Specific heat jump at superconducting transition in the presence of Spin-Density-Wave in iron-pnictides

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We analyze the magnitude of the specific heat jump ΔC at the superconducting transition temperature T_c in the situation when superconductivity develops in the pre-existing antiferromagnetic phase. We show that $\Delta C/T_c$ differs from the BCS value and is peaked at the tri-critical point where this coexistence phase first emerges. Deeper in the magnetic phase, the onset of coexistence, T_c, drops and $\Delta C/T_c$ decreases, roughly as $\Delta C/T_c \propto T_c^2$ at intermediate T_c and exponentially at the lowest T_c, in agreement with the observed behavior of $\Delta C/T_c$ in iron-based superconductors.

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Introduction. The magnitude and the doping dependence of the specific heat jump at the superconducting transition temperature T_c is one of unexplained phenomena in novel iron-based superconductors (FeSCs) [1]. In BCS theory $\Delta C/T_c \simeq 1.43\gamma$, where $\gamma = \pi^2 N_F/3$ is the Sommerfeld coefficient, and N_F is the total quasiparticle density of states (DoS) at the Fermi surface (FS) in the normal state. Although the behavior of FeSCs is in many respects consistent with BCS theory, the experimental values of $\Delta C/T_c$ vary widely between different compounds, ranging between 1 $mJ/(mol \cdot K^2)$ in underdoped $Ba(Fe_{1-x}Ni_x)_2As_2$ [2] and 100 $mJ/(mol \cdot K^2)$ in optimally hole-doped $Ba_{1-x}K_xFe_2As_2$ [3]. Such huge variations may be partly due to differences in γ, which were indeed reported to be larger in hole-doped FeSCs [3, 4]. Yet, even for a given material, e.g., $Ba(Fe_{1-x}Ni_x)_2As_2$ or $Ba(Fe_{1-x}Co_x)_2As_2$ the magnitude of $\Delta C/T_c$ is peaked near optimal doping x_{opt} and rapidly decreases, approximately as $\Delta C/T_c \propto T_c^2$, at smaller and larger dopings [2].

This rapid and non-monotonic variation of $\Delta C/T_c$ over a relatively small range of $0.03 < x < 0.12$ is unlikely to be attributed to change in γ and has to be explained by other effects. According to one proposal [6], $\Delta C/T_c \propto T_c^2$ is caused by interband scattering off non-magnetic impurities, which is pair-breaking for $s^{\pm}$ pairing. However, $\Delta C/T_c \propto T_c^2$ only holds in the gapless superconductivity regime,[6, 13] when T_c is already reduced by more than factor of five as compared to T_c for a clean case. Before that, the reduction of $\Delta C/T_c$ by impurities is rather mild. Experimentally, the reduction is strong immediately away from optimal doping and, moreover, occurs on both sides from the optimal doping. This reduction is difficult to explain by impurity scattering. Large value of $\Delta C/T_c$ at x_{opt} may also be due to strong coupling effects [4]. This is certainly a possibility, but we note that $\Delta C/T_c$ is a non-monotonic function of the coupling [5] and at strong coupling is actually smaller than the BCS value.

We propose a different explanation. We argue that the origin of strong doping dependence of $\Delta C/T_c$ is the coexistence of spin-density-wave (SDW) magnetism and $s^{\pm}$ superconductivity (SC). [7–9] In $Ba(Fe_{1-x}Ni_x)_2As_2$, $Ba(Fe_{1-x}Co_x)_2As_2$ and, possibly, in other FeSCs, optimal doping x_{opt} nearly coincides with the end point of the coexistence region (tri-critical point). [8] We analyzed the behavior of $\Delta C/T_c$ near x_{opt} within a mean-field BCS-like theory and found that $\Delta C/T_c$ is by itself discontinuous and jumps by a finite amount when the system enters the coexistence region, see Figs. 1 and 2. The magnitude of the jump depends on microscopic parameters of the system and for a wide range of parameters, $\Delta C/T_c$ exceeds the BCS value. Beyond a mean-field treatment, paramagnetic fluctuations transform the discontinuity in $\Delta C/T_c$ at x_{opt} into a maximum, such that $\Delta C/T_c$ smoothly decreases on both sides of optimal doping x_{opt}, as illustrated in Fig. 1.

We also examined the behavior of $\Delta C/T_c$ along the entire transition into the coexistence state. We found that $\Delta C/T_c$ decreases together with T_c, and eventually becomes smaller that its BCS value. Deeper in the SDW region, $\Delta C/T_c \propto T_c^2$ and vanishes exponentially at the lowest T_c, see Fig. 2. The explanation of this behavior goes beyond a standard paradigm that T_c and ΔC decrease because FS available for SC is modified by SDW. If that was the only effect, then the DoS would not change significantly and $\Delta C/T_c$ would only weakly depend on T_c. We found, however, that the SC transition line *necessarily* enters the region in which SDW order gaps out the whole FS. In this region, SC appears because the system finds that it is energetically advantageous to decrease the magnitude of the SDW order parameter and develop a non-zero SC order parameter, even in the absence of the FS. Because all low-energy states in this region are gapped at T_c, the thermodynamic characteristics, including $\Delta C/T_c$, are exponentially small. We found that the precursors of this behavior develop at higher T_c, when the reconstructed FS is still present. As a result, $\Delta C/T_c$ decreases as the SC temperature, T_c, drops.

The behavior of $\Delta C/T_c$ outside the coexistence region

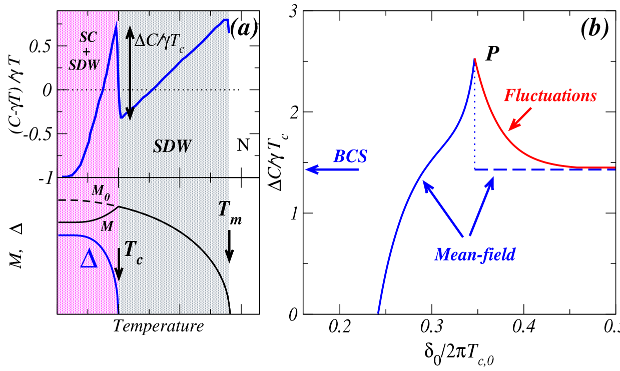

FIG. 1: (Color online) (a) The specific heat $C(T)$ and SC and SDW order parameters Δ and M as functions of T. We consider the jump of $C(T)$ at the onset of SC. (b) The behavior of $\Delta C/(\gamma T_c)$ as a function of δ_0, which scales with doping. In a mean-field theory, $\Delta C/T_c$ is discontinuous at the end point of the coexistence state (P) and jumps back to BCS value $\Delta C/T_c \simeq 1.43\gamma$ at larger dopings (dashed horizontal line). Beyond mean-field, paramagnetic fluctuations smear the discontinuity of $\Delta C/T_c$ and transform it into a maximum, as schematically shown by the solid line.

is likely to be a combination of several effects. When paramagnetic fluctuations weaken, $\Delta C/T_c$ reduces to its BCS value. Further decrease of $\Delta C/T_c$ is partly due to impurities,[6, 13] and partly due to shrinking of the hole FSs and to the fact that at larger x the gap along electron FSs becomes more anisotropic.

The method. To obtain ΔC, we expand the free energy in powers of the SC order parameter Δ to order Δ^4. When the SC transition occurs from a pre-existing SDW state, the expansion reads

$$\frac{\mathcal{F}(\Delta, M_0)}{N_F} = \frac{\mathcal{F}_0}{N_F} + \alpha_\Delta(M_0,T)\Delta^2 + \eta(M_0,T)\Delta^4, \quad (1)$$

where $\mathcal{F}_0 = \mathcal{F}(0, M_0)$ is the free energy of a pre-existing SDW state, $M_0 = M_0(T)$ is the SDW order parameter which minimizes $\mathcal{F}(0, M)$, and η includes the feedback of the finite SC order parameter on the SDW state, $M^2 = M_0^2 - \mathcal{O}(\Delta^2)$, see Fig. 1(a). The T_c is given by $\alpha_\Delta(M_0(T_c), T_c) = 0$ and the specific heat jump is

$$\frac{\Delta C}{T_c} = \frac{3\gamma}{2\pi^2\eta}\left(\frac{d\alpha_\Delta}{dT}\right)^2_{\alpha_\Delta=0}, \quad \frac{d\alpha_\Delta}{dT} = \frac{\partial\alpha_\Delta}{\partial T} + \frac{\partial\alpha_\Delta}{\partial M_0^2}\frac{dM_0^2}{dT}. \quad (2)$$

As $\eta \to 0$, Δ appears discontinuously and the transition between SDW and SC becomes first order.

To obtain actual expressions for α_Δ and η, we need to specify the band structure of a material. Since our goal is to demonstrate the discontinuity of $\Delta C/T_c$ at x_{opt} and the reduction of $\Delta C/T_c$ along the coexistence onset, we adopt a simplified 2D two-band model with the hole-like band near the center of the Brillouin zone (BZ), with $\xi_h = \mu_h - k^2/2m_h$, and electron-like band near the corner of the BZ, with $\xi_e = -\mu_e + k_x^2/2m_x + k_y^2/2m_y$, here

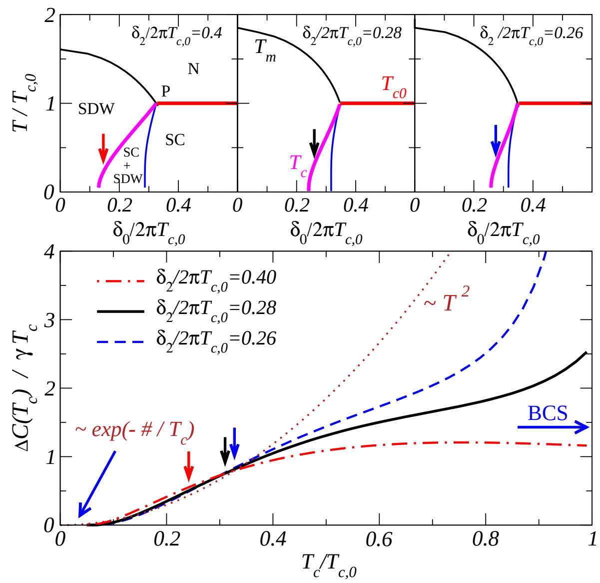

FIG. 2: (Color online) *Top:* The phase diagram in T-δ_0 plane for $T_{m,0}/T_{c,0} = 2$ and several $\delta_2/(2\pi T_{c,0}) = 0.4,\ 0.28,\ 0.26$, corresponding to wide, medium, and narrow doping ranges of the coexistence phase. SDW, SC and the SDW+SC phases meet at the tri-critical point P (in this case also meeting normal (N) state). *Bottom:* The behavior of $\Delta C/\gamma T_c$ vs $T_c/T_{c,0}$ in the coexistence region for these δ_2. The arrows indicate T_c, below which the whole FS is gapped by SDW. As T_c is lowered through this value, $\Delta C/T_c$ decreases, as T_c^2 at intermediate T_c and exponentially at lower T. Near the tri-critical point, $\Delta C/T_c$ may well exceed the BCS value 1.43γ.

k_x and k_y are deviations from (π, π). The same model has been considered in Refs. [8–10] on the coexistence of SDW and SC orders. At perfect nesting, $\xi_e = -\xi_h$, while for a non-perfect nesting $\xi_e = -\xi_h + 2\delta_\varphi$ near the FS, and $\delta_\varphi = \delta_0 + \delta_2 \cos 2\varphi$ captures the difference in the chemical potentials and in electron $m_{x,y}$ and hole m_h masses via δ_0, and anisotropy in m_x and m_y via δ_2. Without loss of generality, we assume that δ_0 changes with doping, but the ellipticity parameter δ_2 remains intact. We use a model with four-fermion interactions in SDW and SC channels [9, 11, 12], decompose them using SDW and SC order parameters M and Δ, and express couplings in terms of transition temperatures $T_{c,0}$ to the SC state in the absence of SDW and $T_{m,0}$ to the perfectly nested SDW state, $\delta_{0,2} = 0$) in the absence of SC. Note that the actual T_m decreases, even in the absence of SC, when δ_0 and δ_2 increase, while $T_{c,0}$ is the transition temperature at the tri-critical point indicated by P in Fig. 2.

The free energy for such a model has the form [9]

$$\frac{\mathcal{F}(\Delta, M)}{N_F} = \frac{\Delta^2}{2}\ln\frac{T}{T_{c,0}} + \frac{M^2}{2}\ln\frac{T}{T_{m,0}}$$
$$-\,2\pi T \sum_{\varepsilon_n>0} \mathrm{Re}\left\langle \sqrt{(E_n + i\delta_\varphi)^2 + M^2} - \varepsilon_n - \frac{\Delta^2 + M^2}{2\varepsilon_n} \right\rangle,$$

where $E_n = \sqrt{\varepsilon_n^2 + \Delta^2}$, $\varepsilon_n = \pi T(2n+1)$ are the Matsubara frequencies ($n = 0, \pm 1, \pm 2, \dots$), and $\langle \dots \rangle$ denotes averaging over φ along FSs. For this functional we find

$$\alpha_\Delta = \frac{\partial \mathcal{F}}{\partial(\Delta^2)} = \frac{1}{2}\ln\frac{T}{T_{c,0}} + \pi T \sum_{\varepsilon_n>0} \frac{1}{\varepsilon_n}(1-K)\ , \qquad \eta(M_0,T) = A - C^2/B, \tag{3}$$

where

$$K = \left\langle \mathrm{Re}\frac{\varepsilon_n + i\delta_\varphi}{\sqrt{(\varepsilon_n + i\delta_\varphi)^2 + M_0^2}} \right\rangle,$$
$$A = \frac{1}{2}\frac{\partial^2 \mathcal{F}}{\partial(\Delta^2)^2} = \sum_{\varepsilon_n>0} \frac{\pi T}{4\varepsilon_n^3}\mathrm{Re}\left\langle \frac{(\varepsilon_n + i\delta_\varphi)^3 + i\delta_\varphi M_0^2}{((\varepsilon_n + i\delta_\varphi)^2 + M_0^2)^{3/2}} \right\rangle,$$
$$B = \frac{1}{2}\frac{\partial^2 \mathcal{F}}{\partial(M^2)^2} \sum_{\varepsilon_n>0} \mathrm{Re}\left\langle \frac{\pi T}{4((\varepsilon_n + i\delta_\varphi)^2 + M_0^2)^{3/2}} \right\rangle,$$
$$C = \frac{1}{2}\frac{\partial^2 \mathcal{F}}{\partial(\Delta^2)\partial(M^2)} = \sum_{\varepsilon_n>0} \mathrm{Re}\left\langle \frac{\pi T(\varepsilon_n + i\delta_\varphi)/4\varepsilon_n}{((\varepsilon_n + i\delta_\varphi)^2 + M_0^2)^{3/2}} \right\rangle. \tag{4}$$

The derivatives are taken at $\Delta = 0$ and $M = M_0$ with M_0 defined by

$$\ln\frac{T_{m,0}}{T} = 2\pi T \sum_{\varepsilon_n>0} \mathrm{Re}\left\langle \frac{1}{\varepsilon_n} - \frac{1}{\sqrt{(\varepsilon_n + i\delta_\varphi)^2 + M_0^2}} \right\rangle. \tag{5}$$

In the absence of SDW, $M_0 \equiv 0$, $d\alpha_\Delta/dT = \partial\alpha_\Delta/\partial T$, $\eta = A(M_0 = 0) = 7\zeta(3)/(32\pi^2 T^2)$, and we reproduce the BCS result $\Delta C/T_c = 1.43\gamma$. To obtain $\Delta C/T_c$ inside SDW phase we solve Eq. (5) for $M_0^2(T)$, insert the result into Eqs. (4), evaluate $d\alpha_\Delta/dT$ and η and finally use Eq. (2). $\Delta C/T_c$ depends on three input parameters δ_0, δ_2, and $T_{m,0}/T_{c,0}$, and generally differs from the BCS value.

Results. We present $\Delta C/T_c$ as function of δ_0 for fixed δ_2 and $T_{m,0}/T_{c,0}$ in Fig. 1(b). It grows from zero value at the low-temperature onset of the coexistence phase and reaches its maximum at the tri-critical point, where SDW order disappears. At this δ_0, T_c reaches $T_{c,0}$ and $\Delta C/T_c$ jumps to the BCS value.

Plotted as a function of $T_c/T_{c,0}$ in Fig. 2, $\Delta C/T_c$ shows exponential behavior at small T_c and approximate T_c^2 behavior at intermediate $T_c/T_{c,0} \lesssim 0.5$. The magnitude of $\Delta C/T_c$ at $T_{c,0}$ increases when the width of the coexistence region shrinks. This can be easily understood, since shrinking of the coexistence region brings the system closer to a first order transition between SDW and SC at which the entropy itself becomes discontinuous at T_c, and $\Delta C/T_c$ diverges. In the opposite limit, when the width of the coexistence range is the largest, the magnitude of $\Delta C/T_c$ is smaller and can even be below the BCS value.

The behavior of $\Delta C/T_c$ at small T_c and at $T_c \approx T_{c,0}$ can be understood analytically. We first focus on the low

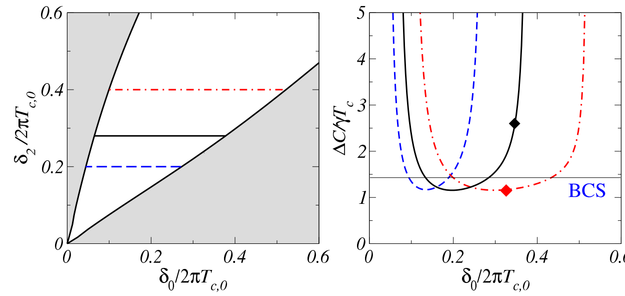

FIG. 3: (Color online) *Left:* the coexistence region (unshaded) in the δ_2-δ_0 plane. Each point corresponds to a particular ratio $T_{m,0}/T_{c,0}$ and this ratio increases monotonically as δ_0 grows at fixed δ_2. *Right:* The value of $\Delta C/\gamma T_c$ at the end point of the coexistence region, at $T_c = T_{c,0} - 0$ for $\delta_2/2\pi T_{c,0} = 0.4, 0.28, 0.2$ Thin solid line is the BCS value $\Delta C/T_c = 1.43\gamma$. Over some range of parameters, $\Delta C/\gamma T_c$ at $T_{c,0} - 0$ significantly exceeds the BCS value. Diamonds represent the values $\Delta C/\gamma T_c$ at $T_c = T_{c,0} - 0$ for the curves for $\delta_2/2\pi T_{c,0} = 0.4$ and 0.28 in Fig. 2

T_c limit, $T_c \ll T_{c,0}$. We argue that at low T_c a conventional reasoning that the mixed SDW/SC state exists because FS reconstruction associated with SDW order still leaves pieces of the FS available for SC does not work because the SDW state immediately above T_c is already fully gapped. Indeed, to a logarithmical accuracy, the condition $\alpha_\Delta(M_0, T_c) = 0$ becomes

$$2\pi T_c \sum_{\varepsilon_n>0} \frac{1}{\varepsilon_n}\left(1 - \mathrm{Re}\left\langle \frac{\delta_\varphi}{\sqrt{\delta_\varphi^2 - M_0^2}} \right\rangle\right) = \ln\frac{T_{c,0}}{T_c} \tag{6}$$

which is only satisfied if $M_0 > \max\{\delta_\varphi\} = \delta_0 + \delta_2$, *i.e.* the SDW state is fully gapped [9].

The coexistence state emerges from the fully gapped SDW state because, when $\eta > 0$ and $\alpha_\Delta > 0$, it is energetically advantageous to gradually reduce the magnitude of the SDW order M below M_0, thus change sign of α_Δ and create non-zero SC order Δ. The contribution to the free energy from SC ordering comes from the rearrangement of quasiparticle states above the gap, and the number of such quasiparticles exponentially decreases with lowering T_c. As a result, the magnitude of the specific heat discontinuity at T_c also becomes exponentially small, $\Delta C/T_c \propto \exp[-(M_0 - \delta_0 - \delta_2)/T_c]$, consistent with Fig. 2. We emphasize that as long as SDW–coexistence transition is of second order, $\eta > 0$, the exponential behavior at low T_c always holds. The behavior of $\Delta C/T_c$ at larger T is less universal, but the reduction of $\Delta C/T_c$ always begins even before the condition $M_0 > \delta_0 + \delta_2$ is reached, see Fig. 2. For smaller η, $\Delta C/T_c$ decreases with T_c over the whole range $T_c < T_{c,0}$.

We next consider $\Delta C/T_c$ near the end point of the coexistence regime, when $T_m \to T_{c,0} + 0$, $T_c \to T_{c,0} - 0$ and M_0 is small. In this case, we expand α_Δ, η, and $\mathcal{F}_0$ in terms of M_0^2, use $\partial\alpha_\Delta(0,T)/\partial T = 1/2T$,

$\partial\alpha_\Delta/\partial M^2 = 2C_0$ and $dM_0^2/dT = -(\partial\alpha_m/\partial T)/2B_0$ and express Eq. (2) as

$$\frac{\Delta C}{T_c} = \frac{3\gamma}{2\pi^2\eta_0}\left(\frac{1}{2T} - \frac{\partial\alpha_m}{\partial T}\frac{C_0}{B_0}\right)^2_{T=T_c}, \tag{7}$$

where $\eta_0 = A_0 - C_0^2/B_0$ and the coefficients A_0, B_0 and C_0 are given by Eqs. (4) with $M_0 = 0$. For dM_0^2/dT we obtain from Eq. (5) $dM_0^2/dT = -(\partial\alpha_m/\partial T)/2B_0$, Eq. (5), with

$$\frac{\partial\alpha_m}{\partial T} = \frac{1}{2T} - 2\pi\sum_{\varepsilon_n>0}\left\langle\frac{\delta_\varphi^2\varepsilon_n}{(\varepsilon_n^2+\delta_\varphi^2)^2}\right\rangle. \tag{8}$$

In the absence of SDW order, $\Delta C/T_c$ does not contain $(C_0/B_0)\partial\alpha_m/\partial T$, $\eta_0 \to A_0$, and $\Delta C/T_c = 1.43\gamma$. Once M_0 is small but finite, $\Delta C/T_c$ is determined by the interplay between $(C_0/B_0)\partial\alpha_m/\partial T$ and C_0^2/B_0 in η_0. Both terms originate from the fact that SDW order is suppressed by SC order, $M^2 = M_0^2 - (C/B)\Delta^2$. As a result, $\Delta C/T_c$ is different from the BCS value already for infinitesimally small SDW order and exhibits discontinuity upon crossing the SDW border. In general, the change in η_0 is more important because $C_0^2 = A_0B_0$ at perfect nesting, $\delta_{0,2} = 0$, and $\eta_0 = 0$ [8, 9]. Reduced value of η leads to generally *larger* $\Delta C/T_c$ at $T_c = T_{c,0} - 0$ than $\Delta C/T_c = 1.43\gamma$ for transition from normal state to a pure SC state. As the coexistence region narrows, $\eta_0 \to 0$ and $\Delta C/T_c$ grows. Figure 3 shows $\Delta C/T_c$ at $T_c = T_{c,0} - 0$ for $\eta_0 > 0$. In a wide range of parameters, $\Delta C/T_c > 1.43\gamma$.

Beyond mean-field. In a mean-field description, $\Delta C/T_c$ is discontinuous at the tri-critical point P, Fig. 2, with $T_m = T_{c,0}$. The free energy $\mathcal{F}_0$ and the specific heat jump depend on the finite *square* of the SDW order, $M_0^2 \propto (T_m - T)$. Although above T_m the average $M_0 = 0$, one expects to replace M_0^2 by the finite *second* moment of SDW order due to Gaussian fluctuations, $\langle M_0^2\rangle_{fluct} \propto (T - T_m)$. These fluctuations enhance $\Delta C/T_c$ and transform the discontinuity in $\Delta C/T_c$ into a maximum, as shown in Fig. 1. As a result, $\Delta C/T_c$ drops for deviations from $T_{c,0} = T_m$ both into the coexistence phase and away from the SDW region. Still, the decrease of $\Delta C/T_c$ should be more rapid within the SDW-ordered phase. An enhancement of $\Delta C/T_c$ by paramagnetic fluctuations was earlier obtained in Ref. [14].

Conclusions. We demonstrated that the specific heat jump $\Delta C/T_c$ across transition from SDW to the coexistence phase significantly deviates from the BCS value. $\Delta C/T_c$ has its maximum for doping at the high-temperature end of the coexistence phase and decreases for doping deviations in both directions. In the coexistence phase, $\Delta C/T_c$ eventually becomes exponentially small as all low-energy states at low T_c are already gapped out by the SDW order. At intermediate $T_c \lesssim T_{c,0}$, $\Delta C/T_c$ scales approximately as T_c^2.

This behavior is quite consistent with the observed doping evolution of $\Delta C/T_c$ in $Ba(Fe_{1-x}Ni_x)_2As_2$ and $Ba(Fe_{1-x}Co_x)_2As_2$ [2]. In these materials $\Delta C/T_c$ is peaked at the tri-critical point, which coincides with the optimal doping x_{opt}, and decreases for deviations from x_{opt} in both directions, faster into the coexistence region. The evolution of $\Delta C/T_c$ there approximately follows T_c^2 behavior.

As doping increases and paramagnetic fluctuations disappear, $\Delta C/T_c$ reduces to the BCS value. Further reduction of $\Delta C/T_c$ at larger dopings $x > x_{opt}$ is, most likely, a combination of several effects: (1) the enhancement of a non-magnetic interband impurity scattering [6, 13]; (2) stronger anisotropy of the gap on the electron FSs that increases η; (3) the reduction of γ due to shrinking of the hole FSs.

How strongly the value of $\Delta C/T_c$ at x_{opt} exceeds the BCS result is difficult to gauge because γ has to be extracted from the normal state $C(T)$ for which γT contribution is only a small portion of the total specific heat. In $Ba(Fe_{1-x}Co_x)_2As_2$, $\Delta C/T_c \sim 26\ mJ/(mol \cdot K^2)$ at x_{opt}, and $\gamma \simeq 20\ mJ/(mol \cdot K^2)$ [4]. In this case, the maximum of $\Delta C/T_c$ is not far from the BCS result, and the reduction of $\Delta C/T_c$ into the coexistence state is mainly due to the gapped low-energy states by SDW order at low T_c. At the same time, a very strong $\Delta C/T_c$ over a $100\ mJ/(mol \cdot K^2)$ near x_{opt} in $Ba_{1-x}K_xFe_2As_2$ is well above the BCS value [3], even if γ is as large as reported [3, 4] $50 - 60\ mJ/(mol \cdot K^2)$. This enhancement can well be due the peak in $\Delta C/T_c$ at the onset of the coexistence regime or strong SDW fluctuations.

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