Manifestations of Strange Metallicity in Inelastic Neutron Studies

S. Acharya¹,‡ M. S. Laad²,† and A. Taraphder¹,‡

¹Department of Physics, Indian Institute of Technology, Kharagpur, Kharagpur 721302, India. 
²Institute of Mathematical Sciences, Taramani, Chennai 600113, India and
³Centre for Theoretical Studies, Indian Institute of Technology Kharagpur, Kharagpur 721302, India.

Emergence of an orbital-selective Mott phase (OSMP) found in multi-band correlated systems leads to a non-perturbative obliteration of the Landau Fermi liquid in favor of a novel metallic state exhibiting anomalous infra-red (branch-cut) continuum features in one- and two-particle responses. We use a combination of (1) dynamical mean-field theory (DMFT) using the continuous-time-quantum Monte-Carlo (CTQMC) solver for a two-band Hubbard model and (2) analytic arguments from an effective bosonized description to investigate strange metal features in inelastic neutron scattering studies for cuprates. Specifically, restricting our attention to symmetry-unbroken metallic phase, we study how emergence of an OSMP leads to qualitatively novel features in (i) the dynamical spin and charge susceptibilities, and (ii) phonon response in the strange metal, in detail. Extinction of theLandau quasiparticle pole in the one-electron propagator in the OSMP mirrors the emergence of critical liquid-like features in the dynamical spin response. This novel finding also underpins truly anomalous features in phonon dynamics, which we investigate by coupling half-breathing phonons in the specific context of cuprates to such a multi-electronic continuum. We find good understanding of various anomalies encountered in experimental inelastic neutron scattering studies in the near-optimally doped cuprates. We also extend these results in a phenomenological way to argue how modification of phonon spectra in underdoped cuprates can be reconciled with proposals for a nematic-plus-d-wave charge modulation order in the pseudogap state. We also study the issue of the dominant “pair glue” contributions to superconductivity, allowing us to interpret recent pump-probe results within a strange metal scenario.

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Quantum Phase Transitions (QPT) of increasingly diverse types continue to present a fundamental challenge to our rapidly evolving understanding of theory of electrons in quantum matter¹,². These range from the famed itinerant type, described by the Hertz-Moriya-Millis (HMM)³ model, to the local type, based on Heisenberg-Kondo⁴ or selective-Mott⁵,⁶ models. Finding of the exotic strange metal phase in cuprates and certain f-electron systems is by now a fundamental problem, related to the issue of how strong electronic correlations can cause a basic transmutation in the nature of elementary excitations in a d > 1 (d is the spatial dimensionality) metallic system, as implied by the change of the analytic structure of the charge- and spin-fluctuation propagators from an infra-red pole to branch-cut structure. Focussing on spin fluctuations, the following issue arises. In a traditional Hertz-Moriya-Millis (HMM) view of QCP, the dynamical spin susceptibility (the Fourier transform of the spin-spin propagator) χ(q, ω) shows the critically overdamped paramagnon form for certain set of critical Qs associated with magnetic order. In stark contrast, anomalous scale-invariant and predominantly ω-dependent response characterizes the strange metal, where χloc(ω) ≃ T−η F(ω/T) with 0 < η < 1 is seen. This form appears in Kondo-RKKY models, but it is necessarily linked to proximity to magnetic order. On the other hand, the FL* theory⁷ does not need such proximity to get this form. Experimentally, while unconventional superconductivity (USC) in f-electron systems indeed maximises near an antiferromagnetic quantum phase transition, USC with high-Tc in hole-doped cuprates sets in and maximises far from an AF-QCP, but close to an optimal doping where a topological Fermi surface reconstruction (FSR) occurs. Thus, proximity to AF-QCP may not be a (uniquely) necessary requirement for generating the soft electronic glue that results in HTSC. This prompts a set of issues: (i) what are the microscopic origins of the anomalous spin-fluctuation spectrum in the normal and the enigmatic pseudogap phases in cuprates, and, in particular, how are we to understand its specific link to equally anomalous fermiology and transport in one picture?, (ii) what non-Landau symmetry-breaking, if any, underlies emergence of strange metallicity and the pseudogapped metal? and (iii) what are its consequences for HTSC that peaks precisely around optimal doping in the strange metal?

These experimental findings and the above discussion motivate our present work. Specifically, here we study these by extending previous work on an extended periodic Anderson model⁸.⁹. Previous works found either a FL* metal or a local QPT between a heavy LFL with very small quasi-particle weight (zFL << 1) and a locally critical metal with zFL = 0 and an anomalous ω/T-scaling of the local propagators as the ratio Vf(e,k)/Uf was varied. Similar behavior was also found, due to JH, even earlier⁸. This was shown to emerge as a direct consequence of effects akin to the orthogonality catastrophe accompanying a selective-Mott localization, a la hidden-FL⁹ or FL* theories. The relevance of the emerging branch-cut singular propagators for understanding strange metallicity in cuprates has long been emphasized by Anderson⁹ in what amounts to a kind of local approximation
in the \( U = \infty \) fixed point for the Hubbard model. In a selective-Mott metal, such features arise for a range of realistic parameters via strong inelastic scattering between Mott-localized and metallic subsets of the dressed spectral function. Here, we show how the same selective-Mottness idea also enables a natural understanding of the unique branch-cut continuum form of spin fluctuations as a consequence of the dualistic (itinerant-localized) character of carriers.

We now describe our formulation for \( \chi(\mathbf{q}, \omega) \) for the EPAM in detail. Begin with the DMFT solution for the one-electron propagators of the EPAM, defined as before\(^{4,6}\)

\[
H = H_{\text{band}} + H_{\text{int}} + H_{\text{hyb}}
\]

where \( H_{\text{band}} = \sum_{k,\sigma} \epsilon_k c_{k,\sigma}^\dagger c_{k,\sigma} + \sum_{k_1<\ldots<k_3} t_{k_1\ldots k_3} f_{k_1,\sigma_1}^\dagger f_{k_3,\sigma_3} \), \( H_{\text{int}} = U_{f}\sum_{i} n_{i\uparrow} n_{i\downarrow} + U_{cc}\sum_{i} n_{i\uparrow} n_{i\downarrow} + \sum_{i,\sigma} U_{f_c \sigma} n_{i\sigma} \), and \( H_{\text{hyb}} = \sum_{k,\sigma} V_{f_c}(k)(f_{k,\sigma}^\dagger c_{k,\sigma} + \text{h.c}) \).

Here \( t_\mathbf{q}, t_{f} \) are kinetic energies, \( U_{c}, U_{f}, U_{f_c} \) are local Hubbard interactions (intra and inter orbital) and \( V_{f_c} \) is inter-orbital hybridization terms for \( c \) and \( f \) electrons respectively. In the \( f \)-electron context, this is an extended periodic Anderson model (EPAM) which incorporates the important effect of \( f \)-valence fluctuations. In the context of high-\( T_c \) cuprates, models very similar to Eq.(1) have a long history: originally proposed\(^{10}\) in the context of marginal-FL theory, they also emerge from ab-initio quantum chemical (QC) calculations\(^{11}\), as effective models for nodal and anti-nodal states\(^{12}\), and in the context of a proposal for the hidden order in the famed pseudogap phase of underdoped cuprates\(^{13}\). Especially interesting is the observation that the two-band Hubbard model in QC calculations closely resembles Eq.(1) if we relabel \( c_{k,\sigma} \to d_{\mathbf{k}2\mathbf{-y2},\sigma} \) and \( f_{\mathbf{k},\sigma} \to d_{\mathbf{k}3\mathbf{-z2},\sigma} \) (the small \( f \to f \) hopping corresponds to the much smaller direct hopping between the \( d_{\mathbf{k}2\mathbf{-y2}} \) states compared to that between \( d_{\mathbf{k}3\mathbf{-z2}} \) states, and the renormalized hybridization is found to be sizable, and to have a \(\mathbf{d}-\text{wave form factor} \).

Interestingly, this is also precisely the model related to the one used by Weber \textit{et al.}\(^{15}\) in the context of loop-current order being a primary candidate for the hidden order in the pseudogap phase of cuprates. Thus, all results and discussions below with model (1) in mind can be applied to cuprates in the light of the above.

Application of our results to cuprates is thus based on: \(i\) applicability of such a two-band model, with \( c = d_{\mathbf{k}2\mathbf{-y2}} \) and \( f = d_{\mathbf{k}3\mathbf{-z2},\sigma} \) rests upon earlier ab-initio results\(^{14}\), \(ii\), where exactly such an effective model was extracted from a quantum chemical calculation, \(ii\) applicability of single-site DMFT, at least for the strange metal without the complication of having either short-ranged spatial correlations (as in cluster-DMFT studies) or broken symmetry, both of which will be relevant at lower \( T \). Finally, in recognition of the fact that strange metal anomalies are seen in optimally doped cuprates, we start out with partially filled \( f, c \) bands (see below for precise numbers). The quasi-local criticality view is implicit in both, hidden-Fermi liquid\(^{9}\) and marginal-Fermi liquid\(^{14}\) views for the cuprates. Thus, our DMFT approach needs extension in the pseudogap (PG) phase in underdoped cuprates. In this work, we adopt a phenomenological approach to study the PG phase, and a full theoretical study of this phase awaits extension of multi-band-DMFT to include spatial correlations. This is a demanding task, and is left for future studies.

Here, with these comments in mind, we investigate the strange metal phase, focussing on dynamical one- and two-particle responses. Our main results are: \(i\) for sizable \( U(U') \), we find that both exhibit a critical continuum with infra-red singular behavior up to high energy, characteristic of the strange metal, \(ii\) we qualitatively describe resistivity, optical conductivity and magnetic fluctuation data in near-optimally doped cuprates without further assumptions, and \(iii\) we build upon these positive features to study phonon responses in detail, providing a novel interpretation of phonon anomalies in INS data in terms of coupling of bond-stretching phonon modes to a critical continuum of multi-particle excitations. Further, motivated by recent pump-probe studies, we also use these results to study the issue of relative importance of such critical electronic vis-a-vis phononic gluons for pairing in cuprates. We conclude by discussing how novel local quantum criticality in the OSMP phase is drastically different from famed Hertz-Moriya-Millis (HMM) views that obtain close to quantum phase transitions to quasi-classical \((e.g., \text{antiferromagnetic})\) order.

It is natural to work in the rotated \( a, b \) fermion basis (linear combinations of \( c, f \) fermionic operators) which diagonalizes the non-interacting part of \( H \) above. For the free band-structure, the \( d\)-wave form of \( V_{f_c}(k) \) generates a pseudogapped one-electron density-of-states (DOS) (not shown). The occupancies of the \( a, b \) bands are found to be 0.52, 1.48 at \( U \) and \( U'(=U_{ab}/3)=0 \). For \( U_{fc}<U_{f'c} \) a stable strongly correlated LFL phase was found in earlier work using iterated perturbation theory (IPT) as an impurity solver in DMFT. However, for \( U_{fc}>U_{f'c} \), a selective-Mott metal with an infra-red branch-cut form of the one-electron propagator, i.e, a local quantum critical metal, emerged as a consequence of the strong scattering induced OC. Given the approximate nature of the IPT solver, it is obviously of interest to ask whether these appealing features survive upon use of a more exact impurity solver. Here, we have solved \( H \) (Eq.1) within DMFT using the much more exact continuous-time quantum Monte Carlo (CT-QMC) solver. The advantage here is that the local component of both, one- and two-particle dynamical responses can be reliably computed, in contrast to IPT where two-particle responses (susceptibilities) need reliable knowledge of the fully dynamical but local irreducible vertex. This is presently a demanding task, unless they can be argued to be irrelevant, as in large-\( N \) approaches to DMFT\(^{15}\).

In the present work, we obtain the full vertex-corrected two-particle dynamical responses for the EPAM using
FIG. 1. $\text{Im}G_{a,b}(\omega)$ and $\text{Im}\Sigma_{a,b}(i\omega_n)$ as a function of $i\omega$ for a two-orbital square lattice with inter orbital hybridization $t_{ab}$ (with a d-wave form factor) are shown as a function of $U$. The hybridization expansion-based CTQMC method as an impurity solver\textsuperscript{16}. This part is based on our earlier study of an OSMP in a generalized two-orbital Hubbard model\textsuperscript{17}. Here, we explicitly show that the spin and charge susceptibilities possess a long-time (in imaginary-time) quantum-critical form, and use a trick inspired by conformal symmetry to extract an effective analytic form in real frequencies. Such a trick has been widely employed in other contexts\textsuperscript{5}. This will allow us to discuss transport and magnetic fluctuations in the strange metal phase, and to discuss underlying microscopic features leading to the specific anomalies, in detail.

In Fig. 1, we show the imaginary parts of the one-fermion Green functions for the $a,b$ orbital states, along with the corresponding self-energies. It is clear thereby that as $U$ and ($U' = U_{ab} = U/3$) increase, the semimetallic behavior for $U = 0$ (due to the $k$-dependent hybridization) changes into a normal, albeit correlated LFL metallicity at moderate $U$. Beyond $U = 4.0$, however, an orbital-selective differentiation of electronic states clearly reveals itself in both $\text{Im}G_{a,b}(i\omega_n)$ and $\text{Im}\Sigma_{a,b}(i\omega_n)$: the $a$-states are in an incoherent metal state, while the $b$-states are in the Mott insulating regime. This dualistic feature exists in the whole parameter region $4.0 < U < 9.0$ for the given set of one-electron parameters in the EPAM, and thus this is an orbital-selective Mott phase, rather than a QC point. For $U > 10.0$, we find that a full Mott insulator phase obtains. Interestingly, the $a,b$ orbital occupancies change continuously as $U$ and $U'$ are raised: at $U = 3.0, U' = 1.0$, we find $n_a = 0.82, n_b = 1.18$. This trend persists throughout the correlated LFL metal regime ($U \leq 4.0$), beyond which ($U = 5.0$) we find that $n_a = 1 = n_b$. Remarkably, this

FIG. 2. $\text{Im}\Sigma_a(i\omega)$ as a function of $i\omega$ for a two-orbital square lattice with inter orbital hybridization $t_{ab}$ and $U = 6.0$ at low $T$. Clear power-law behavior in $\text{Im}\Sigma_a(i\omega) = C(i\omega)^{1-\eta}$ with $\eta = 0.44, 0.49$ for $T = 60\,\text{K}, 30\,\text{K}$ up to high energy $O(0.5)$ eV, is visible. This is a specific characterization of strange metallicity.
is a curious manifestation of emergent particle-hole symmetry in the OSMP. It directly rationalizes the onset of selective-Mott physics: the half-filled narrower band (b states) selectively undergoes a Mott transition, while the broader (a-band) band states remain bad-metallic. It is interesting that there are tantalizing hints of such p-h symmetry around optimal doping from dc Hall data in cuprates.\textsuperscript{18} Within one-band Hubbard model contexts, this has been accounted for by using extended one-electron hopping integrals beyond nearest neighbors, and realizing restoration of p-h symmetry at a critical doping (where the Fermi energy sits at the saddle-point at $K = (\pi, 0)$ in the bare one-electron dispersion). Our multiband model has inbuilt p-h asymmetry, and it is very interesting that restoration of p-h symmetry in the above sense goes hand-in-hand with OSMP and emergence of strange metallic behavior.

Focussing on the OSMP, we now exhibit the $a, b$-fermion self-energy, Im$\chi_{a,b}(i\omega_n)$, and the full local spin susceptibility, Im$\chi_s(i\omega_n)$, for the orbital-selective Mott phase Fig. 1. 2 and Fig. 3. Interestingly, we find clear evidence of anomalous fractional power-law exponents in both. In Fig. 2, we see that $\text{Im}\chi_{a,b}(i\omega_n) \propto (i\omega_n)^{1-\eta}$, with $\eta = 0.44 (T = 60 K)$ and $\eta = 0.49 (T = 30 K)$. In fact, this behavior extends up to rather high energies $O(0.5) \text{ eV}$, which is characteristic of a multi-particle electronic continuum expected to extend to high energies in a quantum critical regime. Remarkably, the local part of the dynamical spin- and charge susceptibilities also exhibit infra-red singular and fractional power-law scaling behavior, characteristic of the strange metal. We see this as follows. Using the DMFT(CTQMC) results, we see that all spin susceptibility ($\chi_s(\tau)$) curves for $U > 4.0$ almost fall on each other and, upon a careful fitting with a scaling function characteristic for quantum criticality, we find that $\chi_s(\tau)/\chi_s(\beta/2)$ scales as $|\sin(\pi\tau/\beta)|^{-\left(1-\alpha_s\right)}$ with $\alpha_s = 0.9$ Fig. 3. This is precisely the scaling form dictated by conformal invariance in the quantum critical region. It exactly corresponds to the scaling form

$$\chi_s''(\omega) \sim \omega^{-\alpha_s} F_s(\omega/T)$$  \hspace{1cm} (2)

with $F_s(x) = x^{\alpha_s}|\Gamma(\frac{1-n}{2} + i\frac{x^2}{2})|^2 \sinh(x/2)$, whence we immediately read off that $T^{-\alpha_s} \chi_s''(\omega)$ is a universal scaling function of $\omega/T$, with a fractional-power-law dependence. Such a unique form for the dynamical spin susceptibility near magnetic QCPs is experimentally seen in more than a few systems by now, specifically in (not obviously proximate to magnetic order), CeCu$_6-\delta$Au,\textsuperscript{19} among others. In cuprates, a similar form has long been known from early studies of dynamical spin fluctuations,\textsuperscript{20} where $\alpha_s \simeq 1$, in good qualitative accord with our extracted exponent. On a theoretical level, extinction of Landau fermionic quasiparticles in $G_0(k, \omega)$ in the OSMP directly manifests in the emergence of a critical branch-cut continuum in (one-spin-flip) spin-fluctuations. Even more interestingly, the dynamical charge susceptibility also exhibits similar scaling form, but with an exponent $\alpha_c \neq \alpha_s$, implying that spin and charge fluctuations propagate with distinct velocities.

![FIG. 3. Im$\chi_{s,c}(\tau)$ as a function of $\tau/\beta$. Both, the dynamical spin ($s$) and charge ($c$) susceptibilities show quantum critical scaling, with $\chi_{s,c}(\tau)/\chi_{s,c}(\beta/2) \propto |\sin(\pi\tau/\beta)|^{-\left(1-\alpha_{s,c}\right)}$, with $\alpha_s(0.9) \neq \alpha_c(0.98)$.](image-url) Within our numerical accuracy, this constitutes a high-$D$ realization of “spin-charge separation”. The inset shows the static local susceptibilities where $\chi_c(T)$ is more singular than $\chi_s(T)$ at low temperatures.
This is an explicit realization of a high-dimensional spin-charge separation. This is our central result, and we show below that it leads to very good accord with the unusual normal-state magnetic fluctuation spectra and transport in strange metals. Physically, these features emerge as a direct manifestation of emergent, critical pseudoparticles driving the extinction of stable Landau-damped FL-like collective modes in the strange metal. This is simply charge and spin fluctuations are themselves constructed from the now incoherent multiparticle continuum, rather than usual Landau quasiparticles.

What is the underlying physical origin of these emergent anomalous features? As in FL* or Kondo breakdown theories, emergence of critical liquid-like features do not need a one-to-one association with proximity to $T = 0$ magnetic order, since DMFT only accesses strong dynamical correlations. In the OSMP, $V_{fc}(k)$ does not need a one-to-one association with proximity to down theories, emergence of critical liquid-like features and anomalous features? As in FL* rather than usual Landau quasiparticles.

structed from the now incoherent multiparticle continuum, because charge and spin fluctuations are themselves constructed from the now incoherent multiparticle continuum, rather than usual Landau quasiparticles.

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The fully renormalized $\chi(q,\omega)$ now reads

$$\chi(q,\omega) = \frac{1}{\Pi(\omega) + J(q)} \quad (3)$$

where $J(q) \approx -c + (q - Q)^2 + ...$ (e.g, $Q = (\pi, \pi)$ for Neel AFM). At finite $T$, $\Pi(\omega,T) = AT^\alpha f(\omega/T)$.

Physical Responses In The Strange Metal

Remarkably, it turns out that our results afford a consistent and surprisingly good quantitative description of both transport and neutron results in the strange metal. Let us consider the consequences of our numerical findings in more detail in this section, with a specific focus on cuprates.

(i) The dynamical spin susceptibility shows an explicit $\omega/T$-scaling with anomalous fractional exponent $\alpha_s$. It is qualitatively consistent with observations in near optimally doped cuprates, and may also be applicable to other $f$-electron systems where there is independent evidence of the relevance of strong, quasilocal liquid-like critical fluctuations near destruction of magnetic order. From the form of the dynamical spin susceptibility, we can also immediately read off that the spin relaxation rate in nuclear-magnetic resonance (NMR) studies will vary very weakly with $T$, as $1/T_1 \approx T^{0.1}$ or that $1/T_1 T \approx T^{-0.9}$. This is quite close to the measured $1/T_1 T \approx T^{-1}$ in near-optimally doped cuprates.

(ii) The fact that $\text{Im} \Sigma_{\alpha,\beta}(i\omega) \approx (i\omega)^{1-\eta}$ with $(1 - \eta) = 0.51, 0.56$ for $T = 30K, 60K$ allows study of $dc$ and $ac$ conductivities without any further approximation within DMFT. This is because irreducible vertex corrections to the current correlation functions for the cuprates in the Bethe-Salpeter equation rigorously vanish in this limit. Transport is now entirely determined by the simple bubble diagram composed of the full DMFT one-electron propagators. Explicitly, the $dc$ resistivity is now $\rho_{dc}(T) \approx T^{2(1-\eta)} = T^{1.02}$ for $T = 30K$ and $T^{1.12}$ for $T = 60K$. Such an unusual resistivity, $\approx T$, has long been known as one of the defining features of the strange metal in cuprates. The optical conductivity can also be readily estimated as $\sigma(\omega) \approx \omega^{-2(1-\eta)} = \omega^{-1.02}, \omega^{-1.12}$. This is indeed consistent with data in underdoped cuprates as well as in the $D = 3$ 122-Fe arsenides.

Interestingly, Akrap et al. associate this with novel self-energy effects for nodal quasiparticles in UD cuprates. In our modelling, the nodal-versus-antinodal aspect enters via the $k$ dependent $f-c$ hybridization. In our model, this would correspond to an inter-site hybridization between $d_{x^2-y^2}$ and $d_{3z^2-r^2}$ orbitals having a $d$-wave form factor. Interestingly, this is precisely the form extracted from ab-initio quantum chemical calculations, which forms the basis for our two-band modelling for cuprates (see earlier discussion in context of our choice of $H$). OSMP are known to be generic in Fe arsenides by now, and transport anisotropy as well as strain and angle-resolved photoemission (ARPES) studies show clear signatures of localization of $d_{xz}$ orbital states in UD Fe-arsenides.
A two-band model such as one we use, but with different hopping matrix elements and a different $k$-space form factor for the non-local $xz - yz$ hybridization could exhibit similar features in its OSMP phase. Our work now explicitly links the anomalous optical response, at least in 122-Fe arsenides, to such an underlying OSMP.

Such results have also been discussed earlier in the context of Kondo-RKKY models and in the FL context. However, our findings are also somewhat different from earlier works.

(i) The above constitutes an important difference from the Kondo-RKKY case, where the power-law fluctuational form is tied down to $D = 2$. In our case, this is not at all necessary, since the excitonic singularity results from the OC that accompanies selective-Mottness in DMFT, which can happen in $D = 3$ as well.

(ii) Moreover, though in both cases, the physical reason behind emergence of the critical metal involves critical Kondo destruction, there is still an important difference: in the Kondo-RKKY case, it is linked to proximity to AF order as a fall-out of the Kondo-RKKY competition. Here, it is caused by the lattice OC due to selective-Mottness and does not necessarily due to proximity to AF order.

(iii) Thus, such behavior can be observed near AF order as a fall-out of selective Mottness, but need not always be so: it could also arise close to a $T = 0$ valence instability ($Q = 0$): e.g., in $\beta$-YbAl$_4$. In fact, strong $U_{fc}$ which is necessary to get the local strange metal also implies strong quantum fluctuations of the $f$-valence. In the latter case, the appropriate charge (valence) susceptibility will diverge in exactly the same way. At finite-$T$, we have

$$\Pi(\omega, T) = AT^\gamma g(\omega/T)$$  \hspace{1cm} (4)$$

with $\gamma = (1 - \alpha)$ and $g(x)$ is a universal scaling function of $x$.

Analytical Insight into DMFT Results

This leads to an insight, first formalized by Anderson$^{9,26}$ that we now use to proceed further. We refer interested readers to Casey and Anderson’s papers for relevant details used in this section.

Since the local impurity problem can be bosonized in radial channels on a $(1 + 1)D$ half-line$^{27}$, $\chi(q, \omega) \simeq \omega^{-\gamma} f(\omega/T)$ can also be understood, using the Schotte et al trick$^{27}$, as arising from a set of radial spin density tomonagons (collective bosonic modes composed of spin- and charge density modes) emanating from every local site in an effective equivalent high-D view of the fermionic system. In fact, these can be identified with the critical bosons. Referring back to Schotte et al., one sees, thanks to the commutation relations $[H, b_q^\dagger] = \omega(q)b_q^\dagger$ in the low-energy subspace spanned by bosons $b, b^\dagger$ defined below, that the latter must in reality represent critical $p$-$h$ spin fluctuation modes: in terms of the $a, b$ fermions, one has $b_{q}^{\dagger} = (1/\sqrt{|N|}) \sum_{k,k',a,b=K} b_{k,\sigma}^{\dagger} a_{k',\sigma'} e^{i(k-k')R_i}$, with $\sigma = \sigma', \sigma' = -\sigma$ for charge $(c)$ and spin $(s)$ respectively: these are precisely the spin- and charge-density (excitonic) variables whose singular fluctuations arise from the lattice OC in a strange metal. Can we use this representation for such novel spin fluctuations to get more physical insight?

We now find it illuminating to use a slick trick$^{27}$ to show how a related analytic procedure can be explicitly carried out in an especially fruitful way in the selective metal. In this case, write-out of heavy-FL screening by the lattice OC is implied by the irrelevant hybridization, $V_{fc}(k)$ as discussed before. Let us consider how this physics reflects itself in the tomonagon variables. Using the definition of the tomonagons as above, we can write$^{9,26}$

$$H' = \sum_{q} \omega(q)b_q^\dagger b_q + (1/\sqrt{L}) \sum_{q} g(q)(b_q + b_q^\dagger)$$ \hspace{1cm} (5)$$

where, crucially, the new aspect that enters in the OSMP is that $g(q) = g(q, t) = g(q)\theta(t)$ is now suddenly switched on and off as a function of $t$ only in the case where $V_{fc}(k)$ is irrelevant, i.e., precisely in the selective-Mott state. This is because only in this case do the fermionic spin fluctuation modes in $H'$ see a fluctuating field that suddenly turns on and off as a function of $t$ (this is the two-particle analogue of the sudden switching-on by $U_{fc}$ in the limit of irrelevant $V_{fc}$ in $H$). In bosonic lore, $H_{res}$ describes spin fluctuation processes: in a scattering process involving two magnons, the potential seen by a magnon ($b_i^\dagger$) is time-dependent and strongly fluctuating in the manner of a step function because the $b$-fermion occupation switches suddenly between $n_a = 0, 1$ as a function of time in the OSMP. The origin of this is that, given an irrelevant $V_{fc}(k)$, an $b$-electron can only be transferred into the bath (making $n_b = 0$, switched off potential) or to the local site ($n_b = 1$, potential switched on). Via the definition $b_q^\dagger = (1/\sqrt{|N|}) \sum_{k,k',\sigma} a_{k,\sigma}^\dagger b_{k',\sigma} e^{i(k-k')R_i}$, and the structure of $H'$, it then follows that this potential is switched on and off in a sudden way as a function of $t$. The second part of $H'$ thus describes dynamic spin fluctuations above a quiescent filled sea of tomonagons$^{9}$, we emphasize that this is, after all, a suitable low-energy representation for spin fluctuations. But $H'$ can now be diagonalized by a$^{27}$ generalized Lee-Low-Pines (LLP) shift transformation, yielding the spectral function $g(t) = \langle T[S_{\uparrow}(t)S_{\downarrow}(0)]\rangle = \exp[\int_{0}^{\Omega} \lambda^2(\omega)N(\omega)(e^{-\omega t} - 1) d\omega]$.

Here, we have introduced a tomonagon DOS, $N(\omega)$ and $\Omega \simeq \max\{\lambda(q)\}$, and interpreted $\lambda^2(\omega)N(\omega)$ as a spectral function of the tomonagons. Interestingly, following Hopfield$^{28}$, the choice $\lambda^2(\omega)N(\omega) \simeq (1 - \alpha)\omega$ reproduces the IR singularity in $\chi_{\uparrow\downarrow}^{-1}(\omega)$. At finite $T$, an explicit calculation gives $g(t) \simeq \left[\sinh(\pi t\beta)/\pi\beta\right]^{-(1-\alpha)}$, implying that $\chi_{\uparrow\downarrow}^{-1}(\omega)$ will show $\omega/T$-scaling. In particular, it turns out that at $T = 0$, we recover precisely
\[ \chi_{loc}(\omega) \simeq \theta(\omega)\omega^{-(1-\alpha)}. \]

In Fig. 4, we show \( \chi(q,\omega) \) for various \( q \) as a function of \( \omega \) at fixed \( T \) and as a function of \( T \) for fixed \( q = Q = (\pi,\pi) \) with \( J(q) \) obtained from the same parameter choice as in earlier EPAM work. In close correspondence with key findings in the normal state spin fluctuation spectrum measured in INS data for strange metals, we observe: (i) anomalously broad continuum response resulting from a branchcut, rather than any conventional pole-like analytic structure of \( \chi(q,\omega) \). Moreover, incoherent magnetic spectral weight piles up at low energy in a way that respects \( \omega/T \)-scaling with \( \text{Im}\chi(q,\omega,T) \sim A(q)T^{-(1-\alpha)} F(\omega/T) \) Simultaneously, the \( q \)-dependence of the INS lineshape is entirely that of the unperturbed Lindhardt susceptibility of the two-band model, since the spin self-energy, \( \Pi(\omega) \) is purely local, (ii) rigorously vanishing magnon residue, namely, \( z_m \simeq (1 - \partial_{\omega}\Pi(\omega)|_{\omega \to 0})^{-1} = 0 \), following from \( \Pi(\omega) \simeq -\alpha(\omega^{1-\alpha} \alpha > 0, \text{ and } (iii) \) a linewidth that nevertheless decays linearly or sub-linearly with \( \omega,T \) as a function of \( q \) if we define the spin fluctuation rate, \( \Gamma_{q}(\omega) = \frac{\omega\chi''(q,\omega)}{\chi''(q,\omega)} = \pi (1 - \alpha)\omega \). Thus, the slope of the spin fluctuation scattering lifetime is simply related to the power-law exponent in \( \chi_{II}^{-}(\omega) \), a feature which can be tested in INS work.

![Graphs showing dynamical spin susceptibility and spin-fluctuation linewidths](image)

**FIG. 4.** The dynamical spin susceptibility and spin-fluctuation linewidths for the strange metal phase of cuprates at various \( q \) in the Brillouin zone \((0,0)(\pi/2,0)(\pi,0)(\pi,\pi/2)(\pi,\pi)(\pi/2,\pi/2)\) of the reduced Brillouin zone at \( \beta = 100 \) (left panel) and 1000 (right panel).

On the other hand, when \( V_{f_{c}}(k) \) is relevant, the local Kondo screening must produce a heavy-FL state at low \( T \): this corresponds to the quantum paramagnetic heavy-FL solution found in DMFT for the EPAM for \( U_{f_{c}} < U_{f_{c}}^{(1)} \) in earlier work. In this case, it is known that one must seek an infra-red solution to \( H' \) with an adiabatically slowly switched on \( g(q,t) \) instead of a suddenly switched one, leading, as required, to heavy-FL metallicity with small \( z_{FL} \). This is because, when \( V_{f_{c}}(k) \) is relevant, an \( a \)-electron can now hop coherently from the site \( i \) into the bath and back. We emphasize that this route to restoration of one-electron Fermi liquid coherence is intimately tied down to the fact that coherent one-electron hybridization \( (V_{f_{c}}) \) in the EPAM now involves both, real charge and spin fluctuations, in contrast to the classical Kondo scenario, where \( b \)-charge fluctuations are suppressed in the infra-red. This manifests itself in a finite recoil of the \( b \)-fermion during scattering, giving it a heavy but finite mass and cutting off the infra-red singularity below a low-energy scale \( T_{coh} \) in both \( \rho_{a}(\omega), \rho_{b}(\omega) \) in the associated impurity model, and this is faithfully reflected in our CTQMC results (where a correlated LFL metal obtains for \( U \leq 4.0 \) eV, as well as in earlier DMFT work).

Finally, there is one more possibility. Since the selective-Mott state must also undergo ordering instabilities at sufficiently low \( T \), if only to relieve its finite \( T = 0 \) entropy (when \( V_{f_{c}}(k) \) is irrelevant), the infra-red singular behavior can also be cut-off by a direct instability to two-particle coherence. This needs an extension of the above framework to explicitly include broken symmetry, and we will present a specific scenario in a phenomenological way when we study phonon responses in the underdoped cuprates below.

**Phonon Dynamics from INS Results**

We now extend the above approach to study various features related to anomalous lattice dynamics in cuprates. In particular, we will focus on (i) inelastic neutron scattering data, which shows clear anomalies in phonon dispersions and lineshapes, (ii) the relative importance of the electronic bosonic and phononic contributions to the pairing glue, and (iii) use of lattice dynamics studies in underdoped cuprates as a test of hidden order in the pseudogap phase that emerges in underdoped cuprates.

Inelastic neutron scattering (INS) studies provide valuable information on lattice dynamics: in particular, the phonon lineshapes, dispersions and linewidths can be extracted from INS data. In the context of high-\( T_{c} \) cuprates, such studies have been extensively performed over the years by various groups. Spurred on by the need to derive quantitative estimates for relevance of electron-lattice coupling in HTSC, special attention has been devoted to various issues. These are

(i) how does the character of lattice dynamics evolve from the strange metal near optimal doping, as one crosses over into the famed pseudogap (PG) regime in the underdoped (UD) regime?

(ii) can changes in phonon spectra provide us with a handle on the important issue of discerning the microscopic nature of the PG state? Characterizing the PG state is an extremely controversial subject, with various competing scenarios extant in literature. These range from preformed \( d \)-wave phase fluctuations without actual SC coherence, nematic instability, circulating-current order, \( d \)-density-wave, and stripes, among others. Appropriate smoking gun scenarios can greatly aid in distinguishing between these. In any case, any plaus-
ble scenario should be constrained by an all-important known fact: namely, that the PG regime with its possible novel symmetry-breaking (or lack thereof) must arise as an instability of the strange metal without Landau quasiparticles.

(iii) study of lattice dynamics in HTSC has long been confronted with a set of well-known, but ill-settled issues. These are:

(1) in UD cuprates, halfway the Brillouin zone, the half-breathing Cu-O vibration mode seems to suddenly dip down to a much lower frequency. The line-width reaches its maximum at a wave-vector somewhat shifted from the frequency-dip position, while it narrows at higher temperatures. A pronounced and little-understood asymmetry in the spectra for UD cases is also visible. In addition, the anomaly has a narrow intrinsic peak width as function of momentum transversal to the mode propagation direction. These rather dramatic observations have been hitherto addressed within fluctuating stripe and $t – J$ model approaches, but revisiting this problem is called for in view of new proposals regarding the order in the pseudo-gap phase. This is because changes in phonon dynamics upon entering the PG phase must, in the final analysis, be tied down to possible electronic order (or lack thereof) in that phase.

(2) For cuprates, a rather weak EPI was found, which alone would not be sufficient to explain the superconductivity. However, the calculated width of the half-breathing phonon is an order of magnitude smaller than the reported experimental value, raising some questions about the accuracy of the LDA in this context. In particular, this points to the need to include strong lifetime effects in the phonon propagator: the latter can only arise from incorporation of dynamical fluctuation effects in the electron-phonon interaction, and the latter is expected to be particularly unconventional in the strange metal (see below).

(3) while signatures of polarons are purportedly seen in undoped cuprates, it is much more challenging to interpret manifestations of electron-phonon coupling in the strange metal. This is because the very untestability of a low-energy Landau quasiparticle description for the strange metal inevitably leads to non-trivial features in extracting such information when the one- and two-fermion propagators exhibit an infra-red branch-cut singular structure. Specifically, observation of anomalous continuum response in the magnetic fluctuation spectrum in the strange metal implies that associated features should manifest in phonon spectra.

Thus, if we wish to extend the analysis of spin and charge fluctuations above to study phonon spectra, the interesting and relevant issue we are faced with is whether (and to what extent) the above issues can be understood within a theoretical scenario where phonons are coupled to a specific critical electronic continuum as worked out above. More importantly, we also ask: can we use changes in phonon dynamics upon entering the pseudo-gap phase as a tool that can offer an additional valuable insight into novel order in the PG state? In this section, we address this issue, as well as the related one of relative importance of intrinsic multi-electronic and phononic gluers for SC, in some detail.

The free phonon propagator for a $D = 2$ square lattice is

$$D(q, \omega) = \frac{2\omega_q}{\omega^2 - \omega_q^2}$$

We choose the electron-phonon coupling to reflect the fact that the coupling reflects electron density modulation by dispersive half-breathing bond-phonons: the coupling Hamiltonian is

$$H_{e-p} = \frac{1}{\sqrt{N}} \sum_{k,q} g(q)c_{k+q,\sigma}c_{k,\sigma}(b_q + b_{-q}^\dagger)$$

where $g(q) = g\sqrt{\sin^2(q_{a}a/2) + \sin^2(q_{b}b/2)}$ and $q = (q_{a}, q_{b})$. Formally, the renormalization of the phonon propagator is caused by coupling to a particle-hole susceptibility, $\chi_{cc}(q, \omega)$ in the charge sector. In a Fermi liquid metal, the latter is evaluated from the fully dressed electronic GFs in a RPA summation involving the fully renormalized GFs and the bare phonon vertex. Effects beyond HF-RPA, which result in a dressing of $g(q)$, do not qualitatively modify that picture. In the quantum critical metal, however, the finding that the density fluctuation spectrum has no pole structure, but rather a branch-cut analytic structure in the infra-red (with a fractional exponent $\alpha_4$ distinct from The exponent $\alpha_4$ in the spin fluctuation spectrum) leads us to expect qualitatively radical deviations from this traditional picture. Thus, given a $\chi_{cc}(q, \omega)$ having similar infra-red branch-cut continuum form as above, we can now readily proceed to discuss the phonon spectra in our case. The dressed phonon GF is, as usual related to the density susceptibility as follows:

$$D(q, \omega) = \frac{2\omega_q}{\omega^2 - \omega_q^2 - 2g^2(q)\omega_q\chi(q, \omega)}$$

with $\chi(q, \omega) = [\chi_0^{-1}(q, \omega) + J(q)\Gamma(q)]^{-1}$ and $\chi_0(q, \omega) = C(q)T^{-\alpha_4}h(\omega/T)$. Here, $h(\omega/T) = \chi_0(iC/2\pi T)^{\alpha_4} T^{-\alpha_4}(x/\Gamma(1/2))$. Here, $J(q) = 2J(\cos q_{a}a + \cos q_{b}b)$ and $\Gamma(x)$ is the digamma function of $x$. In the strange metal, $\alpha_4 = (1/\pi)\tan^{-1}(U_{0}^{\uparrow\downarrow}/W) < 1$ is the anomalous exponent coming from the infra-red singular electronic susceptibility as above, and $\chi_0$ and $C$ are adjustable parameters. The phonon lineshape is now read off as the spectral function of the renormalized phonon propagator, i.e, it is $A_{ph}(q, \omega) = -\frac{1}{\pi}\text{Im} D(q, \omega)$, while the renormalized phonon dispersion is simply given by the equation $\omega^2 - \omega_q^2 - 2g^2(q)\omega_q\chi(q, \omega) = 0$. Finally, the phonon damping, measured as the full-width
at half-maximum of the phonon lineshape, is simply the imaginary part of the phonon self-energy above. We present our results in Fig. 5, 6, 7. Several novel features, germane to extant data, stand out without the need to make any further assumptions about the electronic state:

(1) Phonon dispersions As mentioned above, in at least two families (LSCO and YBCO, the latter at doping levels unrelated to any putative stripe-like instabilities), the half-breathing dispersive bond-phonon mode shows anomalous softening half-way across the Brillouin zone, followed by an anomalous growth of the linewidth at a slightly different wave-vector. This is particularly obvious in Figures (2),(4) of Reznik et al.\textsuperscript{30}, where the phonon dispersion shows a completely unanticipated and severe bending from its LDA counterpart. While this should be interpreted as being caused by coupling of the phonons with appropriate symmetry to electronic fluctuations, large damping and associated asymmetric lineshapes show that this likely involves strong coupling to electronic excitations that are themselves strongly damped. Our contention is that these electronic modes are precisely those associated with the anomalously damped electronic continuum derived above. Our results bear out this expectation quite satisfactorily. It is indeed quite satisfying that the phonon dispersion shows a sharp drop (actually, a jump in $\omega(q)$) precisely somewhat midway across the Brillouin zone, both along $\mathbf{q}_1 = (h,0,0)$ and along $\mathbf{q}_2 = (0,k,0)$, corresponding to Figs.(2),(4) of Reznik \textit{et al}. This feature arises simply due to coupling of the half-breathing phonon to an infrared critical multielectronic continuum in our picture. The attractive feature of the present work is that, apart from coupling to a collective fluctuation spectrum of (anomalously overdamped) fermionic origin, no other assumptions are needed. To the extent that this anomalous fermionic fluctuation spectrum is also consistent with a host of unusual observations in the strange metal, this accord lends additional support to the notion of an anomalous locally critical fluctuation spectrum in the strange metal.
(2) Phonon Lineshapes

Associated anomalous features are also visible in phonon lineshapes, also shown in Fig. 7. A noticeable asymmetry, centered around the (main) phonon peak at 60 meV is visible. In a Fermi liquid, such asymmetry is not expected. More dramatically, an anomalous and incoherent shake-up feature is also found in our calculation around ω = 0, and the phonon spectral function is thus composed of (i) a strong feature around the phonon frequency, shifted somewhat from its bare value and anomalously broadened, especially at lower T. This is the direct effect of the phonon self-energy. A direct prediction following herefrom is that the phonon linewidth should show appreciable damping at a wave-vector somewhat different from that where the dispersion shows the anomaly in (1) above. Thus, the direct effect of coupling to a critical multielectronic continuum is that the phonon lineshapes will also exhibit anomalies. It would be very interesting to analyze the prediction of a specific Fano-like shake-up feature in phonon lineshapes, but we remain unaware of systematic studies along these lines. The key stumbling block seems to be the limit of resolution in actual INS studies: since the shake-up feature is very small compared to the main phonon peak, it will probably be completely obscured by the background signal in reality. But another key prediction, that of measurable asymmetry in the main phonon lineshape, could be more readily resolved with state-of-the-art facilities. Appreciable phonon damping is also clearly seen in our results, and is qualitatively consistent with the large order-of-magnitude discrepancy between LDA estimates and neutron data for phonon linewidths.30

(3) Finally, our results for the electronic susceptibility and phonon lineshape can be directly used to estimate the pairing glue function contribution from both processes. The relative contributions from purely electronic and phononic channels to the high-Tc values in cuprates has been a subject of various detailed analyses.30,37 However, the relative importance of these processes has never, to our best knowledge, been considered within the strange metal hypothesis, though cluster-DMFT studies indeed go a long way toward showing the dominant importance of a purely electronic pairing glue. Clearly, this is an important constraint on theoretical scenarios, and here, we present our attempt to fill in this breach.

Within our analysis above, the pair glue function is simply a sum of two contributions, (i) from the purely electronic collective modes, written as

\[ \alpha_p^2 F_e(\omega) = J^2 \sum_q \Im \chi(q, \omega), \]

and a phononic part, which is simply

\[ \alpha_p^2 F_p(\omega) = \sum_q g^2(q) \Im D(q, \omega). \]

In Fig. 8, we show these contributions and the total pair glue function, which exhibits several interesting features.

First, \( \alpha_p^2 F_e(\omega) \) at low T clearly exhibits the singular branch-cut continuum form \( \sim \omega^{-\nu} \) inherited from the strange metal. This is precisely the contribution expected from a quantum critical fluctuation spectrum, whose origin (in our picture) is the critical (incoherent) continuum that arises due to the underlying inverse orthogonality catastrophe in the selective-Mott state in the fermionic (DMFT) theory. Interestingly, though the phononic contribution is not negligible, it is clearly much smaller (almost by an order of magnitude) than the purely electronic one. Though a full theoretical estimate of these glue to \( T_c \) must involve treatments beyond the Eliashberg scenario,38 we can readily make qualitatively

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**FIG. 7.** Renormalized Phonon lineshapes and linewidths as functions of various \( q \) in the Brillouin zone. \([0,0)(\pi/2,0)(\pi,0)(\pi,\pi/2)(\pi,\pi)(\pi/2,\pi/2)\) of the reduced Brillouin zone at \( \beta = 100 \) (left panel) and 1000 (right panel). Asymmetry in the lineshapes as well as a “Fano”-like peak at low energy is also clearly visible.

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**FIG. 8.** Multi-electronic and bosonic contributions to the pair-glue functions, along with the total glue function at \( \beta = 100 \) (left panel) and 1000 (right panel). At low T, the contribution of the multi-electronic glue is an order-of-magnitude larger than that due to bond-stretching phonons, in good accord with quantitative estimations from pump-probe data (see text).
reasonable order-of-magnitude estimates using the above results. However, one needs to take into account the fact that having $\lambda_\omega = \alpha^2 F_c(\omega)/\omega \simeq J^2 \text{Im}(\chi(\omega))/\omega$ makes this case qualitatively different from a BCS-Eliashberg one, where $\lambda(\omega)$ is constant at low energy. Specifically, retardation effects are much more subtle when the pair glue is dominated by a massless (critical) electronic boson. Fortunately, the singular-glue case has been recently analyzed by Moon et al. The pairing scale, denoted $T^\text{el}_p$, increases monotonically as the quantum critical regime is approached from the disordered side. However, the contribution to the actual SC $T^\text{el}_c$ from the electronic continuum, estimated following Moon et al., is given by $T^\text{el}_c \simeq E_F \cdot e^{-\pi/2\sqrt{\lambda}}$, enhanced above its BCS value. Thus, this strong coupling view gives two different scales: one associated with pair formation without pair coherence (at $T_p$) and the second with long-range pair coherence ($T^\text{el}_c < T_p$), where actual SC occurs. However, the contributions from phonons can be qualitatively estimated within a more traditional BCS-Eliashberg formalism, since $F_p(\omega)$ does not exhibit low-energy singular behavior. Inserting the order-of-magnitude values from Fig. 8, it is easy to convince oneself that the contribution of the electronic (“bosonic”) continuum to $T_c$ is about an order-of-magnitude higher than that of phonons. Thus, our findings are also in full accord with other theoretical and experimental estimations on relative importance of electronic and phononic glue in cuprates.

Pseudogap Regime

Our treatment has hitherto relied on the existence of strange metallicity, and thus restricted to the near-optimally doped regime. Upon underdoping, even more drastic deviations from Fermi liquid theory in thermal and transport responses characterize the famed pseudogap regime.

(1) inelastic neutron scattering clearly reveal sizable 1D-like anisotropy in magnetic excitations around the AF ordering wave-vector $Q = ((\pi/2, \pi/2)$, in a magnetically disordered phase below 150 K in the UD phase. That this anisotropy is most likely associated with an intrinsic electronic instability is suggested by the observation that it greatly exceeds estimates based on purely structural anisotropy, and, more crucially, by the finding that it follows the $T$ and $x$ dependence of the inplane resistivity anisotropy.

(2) more recent structural measurements by Fujita et al. also finds a $d$-wave modulation of the charge density distribution in the UD cuprates. Interestingly, both, this modulation and nematic signatures in (1) above, appear to vanish precisely around the same doping close to optimal doping, making them attractive candidates for the hidden order in the UD cuprates. It must be emphasized that both these orders can co-exist on purely symmetry grounds, and, indeed, that one follows the other.

(3) simultaneously, however, Nernst effect data appear to indicate a strongly fluctuating, preformed cooper pair phase without actual superconductive order. This has been studied in detail by various groups with good success.

(1) – (3) pose an additional set of questions. How can we conceive of (1), (2) arising as direct instabilities of the strange metal found around optimal doping? Are they in irreconcilable conflict with (3), which has also been successfully used to rationalize a variety of data?

Within our approach as described above, we proceed as follows. Since the local strange metal found within DMFT has a finite residual entropy, this state must eventually find a way to relieve this entropy as $T \to 0$. If one-electron hybridization were eventually relevant, quenching the entropy would necessarily involve eventual screening of the selectively Mott-localized magnetic moment via the local Kondo effect (this is indeed what happens in the EPAM for small enough $U_{fc}$). However, since $V_{fc}(k)$ is irrelevant in the strange metal, the system must quench its residual entropy by generating a long-range ordered state via a two-particle instability, directly from the strange metal. In analogy with what happens in coupled $D = 1$ Luttinger liquids and following earlier ideas of Anderson, we have proposed that increasing relevance of inter-site correlations between neighboring impurities of the DMFT problem generates an effective residual and non-local two-particle interaction in the local version of the strange metal. As in the coupled $D = 1$ chains case, this allows for a direct instability of the local critical metal to ordered states. As worked out before, this residual two-particle interaction is

$$H_{\text{res}} \simeq -\frac{V_{fc}^2}{U_{fc}} \sum_{k,k'} \gamma(k)\gamma(k') \langle b_{k\sigma}^\dagger a_{k'\sigma}^\dagger b_{k'\sigma'}^+ + h.c \rangle$$

(9)

which is also

$$H_{\text{res}} \simeq -\frac{V_{fc}^2}{U_{fc}} \sum_{k,k'} \gamma(k)\gamma(k') \langle b_{k\sigma}^\dagger \delta_{kk'}\delta_{\sigma\sigma'} - a_{k'\sigma}^\dagger a_{k\sigma} b_{k'\sigma'}^+ + h.c \rangle$$

(10)

and has a separable form in $k$-space. Within the local approximation, it is now fully legitimate to decouple $H_{\text{res}}$ (which scales like $1/D$) in a Hartree-Fock approximation in both particle-hole (p-h) and particle-particle (p-p) channels. The result is

$$H_{\text{res}}^{mf} = -J' \sum_k [\Delta_{ph}(k)b_{k\sigma}^\dagger a_{k\sigma} + \Delta_{pp}(k)b_{k\sigma}^\dagger a_{k\sigma}^\dagger a_{-k\sigma} + (1 - \langle n_{k,\sigma}\rangle) n_{k,b\sigma}]$$

(11)

and, since both $\Delta_{ph}(k), \Delta_{pp}(k)$ arise from the same set of $a, b$ fermionic states involved in $H_{\text{res}}$, it follows that they necessarily represent competing p-h (density-wave) and p-p (superconductive) orders. Additionally, the
last term in $H_{res}$ above results in electronic anisotropy infrom the outset, yielding an electronic nematic that co-exists with $\Delta_{ph} \neq 0$. It is crucial to notice that, with $\gamma(k) = (\cos k_x - \cos k_y)$, both p-h and p-p instabilities are of d-wave type. The p-h order parameter is the average $\Delta_{ph}(k) = \langle \gamma(k) \hat{a}_{k}^{\dagger} \hat{a}_{k} \rangle$ while the p-p order parameter is $\Delta_{pp}(k) = \langle \gamma(k) \hat{a}_{k\sigma}^{\dagger} \hat{a}_{k\sigma} \rangle$. The first represents a d-wave charge density modulated order. As advertized above and previously noted by Kee et al., such a d-density modulation, expressed as $\Delta_{d,ch}(\mathbf{q}) = \sum_{k} \gamma(k) \hat{b}_{k+\mathbf{q}}^{\dagger} a_{k\sigma}$, will also necessarily follow a finite $\Delta_{ph}(k)$ (and vice-versa) on purely symmetry grounds. Thus, starting from the strange metal, we have derived an effective residual interaction which exposes both, the instability to a d-wave superconductor, as well as to a competing p-h or excitonic instability to a state with a d-wave density modulation and intra-cell nematicity, in qualitative accord with recent structural analyses.\(^{34}\)

With this insight, we now return to the question posed before: can we use the changes in phonon spectra in the PG phase to gain insight into possible novel electronic order (or lack thereof) in UD cuprates? From the above analysis, it is clear that, if a hidden order related to $\Delta_{ph}(k) \neq 0$ indeed develops in the PG state, now to be interpreted as a direct instability of the strange metal, we have derived an effective residual in- \(\ldots \)

**Inelastic Neutron Scattering Lineshape** Our main results for $\chi^0(q, \omega)$ are shown in Fig. 9. The first observation is that the infra-red singular feature seen for the strange metal is immediately cut-off by the appearance of the d-wave pseudogap scale (which is of order $j\delta$ on the scale of 50 meV in actual UD cuprates), the latter now being introduced by a finite $\Delta_{ph}(k)$, $\Delta_{d,ch}$ as above. As also expected, the d-wave nature inherent in $H_{res}$ leads to significant variation with $\mathbf{q}$, and the resulting anisotropy in the magnetic fluctuation spectrum with respect to $q_x$ and $q_y$ is clearly reflected in the results. Specifically, the response around $\mathbf{Q} = (\pi, \pi)$ remains sharply peaked, but significant supression of magnetic spectral weight for $\mathbf{q} \neq \mathbf{Q}$ stands out as a manifestation of anisotropic spin-gap formation. Concomitantly, increased damping, resulting in even less well-defined spin fluctuation modes, except for $\mathbf{q} = \mathbf{Q}$, is also visible. These are direct consequences of the proposed d-wave nematic-plus bond-order, which spontaneously breaks the discrete four-fold $C_4$ rotation symmetry. It is important to point out, however, that all we need to obtain such a result is a finite intra-cell nematicity, but not necessarily a true long-range nematic order (sometimes dubbed fluctuating order in literature). So strictly speaking, this accord in our phenomenology cannot distinguish between strongly dynamically fluctuating nematic correlations and nematic order, but it is not inconsistent with true electronic nematic order either. More analysis is thus needed to clinch this issue.

**Phonon Spectra in the d-PG state** Concomitantly, phonon dynamics is also drastically modified by emergence of d-wave p-h instabilities in the PG phase. We show the phonon dispersions Fig. 10, 11, lineshapes, and linewidths Fig. 12 assuming finite $\Delta_{ph}(k)$. In particular, we focus on the change in phonon dispersion within the scenario of an instability to d-wave nematic-plus d-wave density modulation. The Fig. 10 clearly shows that the main effect of this instability is to introduce a clear anisotropy in phonon dispersions. Since $j\delta > 0$, the dispersion of magnetic excitations (neglecting lifetime effects coming from the anomalous spin self-energy) will be $J(q_x, q_y) = (J + j\delta)\cos q_x + (J - j\delta)\cos q_y$. This means magnetic excitations are more dispersive along the $a$-axis and less so along $b$: this is a consequence of the d-wave form of the residual interaction derived above. One thus
FIG. 10. Renormalized Phonon dispersion relations in the pseudogap phase in the Brillouin zone, \( \omega(q_x, q_y) \) at \( \beta = 1000 \). Clear momentum-dependent anisotropy, along with clear anomaly in the dispersion along \( q_y \) in good accord with data of Pintschovius et al.\(^{42}\) is clearly visible. Standard color function has been used for dispersion intensity (violet having least value and red having highest value).

expects that the bond-stretching phonon mode will couple more efficiently to electronic excitations along \( b \), and this is fully borne out by our results. Remarkably, we find a clear anomaly in the phonon dispersion along \( b \) but not along \( a \). It is very interesting to observe that the anomaly occurs in a direction perpendicular to the one along which electronic excitations are more dispersive, a finding fully consistent with that of Pintschovius et al.\(^{42}\). As they have emphasized, this is inconsistent with a stripe scenario. However, we have now shown that it is qualitatively fully consistent with having intracell nematic-plus \( d \)-bond charge density modulated order in the UD phase. Thus, our results offer an attractive possibility to distinguish between different scenarios for the hidden order of the PG phase by appealing to analysis of phonon spectra. In the specific context of cuprates, the accord we find is corroborating evidence in favor of a coupled \( d \)-nematic-plus \( d \)-bond charge density modulated order in the UD cuprates, and reconciles phonon spectra with recent structural findings\(^{34}\).

**What about Preformed-Pairs?**

How does one reconcile extensive observations of pre-formed cooper-pair regime with findings above? Extensive evidence of pre-formed cooper paired bad-metallic state is well documented in the PG phase. Let us now discuss a possible resolution of this seemingly irreconcilable conflict within our idea. Focussing on the form of \( H_{res} \) or \( H_{res}^{mf} \), we see a remarkable emergent symmetry that may hold the key to our argument. Introducing a \( s \)-wave spin-singlet pairing operator, \( \Delta_{s,sc} = \frac{1}{\sqrt{2}} \sum_{k,\sigma} \sigma b_{-k,-\sigma} b_{k\sigma} \), we easily see that it rotates \( \Delta_d \) above into \( \Delta_{d,sc} \):

\[
\{\Delta_{s,sc}, \Delta_d\} = \Delta_{d,sc} \quad (12)
\]

The crux is now that short-range correlations associated with \( \Delta_{s,sc} \) also appear in the PG phase, thanks to the two-particle couplings between \( a, b \) fermions in \( H_{res} \) (remember that the sum is over both \( a, b \) orbital indices). So having finite intra-cell nematic correlations in the PG
The changes in the magnetic fluctuation and phonon spectra upon emergence of intracell nematic-plus d-wave density modulation order in UD cuprates must affect the total glue function, \( \alpha^2 F(\omega) = J^2 \text{Im} \chi(\omega) + g^2 \text{Im} D(\omega) \) defined before. That this is indeed the case is shown in Fig. 13. As one would expect, the cut-off of the infra-red divergence in \( \chi(q, \omega) \) in the PG phase cuts off the corresponding feature in the glue function contribution from electronic bosonic excitations. By itself, this directly implies a reduction in the SC \( T_c \) upon underdoping. The underlying reason for this is clear from the observation that intracell nematic-plus d-charge density modulation competes with d-wave SC, since both instabilities arise from the same set of carriers, via the residual interaction term. It must be mentioned that though we have been able to rationalize the reduction of \( T_c \) within our semi-phenomenological approach, a definitive resolution of this issue awaits a fully microscopic calculation including \( H_{\text{mix}} \) in the corresponding fermionic model within DMFT or cluster-DMFT approaches. This remains out of scope of the present study. However, it is encouraging that a nematic instability as proposed here is indeed found in recent cluster-DMFT studies of the \( D = 2 \) Hubbard model\(^{43} \). In view of our analysis, an attractive feature is that such a hidden order in the PG phase arises as a natural instability of the strange metal via the preferential dominance of intersite pair-hopping interactions in the p-h channel.

**Discussion and Implications**

What distinguishes our view from extant ones? In itinerant HMM views, the spatio-temporal build-up of AF spin correlations near a \( T = 0 \) AF QCP can, under certain conditions, give \( \chi_{\text{loc}}(\omega) \simeq \omega^{-\eta} \) with \( \eta = 1/2, 1/3 \)\(^{38} \). Alternatively, in a Kondo-RKKY formalism, one finds \( \chi_{\text{loc}}(\omega) \simeq \omega^{-\gamma} \) with an interaction-dependent \( \gamma \). In both cases, however, this behavior is intimately tied down to proximity to a \( T = 0 \) AF QCP, even though it is accompanied by breakdown of the Kondo effect by competing intersite RKKY couplings in the latter case. In stark contrast, similar behavior found in our selective-Mott mechanism is not necessarily associated with proximity to any \( T = 0 \) AF criticality: the only quantum criticality involved here is that of proximity to the \( T = 0 \) end-point of the line of first-order (liquid-gas universality) selective-Mott transition: this implies a divergent compressibility and leads to destruction of Fermi liquid theory by coupling fermions to the associated soft collective electronic excitations. What we have shown here is that the inverse orthogonality catastrophe that acquires a rigorous meaning in the local problem of DMFT for the selective metal.

**Electronic and Phononic Pair Glues**

FIG. 12. Renormalized Phonon lineshapes and linewidths at different \( q \) points \((0,0)(\pi/2,0)(\pi,0)(\pi,\pi/2)(\pi,\pi)(\pi/2,\pi/2)\) of the reduced Brillouin zone at \( \beta = 100 \) (left panel) and 1000 (right panel).

FIG. 13. Multi-electronic and phononic contributions, and the total glue function for the underdoped case at \( \beta = 100 \) (left panel) and 1000 (right panel). Clear reduction in the critical multi-electronic occurs as a result of depletion of low-energy spectral weight, compared to the case for the strange metal. Reduction of SC \( T_c \) upon underdoping could be driven by this effect.
also provides, remarkably enough, a natural explanation for the anomalous scale-invariant magnetic fluctuations of the strange metal without having to invoke proximity to any $T = 0$ AF QCP. Further, since DMFT can yield a strange metal phase for a range of parameters in the EPAM, such anomalous spin correlations can exist over a range of tuning parameters in practice. This is an attractive option when one considers cases like the optimally (hole)-doped cuprates and $\beta$-YbAl$_4$, which show features consistent with a quasi-locally critical $\chi(q, \omega)$ without any obvious proximity to $T = 0$ AF order. On the other hand, evidence for Fermi surface reconstruction (FSR) in both the above cases\cite{2,44} supports our argument linking these anomalies with selective-Mottness, where such FSR must indeed occur. Though such FSR can also be rationalized within HMM and Kondo-RKKY views, they must be associated with the $T = 0$ AF QCP in those cases, as mentioned before. In our case, the FSR involves a topological aspect of Mott physics, namely, penetration of zeros of $G_{bb}(k, \omega)$ in EPAM to where poles would have been in the normal metal\cite{12}, and has nothing to do with the FSR involving AF order. However, in cases where the unquenched local moments in the OSMP can (as mostly happens) order, the FSR will coincide with the magnetic instability. Since it is ubiquitous for spins to order in (insufficiently geometrically frustrated) real cases like cuprates and $f$-electron systems, it is hard to disentangle the roles of OSM physics vis-a-vis AF order in the FSR that is widely known to occur near QCPs in those cases.

The anomalous spin- and charge-fluctuation continuum responses we find are an attractive and novel choice for an intrinsically multi-electronic glue that can induce an unconventional superconductive (USC) coherent state. Indeed, suggestions for unconventional $d$-wave SC due to diverging AF spin correlations with an effective dynamic pairing interaction of the form $V_{eff} \approx J^2 \chi(\omega) \approx 1/\omega^q$ exist\cite{38}. Once again, in contrast to views where such a bosonic glue is associated with quantum critical fluctuations linked to destruction of AF order, the multiparticle incoherent glue function proposed here bears an intimate connection to breakdown of LFL theory at an OSMP. It is intrinsically quantum critical in the sense of being a two-particle continuum that is inherently unstable to a $T = 0$ USC state. Finally, in contrast to a normal BCS instability, involvement of selective-Mott physics in emergence of local critical features (implying that both incoherent metallic and Mott localized fermions participate in pairing via $H_{rel}$) naturally means wild pair-phase fluctuations from number-phase uncertainty principle, suppression of the mean-field SC $T_c$ while preserving the pair amplitude, and thus strong preformed pair fluctuation regime above $T_c$: thus, this is, as expected, an intrinsically strong-coupling (non-BCS-Eliashberg type\cite{38}) instability of the strange metal. Actual computation of the instability is much more involved in this case, owing to the fact that the pairing kernel requires the full form of $\chi(q, \omega)$ over the entire energy range: this is out of scope of our analytic approach.

There are more ways to further elucidate the unconventional nature of the underlying quantum criticality in our case. In the selective-Mott state, below the selective-Mott gap, we find an emergent local $Z_2$ symmetry [$\exp(i\pi n_{i,b}), H] = 0$ for all $i$, arising from $[n_{i,b}, H] = 0$ for all $i$. This is an effective low-energy symmetry in the $b$-fermion sector in the OSMP. This feature is reminiscent of what happens in the celebrated Kitaev model\cite{45}, where a $Z_2$ symmetry is exact rather than emergent, and maybe it is now no surprise that extreme short-range spatial correlations and X-ray-edge related behavior in $\chi(q, \omega)$ rigorously characterize spin correlations there as well\cite{46,47}. However, in this case, infra-red power-law singular behavior results in stark contrast to the Kitaev case, where the Dirac fermion spectrum suppresses singular behavior. Nevertheless, there are deeper analogies and connections with confinement-deconfinement (C-DC) transition(s): in our case, lack of $a$-fermion quasiparticles requires Mott localization of $b$-fermions, while itinerant $b$-fermions imply a correlated FL metal. In the language of fermions coupled to a fluctuating $Z_2$ gauge field as defined above, the former corresponds to a quasistatic gauge field, while the latter corresponds to the gauge field fluctuations acquiring dynamics with a timescale set by $h/k_B T_{coh}$ (recollect that $T_{coh}$ is finite only when $V_{fc}(k)$ is relevant at one-particle level). The exotic confinement-deconfinement (quantum) criticality that should be linked to this is thus once again - unsurprisingly - related to relevance or otherwise of $V_{fc}(k)$: As long as $V_{fc}$ remains irrelevant (this can well be the case up to very low $T$ in practice, and often pre-empted by direct instabilities of the incoherent metal we find to ordered state(s)), this local $Z_2$ symmetry will control the physical response of the system. An interesting issue is to inquire about a possible link to fractionalization ideas. Since we have seen that non-FL vis-a-vis FL metallicity is caused by an irrelevant (non-FL) vis-a-vis relevant (FL) $V_{fc}(k)$, the confinement-deconfinement transition in the $b$-fermion sector is now tied down to the underlying selective-Mott transition in the $b$-fermion sector, since there is no question of having fractionalization in the heavy FL phase. More work is called for to see whether this is correct, or whether the exotic excitations represented by the emergent branch-cut form of $\chi_{\text{res}}^+(\omega)$ at the OSMT admit no particle description at all\cite{48} - this is also a known generic tendency at QCPs. However, along with Fermi surface reconstruction (involving penetration of zeros of the Green function to where poles would have been in the heavy-FL), the above arguments hint at an exotic topological criticality underlying our findings. These connections will be explored separately.
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* swagata@phy.iitkgp.ernet.in
† mslaad@imsc.res.in
‡ arghya@phy.iitkgp.ernet.in

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