Effect of spin-density wave fluctuations on the specific heat jump in iron pnictides at the superconducting transition

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Measurements of the specific heat jump at the onset of superconducting transition in the iron-pnictide compounds revealed strong variation of its magnitude as a function of doping that is peaked near the optimal doping. We show that this behavior is a direct manifestation of the coexistence between spin-density wave and superconducting orders and the peak originates from thermal fluctuations of the spin-density waves near the end point of the coexistence phase—a tetracritical point. Thermal fluctuations result in a power-law dependence of the specific heat jump that is stronger than the contribution of mass renormalization due to quantum fluctuations of spin-density waves in the vicinity of the putative critical point beneath the superconducting dome.

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I. INTRODUCTION

The concept of quantum criticality is at the forefront of the physics of strongly correlated materials [1]. The discovered superconductivity in the iron-pnictide compounds [2–5] that emerges in the close proximity to magnetic instability [6–9] provides new opportunities to study quantum critical phenomena in the system with multiple order parameters. The observed microscopic coexistence between spin-density wave (SDW) and superconducting (SC) orders in iron-pnictide superconductors (FeSC) [8–18] implies that the SDW transition line extends into the superconducting state. If this line reaches zero temperature the system develops a quantum critical point (QCP) beneath the superconducting dome. Such a scenario is further complicated by the fact that besides the SDW transition, there is also a nematic transition, below which the tetragonal symmetry of the system is spontaneously broken down to an orthorhombic [19–21]. The transition line of the nematic order also enters the superconducting dome, which may lead to yet another QCP. A magnetic QCP without superconductivity and in the case of nodal fermions in d-wave superconductors has been a subject of intensive study and is known to give rise to non-Fermi liquid behavior, and to singularities in various thermodynamic and transport characteristics [22–25]. The multi-band unconventional superconductivity in FeSC brings new intriguing questions concerning the role of QCP in thermodynamic and transport properties of correlated materials [26–33].

Recently we have received compelling experimental evidence that superconductivity in FeSCs indeed hosts quantum criticality. Low-temperature measurements of the doping dependence of the London penetration depth $\lambda(x)$ in clean samples of isovalent $\text{BaFe}_2(\text{As}_1-x\text{P}_x)_2$ revealed a sharp peak in $\lambda(x)$ near the optimal doping $x_\text{o} \approx 0.3$ [27]. Magnetooscillations data show an increase in the effective mass $m^*(x)$ on one of the electron Fermi surfaces as $x$ approaches $x_c$ [34]. Nuclear magnetic resonance (NMR) experiments show that the magnetic ordering temperature approaches zero at $x_c$ [35]. Specific heat jump $\Delta C$ displays a nonmonotonic dependence on $x$ when measured across $x_c$ at the superconducting critical temperature $T_c$ [29]. Finally, the system obeys a linear temperature dependence of the resistivity close to $x_c$ [36]. The observation of the same set of features in the other families of FeSCs has been elusive so far since quantum critical effects are easily masked by inhomogeneity and impurity scattering. $\text{BaFe}_2(\text{As}_1-x\text{P}_x)_2$ is particularly useful in this regard since the substitution of As by the isovalent P does not change the electron/hole balance and does not induce appreciable scattering, unlike in the electron-doped $\text{Ba(Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ compound [28].

Measurements of the magnitude and the doping dependence of the specific heat jump were instrumental for determining and understanding the phase diagram of iron-pnictide superconductors. Experiments [37–39] revealed that $\Delta C/T_c$ vary greatly between underdoped $\text{Ba(Fe}_{1-x}\text{Ni}_x)_2\text{As}_2$ and optimally hole-doped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$, but even for the given material, e.g., $\text{Ba(Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ or $\text{BaFe}_2(\text{As}_1-x\text{P}_x)_2$, the value of $\Delta C/T_c$ has its maximum near the optimal doping and then decreases, approximately as $\Delta C/T_c \propto T^2_c$ at smaller and larger dopings. It is useful to recall that in BCS theory the specific heat jump $\Delta C/T_c \approx 4\pi^2 N_f/7\xi^3(3)$ is universally determined by the total quasiparticle density of states $N_f$ at the Fermi surface. The origin of the strong doping dependence of $\Delta C(x)$ was rooted [40] to the coexistence of SDW magnetism and $s^\pm$ superconductivity and the mean-field theory is in general consistent with experimental observations. However, the sharply peaked and highly nonmonotonic variation of $\Delta C/T_c$ near $x_c$ as seen in the experiment [29] is beyond the mean-field treatment and is clearly related to fluctuation effects.

Combined accurate data analysis [27,29,34] on the magnetooscillations, specific heat jump, and magnetic penetration depth near the optimal doping lead to the conjecture that the quasiparticle mass renormalization expected close to a QCP is the main factor that is causing the observed sharp features. Although this is certainly the case for the explanation of the low-temperature $\lambda(x)$ measurements, we take the point of view that the interpretation of the $\Delta C(x)$ data obtained near the critical temperature requires an account of thermal fluctuations.

In this work, we find that thermal SDW fluctuations lead to a dominant contribution to the specific heat jump at the onset of the superconducting transition that scales as a power law $\Delta C/T_c \propto |x-x_c|^{-\alpha}$. The value of the exponent $\alpha = 1 \div 3/2$ depends on whether the SDW transition is commensurate
or incommensurate. We recall that in the 122 family of iron pnictides, and possibly in other FeSCs, optimal doping \( x_c \) nearly coincides with the end point of the coexistence region—a tetracritical point \( P \). Once the system is tuned to the proximity of the tetracritical point both the SDW and SC order parameters develop strong fluctuations. In the quantum case of \( T = 0 \), when the whole FS, except possibly for isolated hot points, is gapped by the nonzero SC order parameter \( \Delta \neq 0 \), fluctuation effects are reduced [28]. On the contrary, near \( T = T_c \), the SC order parameter vanishes \( \Delta = 0 \), and SDW fluctuations are not suppressed, giving rise to large thermal corrections.

The rest of the paper is organized as follows. In Sec. II we introduce the minimal two-band model of FeSCs and discuss the emergent phase diagram at the mean-field level. In Sec. III we incorporate fluctuation effects and compute the renormalized free energy of the system. In Sec. IV we use this free energy to address the scaling of the specific heat jump near the tetracritical point and compare our calculations to the recent experimental findings. In Sec. V we summarize our main results and draw final conclusions.

II. MODEL OF FeSC AND PHASE DIAGRAM

We consider the minimal two-band low-energy model consisting of one circular hole pocket near the center of the Brillouin zone (BZ) and an electron pocket near its corner [41,42]. Away from the perfect nesting electron-like band can be parametrized as follows \( \xi_n = -\xi_0 + 2\delta\phi_q \), where hole band dispersion is assumed quadratic \( \xi_n = \mu_n - p^2/2m_n \), with \( \delta\phi_q = \delta_0 + \delta_2 \cos(2\phi) + (v_F q/2) \cos(\phi - \phi_0) \). The parameter \( \delta\phi_q \) captures the relative shift in the Fermi energies, and the difference in the effective masses of the electron and hole bands, via \( \delta_0 \), and an overall ellipticity of the electron band, via \( \delta_2 \) [41]. In addition, \( \delta\phi_q \) also captures the incommensurability of the SDW order with vector \( q \), where \( \phi \) and \( \phi_0 \) are the directions of Fermi velocity \( v_F \) and \( q \), respectively. For isovalent doping (As \( \rightarrow \) P) both \( \delta_0 \) and \( \delta_2 \) change, as the shape of the bands changes with doping \( x \). Earlier calculations showed [42] that there was a broad parameter range \( \delta_2/\delta_0 \) for which SDW order emerges gradually, and its appearance did not destroy the SC order; i.e., the SDW and SC orders coexist over some range of dopings. For simplicity, in our analysis we assume that only \( \delta_2 \) changes, while the ellipticity parameter \( \delta_0 \) is fixed, although the picture is expected to stay similar for different choices of dependence of \( (\delta_0,\delta_2) \) on doping. The incommensurability vector \( q \) is an adjustable parameter that minimizes the system free energy in the SDW phase or describes inhomogeneous SDW fluctuations in nonmagnetic phases.

The basic Hamiltonian for the electron-electron interaction includes the free fermion part, and four-fermion interaction terms. The interaction terms in the band basis are Hubbard, Hund, and pair-hopping interactions, dressed by coherence factors from the diagonalization of the quadratic form. There are five different interaction terms in the band basis [44]: two density-density intrapocket interactions (these interactions are often treated as equal), density-density interpocket interaction, exchange interpocket interaction, and interpocket pair hopping. These five interactions can be rearranged into interactions in the particle-particle channel, and spin- and charge-density wave particle-hole channels. For repulsive interactions, the SDW and SC channels are the two most relevant ones. We decompose these four-fermion interactions by using the SDW and SC order parameters \( M_q \) and \( \Delta \), and express the corresponding couplings in terms of the bare transition temperatures \( T_{c0} \) to the SC state in the absence of SDW and \( T_{d0} \) to the perfectly nested FS in the absence of SC. Thus we arrive at the following free energy density:

\[
\mathcal{F}(\Delta, M_q) = \frac{\Delta^2}{2} \ln \left( \frac{T}{T_{c0}} \right) + \frac{|M_q|^2}{2} \ln \left( \frac{T}{T_{d0}} \right) - 2\pi T \sum_{n>0} \left[ \text{Re} \left( \sqrt{\epsilon_n^2 + |M_q|^2} \right) - \epsilon_n - \frac{\Delta^2 + |M_q|^2}{2\epsilon_n} \right],
\]

where \( \langle \cdots \rangle_\phi \) denotes the averaging over \( \phi \) along Fermi surfaces, \( \epsilon_n = E_n + i\delta\phi_q \), \( E_n = \sqrt{\epsilon_n^2 + \Delta^2} \), and \( \epsilon_n = \pi T (2n + 1) \) are the fermionic Matsubara frequencies (\( n = 0, \pm 1, \pm 2, \ldots \)). In Eq. (1) we allowed \( M_q \) to be a vector that has freedom in orientation as well as in the choice of the nesting vector \( q \).

The transition temperatures from a normal phase to SDW or SC phases as well as from SDW to the coexistence phase as functions of \( \delta_0 \) are depicted in the upper panels of Fig. 1 and have been studied in the entire range of parameters [42,43]. One spurious property of the mean-field analysis when applied to the calculation of the specific heat jump is the apparent discontinuity of \( \Delta C \) occurring when the system enters the coexistence region, see the lower panels of Fig. 1. The key point to emphasize here is that this singularity gets rounded up and transforms into a sharp peak once we include fluctuations of the SDW order in the paramagnetic phase. Indeed, thermodynamic fluctuations are nonzero on both sides of the tetracritical point, and the averages \( \langle |M_q|^2 \rangle \) effectively renormalize the superconducting part of the free energy. A similar mechanism of enhancement of \( \Delta C \) has been explored in the context of the heavy fermion superconductors CeCoIn5 and UBe13, which occurs due to the coupling of the SC order parameter to the fluctuating magnetization of the uncompensated part of the localized f moments [45]. However, such a scenario is not directly applicable to FeSCs since their magnetism is itinerant and spatial fluctuations of SDW order have a long correlation length. Another important remark is that in our free energy, Eq. (1), we neglected the gradient terms of SC order \( \delta \phi_q \) since they give rise only to subleading corrections to \( \Delta C \). In other words, the region of fluctuations is narrower for SC order than for SDW order.

III. RENORMALIZED FREE ENERGY FROM SDW FLUCTUATIONS

To find an effective free energy functional \( \mathcal{F}(\Delta) \) near the tetracritical point, we need to integrate out magnetic fluctuations \( M_q \) in Eq. (1). The overdoped case \( x > x_c \) differs by the absence of the finite \( \langle M_q^2 \rangle \) from the underdoped case \( x < x_c \). However, as \( \langle M_q^2 \rangle \) vanishes at the tetracritical point,
we expect approximately the same results in both cases. According to the general picture of fluctuations near the second-order phase transition, we expect the same power-exponent scaling of \( \Delta C/T \) versus \( x - x_c \) for the underdoped and the overdoped regions of the phase diagram, but with the different prefactors.

Expanding Eq. (1) to the leading order in \( |M_q|^2 \) and performing integration at the Gaussian level we find

\[
\mathcal{F}(\Delta) = -T \ln \left[ \int \mathcal{D}[M_q] \exp(-\mathcal{F}(\Delta, M_q)/T) \right] = \mathcal{F}_{SC}(\Delta) + \delta \mathcal{F}_{SDW}(\Delta).
\]

The first term in the right-hand side of Eq. (2) is simply the superconducting part of the free energy that follows directly from Eq. (1) by setting \( M_q \) and \( \delta \) to zero, which thus reads

\[
\frac{\mathcal{F}_{SC}(\Delta)}{N_F} = A \Delta^2 + \frac{B}{2} \Delta^4
\]

With the coefficients \( A = (1/2) \ln(T/T_c) \) and \( B = (\pi T/2) \sum_{\epsilon_n>0} \frac{\epsilon_n^3}{T} \), from the general thermodynamic relation \( C = -T \partial^2 F/\partial T^2 \) we find from Eq. (4)
that the jump of the specific heat at the SC transition is 
\[ \Delta C = N_F T_c [\delta_\phi A]^2 / B ]_{T=T_c}, \]
which reproduces the BCS value \[ \Delta C / T_c = 1.43 (\pi^2 / 3) N_F. \]

The second term in Eq. (2) is the correction to the free energy due to SDW fluctuations
\[ \frac{\delta F_{SDW}(\Delta)}{N_F} = \frac{3T}{2N_F} \sum_q \ln \left( \frac{K_q(T, \Delta)}{K_q(T,0)} \right), \]
where
\[ K_q(T, \Delta) = \ln \left( \frac{T}{T_{q0}} \right) - 2\pi T \sum_{\epsilon_n > 0} \left[ \frac{1}{\epsilon_n} - \frac{1}{\epsilon_n + \epsilon_n} \right]. \]

An expansion of the correction term Eq. (5) in powers of \( \Delta \)
\[ \frac{\delta F_{SDW}(\Delta)}{N_F} = \delta A \Delta^2 + \frac{\delta B}{2} \Delta^4, \]
leads to the renormalization of the coefficients \( A \) and \( B \) in Eq. (4) that acquire corrections
\[ \delta A = \frac{3T}{2N_F} \sum_q D_1 \Gamma, \quad \delta B = \frac{3T}{2N_F} \sum_q \left( \frac{D_2}{\Gamma} - \frac{T^2}{\Gamma^2} \right). \]

The expressions that enter into Eq. (8) are given by
\[ \Gamma \equiv K_q(T,0) = \ln \left( \frac{T}{T_{q0}} \right) - \psi \left( \frac{1}{2} \right) + \text{Re} \left( \psi \left( \frac{1}{2} + \frac{i\delta_\phi}{2\pi T} \right) \right), \]
\[ D_1 = \text{Re} \left( \frac{\psi \left( \frac{1}{2} \right) - \psi \left( \frac{1}{2} + \frac{i\delta_\phi}{2\pi T} \right)}{2\delta^2 \phi} \right) - \text{Im} \left( \frac{\psi \left( \frac{1}{2} + \frac{i\delta_\phi}{2\pi T} \right)}{4\pi T \delta^2 \phi} \right), \]
\[ D_2 = \frac{3}{4} \text{Re} \left( \frac{\psi \left( \frac{1}{2} + \frac{i\delta_\phi}{2\pi T} \right) - \psi \left( \frac{1}{2} \right)}{\delta^2 \phi} \right) - 3\text{Im} \left( \frac{\psi \left( \frac{1}{2} + \frac{i\delta_\phi}{2\pi T} \right)}{8\pi T \delta^3 \phi} \right), \]
where \( \psi \) and \( \psi [n] \) are the digamma and polygamma functions, respectively. The terms representing fluctuation corrections in the free energy lead to the smearing of the discontinuity in the specific jump near the transition \[ \delta(\Delta C) / \Delta C = \delta T_c / T_c + 2\gamma \delta A / \partial T_c A - \delta B / B \] \( \delta T_c = -2\gamma \delta A(T_c) \). Computing the temperature derivative of the \( A \) and collecting all the terms together we obtain the following expression for the relative correction of the specific heat jump
\[ \frac{\delta(\Delta C)}{\Delta C} = \frac{3T_c}{2N_F} \sum_q \left[ \frac{1}{\Gamma^2} \left( \frac{16\pi^2 T_c^2}{7\zeta(3)} D_1^2 - 4T_c D_1 \delta_T \Gamma \right) + \frac{1}{\Gamma} \left( 2D_1 + 4T_c \delta_T D_1 - \frac{16\pi^2 T_c^2}{7\zeta(3)} D_2 \right) \right], \]
which constitutes the main result of this work. To study the most singular contribution to the specific heat jump correction in the vicinity of the tetracritical point, we note that a second-order transition to the SDW phase is defined as the value of the detuning parameters for which the global minimum of \( \Gamma \) defined in Eq. (9) becomes equal to zero. Since \( \Gamma \) is in the denominator in Eq. (12), the most singular contribution comes from terms proportional to \( 1 / \Gamma^2 \).

IV. SCALING OF \( \Delta C \) NEAR THE TETRACRITICAL POINT

Since the \( q \) dependence of any coefficient comes from \( \delta_\phi \), some general symmetries of the function \( \Gamma(q_x, q_y, \delta_0, \delta_2) \) follow straightforwardly. First, \( \Gamma \) is symmetric in each \( q \) component separately, i.e., \( \Gamma(q_x, q_y) = \Gamma(-q_x, q_y) = \Gamma(q_x, -q_y) \). Second, a change in the sign of \( \delta_2 \) is equivalent to the exchange \( q_x \leftrightarrow q_y \). We checked numerically that if there are any local minima of \( \Gamma \) at \( (q_x, \pm q_y) \) for a nonzero \( q_y \), these minima merge as \( q_y \) increases until a value \( q_y = q_0 \), which in this case is the point of a global minimum. To model such a behavior, it is convenient to expand \( \Gamma \) in Eq. (9) up to the fourth order in powers of \( q_{x,y} \), in the following form:
\[ \Gamma(q_x, q_y) \approx A_M + \left( |q_x^2 - q_0^2|^m |q_y^2|^n \right) \left( \frac{u}{v} \right) \left( \frac{v^2}{u^2} \right), \]
assuming that \( u + w > 0 \) and \( u w - v^2 > 0 \), so that both of the eigenvalues of the matrix are positive, and \( \Gamma \) is bounded from below by \( A_M \). The power exponents \( m \) and \( n \) are to be chosen so that there is a quadratic dispersion around the global minimum, unless there is a crossing from commensurate \( (q_y = 0) \) to incommensurate \( (q_y \neq 0) \) SDW order, in which case the quartic terms are to be retained. In Eq. (13) \( A_M = a_M |T - T_c(x)| \) near the SDW-normal phase transition. The coefficient \( a_M > 0 \) is positive for temperatures higher than the transition temperature and \( \Gamma > 0 \). The tetracritical point is determined for doping \( x \), where the condition \( T_c(x_c) = T_c \) is satisfied. This leads to \( A_M \approx -a_M T_c(x_c)(x - x_c) \). The derivative \( T_c(x_c) < 0 \) is negative because doping leads to a decrease in the SDW transition temperature. Thus, the exponent in the scaling of the specific heat jump with \( A_M \) is the same as the exponent with \( x - x_c \). We estimate the momentum integral in Eq. (12) by estimating the area \( S \) in the \( q \) plane where
\[ \left( |q_x^2 - q_0^2|^m \right) \left( |q_y^2|^n \right) \cdot \hat{M} \left( \left( \frac{q_x^2 - q_0^2}{|q_y^2|^n} \right) \right) \leq A_M, \]
with
\[ \hat{M} = \left( \begin{array}{cc} u & v \\ v & w \end{array} \right). \]

We diagonalize the matrix \( \hat{M} \) by an orthogonal matrix
\[ \hat{O} = \left( \begin{array}{cc} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{array} \right), \]
so that \( \hat{M} \cdot \hat{O} = \hat{O} \cdot \hat{A} \), and \( \hat{A} = \text{diag}(\lambda_1, \lambda_2) \) is a diagonal matrix with positive eigenvalues. The angle \( \theta \) is found from the condition
\[ \tan 2\theta = \frac{2v}{u - w}. \]
and the eigenvalues are

$$\lambda_{1,2} = \frac{u + w}{2} \pm \sqrt{\left(\frac{u - w}{2}\right)^2 + v^2}.$$  \hfill (18)

If we introduce the substitution

$$|q_x^2 - q_0^2|^m = \rho A_M^{1/2} \left[\frac{\cos \theta \cos t}{\sqrt{\lambda_1}} - \frac{\sin \theta \sin t}{\sqrt{\lambda_2}}\right],$$  \hfill (19a)

$$|q_y^2|^m = \rho A_M^{1/2} \left[\frac{\sin \theta \cos t}{\sqrt{\lambda_1}} + \frac{\cos \theta \sin t}{\sqrt{\lambda_2}}\right],$$  \hfill (19b)

then the region where \( \Gamma \approx A_M \) is delimited by \( \rho \lesssim 1 \). It is further convenient to introduce

$$\cos \theta = K_x \cos \alpha, \quad \sin \theta = K_x \sin \alpha,$$  \hfill (20a)

$$\cos \theta = K_y \cos \beta, \quad \sin \theta = K_y \sin \beta.$$  \hfill (20b)

Using the definitions of \( \theta \), and \( \lambda_{1,2} \) from above, we obtain

$$K_{x,y}^2 = \frac{1}{u w - v^2} \left(\frac{w}{u}\right), \quad \sin (\alpha - \beta) = \frac{v}{\sqrt{u w}}.$$  \hfill (21)

Performing the final substitutions \( t \to t - \alpha \), and \( \beta \to -\beta + \alpha \), Eq. (19), for the first quadrant of the \( q \) plane goes over to

$$q_x^{(1/2)} = \left[q_0^2 \pm (K_x \rho A_M^{1/2} \cos t)^{1/2}\right],$$  \hfill (22a)

$$q_y = (K_y \rho A_M^{1/2} \sin(t - \beta))^{1/2},$$  \hfill (22b)

where \( \sin \beta \) should now stand for what was \( \sin (\alpha - \beta) \), i.e.,

$$\sin \beta = \frac{v}{\sqrt{u w}}, \quad -\pi/2 < \beta < \pi/2.$$  \hfill (23)

The parameter \( t \) is limited by \( \beta \leq t \leq \frac{\pi}{2} \), unless \( |q_x^2|^m < K_x A_M^{1/2} \cos \beta \). But since we are concerned in the regime where \( A_M \to 0^+ \), this is only viable when \( q_0 = 0 \), in which case the branch \( q_x^{(2)} \) does not exit. The area \( S \) of this region may be approximated by the area of a polygon for some specific values of the parameter \( t \).

**Case 1.** When \( |q_x^2|^m \gg K_x A_M^{1/2} \) the area is approximated by the area of the triangle with vertices at points obtained for points on the two branches \( q_x^{(1/2)}, q_y = 0 \), for \( t = \beta \), and the point \( q_x^{(1/2)} = q_0 \), and \( q_y \), for \( t = \pi/2 \).

$$S \approx 2 K_x^2 K_y^2 (A_M \cos \beta)^{\frac{1}{1/2}}.$$  \hfill (24)

**Case 2.** If \( q_0 \to 0^+ \), then the area is approximately that of a right-angled triangle with the sides equal to the \( q_x \) and \( q_y \) intercepts, obtained for \( t = \beta \), and \( t = \pi/2 \), respectively.

$$S_q \approx 2 K_x^2 K_y^2 (A_M \cos \beta)^{\frac{1}{1/2}}.$$  \hfill (25)

The behavior of the integral is then

$$\int \int \frac{d^2 q}{\Gamma^2(q)} \approx \frac{S}{A_M^3}.$$  \hfill (26)

There is one limiting situation that arises for the choice of parameter \( \delta_2 = 0 \). In that case \( \Gamma \) is independent on the azimuthal angle \( \phi_0 \) of the wave vector \( q \). It only depends on the magnitude. Expanding Eq. (9) up to the leading order around the value \( q = q_0 \) for which the global minimum is obtained we get

$$\Gamma(q) \approx A_M + u|q^2 - q_0^2|^p,$$  \hfill (27)

where the power exponent \( p \) is equal to either 1 or 2, see Table I for the summary. The integral is then easily evaluated in the polar coordinates \( \int \int \frac{d^2 q}{\Gamma^2(q)} = \int_0^\infty \frac{4 \pi q d q}{\Gamma^2(q)} \). Considering two limiting cases as above, namely \( u|q_0|^p \gg A_M \), and \( q_0 \to 0^+ \), one may show that the asymptotic behavior is as follows:

$$\int \int \frac{d^2 q}{\Gamma^2(q)} \approx \frac{c}{u^{1/p} A_M^{1/p - 2}},$$  \hfill (28)

and the difference between the two cases is only in the numerical prefactor \( c = 2\pi \) and \( c = \frac{4\pi}{\sin(\pi/p)} \), respectively.

A summary of the scaling exponents is given in Table I.

Having the above analytical arguments, we evaluate the correction to the specific heat jump numerically and present our results in Fig. 2 on a log-log plot for the same choice of parameters as in Fig. 1. A useful dimensionless parameter that characterizes the deviation from the tetracritical point, and one that is customarily chosen is

$$\tau = \frac{T_e - T_e^*(\delta_0)}{T_e}.$$  \hfill (29)

Here \( T_e^*(\delta_0) = T_e(\delta_0) + T_e^*(\delta_0 - \delta_0) \) is the linearized SDW transition temperature dependent on the isotropic detuning parameter \( \delta_0 \) near the tetracritical point, defined as \( T_e(\delta_0) = T_e \). We use the linearized temperature dependence to cancel any additional power-law scaling coming from the nonlinear dependence. Assuming that \( \delta_0 \) is a linear function of \( x \), this enables us to study scaling in terms of experimentally measurable \( x - x_c \). In this way, we obtain the following numerical law

$$\frac{\delta(\Delta C)_{\text{hang}}}{\Delta C} = \kappa \left(\tau, \delta_2, \frac{T_e}{T_{e_0}}\right).$$  \hfill (30)
that scales logarithmically is due to inessential band structure effects for the topic at hand. For the term in Eq. (12), one would naturally obtain a correction prominent when the effects of details in the band structure certainly become inapplicable. The fact that the correction Eq. (12) becomes inapplicable. The fact that the ratio \( T_c / T_\text{iso} \) takes a numerical value of the order of \( 10^{-2} \) to \( 10^{-1} \) in the iron-pnictide compounds, limits the validity of the mean-field approximation scheme. When \( \kappa F \sim 1 \), the contribution to the specific heat jump from fluctuations becomes comparable to the mean-field contribution, indicating that this corresponds to underdoped samples and are not taken into account for fitting curves.

Furthermore, there are contributions from the four-point SC correlator of the SC fluctuation correction of the two-point correlator of the SC action for the two order parameters from the very beginning, giving the possibility for a SDW order. In the incommensurate SDW phase in our model (see Fig. 1), using ten points for overdoped samples, as shown in Fig. 3. Equation (32) incorporates a constant ("BCS") and a logarithmically dependent ("QCP") term, as well as a power-law dependence (\( (x - x_c)^{-1} \)). As for the choice of the exponent, the experimental evidence for real materials would suggest that \( T_\text{so}/T_\text{iso} \gg 1 \). This would place the tetracritical point deep in the incommensurate SDW phase in our model (see Fig. 1 for illustration), rendering the possibility for a SDW order develops at low temperatures.

It corresponds to the well-separated global minima of the function \( \Gamma_q \) and an anisotropic band dispersion. Table I shows that this corresponds to \( p = -1 \), as in Fig. 1(b). The critical doping \( x_c = 0.3 \) corresponds to the optimally doped sample and is held fixed. The fit gives the following values:

\[
\alpha = -14.4, \quad \beta = -16.9, \quad \gamma = 1.7,
\]

with a reduced chi-squared \( \chi^2 = 0.91 \) for \( v = 10 - 3 = 7 \) degrees of freedom. This is a statistically significant reduction in \( \chi^2 \) from the value \( \chi^2 = 3.00 \) if the power-law term is omitted. From these numerical values, one can conclude that the power-law contribution is larger than the logarithmic term for doping \( x_c < x < x_c + 0.03 \). This places four of the ten

where \( \kappa \) is a dimensionless combination of several constants characterizing the system

\[
\kappa = \frac{6}{\pi^2} \frac{T_{\text{c},0}}{N_F v_F^2} = \frac{3}{2\pi} \frac{T_{\text{c},0}}{T_F}. \tag{31}
\]

In the last step, we use the fact that for a parabolic dispersion in two dimensions, \( N_F v_F^2 = 2bT_F / \pi \), where \( b \) is the number of FS pockets (in our case \( b = 2 \)). This prefactor plays the role of a small parameter in our approximation scheme. When \( \kappa F \sim 1 \), the contribution to the specific heat jump from fluctuations becomes comparable to the mean-field contribution, indicating that the logarithmic derivative approximation to derive the correction Eq. (12) becomes inapplicable. The fact that the ratio \( T_{\text{c},0}/T_F \) takes a numerical value of the order of \( 10^{-2} \) in the iron-pnictide compounds, limits the validity of the correction to lower values of \( \tau \) in the region of \( 0.05 - 0.5 \), while the effects of details in the band structure certainly become prominent when \( \tau \sim 1 \).

If one performs a similar analysis for the subdominant term in Eq. (12), one would naturally obtain a correction that scales logarithmically \( \propto \ln(x - x_c) \) for the most typical \( q \) dependence of \( \Gamma \). Since our analysis deals with an effective action for the two order parameters from the very beginning, we interpret this correction as arising due to the SDW fluctuation correction of the two-point correlator of the SC order parameter. Drawing skeleton diagrams with the explicit appearance of fermion lines and SC-fermion interaction vertices, and “dressing them” with SDW fluctuations, one sees that, aside from the self-energy (mass) renormalization of the fermions, there are also vertex-correction contributions. Furthermore, there are contributions from the four-point SC correlator that involve even more complicated constructs in terms of language of fermions and our analysis captures all these effects.

**V. COMPARISON TO EXPERIMENT**

We perform a weighted least-squares fit, including the combined errors in \( \Delta C/T_c \), as well as \( x_c \), of the model

\[
\frac{\Delta C}{T_c} = \alpha + \beta \ln(x - x_c) + \gamma (x - x_c)^{-1}, \tag{32}
\]

to data from the recent experiment of Walmsley *et al.* [29], using ten points for overdoped samples, as shown in Fig. 3. Equation (32) incorporates a constant ("BCS"), and a logarithmically dependent ("QCP") term, as well as a power-law dependence (\( (x - x_c)^{-1} \)). As for the choice of the exponent, the experimental evidence for real materials would suggest that \( T_{\text{so}}/T_{\text{iso}} \gg 1 \). This would place the tetracritical point deep in the incommensurate SDW phase in our model (see Fig. 1 for illustration), rendering the possibility for a SDW order develops at low temperatures. This corresponds to the well-separated global minima of the function \( \Gamma_q \) and an anisotropic band dispersion. Table I shows that this corresponds to \( p = -1 \), as in Fig. 1(b). The critical doping \( x_c = 0.3 \) corresponds to the optimally doped sample and is held fixed. The fit gives the following values:

\[
\alpha = -14.4, \quad \beta = -16.9, \quad \gamma = 1.7,
\]

\[\chi^2 = 0.91 \text{ for } v = 10 - 3 = 7 \text{ degrees of freedom}.\] This is a statistically significant reduction in \( \chi^2 \) from the value \( \chi^2 = 3.00 \) if the power-law term is omitted. From these numerical values, one can conclude that the power-law contribution is larger than the logarithmic term for doping \( x_c < x < x_c + 0.03 \). This places four of the ten
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data points corresponding to overdoped samples in a region where the logarithmic and power-law terms have comparable contributions.

These fitting arguments should be taken carefully, as the lack of data points very close to the tetracritical point and the effect of inhomogeneity in doping do not permit to investigate the discontinuity of band structure. We have found that beyond the mean-field level the discontinuity of \( \Delta C / T_c \) at the tetracritical point (the end point of the coexistence phase) transforms into the sharp maximum. As a result, \( \Delta C / T_c \) drops for deviations from \( T_c(x) = T_c(x_c) \) away from the SDW region. We expect the decrease of \( \Delta C / T_c \) to be more rapid within the SDW-ordered phase. In the vicinity of the optimal doping \( x_c \), the scaling of \( \Delta C / T_c \) versus \( x - x_c \) is governed by the effect of thermal

VI. CONCLUSION

We have studied the doping dependence of the specific heat jump in FeSCs based on a minimal two-band model of electron band structure. We have found that beyond the mean-field level the discontinuity of \( \Delta C / T_c \) at the tetracritical point transforms into the sharp maximum. As a result, \( \Delta C / T_c \) drops for deviations from \( T_c(x) = T_c(x_c) \) away from the SDW region. We expect the decrease of \( \Delta C / T_c \) to be more rapid within the SDW-ordered phase. In the vicinity of the optimal doping \( x_c \), the scaling of \( \Delta C / T_c \) versus \( x - x_c \) is governed by the effect of thermal

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[1] S. Sachdev, Quantum Phase Transitions (Cambridge University Press, Cambridge, England, 2011).

[2] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, J. Am. Chem. Soc. 130, 3296 (2008).

[3] X. H. Chen, T. Wu, G. Wu, R. H. Liu, H. Chen, and D. F. Fang, Nature (London) 453, 761 (2008).

[4] G. F. Chen, Z. Li, D. Wu, G. Li, W. Z. Hu, J. Dong, P. Zheng, J. L. Luo, and N. L. Wang, Phys. Rev. Lett. 100, 247002 (2008).

[5] M. Rotter, M. Tegel, and D. Johrendt, Phys. Rev. Lett. 101, 107006 (2008).

[6] H. Luetken, H.-H. Clauss, M. Kraken, F. J. Litterst, T. Dellmann, R. Klingeler, C. Hess, R. Khasanov, A. Amato, C. Baines, M. Kosmala, O. J. Schumann, M. Braden, J. Hamann-Borrero, N. Leps, A. Kondrat, G. Behr, J. Werner, and B. Büchner, Nat. Mater. 8, 305 (2009).

[7] A. J. Drew, Ch. Niedermayer, P. J. Baker, F. L. Pratt, S. J. Blundell, T. Lancaster, R. H. Liu, G. Wu, X. H. Chen, I. Watanabe, V. K. Malik, A. Dubroka, M. Rossl, K. W. Kim, C. Baines, and C. Bernhard, Nat. Mater. 8, 310 (2009).

[8] N. Ni, M. E. Tillman, J.-Q. Yan, A. Kracher, S. T. Hannahs, S. L. Bud’ko, and P. C. Canfield, Phys. Rev. B 78, 214515 (2008).

[9] J.-H. Chu, J. G. Analytis, C. Kucharczyk, and I. R. Fisher, Phys. Rev. B 79, 014506 (2009).

[10] Y. Laplace, J. Bobroff, F. Rullier-Albenque, D. Colson, and A. Forget, Phys. Rev. B 80, 140501(R) (2009).

[11] M.-H. Julien, H. Mayaffre, M. Horvatic, C. Berthier, X. D. Zhang, W. Wu, G. F. Chen, N. L. Wang, and J. L. Luo, Europhys. Lett. 87, 37001 (2009).

[12] C. Bernhard, A. J. Drew, L. Schulz, V. K. Malik, M. Rossle, C. Niedermayer, T. Wolf, G. D. Varma, G. Mu, H. H. Wen, H. Liu, G. Wu, and X. H. Chen, New J. Phys. 11, 055050 (2009).

[13] F. Ning, K. Ahilan, T. Imai, A. S. Sefat, R. Jin, M. A. McGuire, B. C. Sales, and D. Mandrus, J. Phys. Soc. Jpn. 78, 013711 (2009).

[14] C. Lester, J.-H. Chu, J. G. Analytis, S. C. Capelli, A. S. Erickson, C. L. Condron, M. F. Toney, I. R. Fisher, and S. M. Hayden, Phys. Rev. B 79, 144523 (2009).

[15] D. K. Pratt, W. Tian, A. Kreyssig, J. L. Zarestky, S. Nandi, N. Ni, S. L. Bud’ko, P. C. Canfield, A. I. Goldman, and R. J. McQueeney, Phys. Rev. Lett. 103, 087001 (2009).

[16] H. Chen, Y. Ren, Y. Qiu, W. Bao, R. H. Liu, G. Wu, T. Wu, Y. L. Xie, X. F. Wang, Q. Huang, and X. H. Chen, Europhys. Lett. 85, 17006 (2009).

[17] M. Rotter, M. Tegel, I. Schellenberg, F. M. Schappacher, R. Pöttgen, J. Deisenhofer, A. Günter, F. Schrettle, A. Loidl, and D. Johrendt, New J. Phys. 11, 025014 (2009).

[18] Z. Li, R. Zhou, Y. Liu, D. L. Sun, J. Yang, C. T. Lin, and Guo-qing Zheng, Phys. Rev. B 86, 180501(R) (2012).

[19] R. M. Fernandes, A. V. Chubukov, J. Knolle, I. Eremeev, and J. Schmalian, Phys. Rev. B 85, 024534 (2012).

[20] I. R. Fisher, L. Degiorgi, and Z. X. Shen, Rep. Prog. Phys. 74, 124506 (2011).

[21] S. Karasawa, H. J. Shi, K. Hashimoto, S. Tonegawa, Y. Mizukami, T. Shibauchi, K. Sugimoto, T. Fukuda, T. Terasima, A. H. Nevidomskyy, and Y. Matsuda, Nature (London) 486, 382 (2012).

[22] A. Aibanov, A. V. Chubukov, and J. Schmalian, Adv. Phys. 52, 119 (2003).

[23] M. A. Metlitski and S. Sachdev, Phys. Rev. B 82, 075128 (2010).

[24] A. Pelissetto, S. Sachdev, and E. Vicari, Phys. Rev. Lett. 101, 027005 (2008).

[25] K. B. Efetov, H. Meier, and C. Pépin, Nat. Phys. 9, 442 (2013).

[26] T. Shibauchi, A. Carrington, and Y. Matsuda, Annu. Rev. Condens. Matter Phys. 5, 113 (2014).
A. Levchenko, M. G. Vavilov, M. Khodas, and A. V. Chubukov, Phys. Rev. Lett. 110, 177003 (2013).

P. Walmsley, C. Putzke, L. Malone, I. Guillamon, D. Vignolles, C. Proust, S. Badoux, A. I. Coldea, M. D. Watson, S. Kasahara, Y. Mizukami, T. Shibauchi, Y. Matsuda, and A. Carrington, Phys. Rev. Lett. 110, 257002 (2013).

R. Zhou, Z. Li, J. Yang, D. L. Sun, C. T. Lin, and G.-Q. Zheng, Nat. Commun. 4, 2265 (2013).

D. Chowdhury, B. Swingle, E. Berg, and S. Sachdev, Phys. Rev. Lett. 111, 157004 (2013).

T. Nomoto and H. Ikeda, Phys. Rev. Lett. 111, 167001 (2013).

R. M. Fernandes, S. Maiti, P. Wölfle, and A. V. Chubukov, Phys. Rev. Lett. 111, 057001 (2013).

H. Shishido, A. F. Bangura, A. I. Coldea, S. Tonegawa, K. Hashimoto, S. Kasahara, P. M. C. Rourke, H. Ikeda, T. Terashima, R. Settai, Y. Onuki, D. Vignolles, C. Proust, B. Vignolles, A. McCollam, Y. Matsuda, T. Shibauchi, and A. Carrington, Phys. Rev. Lett. 104, 057008 (2010).

Y. Nakai, T. Iye, S. Kitagawa, K. Ishida, H. Ikeda, S. Kasahara, H. Shishido, T. Shibauchi, Y. Matsuda, and T. Terashima, Phys. Rev. Lett. 105, 107003 (2010).

S. Kasahara, T. Shibauchi, K. Hashimoto, K. Ikada, S. Tonegawa, R. Okazaki, H. Shishido, H. Ikeda, H. Takeya, K. Hirata, T. Terashima, and Y. Matsuda, Phys. Rev. B 81, 184519 (2010).

S. L. Bud’ko, N. Ni, and P. C. Canfield, Phys. Rev. B 79, 220516 (2009).

Z. S. Wang, H.-Q. Luo, C. Ren, and H.-H. Wen, Phys. Rev. B 78, 140501 (2008); N. Ni, S. L. Bud’ko, A. Kreyssig, S. Nandi, G. E. Rustan, A. I. Goldman, S. Gupta, J. D. Corbett, A. Kracher, and P. C. Canfield, ibid. 78, 014507 (2008); G. Mu, H. Luo, Z. Wang, L. Shan, C. Ren, and H.-H. Wen, ibid. 79, 174501 (2009); P. Popovic, A. V. Boris, O. V. Dolgov, A. A. Golubov, D. L. Sun, C. T. Lin, R. K. Kremer, and B. Keimer, Phys. Rev. Lett. 105, 027003 (2010); J. S. Kim, G. R. Stewart, S. Kasahara, T. Shibauchi, T. Terashima, and Y. Matsuda, J. Phys.: Condens. Matter 23, 222201 (2011).

F. Hardy, T. Wolf, R. A. Fisher, R. Eder, P. Schweiss, P. Adelmann, H. V. Löhnysen, and C. Meingast, Phys. Rev. B 81, 060501(R) (2010); F. Hardy, P. Burger, T. Wolf, R. A. Fisher, P. Schweiss, P. Adelmann, R. Heid, R. Fromknecht, R. Eder, D. Ernst, H. V. Löhnysen, and C. Meingast, Europhys. Lett. 91, 47008 (2010).

M. G. Vavilov, A. V. Chubukov, and A. B. Vorontsov, Phys. Rev. B 84, 140502(R) (2011); M. G. Vavilov and A. V. Chubukov, ibid. 84, 214521 (2011).

M. G. Vavilov, A. V. Chubukov, and A. B. Vorontsov, Supercond. Sci. Technol. 23, 054011 (2010).

A. B. Vorontsov, M. G. Vavilov, and A. V. Chubukov, Phys. Rev. B 81, 174538 (2010); R. M. Fernandes and J. Schmalian, ibid. 82, 014521 (2010).

We note that the SDW-normal phase transition curve in Figs. 1(a) and 1(b) differs from the one in Ref. [42] (see their Fig. 5), while Fig. 1(c) is identical. The reason for this is that in the presence of anisotropic detuning, there is partial compensation of the detrimental effects of anisotropy and incommensurability for the survival of the SDW phase, extending the SDW \( q \) phase above the critical value \( \delta_0 = e^{-\gamma E/2} \) = 0.2807 valid in the case when either \( \delta_2 = 0 \), or \( q = 0 \).

A. V. Chubukov, D. V. Efremov, and I. Eremin, Phys. Rev. B 78, 134512 (2008).

S. Kos, I. Martin, and C. M. Varma, Phys. Rev. B 68, 052507 (2003).