# Non-Fermi liquid due to orbital fluctuations in iron pnictide superconductors

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We study the influence of quantum fluctuations on the electron self-energy in the normal state of iron pnictide superconductors using a five-orbital tight-binding model with generalized Hubbard on-site interactions. Within a one-loop treatment, we find that an overdamped collective mode develops at low frequency in channels associated with quasi-one-dimensional $d_{xz}$ and $d_{yz}$ bands. When the critical point for the $C_4$-symmetry-broken phase (structural phase transition) is approached, the overdamped collective modes soften, and acquire increased spectral weight, resulting in non-Fermi-liquid behavior at the Fermi surface characterized by a frequency dependence of the imaginary part of the electron self-energy of the form $\omega^{\lambda}$, $0 < \lambda < 1$. We argue that this non-Fermi-liquid behavior is responsible for the recently observed zero-bias enhancement in the tunneling signal in point-contact spectroscopy. A key experimental test of this proposal is the absence of non-Fermi-liquid behavior in the hole-doped materials. Our result suggests that quantum criticality plays an important role in understanding the normal-state properties of iron pnictide superconductors.

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## I. INTRODUCTION

Whether or not the iron pnictide superconductors are strongly correlated materials is hotly debated. Certainly a clean association of non-Fermi-liquid behavior, either experimentally or theoretically, with any part of the phase diagram would suffice to settle this debate. While parallels with the cuprates are suggestive,[1–5] they have not resulted in a decisive answer to this problem. In fact, to our knowledge, the possibility of non-Fermi-liquid behavior other than Mott physics[6] has not been discussed to date.

A feature common to the parent and underdoped compounds of the iron pnictide superconductors is the structural phase transition (SPT) from tetragonal to orthorhombic symmetry occurring around 150 K.[7] For most members of the 1111 and 122 families, in-plane anisotropy in the resistivity commences near the structural transition, and stripelike antiferromagnetism develops if the temperature is further lowered. The quasiparticle interference in scanning tunneling microscopy[8] also showed aniostropic electronic states at low temperature. Despite the controversy as to whether the SPT is induced by magnetic fluctuations as a result of the onset of stripelike antiferromagnetism[9–13] or if orbital ordering in quasi-one-dimensional (1D) $d_{xz}$ and $d_{yz}$ bands[14–17] is the efficient cause, the phase below the SPT breaks $C_4$ symmetry, and quantum fluctuations associated with this phase are nematic in character. A recent measurement of photoexcited quasiparticle relaxation[18] reveals the existence of strong nematic fluctuations up to 200 K, well above the SPT temperature. Moreover, in electron-doped $Ba(Fe_{1-x}Co_x)_2As_2$ (Ba122), an unexpected enhancement of the zero-bias signal[19,20] in the tunneling data measured in point-contact spectroscopy has been observed at an onset temperature higher than $T_{\mathrm{SPT}}$. The excess conductance appears at temperatures around 175 K, increasing in magnitude through the structural, antiferromagnetic, and, in materials exhibiting superconductivity, the superconducting transitions. It is not seen in overdoped Ba122. It is important to study how these strong orbital (nematic) fluctuations affect the physical properties in both the normal and orthorhombic states of the iron pnictide superconductors.

In this paper, we develop a microscopic theory for the orbital fluctuations and show that they give rise to non-Fermi-liquid behavior. In particular, we find a branch of overdamped collective modes in the scattering channels associated with quasi-1D $d_{xz}$ and $d_{yz}$ bands in the normal state at a temperature higher than $T_{\mathrm{SPT}}$. In the vicinity of the SPT critical point, these overdamped collective modes dominate the low-energy physics, resulting in a strong modification of the electron self-energy and a breakdown of Fermi-liquid theory even in the symmetric normal state.

## II. RANDOM-PHASE APPROXIMATION THEORY FOR ELECTRON SELF-ENERGY

Since the random-phase approximation (RPA) represents a perturbative treatment of the fluctuations, it represents a zeroth-order theory. If deviations from Fermi-liquid theory are found at this level of theory, then a Fermi-liquid description is most likely invalid. This line of reasoning has been used previously in the continuum limit to establish the existence of the nematic phase.[21] Thus far, a similar analysis appears to be lacking for a multiorbital model. We use this approach here to show that at the RPA level, the fluctuations are inherently non-Fermi liquid in nature. Our starting point is the Hamiltonian $H = H_t + H_I$, where $H_t = \sum_{\vec{k}} H_k$ is the five-band tight-binding model proposed in Ref. 22 which can reproduce correctly the Fermi surfaces of hole $\alpha_1$,$\alpha_2$ and electron $\beta_1$,$\beta_2$ pockets in the unfolded Brillouin zone. The interaction terms are given by $H_I$,

$$H_I = \sum_{ia} U n_{ia\uparrow} n_{ia\downarrow} + \sum_{i,b>a} \left(U' - \frac{J}{2}\right) n_{ia} n_{ib} - \sum_{i,b>a} 2J \vec{S}_{ia} \cdot \vec{S}_{ib} + J'(p^{\dagger}_{ia} p_{ib} + \mathrm{H.c.}), \quad (1)$$

where $U' = U - 2J$, $J$ is the Hund coupling, $J' = J$, and $a$ ($b$) refers to the orbital index, $1 = xz$, $2 = yz$, $3 = xy$, $4 = x^2 - y^2$, and $5 = 3z^2 - r^2$. $n_{ia} = \sum_{\sigma} c^{\dagger}_{ia\sigma} c_{ia\sigma}$ is the number operator on site $i$ in orbital $a$, and $p_{ia} = c_{ia\downarrow} c_{ia\uparrow}$. Energies

 

are measured in eV, in line with the units used in recent tight-binding models.[22] $J = 0.2U$ throughout this paper. This model has been shown to have stripelike antiferromagnetism together with orbital ordering in a previous study.[23,24] We introduce a unitary transformation $\hat{U}_{\vec{k}}$ such that $(\hat{U}_{\vec{k}})^{\dagger}\hat{H}_{\vec{k}}\hat{U}_{\vec{k}} = \mathrm{diag}[E_{\vec{k},1},\ldots,E_{\vec{k},5}]$, and it is straightforward to obtain the noninteracting response functions,

$$\chi^{(0)}_{ab;cd}(\vec{q},i\omega_n) = -\frac{1}{N}\sum_{\vec{k}}\sum_{l,m}(\hat{U}_{\vec{k}+\vec{q}})_{a,l}(\hat{U}_{\vec{k}+\vec{q}})^{*}_{c,l}(\hat{U}_{\vec{k}})_{d,m}(\hat{U}_{\vec{k}})^{*}_{b,m} \times \frac{n_F(E_{\vec{k}+\vec{q},l}) - n_F(E_{\vec{k},m})}{E_{\vec{k}+\vec{q},l} - E_{\vec{k},m} - i\omega_n}, \quad (2)$$

in the symmetric normal phase, where $\chi^{(0)}_{ab;cd}(\vec{q},i\omega_n)$ is a $25 \times 25$ matrix. The convention on the indices is that in Ref. 22. Adopting the interaction kernels for the spin-spin ($\hat{V}^s$) and density-density ($\hat{V}^c$) fluctuations derived in Ref. 25, we obtain the electron self-energy at the random-phase-approximation level,

$$\Sigma^{\mathrm{orbital}}_{ab}(\vec{k},ip_n) = \frac{1}{\beta N}\sum_{\vec{q}}\sum_{ik_m}\hat{\Gamma}_{ai;jd} \times (\vec{q},ip_n - ik_m)\hat{G}^0_{ij}(\vec{k}-\vec{q},ik_m), \quad (3)$$

where $ik_m$ and $ip_n$ are Matsubara frequencies for fermions, $\hat{G}^0(\vec{k},ip_n) = [ip_n - \hat{H}_t + \mu]^{-1}$ is the bare Green function, and $\hat{\Gamma}_{ab;cd}(\vec{q},ip_n - ik_m)$ is the effective interaction,

$$\hat{\Gamma}(\vec{q},ip_n - ik_m) = \tfrac{1}{2}\{3[1 - \hat{V}^s\hat{\chi}_0(\vec{q},ip_n - ik_m)]^{-1}\hat{V}^s - [1 + \hat{V}^c\hat{\chi}_0(\vec{q},ip_n - ik_m)]^{-1}\hat{V}^c\} \quad (4)$$

within one loop.

## III. CRITICAL BEHAVIOR ABOVE THE STRUCTURAL PHASE TRANSITION

Since our focus is on the critical region above the structural phase transition, throughout this paper the temperature is set to $k_BT = 0.02$ eV at which the system is in a normal state without any symmetry breaking. The case of ordered states will be discussed in the next section.

We start by studying the mean-field phase diagram of our model using the formalism outlined in Ref. 23, as shown in Fig. 1. Then we can fix the temperature and change $U$ to investigate how the self-energy changes as the critical region is approached. Consider first the spectral functions for the effective interactions $-\mathrm{Im}\hat{\Gamma}(\vec{q},\omega + i\eta)$ displayed in Fig. 2. As is evident, the spectral functions for the intraorbital effective interactions $-\mathrm{Im}\Gamma_{aa;aa}(\vec{q}_1,\omega)$ dominate the electron self-energy. Also of interest are the spectral functions for momenta $\vec{q}$ along the diagonal direction so that $\Gamma_{11;11}(\vec{q},\omega) = \Gamma_{22;22}(\vec{q},\omega)$. It can be seen in Fig. 2 that the spectral functions at low frequency are dominated by an overdamped collective mode in $\Gamma_{11;11}$ ($\Gamma_{22;22}$). When $U$ is tuned to approach the critical point ($U_c \approx 2.1$ eV at this temperature), this mode gains more spectral weight and moves to even lower energy as shown in Fig. 3. Note that although the shift of the spectral weight upon approaching the critical point is shown to follow the typical behavior for an overdamped continuum

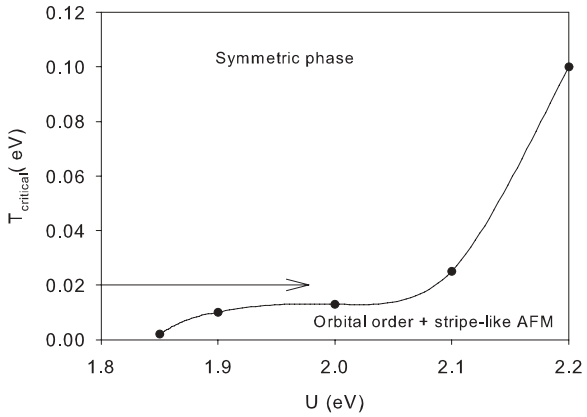


FIG. 1. Mean-field phase diagram of the model used in this paper. The arrow indicates the direction from which the critical region is approached in this paper. At $T = 0$, the orbital ordering transition is driven entirely by changing the strength of the interaction.

of collective excitations, our calculations do not have the accuracy to demonstrate the shift of the peak position toward zero frequency as expected. We attribute this to the fact that the model considered here generally has both orbital ordering and stripe-antiferromagnetic (AFM) phases occurring together. In this case, it is hard to distinguish whether the transition is first

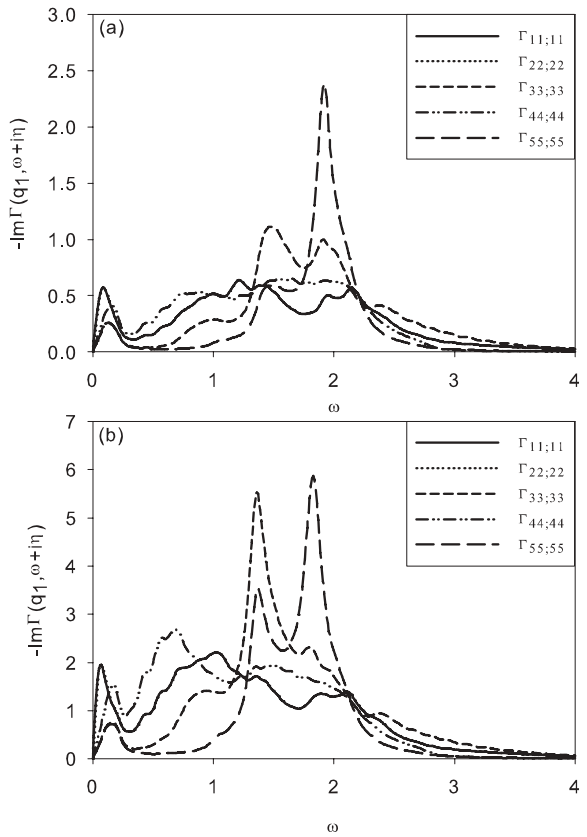


FIG. 2. Spectral functions for effective interactions in intraorbital channels $[\Gamma_{aa;aa}(\vec{q},\omega)]$ at $\vec{q}_1 = (0.04\pi, 0.04\pi)$ for (a) $U = 1.3$ and (b) $U = 2.0$. $\Gamma_{11;11}(\vec{q},\omega) = \Gamma_{22;22}(\vec{q},\omega)$ for $\vec{q}$ along the diagonal direction as expected, and an overdamped collective mode appearing at low energy in $\Gamma_{11;11}(\vec{q},\omega)$ $[\Gamma_{22;22}(\vec{q},\omega)]$ can be observed.

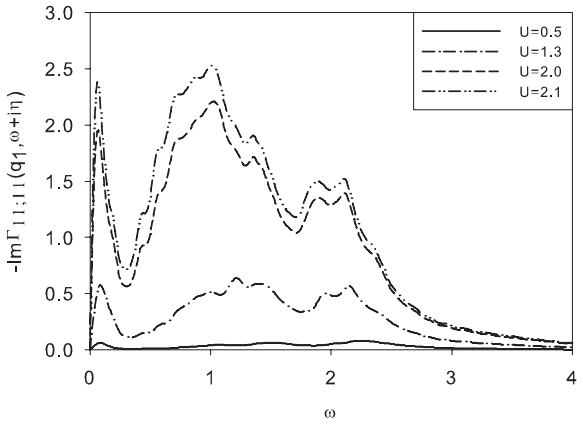


FIG. 3. Spectral functions of effective interactions $\Gamma_{11;11}(\vec{q}_1,\omega)$ at $\vec{q}_1 = (0.04\pi,0.04\pi)$ for different $U$. The overdamped collective mode at low energy acquires increased spectral weight as the critical point ($U_c \approx 2.1$ eV at the temperature we are considering, $k_BT = 0.02$ eV) is approached.

or second order as discussed in Ref. 26, which is beyond the accuracy of our calculation on a finite-size square lattice.

These overdamped modes, emergent at low frequency and small $\vec{q}$, resemble the collective modes observed in the *quadrupole density spectral function*,[21,27–29] that is, the spectral function related to the interactions in the $d$-wave channel in a quantum nematic Fermi fluid. As shown in Ref. 30, in a system containing quasi-1D $d_{xz}$ and $d_{yz}$ bands, hybridization enhances significantly the strength of the interaction in the $d$-wave channel. As a result, the nematic order in such multiorbital systems is completely equivalent to orbital ordering in quasi-1D bands, and the spectral functions due to quantum fluctuations associated with the quasi-1D bands naturally acquire the same properties of the quadrupole density spectral function discussed in the context of the quantum nematic fluid mentioned above. It has been shown[21,27,29] that these overdamped collective modes could lead to a non-Fermi liquid near the critical region and also in the nematic phase. The reason is that in the vicinity of the nematic critical point, these overdamped collective modes become soft. Electrons scatter strongly with these soft overdamped collective modes, which modify the electron self-energy away from the Fermi-liquid behavior in the vicinity of the nematic critical point.

It is intriguing to check whether the same physics discussed above occurs in the iron pnictide superconductors since the SPT signals a transition from their symmetric normal phase to a state which breaks $C_4$ symmetry. We performed a numerical evaluation of Eq. (3). To compute the self-energy of the retarded Green function of a single-particle state on the Fermi surface, we need to do one more transformation and also an analytical continuation of Eq. (3) to obtain

$$\Sigma^{\text{band}}_{\alpha\alpha}(\vec{k}_F,\omega+i\eta) = [\hat{U}_{\vec{k}_F}\hat{\Sigma}^{\text{orbital}}(\vec{k}_F,\omega+i\eta)\hat{U}^{\dagger}_{\vec{k}_F}]_{\alpha\alpha}, \quad (5)$$

which is the self-energy of the electron with momentum $\vec{k}_F$ on the Fermi surface sheet $\alpha$.

Because we study the normal state at finite temperature, $\Sigma^{\text{band}}_{\alpha\alpha}(\vec{k}_F,\omega+i\eta)$ contains contributions from both thermal and quantum fluctuations which cannot be separated in RPA-type calculations.[29] Nevertheless, it is generally expected that

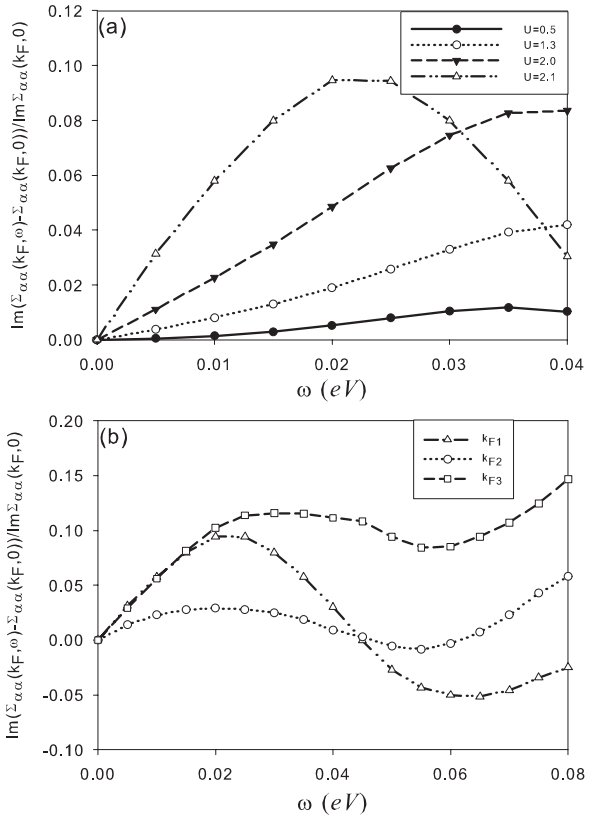


FIG. 4. (a) Normalized self-energy of electron with momentum $\vec{k}_F = (0.12\pi,0.12\pi)$ on the hole Fermi pocket $\alpha_1$ for different $U$. A crossover from Fermi liquid ($\lambda = 2$) to non-Fermi liquid ($\lambda \leqslant 1$) can be seen as $U$ increases from $U = 0.5$ to the critical point $U = 2.1$ eV. (b) Normalized self-energy of electron in the critical region ($U = 2.1$ eV) with momenta $\vec{k}_{F1} = (0.12\pi,0.12\pi)$, $\vec{k}_{F2} = (0.2\pi,0)$ on hole Fermi pocket $\alpha_1$, and $\vec{k}_{F3} = (0.88\pi,0.16\pi)$ on electron Fermi pocket $\beta_1$.

the contribution from quantum critical fluctuations should be expanded in powers of $\omega/T$ and the thermal fluctuations should be most dominant at $\omega = 0$. In order to see the frequency dependence due to the quantum critical fluctuations more clearly, we plot in Fig. 4 the normalized imaginary part of the self-energy defined as

$$\text{Im}\Sigma^{\text{nor}}_{\alpha\alpha}(\vec{k}_F,\omega) \equiv \frac{[\text{Im}\Sigma^{\text{band}}_{\alpha\alpha}(\vec{k}_F,\omega) - \text{Im}\Sigma^{\text{band}}_{\alpha\alpha}(\vec{k}_F,0)]}{\text{Im}\Sigma^{\text{band}}_{\alpha\alpha}(\vec{k}_F,0)}. \quad (6)$$

Generally, it is expected that at finite temperature the self-energy is analytical for $\hbar\omega \ll k_BT$, which gives the $\omega^2$ term. We find the crossover from a Fermi liquid with $\omega^2$ at small frequency to a non-Fermi liquid in which the $\omega^\lambda$ term with $\lambda \leqslant 1$ dominates over the $\omega^2$ term as $U$ is increased to approach the critical point. Similar results have been seen in Ref. 29. In the critical region, non-Fermi-liquid behavior exists on a large part of the Fermi surface with strong angular dependence of $\text{Im}\Sigma$, as expected, due to the critical fluctuations near orbital ordering (now termed nematicity).[27] As the temperature is lowered, the critical point $U_c$ shifts to a lower value but the non-Fermi-liquid behavior remains robust near the critical point. This strongly suggests that this non-Fermi-liquid behavior should

be observable in iron pnictide superconductors at a temperature above the SPT.

One subtle point is that the effective interaction $\Gamma$ in Eq. (4) contains contributions from both the charge and spin channels. While for large momentum [e.g., $(\pi,0)$ or $(0,\pi)$] there is no doubt that the contribution from spin channels is dominant, as seen from previous calculations[22,25] and also in our calculations, for small momentum, which we focus on here, the contributions from both charge and spin channels become comparable. As a result, we cannot completely rule out the effects from the spin channels. However, since it has been shown[26] that the spin nematicity could also induce orbital ordering, the critical collective modes associated with the orbital ordering discussed above will be still present in that case, despite the fact that the spectral weight might be reduced due to the coupling to the collective modes associated with spin nematic order. As a result, the non-Fermi-liquid behavior discussed above will be most prominent if the contribution from charge channels in Eq. (4) is dominant. We find, in general, that the charge channels become much stronger for $U \approx U'$, which is consistent with previous studies of orbital ordering in $Sr_3Ru_2O_7$.[31,32] Moreover, it has been shown that the inclusion of electron-phonon coupling can also enhance the instability in the charge channels.[33] Since it is well known that physical properties of iron-based superconductors could vary significantly for different families due to differences in details, we expect that the non-Fermi-liquid behavior discussed above might not be visible in some families of the iron-based superconductors. This is actually what is seen in point-contact spectroscopy and other experiments which will be discussed in Sec. V.

## IV. NON-FERMI-LIQUID BEHAVIOR BELOW THE STRUCTURAL PHASE TRANSITION

In this section, we discuss the fate of the non-Fermi-liquid behavior in the $C_4$-symmetry-broken phase. For the nematic phase in a continuous model, these overdamped collective modes induced by the $d$-wave interaction evolve into Goldstone modes but remain overdamped and dominate the low-energy physics. Consequently, the non-Fermi liquid persists in the nematic phase. In the multiorbital model studied here, the situation is complicated by the fact that since the continuous rotational symmetry is absent in a lattice model, there are no gapless Goldstone modes in general. Nevertheless, these overdamped collective modes remain, existing with a gap $\Delta$ due to the breaking of the discrete symmetry from $C_4$ to $C_2$. Consequently, the non-Fermi-liquid behavior will be present as long as the temperature energy scale $k_BT$ is larger than $\Delta$. Note that $\Delta$ is a gap in the density-density correlation function, not in the single-particle spectrum, since the orbital order (like the nematic order) does not gap out the Fermi surfaces. As a result, it is expected that the non-Fermi liquid will persist for a while as the temperature is lowered below $T_{\mathrm{SPT}}$ and then gradually disappear at very low temperature where the orbital order is strong. This is analogous to the case of the ferromagnetic quantum critical point with a magnetic field where the critical fluctuations are gapped by the Zeeman energy.[34]

## V. EXPERIMENTAL CONSEQUENCES

A direct consequence of non-Fermi-liquid behavior is the temperature dependence of the resistivity. It has been pointed out[35] from studies on various iron pnictide superconductors that a strong deviation from the Fermi-liquid $T^2$ behavior of the resistivity above the SPT temperature will occur if a large anisotropy in the in-plane resistivity exists below the SPT temperature. Since the anisotropy in resistivity is intimately related to orbital ordering, this observation provides direct evidence for our claim that non-Fermi-liquid behavior is due to orbital fluctuations. An independent calculation including electron-phonon coupling to enhance the effect of orbital fluctuations by Onari and Kontani[33] also showed unusual temperature dependence of the resistivity above the structural transition temperature.

What about the zero-bias anomaly seen in point-contact tunneling experiments[19,20] on electron-doped $Ba(Fe_{1-x}Co_x)_2As_2$? Intriguingly, this zero-bias enhancement starts to appear at temperatures roughly 30 K higher than $T_{\mathrm{SPT}}$ and remains robust well below $T_{\mathrm{SPT}}$. This observation is also consistent with our theory. It has been shown by Lawler *et al.*[21] that the single-particle density of states has the form of

$$N^*(\omega) = N^*(0) + B\omega^{2/3}\ln\omega + \cdots \tag{7}$$

in the nematic critical region and also in the nematic phase. In fact, $N^*(\omega)$ obtains extra contributions due to the non-Fermi-liquid self-energy, giving rise to a cusp at zero frequency and a subsequent decrease as the frequency increases. This provides a direct explanation for the zero-bias enhancement observed in point-contact spectroscopy since the conductance $dI/dV$ roughly measures the single-particle density of states for small frequency. Moreover, since the form of the single-particle density of states is the same up to some mild modifications in the vicinity of the critical point and also in the $C_4$-symmetry-broken phase, the zero-bias enhancement should have a smooth crossover as $T_{\mathrm{SPT}}$ is crossed, which in fact has been noticed in quantum point-contact measurements.[36] We predict that for hole-underdoped $Ba_{1-x}K_xFe_2As_2$, which does not have an in-plane resistivity anisotropy,[35] the zero-bias enhancement should be either nonexistent or much weaker than that in electron-doped $Ba(Fe_{1-x}Co_x)_2As_2$.

## VI. CONCLUSION

In this paper we have presented a theory of non-Fermi-liquid behavior in a five-band model with generalized Hubbard on-site interactions for iron pnictide superconductors. At the level of the random-phase approximation, we found a branch of overdamped collective modes emergent at low frequency in channels associated with quasi-1D $d_{xz}$ and $d_{yz}$ bands, and we have shown that these modes become dominant at low energies near the critical point for the $C_4$-symmetry-broken phase, leading to non-Fermi-liquid behavior. Our theory indicates that quantum criticality through the evolution of a non-Fermi-liquid phase plays an important role in understanding the normal-state properties of iron pnictide superconductors.

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[36] As mentioned in Sec. IV, the non-Fermi-liquid behavior will eventually disappear when the temperature is low enough, and the point-contact spectroscopy described in Refs. 19 and 20 indeed revealed more complicated structures for very low temperature. These complicated structures might result from an interplay between the orbital order and also stripelike AFM order, which cannot be captured by the present theory.