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# Jump in specific heat in the presence of a spin-density wave at the superconducting transition in iron pnictides

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Many experiments reveal that in iron-based superconductors the jump of the specific heat $\Delta C$ at the superconducting $T_c$ is not proportional to $T_c$, as expected in BCS theory. Rather, $\Delta C/T_c$ varies with $T_c$, and has a peak near optimal doping and decreases at smaller and larger dopings. We show that this behavior can be naturally explained by the interplay between superconductivity and antiferromagnetism. We demonstrate on general grounds that $\Delta C/T_c$ peaks at the doping where the coexistence phase with antiferromagnetism develops, and decreases at deviations from this doping in both directions. Our results are in quantitative agreement with the experiments.

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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 the unexplained phenomenas in 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). 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 K$^2$) in underdoped $Ba(Fe_{1-x}Ni_x)_2As_2$ (Ref. 2) and 100 mJ/(mol K$^2$) in optimally hole-doped $Ba_{1-x}K_xFe_2As_2$.[3] Such huge variations may be partly due to differences in $\gamma$, 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 $\Delta C/T_c$ peaks near optimal doping $x_{\rm opt}$ and rapidly decreases, approximately as $\Delta C/T_c \propto T_c^2$, at smaller and larger dopings.[2,4]

This rapid and nonmonotonic variation of $\Delta C/T_c$ over a relatively small range of $0.03 < x < 0.12$ is unlikely to be attributed to a change in $\gamma$ and has to be explained by other effects.[2] The reduction of $\Delta C/T_c$ in the overdoped regime may be caused by interband scattering off non-magnetic impurities,[5] which is pair-breaking for $s^{\pm}$ pairing, and the reduction of $\Delta C/T_c$ in the underdoped region may be due to phase separation. However, the near-symmetric reduction on both sides from the optimal doping is difficult to explain either by impurity scattering or by phase separation. Strong coupling effects do increase $\Delta C/T_c$ over some range of couplings,[6] although they are unlikely to explain non-monotonic behavior of $\Delta C/T_c$ around optimal doping.

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 $x_{\rm opt}$ nearly coincides with the end point of the coexistence region (tetracritical point).[8] We analyze the behavior of $\Delta C/T_c$ near $x_{\rm opt}$ within BCS theory and find that $\Delta C/T_c$ is by itself discontinuous and jumps by a finite amount when the system enters the coexistence region (see Fig. 1). For a wide range of parameters $\Delta C/T_c$ immediately after the jump well exceeds the BCS value. Beyond a mean-field treatment, paramagnetic fluctuations transform the discontinuity in $\Delta C/T_c$ at $x_{\rm opt}$ into a maximum, such that $\Delta C/T_c$ decreases on both sides of optimal doping, as illustrated in Fig. 1.

We also examine the behavior of $\Delta C/T_c$ along the entire $T_c$ line in the coexistence region. In our two-pocket model we find that $\Delta C/T_c$ decreases together with $T_c$, follows $\Delta C/T_c \propto T_c^2$ over some range of $T_c$, and becomes exponentially small at the lowest $T_c$. The explanation for this behavior goes beyond a standard paradigm that $T_c$ and $\Delta C$ decrease because the FS available for superconductivity is modified by the SDW. If that were the only effect, then the DOS would not change significantly and $\Delta C/T_c$ would only weakly depend on $T_c$. We find that the strong decrease of $\Delta C/T_c$ originates from the fact that the $T_c$ line *necessarily* crosses over into the region in which the SDW order gaps out the hole and the electron FSs which are reconstructed by SDWs.[10] In this situation, all states are gapped at $T_c$ and $\Delta C/T_c$ is exponentially small. We find that the precursors of this behavior develop at a higher $T_c$, when the reconstructed FS is still present, and $\Delta C/T_c$ decreases in the entire coexistence phase. In more realistic four- or five-pocket models, the system still remains a metal even at the lowest $T_c$ because at least one FS is not involved in SDW reconstruction.[11] That FS accounts for a metallic behavior and a nonzero $\Delta C/T_c$. Still, the total $\Delta C/T_c$ is well below the BCS value.

The behavior of $\Delta C/T_c$ outside the coexistence region is likely to be a combination of several effects. When paramagnetic fluctuations weaken, $\Delta C/T_c$ reduces to its BCS value. A further decrease of $\Delta C/T_c$ is partly due to impurities,[5,12] and partly due to the 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 $\Delta C$, we expand the free energy in powers of the SC order parameter $\Delta$ to order $\Delta^4$. When the SC transition occurs from a preexisting SDW state, the expansion reads

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

 

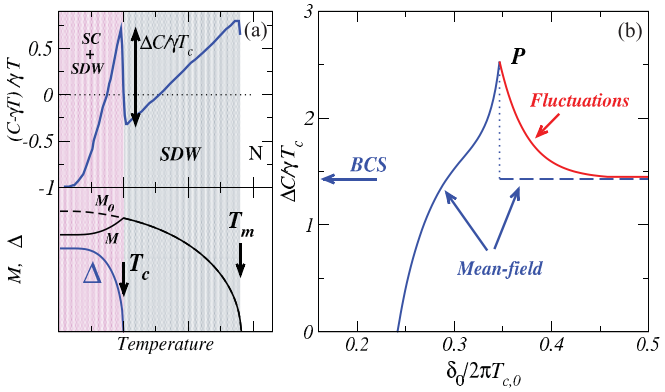


FIG. 1. (Color online) (a) The specific heat $C(T)$ and SC and SDW order parameters $\Delta$ and $M$ as functions of $T$. We consider the jump of $C(T)$ at the onset of SC. (b) The behavior of $\Delta C/(\gamma T_c)$ as a function of $\delta_0$, which scales with doping. In a mean-field theory, $\Delta C/T_c$ is discontinuous at the end point of the coexistence state ($P$) and jumps back to the BCS value $\Delta C/T_c \simeq 1.43\gamma$ at larger dopings (dashed horizontal line). Beyond the 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.

where $\mathcal{F}_0 = \mathcal{F}(0,M_0)$ is the free energy of a preexisting SDW state, $M_0 = M_0(T)$ is the SDW order parameter which minimizes $\mathcal{F}(0,M)$, and $\eta$ includes the feedback of the finite SC order parameter on the SDW state, $M^2 = M_0^2 - O(\Delta^2)$ [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

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

To obtain actual expressions for $\alpha_\Delta$ and $\eta$, we need to specify the band structure of a material. Since our goal is to demonstrate the discontinuity of $\Delta C/T_c$ at $x_{\rm opt}$ and the reduction of $\Delta C/T_c$ along the coexistence onset, we adopt a simplified two-dimensional, two-band model with a holelike band near the center of the Brillouin zone (BZ), with $\xi_h = \mu_h - k^2/2m_h$, and an electronlike band near the corner of the BZ, with $\xi_e = -\mu_e + k_x^2/2m_x + k_y^2/2m_y$, where $k_x$ and $k_y$ are deviations from $(\pi,\pi)$. The same model was earlier considered in Refs. 8,9, and 13. At perfect nesting $\xi_e = -\xi_h$, while for a non-perfect nesting $\xi_e = -\xi_h + 2\delta_\varphi$, where $\delta_\varphi = \delta_0 + \delta_2\cos 2\varphi$ captures the difference in the chemical potentials and in electron and hole masses, via $\delta_0$, and ellipticity ($m_x \neq m_y$), via $\delta_2$. Without loss of generality, we assume that $\delta_0$ changes with doping, but the ellipticity parameter $\delta_2$ is doping independent. We consider an effective low-energy theory with angle-independent interactions in the SDW channel and in the $s^\pm$ SC channel.[9,14,15] We assume that the pairing interaction is attractive without specifying its origin.

We decompose these four-fermion interactions using SDW and SC order parameters $M$ and $\Delta$, 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 $T_m$ differs from $T_{m,0}$ even in the absence of SC and decreases when $\delta_0$ and $\delta_2$ increase.

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 ($n = 0, \pm 1, \pm 2, \ldots$), and $\langle\cdots\rangle$ denotes averaging over $\varphi$ 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

$$K = \left\langle\mathrm{Re}\frac{\varepsilon_n+i\delta_\varphi}{\sqrt{(\varepsilon_n+i\delta_\varphi)^2+M_0^2}}\right\rangle,$$

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

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

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

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, $M_0 \equiv 0$, $d\alpha_\Delta/dT = \partial\alpha_\Delta/\partial T$, $\eta = A(M_0=0) = 7\zeta(3)/(32\pi^2T^2)$, and we reproduce the BCS result $\Delta C/T_c = 1.43\gamma$. To obtain $\Delta C/T_c$ inside the SDW phase we solve Eq. (5) for $M_0^2(T)$, insert the result into Eq. (4), evaluate $d\alpha_\Delta/dT$ and $\eta$, and substitute them into Eq. (2). $\Delta C/T_c$ depends on three input parameters $\delta_0,\delta_2$, and $T_{m,0}/T_{c,0}$, and generally differs from the BCS value.

*Results*. We present $\Delta C/T_c$ as function of $\delta_0$ for fixed $\delta_2$ 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 tetracritical point, where $T_c$ reaches $T_{c,0}$. At this point, $\Delta C/T_c$ jumps back 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 the 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

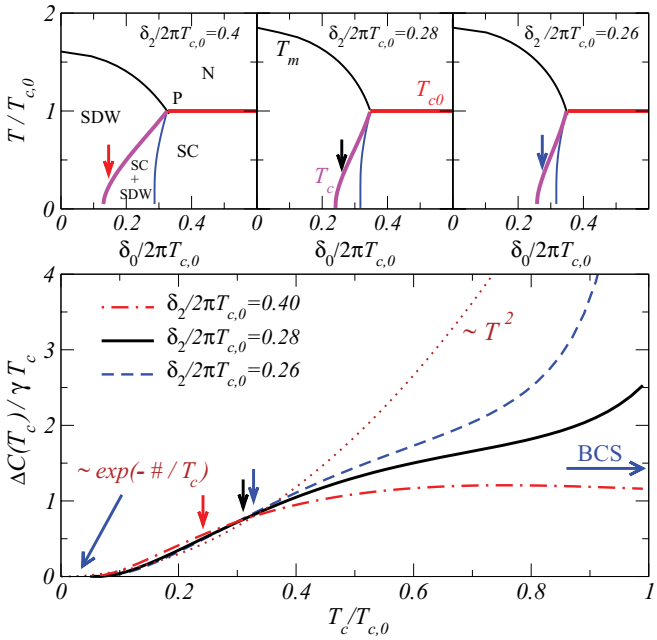


FIG. 2. (Color online) Top: The phase diagram in the $T$-$\delta_0$ plane for $T_{m,0}/T_{c,0} = 2$ and $\delta_2/(2\pi T_{c,0}) = 0.4$, 0.28, 0.26, corresponding to wide, medium, and narrow doping ranges of the coexistence phase. The SDW, SC, SDW+SC and normal (N) phases meet at the tetracritical point $P$. Bottom: The behavior of $\Delta C/\gamma T_c$ vs $T_c/T_{c,0}$ in the coexistence region for these $\delta_2$. 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 tetracritical point, $\Delta C/T_c$ may well exceed the BCS value $1.43\gamma$.

the largest, $\Delta C/T_c$ is much smaller and can even be below the BCS value.

The decrease of $\Delta C/T_c$ at small $T_c \ll T_{c,0}$ and the discontinuity at $T_c \approx T_{c,0}$ can be understood analytically. In the low-$T_c$ limit, it turns out that the SDW state immediately above $T_c$ is fully gapped (in the two-band model). To see this we note that at low $T$ the condition on $T_c$ becomes, to a logarithmical accuracy,

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

This equation is satisfied only if $M_0 > \max\{\delta_\varphi\} = \delta_0 + \delta_2$, which is the condition that the SDW state gaps fermionic excitations.[9] Superconductivity emerges from this fully gapped SDW state by purely energetical reasons—below $T_c$ it becomes energetically advantageous to gradually reduce the magnitude of the SDW order $M$ below $M_0$, and create a nonzero SC order $\Delta$. The contribution to the free energy from SC ordering comes from the rearrangement of quasiparticle states above the gap. As a result, the magnitude of the specific-heat discontinuity at $T_c$ in the two-band model becomes exponentially small. In more realistic four- and five-band models, $\Delta C/T_c$ also decreases exponentially but tends to a finite value because at least one FS is not involved in the SDW reconstruction.[11]

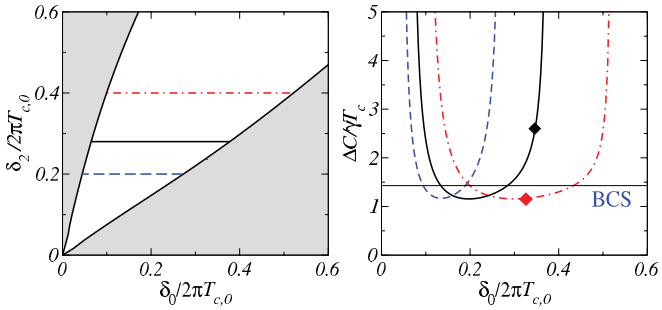


FIG. 3. (Color online) Left: The coexistence region (unshaded) in the $\delta_2$-$\delta_0$ plane. Each point corresponds to a particular ratio $T_{m,0}/T_{c,0}$, and this ratio increases monotonically as $\delta_0$ grows at fixed $\delta_2$. Right: The value of $\Delta C/\gamma T_c$ at the end point of the coexistence region for $\delta_2/2\pi T_{c,0} = 0.4, 0.28, 0.2$. The thin solid line is the BCS value $\Delta C/T_c = 1.43\gamma$. 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.

We next consider $\Delta C/T_c$ near the end point of the coexistence regime, when $T_m \to T_{c,0} + 0$, and $M_0$ is small. In this limit we expand $\alpha_\Delta$, $\eta$, and $\mathcal{F}_0$ in terms of $M_0^2$ and express Eq. (2) as

$$\frac{\Delta C}{T_c} = \frac{3\gamma}{8\pi^2 A_0 T_c^2} \frac{\left(1 - 2T_c \frac{\partial \alpha_m}{\partial T} \frac{C_0}{B_0}\right)^2}{\left(1 - \frac{C_0^2}{A_0 B_0}\right)}, \quad (7)$$

where the derivative is taken at $T_c$, the coefficients $A_0$, $B_0$, and $C_0$ are given by Eqs. (4) with $M_0 = 0$, and

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

The terms containing $C_0/B_0$ originate from the fact that SDW order is suppressed by SC order $M^2 \approx M_0^2 - (C_0/B_0)\Delta^2$. In the absence of SDW order, these terms are absent and $\Delta C/T_c$ reduces to the BCS result. Once $M_0$ is small but finite, $\Delta C/T_c$ changes discontinuously and its value is now determined by the interplay between the additional $(C_0/B_0)$ terms in the numerator and the denominator in Eq. (7). In general, the additional term in the denominator is more important because at perfect nesting ($\delta_{0,2} = 0$) $C_0^2 = A_0 B_0$.[8,9] As a result $\Delta C/T_c$ at $T_c = T_{c,0} - 0$ is generally *larger* than at $T_c = T_{c,0} + 0$. In Fig. 3 we show $\Delta C/T_c$ at $T_c = T_{c,0} - 0$ for various $\delta_0$ and $\delta_2$. Over some range of parameters, $\Delta C/\gamma T_c$ at $T_{c,0} - 0$ significantly exceeds the BCS value.

*Beyond the mean field*. In a mean-field description, $\Delta C/T_c$ is discontinuous at the tetracritical 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 $\langle M_0^2 \rangle_{\mathrm{fluct}} \propto (T - T_m)$. These fluctuations modify the mean-field result for $\Delta C/T_c$ on both sides around the tetracritical point, and transform the discontinuity in $\Delta C/T_c$ into a maximum, as illustrated in Fig. 1. As a result, $\Delta C/T_c$ enhances upon approaching optimal doping both from the coexistence phase and from higher dopings. Still, the increase of

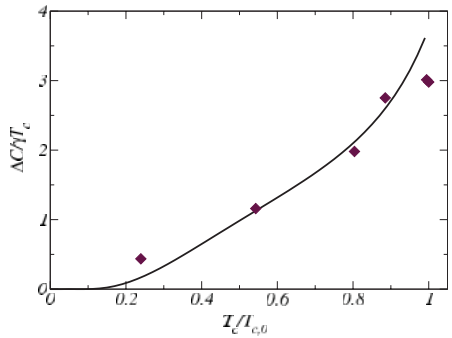


FIG. 4. (Color online) A comparison between the calculated $\Delta C/T_c$ and the experimental data from Ref. 4 for $Ba(Fe_{0.925}Co_{0.075})_2As_2$ for dopings below the optimal one. We used $T_{m,0}/T_{c,0} = 1.45$ and $\delta_2/2\pi T_{c,0} = 0.174$.

$\Delta C/T_c$ should be more rapid within the SDW-ordered phase. An enhancement of $\Delta C/T_c$ by paramagnetic fluctuations was earlier obtained in Ref. 16.

*Comparison with experiments*. The theoretical behavior of $\Delta C/T_c$ is quite consistent with the observed doping evolution of $\Delta C/T_c$ in $Ba(Fe_{1-x}Ni_x)_2As_2$ and $Ba(Fe_{1-x}Co_x)_2As_2$.[2,4] In these materials $\Delta C/T_c$ is peaked at the tetracritical point, which coincides with the optimal doping $x_{opt}$, and decreases for deviations from $x_{opt}$ in both directions, faster into the coexistence region. To make the comparison quantitative, in Fig. 4 we plot our results together with the measured $\Delta C/T_c$ in $Ba(Fe_{0.925}Co_{0.075})_2As_2$.[4] We see that the agreement is quite reasonable.

How strongly the value of $\Delta C/T_c$ at $x_{opt}$ exceeds the BCS result is difficult to gauge because $\gamma$ has to be extracted from the normal state $C(T)$ for which the $\gamma T$ 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 K$^2$) at $x_{opt}$, and $\gamma \simeq 20$ mJ/(mol K$^2$).[4] In this case, the maximum of $\Delta C/T_c$ is not far from the BCS result. At the same time, in $Ba_{1-x}K_xFe_2As_2$ $\Delta C/T_c$ is over 100 mJ/(mol K$^2$) near $x_{opt}$, well above the BCS value,[3] even if $\gamma$ is as large as reported,[3,4] 50–60 mJ/(mol K$^2$).

*Conclusions*. We demonstrated that the specific-heat jump, $\Delta C/T_c$, across the transition from the SDW to the coexistence phase significantly deviates from the BCS value. The key result is that $\Delta C/T_c$ peaks at the onset of the coexistence phase and decreases for doping deviations in both directions. In the coexistence phase, $\Delta C/T_c$ decreases as $T_c^2$ at intermediate $T_c$ and even faster at smallest $T$. Outside the coexisatence phase $\Delta C/T_c$ reduces in our model to the BCS value. A 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;[5,12] (2) strong anisotropy of the gap on the electron FSs that increases $\eta$; and (3) the reduction of $\gamma$ due to the shrinking of the hole FSs. Our theoretical results agree quantitatively with the experimental data.

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[10] This holds assuming that the SDW interaction is angle independent along the FSs. It has been argued [Y. Ran, F. Wang, H. Zhai, A. Vishwanath, and D.-H. Lee, Phys. Rev. B **79**, 014505 (2009)] that, at least, in some orbital models for Fe pnictides, SDW interaction must vanish along a particular direction. In this case, small FSs survive even if the SDW order is strong.

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