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

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Many experiments reveal that in iron-based superconductors the jump of the specific heat ΔC 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 $\Delta C/T_c$ is peaked 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.

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). 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)₂As₂² 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^{2,4}.

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 effects². The reduction of $\Delta C/T_c$ in the overdoped regime may be caused by interband scattering off non-magnetic impurities⁶, 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 couplings⁵, 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).^{7,11,12} In Ba(Fe_{1-x}Ni_x)₂As₂, Ba(Fe_{1-x}Co_x)₂As₂ and, possibly, in other FeSCs, optimal doping x_{opt} nearly coincides with the end point of the coexistence region (tetra-critical point).¹¹ We analyze the behavior of $\Delta C/T_c$ near x_{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_{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 of this behavior goes beyond a standard paradigm that T_c and ΔC decrease because FS available for superconductivity 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 find that the strong decrease of $\Delta C/T_c$ originates from the fact that T_c line necessarily crosses over into the region in which SDW order gaps out the hole and the electron FSs which are reconstructed by SDW^8 . 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 co-existence phase. In more realistic 4 or 5-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.⁹. That FS accounts for a metallic behavior and a non-zero $\Delta C/T_c$. Still, the total $\Delta C/T_c$ is well below 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. Further decrease of $\Delta C/T_c$ is partly due to impurities,^{6,10} 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

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

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 $\xi_e = -\mu_e + k_x^2/2m_x + k_y^2/2m_y$, where k_x and k_y are deviations from (π, π) . The same model was earlier considered in Refs.^{11–13}. 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 δ_0 , and ellipticity $(m_x \neq m_y)$, via δ_2 . Without loss of generality, we assume that δ_0 changes with doping, but the ellipticity parameter δ_2 is doping independent. We consider an effective low-energy theory with angleindependent interactions in the SDW channel and in the s^{\pm} SC channel, ^{12,14,15}. 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 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 differs from $T_{m,0}$ even in the absence of SC and decreases when δ_0 and δ_2 increase.

The free energy for such a model has the form¹²

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

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

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

where

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

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

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

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

(4)

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

$$\ln \frac{T_{m,0}}{T} = 2\pi T \sum_{\varepsilon_n > 0} \operatorname{Re} \left\langle \frac{1}{\varepsilon_n} - \frac{1}{\sqrt{(\varepsilon_n + i\delta_{\varphi})^2 + M_0^2}} \right\rangle.$$
(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 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 substitute them into 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 tetra-critical 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 $T_c/T_{c,0} \leq 0.5$. 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, $\Delta C/T_c$ is much smaller and can even be below the BCS value.

The decrease of $\Delta C/T_c$ at 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 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,

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

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.¹² 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 non-zero SC order Δ . 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 4 band and 5 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.⁹

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 α_{Δ} , η , and \mathcal{F}_0 in terms of M_0^2 and express Eq. (2) as

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

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

$$\frac{\partial \alpha_m}{\partial T} = \frac{1}{2T} - 2\pi \sum_{\varepsilon_n > 0} \left\langle \frac{\delta_{\varphi}^2 \varepsilon_n}{(\varepsilon_n^2 + \delta_{\varphi}^2)^2} \right\rangle.$$
(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 is value is now determined by the interplay between the additional (C_0/B_0) terms in the numerator and the denominator in 7. In general, the additional term in the demoninator is more important because at perfect nesting $(\delta_{0,2} = 0) C_0^2 = A_0 B_0$.^{11,12}. 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 varios δ_0 and δ_2 . Over a wide range of parameters, $\Delta C/T_c$ over some range of parameters, $\Delta C/\gamma T_c$ at $T_{c,0} - 0$ significantly exceeds the BCS value.

Beyond mean-field. In a mean-field description, $\Delta C/T_c$ is discontinuous at the tetra-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 modify the mean-field result for $\Delta C/T_c$ on both sides around the tetra-critical 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 $\Delta C/T_c$ 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)₂As₂ and Ba(Fe_{1-x}Co_x)₂As₂^{2,4}. In these materials $\Delta C/T_c$ is peaked at the tetra-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. 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})₂As₂ (Ref.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 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)₂As₂, $\Delta C/T_c \sim 26 \ mJ/(mol \cdot K^2)$ at x_{opt} , and $\gamma \simeq 20 \ mJ/(mol \cdot K^2)^4$. In this case, the maximim of $\Delta C/T_c$ is not far from the BCS result. At the same time, in Ba_{1-x}K_xFe₂As₂ $\Delta C/T_c$ is over a 100 $mJ/(mol \cdot K^2)$ near x_{opt} , well above the BCS value³, even if γ is as large as reported^{3,4} 50 - 60 $mJ/(mol \cdot K^2)$.

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. The key result is that $\Delta C/T_c$ is peaked 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 co-existence phase $\Delta C/T_c$ reduces in our model 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^{6,10}; (2) stronge anisotropy of the gap on the electron FSs that increases η ; (3) the reduction of γ due to shrinking of the hole FSs. Our theoretical results agree quantitatively with the experimental data

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Figures



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.



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 tetra-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 tetra-critical point, $\Delta C/T_c$ may well exceed the BCS value 1.43γ .



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 for $\delta_2/2\pi T_{c,0} = 0.4, 0.28, 0.2$ Thin solid line is the BCS value $\Delta C/T_c = 1.43\gamma$. 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



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})₂As₂ for dopings below the optimal one. We used $T_{m,0}/T_{c,0} = 1.45$ and $\delta_2/2\pi T_{c,0} = 0.174$.