q),
$$

(S.16)

where we defined the vertex quantity

$$
\tilde{\Gamma}(\nu, q) = \sum_{k'} \Gamma(k', q) \tilde{X}^0(k', q) f^{\text{sp}}(\nu', \nu, \omega).
$$

(S.17)

In a perturbation theory for real fermions with the bare vertex $U$ this diagram would correspond to the polarization times $U^{\text{sp}}$ and using the Dyson equation for $W$ Eq. (S.16) would assume a GW-like form. However, in the dual formalism the bare vertex $f$ depends on three frequencies and Eq. (S.17) is not the polarization diagram [cf. Eq. (S.13)]. We therefore have to include the above-defined $\tilde{\Gamma}$ into the discussion which is similar to $\Gamma$ but does not depend on $k$.

We take the imaginary part of Eq. (S.16) and separate by real and imaginary part of $\tilde{\Gamma}$

$$
\tilde{\Sigma}''_{\text{sp}}(k) = \frac{3}{2} \sum_{q} \left[ \tilde{G}_{k+q} \left( \Gamma'_{kq} \tilde{\Gamma}''_{\nu q} + \Gamma''_{kq} \tilde{\Gamma}_{\nu q} \right) + \tilde{G}''_{k+q} \left( \Gamma'_{kq} \tilde{\Gamma'}_{\nu q} - \Gamma''_{kq} \tilde{\Gamma}''_{\nu q} \right) \right] W_q.
$$

(S.18)

This is the dual analog to the model self-energy GW used in the main text. The key feature that they share is that the real part $\tilde{G}'$ of the dual Green’s function contributes to $\tilde{\Sigma}''_{\text{sp}}$ only via the imaginary part of a vertex. A difference is that in Eq. S.18 both $\Gamma$ or $\tilde{\Gamma}$ enter. However, the latter is anyhow defined in terms of the former via Eq. S.17. Hence, in the dual fermion theory we also have a kind of GW form as in the spin-fermion ansatz [Eq. (2) main text], just with a few complications: (i) the denominator in Eq. (S.14) is a complex number, (ii) we had to introduce a second vertex $\tilde{\Gamma}$, (iii) the imaginary part $\tilde{\Gamma}''$ of the dual Green’s function can be positive, (iv) the imaginary parts $\Gamma''$, $\tilde{\Gamma}''$ couple not only to $\tilde{G}'$ but (in their combination) also to $\tilde{G}''$. Despite these complications our numerical results presented in the main text show full consistency with the qualitative predictions based on the model self-energy GW for real fermions.

E. Convergence in the pseudogap regime

Technical details and implementation notes for our method are provided in Ref. [1]. We add here a note to explain how calculations are converged in the pseudogap regime using Anderson/Pulay mixing.

In the parquet iterations the following large vector of quantities is updated self-consistently:

$$
\mathbf{x}_i = (\tilde{\Sigma}_i, \Pi^i, \Gamma^\alpha, \Lambda^{\text{Uirr}, \alpha}).
$$

(S.19)

As an initial guess for $\mathbf{x}_0$, in most cases a converged ladder dual fermion calculation is used where the ladder self-energy $\tilde{\Sigma}_0$ in Eq. (S.8) yields $\Gamma_0$ and then $\Pi_0$ via Eq. (S.13): $\Lambda^{\text{Uirr}}_0 = 0$ is a reasonable initial guess. As discussed in relation with Eq. (S.8), $\Gamma_0(\nu, q)$ does not depend on $k$ in the ladder approximation, but $\Gamma_1$ acquires this dependence already after the first parquet iteration.

In Eq. (S.19) $\tilde{\Sigma}(k), \Pi(q)$, and $\Gamma(k, q)$ carry the full momentum and frequency dependence, but not $\Lambda^{\text{Uirr}}$ which represents a set of vertex functions (the multi-boson exchange, cf. Fig. S.1). These vertices are parameterized in
terms of the truncated form-factor basis [cf. right-hand-side of Eq. (S.10)], which drastically reduces the required memory. In our calculations outside of the pseudogap regime linear mixing converges fast, which is defined as,

\[ x_{i+1} = (1 - \xi)x_i + \xi g[x_i], \quad (0 < \xi \leq 1), \]

where \( g \) is the result of the parquet iteration. However, at smaller dopings, as soon as the quasiparticle weight is suppressed near the antinodes, convergence deteriorates and linear mixing fails.

Slow convergence often has a physical origin, for example, critical slowing down of the iterative cycle of DMFT sets in near the Mott transition when a solution turns from stable to unstable as a function of a control parameter (interaction, temperature, doping, ...). The free energy landscape around the minimum is then very flat. For DMFT it was shown that stability of the iterative cycle is determined by the dual Bethe-Salpeter kernel \( \sum_{\nu\nu'} \langle \bar{\nu}\bar{\nu}'|0\rangle \tilde{X}_{\nu\nu'}^{\bar{\nu}\bar{\nu}'} \) [16], which highlights the dual fermion approach [2] as a natural extension of diagrammatic perturbation theory to the strong-coupling regime, and serves as a further justification of our numerical method.

To improve the convergence of the parquet solver we employ Anderson/Pulay mixing which has been used previously to accelerate the iterative cycle of DMFT [57, 58] and its diagrammatic extensions [59]. In the improved mixing scheme one defines a fixed-point function,

\[ f[x_i] = g[x_i] - x_i \equiv f_i, \]

and the solution \( x^* \) hence satisfies \( f[x^*] = 0 \). Convergence of an iterative scheme is determined by the eigenvalues of the Jacobian \( J = \frac{df}{dx} \). Convergence of linear mixing deteriorates if an eigenvalue approaches unity. An improved mixing scheme approximates \( J \), based on \( f_i, f_{i-1}, ... \) evaluated at previously traversed points \( x_i, x_{i-1}, ... \), and constructs an update \( x_{i+1} \) taking into account the slope of \( f \). Extrapolating from a sequence of \( n+1 \) parquet iterations \( x_{i-n}, ..., x_i \), the updated vector is given through the Anderson/Pulay mixing as (cf., e.g., Ref. [60]),

\[ x_{i+1} = x_i + \tilde{C}_i f_i, \]

\[ \tilde{C}_i \equiv 1 - (R_i + \xi F_i)(F_i)^{-1}, \]

\[ R_i = [x_{i-n+1} - x_{i-n}, x_{i-n+2} - x_{i-n+1}, ..., x_i - x_{i-1}], \]

\[ F_i = (f_{i-n+1} - f_{i-n}, f_{i-n+2} - f_{i-n+1}, ..., f_i - f_{i-1}). \]

Unfortunately, due to the full momentum and frequency dependence of \( \Gamma(k, q) \) it is not feasible to store this quantity for many iterations. Therefore, we apply linear mixing in the subspace of \( \Gamma \), where the respective matrix elements of \( C_i \) are set to \( \xi \). Similarly, we apply the improved mixing only to the smallest frequencies of \( \Lambda^{\text{Uirr}} \) and linear mixing to higher frequencies.

Using the improved mixing scheme we are able to converge also in the pseudogap regime. The left panel of Fig. S.2 shows the distance \( d_i = |\hat{\Sigma}_i - \hat{\Sigma}_{i-1}| \) (normalized by the length of the array) as a function of \( i \) for temperature \( T/t = 0.15 \) and doping \( \delta = 0.01 \), the most extreme parameters we accessed so far with the described optimizations. Since we have to use linear mixing for \( \Gamma \), the improved mixing scheme does not unfold its full power and \( d_i \) shows an erratic, weakly exponential decay. Even for well converged solutions we observe sporadically a strong increase of \( d_i \), followed by a return to the convergent track.

Overall convergence of the iterative scheme is tightly connected to convergence of the leading eigenvalues [40] of the ladder equations that are discussed in more detail in Ref. [1]. In the strongly correlated regime the leading eigenvalue is in the charge channel, connected to the momentum and energy \( q = (q = 0, \omega = 2\pi T) \), as discussed below Eq. (S.9). We find that this eigenvalue is the origin of the convergence problems in the pseudogap regime at strong coupling. In contrast, in the pseudogap regime at weak coupling [35] this eigenvalue is small, which shows that strong correlations have a destabilizing effect on diagrammatic perturbation theory. The center panel of Fig. S.2 shows the large eigenvalue as a function of the iterations.

At the level of the vertex the large eigenvalue leads to an enhancement of \( \Gamma^{\text{ch}}(k, \nu, q = 0, \omega = 2\pi T) \), shown in the right panel of Fig. S.2 for \( k \) corresponding to the antinode (but \( k \)-dependence of the feature is weak). The spin-fermion vertex \( \Gamma^{\text{sp}} \) shows a much smaller enhancement, a disparity also observed in Ref. [23]. The enhancement of the charge vertex and its relation to electron-phonon coupling, phase separation, superconductivity, and charge density waves has been discussed by many authors, see, for example, Refs. [61, 62]. In agreement with Ref. [61] we observe the enhancement only for \( |q| \ll \omega \), where screening is ineffective. Notice that instability of \( \Gamma \) is rather the exception than the rule, for example, in the case of strong spin fluctuations \( \Gamma^{\text{sp}} \) is even suppressed near \( Q \) (see main text).

In contrast to Ref. [40] we do not encounter convergence problems connected to a violation of the crossing symmetry. This may be a benefit of our bosonized parquet approach, which explicitly preserves the crossing symmetry at the level of the SBE diagrams [cf. Fig. S.1] (the truncated-unity approximation violates the crossing symmetry of \( \Lambda^{\text{Uirr}} \)).
Our parquet calculations were performed on a lattice of size $N = 16 \times 16$, as a good compromise between resolution and computational feasibility. The self-energy $\Sigma_{\nu}^{DMFT}$ of the self-consistent AIM (S.1) of DMFT was evaluated at $N_{\nu}^{(1)} = 64$ positive Matsubara frequencies. The four-point vertex $f_{\nu'\nu'\omega}$ was evaluated at $N_{\nu} = 14$ bosonic frequencies $\omega_{m} \geq 0$ and $N_{\nu}^{(2)} = 14$ fermionic frequencies $\nu_{n}$ with index $-7 \leq n \leq 6$. The three-point vertices $\Gamma_{\text{loc}}(\nu, \omega)$ are evaluated in the same window. The vertices at negative bosonic frequencies $\omega < 0$ can be obtained from the positive frequencies, $f(\nu, \nu', \omega) = f^*(\nu', -\nu, -\omega)$ and $\Gamma_{\text{loc}}(\nu, \omega) = \Gamma_{\text{loc}}^*(\nu, -\omega)$, and hence for the chosen $N_{\nu}^{(2)}$ and $N_{\nu}$ the window for bosonic frequencies is twice as large as for fermionic ones. This reduces the cutoff error for fermionic observables, whereas a cutoff error is visible in bosonic observables near $\omega \approx N_{\nu}^{(2)}/2$. If instead our focus was to evaluate bosonic correlation functions the window for fermionic frequencies should be twice larger than for bosonic ones. While these cutoffs may seem small, our method presented in Ref. [1] is heavily optimized in this respect. Purely local quantities are measured directly by the impurity solver [9, 10], avoiding for example summation over local charge observable.

F. Calculation details

Our parquet calculations were performed on a lattice of size $N = 16 \times 16$, as a good compromise between resolution and computational feasibility. The self-energy $\Sigma_{\nu}^{DMFT}$ of the self-consistent AIM (S.1) of DMFT was evaluated at $N_{\nu}^{(1)} = 64$ positive Matsubara frequencies. The four-point vertex $f_{\nu'\nu'\omega}$ was evaluated at $N_{\nu} = 14$ bosonic frequencies $\omega_{m} \geq 0$ and $N_{\nu}^{(2)} = 14$ fermionic frequencies $\nu_{n}$ with index $-7 \leq n \leq 6$. The three-point vertices $\Gamma_{\text{loc}}(\nu, \omega)$ are evaluated in the same window. The vertices at negative bosonic frequencies $\omega < 0$ can be obtained from the positive frequencies, $f(\nu, \nu', \omega) = f^*(\nu', -\nu, -\omega)$ and $\Gamma_{\text{loc}}(\nu, \omega) = \Gamma_{\text{loc}}^*(\nu, -\omega)$, and hence for the chosen $N_{\nu}^{(2)}$ and $N_{\nu}$ the window for bosonic frequencies is twice as large as for fermionic ones. This reduces the cutoff error for fermionic observables, whereas a cutoff error is visible in bosonic observables near $\omega \approx N_{\nu}^{(2)}/2$. If instead our focus was to evaluate bosonic correlation functions the window for fermionic frequencies should be twice larger than for bosonic ones. While these cutoffs may seem small, our method presented in Ref. [1] is heavily optimized in this respect. Purely local quantities are measured directly by the impurity solver [9, 10], avoiding for example summation over local charge observable.

S.2. FURTHER SUPPORTING RESULTS

A. Additional parquet dual fermion observables

To put the results shown in the main text into a broader context we report here several more observables. We first note, however, that diagrammatic approximations based on the dual fermion formalism, including stochastic summation of diagrams, are not fully consistent internally, see Refs. [18, 22] for discussions. This puts some uncertainty on the actual doping level $\delta$, which we obtain from summation over the lattice Green’s function $\sum_{k} G_{k}$. Further, since the dual formalism heavily relies on directly measured impurity correlation functions [cf. Eqs. (S.2)-(S.4)], the choice of the hybridization function $h_{\nu}$ becomes important. The best quantitative agreement with numerically exact results has so far been achieved using the prescription $G_{\text{loc}} = 0$ [22, 35]. Here we use however the DMFT hybridization $h^{DMFT}$ which yields good results in combination with stochastic sampling [22] and our parquet approach in turn shows good agreement with stochastic sampling where it can be converged in the perturbation order [1]. We emphasize that our goal here is to investigate the strongly coupled Hubbard model for cuprates qualitatively; benchmarks against numerically exact methods in this or a similar regime will be presented elsewhere.
Fig. S.3 shows various quantities for our hole-doping scan at $T/t = 0.15$. Panel (a) shows $\Delta \Sigma(k) = \Sigma(k, \pi T) - \Sigma(k, 3\pi T)$ for different $k$ as a function of $\delta$. This quantity serves as a rough marker for metallic ($\Delta \Sigma > 0$) or insulating ($\Delta \Sigma < 0$) behavior and confirms the gap opening at the point PG, corresponding in the noninteracting system to the intersection of the curve $\varepsilon(k) = \mu$ with the Brillouin zone boundary. As discussed in the main text, the ARC momentum inside of the antiferromagnetic zone boundary is made more metallic by spin fluctuations down to the smallest dopings. The small slope of $\mu(\delta)$ in panel (c) of Fig. S.3 at small dopings indicates an enhanced compressibility $\partial \delta / \partial \mu$. The latter is often observed near the critical point of the phase separation instability of strongly correlated Hubbard models [64–72].

Fig. S.3 (b) shows the leading eigenvalues as a function of doping. As discussed above, the largest eigenvalue corresponds to the charge channel at $q = 0$ and $\omega = 2\pi T$. In our physical setting it can be interpreted as a measure of ‘Mottness’ [cf. Eq. (S.9)], as it leads to a divergence of the charge vertex at the zero temperature Mott transition [23]. This eigenvalue increases when approaching half-filling, even more steeply as the pseudogap opens. The next largest eigenvalue is in the spin channel for $\omega = 0$ where the corresponding momentum depends on doping, leading to a relay race of incommensurate momenta with decreasing $\delta$. The commensurate momentum $Q = (\pi, \pi)$ [(8, 8) in Fig. S.3 b)] becomes the leading instability at roughly $\delta = 0.03$. Panel (d) shows the screened interaction $W(q, \omega = 0)$ on the high-symmetry path ($W = W^{\text{sp}}$). Corresponding to the crossover from incommensurate to commensurate momenta $W$ develops from a two-peak structure to a single large peak (corresponding to 8 and 4 peaks in the Brillouin zone, respectively). The correlation length, estimated from the width of the peak, is indicated for dopings $\delta = 0.05, 0.04, 0.03, 0.02$, and 0.01.

Finally, panels (e) and (f) show the real, respectively imaginary part of self-energy for various dopings. At large doping the self-energy is almost local but acquires a strong momentum dependence closer to half-filling. The spatial resolution is sufficient to differentiate the antinode $X = (\pi, 0)$ from the position PG where the pseudogap opens first, which lies two units away from X. Similarly, a second peak is located not at the node $M/2 = (\pi/2, \pi/2)$ but instead lies closer to the corner of the Brillouin zone, $(\pi/2 + \epsilon, \pi/2 + \epsilon)$.
FIG. S.4. Left: Ratio of imaginary over real part of the spin-fermion vertex calculated in the ladder approximation (full lines) for various $U$ and $\delta$ ($t = 1$, $t' = -0.2 t$, $t'' = 0.1 t$). Frequencies are set to $\nu = \pi T$, $\omega = 0$, the bosonic momentum to $Q = (\pi, \pi)$. In the ladder approximation the vertex does not depend on the fermionic momentum $k$. Dashed lines correspond to the momentum-independent spin-fermion vertex $\Gamma_{\text{loc}}$ of the AIM. A large $\Gamma''$ is a hallmark of the strong-coupling regime, nonlocal correlations further enhance this quantity. Top right: Approximation Eq. (S.27) for the imaginary part of the local spin-fermion vertex calculated numerically by continuous-time quantum Monte Carlo.

B. Imaginary part of the spin-fermion vertex in the ladder approximation

In the main text the imaginary part of the spin-fermion vertex $\Gamma$ plays an important role, because it facilitates the strong-coupling mechanism that allows spin fluctuations to open the pseudogap beginning near the antinodes. In the weak-coupling picture the gap opens first at the hot spots [73] and hence $\Gamma''$ is large only for strong coupling. To show this we calculate $\Gamma$ within the ladder dual fermion approximation according to Eq. (S.8), which is cheap and easy to converge. As before, the temperature is set to $T/t = 0.15$. The left panel of Fig. S.4 shows the ratio,

$$\frac{\Gamma''(\nu = \pi T, q = Q, \omega = 0)}{\Gamma'(\nu = \pi T, q = Q, \omega = 0)}.$$ (S.26)

Large negative values near half-filling indicate that the strong-coupling mechanism may play a role in the formation of the pseudogap. Notice that the ratio $\Gamma''/\Gamma'$ corresponds to an odd function of $\nu$ (see main text), its value at fixed $\nu_0 = \pi T$ therefore decreases with $T$ (unless it develops a pole at zero which we do not observe in our parquet and ladder calculations).

C. Diagrammatic analysis of the local spin-fermion vertex

We derive an approximation for the imaginary part of the static spin-fermion vertex $\Gamma_{\text{loc}}(\nu, \omega = 0)$ of the AIM and test it in practice. According to Ref. [74] the vertex correction due to single-boson exchange in the vertical particle-hole channel is given as,

$$\Gamma_{1-\text{boson}}(\nu, \omega = 0) = 1 + \sum_{\nu'} [\nabla_{\text{ph}}(\nu, \nu') + U]g(\nu')g(\nu'),$$ (S.27)

$$\nabla_{\text{ph}}(\nu, \nu') = -\frac{1}{2}\Gamma_{\text{loc}}(\nu, \nu' - \nu)w(\nu' - \nu)\Gamma_{\text{loc}}(\nu, \nu' - \nu) + \frac{1}{2}\Gamma_{\text{loc}}(\nu, \nu' - \nu)w(\nu' - \nu)\Gamma_{\text{loc}}(\nu, \nu' - \nu).$$ (S.28)
We are interested in a rough estimate of the imaginary part. To this end, we introduce a few further approximations: the contribution due to charge fluctuations is neglected, $\Gamma_{loc}^{\text{ch}}(\nu, \nu'-\nu)w_{loc}(\nu'-\nu)\approx U$, the spin-fermion vertex is set to 1 on the right-hand-side of Eq. (S.27), and only contributions of static spin fluctuations are taken into account, $w(\omega) \approx -U - \frac{U^2}{2} \chi^sp(\omega = 0)\delta_{\omega}$. With these simplifications Eq. (S.27) reads,

$$\Gamma_{1-\text{boson}}(\nu, \omega = 0) \approx 1 - \frac{T U^2}{4} \chi^sp(\omega = 0) g(\nu)g(\nu),$$

where the factor $T$ was implicit in the Matsubara summation. Taking the imaginary part we arrive at the approximation discussed in the main text.

Here we test this approximation in the DMFT calculations which serve as the basis for the dual parquet solver. For implementation reasons we evaluate Eq. (S.27) instead of (S.29). The ratio $\Gamma_{1-\text{boson}}^{\nu}(\nu, \omega = 0)/\Gamma_{loc}^{\nu}(\nu, \omega = 0)$ is drawn on the top right panel of Fig. S.4. Actually, it is close to unity only for small frequencies and values of the chemical potential where the pseudogap opens ($\mu \approx 1.8$). The drastic change of the approximation quality is remarkable in view of the weak $\mu$-dependence of the numerically exact $\Gamma_{loc}^{\nu}$ shown in the bottom right panel [75]. In any case, we employ Eq. (S.29) in the main text only for the smallest Matsubara frequencies to underline that $\Gamma$ develops a large imaginary part at strong coupling.

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