Anomalous scaling of $\Delta C$ versus $T_c$ in the Fe-based superconductors: the $S_{\pm}$-wave pairing state model

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Abstract

The strong power law behavior of the specific heat jump $\Delta C$ versus $T_c$ ($\Delta C / T_c \sim T_c^{\alpha}$, $\alpha \approx 2$), first observed by Bud’ko et al (2009 Phys. Rev. B 79 220516), has been confirmed with several families of the Fe-based superconducting compounds with various dopings. We have tested a minimal two band BCS model to understand this anomalous behavior and showed that this non-BCS relation between $\Delta C$ versus $T_c$ is a generic property of the multiband superconducting state paired by a dominant interband interaction ($V_{\text{inter}} > V_{\text{intra}}$) reflecting the relation $\Delta C / T_c \sim \sqrt{N_f / N_e}$ near $T_c$ as in the $S_{\pm}$-wave pairing state.

We also found that this $\Delta C$ versus $T_c$ power law can continuously change from the ideal BNC scaling to a considerable deviation by a moderate variation of the impurity scattering rate $\Gamma_0$ (non-pair-breaking). As a result, our model provides a consistent explanation why the electron-doped Fe-based superconductors follow the ideal BNC scaling very well while the hole-doped systems often show varying degree of deviations.

1. Introduction

The specific heat (SH) jump $\Delta C$ is the most well known thermodynamic signature of the second order phase transition and hence contains the generic information of the transition as well as the material specific information. For example, the BCS theory of superconductivity predicts the universal ratio $\Delta C / C_{\text{dil}} \sim 1.43$, hence $\Delta C / T_c \sim 1.43 \gamma$ is a temperature independent constant and tells us the material specific quantity $\gamma$, the Sommerfeld coefficient of the normal state $\gamma = \frac{\pi^2}{3} N (0) (N(0)$ density of states (DOSs) at Fermi level). In view of this BCS prediction of $\Delta C / T_c = \text{const.}$, the experimental observation by Bud'ko, Ni, and Canfield (BNC) [1], $\Delta C / T_c \sim T_c^2$ for a family of doped Ba(Fe$_{1-x}$TM$_x$)$_2$As$_2$ compounds with TM = Co, Ni is a very intriguing behavior and stimulated active investigations both experimentally and theoretically. After the work of [1], this so-called BNC scaling relation was expanded with an increasing list of the iron pnictide and iron chalcogenide (FePn/Ch) superconducting (SC) compounds [2–9], hence strengthens the speculation that some generic mechanism must exist behind this unusual scaling behavior.

However, recently a few cases—all hole-doped systems—were also reported that they do not follow the ideal BNC scaling behavior. For example, the observation of a strong deviation from the BNC scaling in the K-doped Ba$_{1-x}$K$_x$Fe$_2$As$_2$ for $0.7 < x < 1$ [10] is contrasted to the Na-doped Ba$_{1-x}$Na$_x$Fe$_2$As$_2$ (0.1 $\leq x \leq 0.9$) [8] which displays an excellent BNC scaling. Furthermore, in a more recent measurement [11] on Na-doped K$_{1-x}$Na$_x$Fe$_2$As$_2$, the authors claimed that $\Delta C \sim T_c^\rho$ fits the data instead of $\sim T_c^2$ although data of this compound is limited to a very narrow range of $T_c$ variation. Summarizing the experimental situation, it is fair to say that the large majority of Fe-pnictide superconductors fits the BNC scaling $\Delta C \sim T_c^2$ but there exists a small subset of Fe-pnictide systems showing some deviation of varying degrees. In any case, all reported data of the Fe-pnictide
superconductors up to now universally exhibit anomalously strong non-BCS dependence\(^4\) between \(\Delta C\) versus \(T_c\), and it deserves a theoretical understanding.

For the theoretical investigations, there are three attempted explanations. Kogan [13] argued that strong pair-breaking can cause \(\Delta C/T_c \propto T^2\). The essence of this theory is a dimensional counting. The free energy difference near \(T_c\), \(\Delta F = F_i - F_n\), can be expanded in powers of \(\Delta^2/\Delta_c^2\): the SC order parameter (OP). In the BCS theory, \(\Delta F \propto -N(0) \frac{\Delta^f}{\Delta_c^2}\). Using the BCS result of \(\Delta^2(T) \sim T^2\left(1 - \frac{T}{T_c}\right)\), we get \(\Delta C/T_c \propto \frac{\partial^2 \Delta F}{\partial \Delta^2} \sim N(0)\), the well known BCS prediction. In the case of the strong pair-breaking limit, \(\Gamma_i \gg T_c\) (\(\Gamma_i = \text{pair-breaking rate}\)), considered by Kogan, \(\Delta F \propto -N(0) \frac{\Delta^f}{\Gamma_i^2}\) by a dimensional counting. Substituting the same BCS behavior of \(\Delta^2(T) \sim T^2\left(1 - \frac{T}{T_c}\right)\), we immediately recover Kogan’s result \(\Delta C/T_c \sim N(0) \frac{T_c^2}{\Gamma_i^2} \sim T^2\). However, we believe that this result is the consequence of an inconsistent approximation\(^5\). The theory of Vavilov et al [15] mainly studied the coexistence region with magnetic order \(M\) and SC order \(\Delta\). It is a plausible theory that the coexisting magnetic order over the SC order can substantially reduce \(\Delta C\), hence develops a steep variation of \(\Delta C\) versus \(T_c\). However this theory did not reveal any generic mechanism as to why \(\Delta C/T_c\) follows the BNC scaling \(\sim T^2\). Finally, Zannen [16] attributed the origin of \(\Delta C \propto T^2\) to the anomalous temperature dependence of the normal state electronic SH with the scaling form \(C^\text{elec}_{\text{Ni}} \propto T^3\) due to the critical fluctuations near the quantum critical point (QCP). A problem of this theory is that there is no evidence of \(C^\text{elec}_{\text{Fe}} \propto T^3\) for a wide doping range of the FePn/Ch superconductors. Moreover all three theories mentioned above are single band theories and do not particularly utilize the unique properties of the FePn/Ch superconductors. In this paper, we propose a theory in which the multi-band nature of the FePn/Ch superconductors is the root cause for producing the BNC scaling behavior.

2. Minimal two band model for the SH jump \(\Delta C\)

The SH jump \(\Delta C\) in any 2nd order phase transition is an indication of the entropy change through the phase transition at \(T_c\). For SC transition, regardless of pairing mechanism, \(\Delta C\) is due to the opening of the SC gap on Fermi surface and its magnitude is proportional to how rapidly the gap opens\(^6\). We also note that the Fe-based superconductors are multi-band superconductors, hence the total SH jump \(\Delta C\) should be a summation of the SH jump contribution of each band. Therefore, the standard single band formula [17] should be generalized for many bands as

\[
\Delta C = \sum_{i=\text{h,e}} N_i(0) \left(-\frac{d\Delta_i^2}{dT}\right)_{T_c}.
\]

where the band index \(i\) counts the different bands, and \(N_i\) are the DOSs and \(\Delta_i\) are the SC OPs of each band. For the minimal two band model, which will be used in this paper, \(i\) counts the hole and electron bands typical in the Fe-based superconductors.

In the one band BCS superconductor, using \(\Delta^2(T) \sim T^2\left(1 - \frac{T}{T_c}\right)\), the above equation yields the BCS result \(\Delta C/T_c \propto N(0) = \text{const.}\). However, in the case of a multiband superconductor, with the same BCS pairing mechanism but generalized to multiband, the standard single band BCS result can strongly deviate for the following reasons. First, each \(\Delta_i^2 \propto a_i T^2\) has non-universal and strongly band dependent coefficient \(a_i\) because \(a_i\) is determined by the combination of \(N_i\) of several bands and the inter- and intra-band pairing interactions \(V_{ij}\) among them. Second, the size of \(\Delta_i\) and \(N_i\) is inversely correlated when the interband pairing is dominant [18], hence equation (1) is not a simple summation of the BCS behavior of many bands. Therefore, the behavior of equation (1) for the multi-band superconductors can reveal more information about the pairing interactions as well as the pairing state.

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\(^4\) According to the standard single band BCS theory, \(\Delta C/T_c \sim N_{\text{elec}}(0)\). If we adopt this single band BCS formula to understand the typical BNC scaling data, it would require that the total DOS \(N_{\text{elec}}(0)\) of Fe-pnictides should change by two orders of magnitude by doping. Although there is a large uncertainty in the experimental data, the variation of \(N_{\text{elec}}(0)\) by doping is less than a factor 3 (within the hole and electron doping regions, respectively) [12].

\(^5\) In the strong pair-breaking limit (\(\Gamma_i > T_c\)) where \(\Delta F \propto -N(0) \frac{\Delta^f}{\Gamma_i^2}\) is valid, the behavior of \(\Delta(T)\) should also change to \(\Delta^2(T) \propto T^2\left(1 - \frac{T}{T_c}\right)\) instead of the BCS behavior \(\Delta^2(T) \propto T^2\left(1 - \frac{T}{T_c}\right)^2\). Then the SH jump in this limit becomes \(\Delta C/T_c \propto N(0) \frac{T_c^2}{\Gamma_i^2} \sim T^2\), quite opposite to the BNC scaling.

\(^6\) One assumption for this statement is that fermionic quasiparticles are defined as low energy excitations both at normal state and superconducting state, of course, with different contents for each phase. Then, the general form of entropy can always be written as \(S = -2k_a \sum \{(1 - f_i) \ln(1 - f_i) + f_i \ln f_i\} (f_i = \text{Fermi–Dirac distribution function}).\) This statement is more general than the BCS theory and holds regardless of pairing mechanism. The SH jump \(\Delta C\) is derived by taking a differentiation as \(\frac{\partial S}{\partial T}\).
At present the most widely accepted pairing state in the Fe-based superconductors is the sign-changing $s$-wave state ($s_\pm$-wave) mediated by a dominant interband repulsive interaction ($V_{\text{inter}} > V_{\text{intra}}$) between the hole band(s) around $\Gamma$ point and the electron band(s) around $M$ point [19]. In real compounds, there exist multiple hole and multiple electron bands with their corresponding SC OP's $\Delta_i$ [20] and there should exist a multitude of inter- and intra-band pairing interactions $V_{ij}$ among them. However, we notice that the SH and $T_c$ studied in this paper, are the thermodynamically averaged quantities and these two quantities do not sensitively depend on the details of the multiple hole bands and multiple electron bands. Instead, the total SH and $T_c$ are determined by the interaction between the averaged hole bands and the averaged electron bands in the following way:

$$N_0 = N_{h1} + N_{h2} + \ldots$$

and

$$\Delta_0 = [N_{e1} \Delta^e_{h1} + N_{e2} \Delta^e_{h2} + \ldots]/N_0 \quad (\text{when } T \to 0)$$

and a similar definition for the electron bands. Therefore, as far as we are interested in the relation between the total SH jump $\Delta C$ and $T_c$, the minimal two band model is sufficient and the values of $N_{b(i)e}$ and $\Delta_{b(i)e}$ in our two band model should be understood as the thermodynamically averaged quantities as above.

Having justified the two band model for the study of the SH jump $\Delta C$ versus $T_c$, we again emphasize that our purpose of this paper is not to prove any pairing mechanism or model for the Fe-based superconductors but to test a minimal model to see how much we can understand the BNC scaling with it. The essential physics of the two band $s_\pm$-wave state can be studied with the two coupled gap equations [21]

$$\Delta_h = - [V_{he} N_h \chi] \Delta_h - [V_{he} N_e \chi] \Delta_e,$$

$$\Delta_e = - [V_{eh} N_e \chi] \Delta_e - [V_{eh} N_h \chi] \Delta_h,$$

(2)

where the pair susceptibility $\chi$ at $T_c$ is defined as

$$\chi(T_c) = \frac{\pi}{2} \sum_\alpha \int_{-\delta_0}^{\delta_0} d\xi \frac{1}{\omega_\alpha + \xi} \approx \ln \left[ \frac{1.14 \Lambda_0}{T_c} \right],$$

(3)

where $\omega_\alpha = \pi T_c (2n + 1)$ and $\delta_0$ is a pairing energy cut-off. The pairing potentials $V_{ab}$ ($a,b = h,e$) are all positive and further simplified in this paper as $V_{he} = V_{he} = V_{\text{int}}$ and $V_{eh} = V_{eh} = V_{\text{intra}}$ without loss of generality.

In the limit $V_{\text{intra}}/V_{\text{inter}} \to 0$, equation (2) can be analytically solved and provides the interesting kinematic constraint relation [18]

$$\frac{\Delta_h}{\Delta_e} \sim \sqrt{\frac{N_e}{N_h}} \quad \text{as } T \to T_c,$$

(4)

and the critical temperature is given by

$$T_c \approx 1.14 \Lambda_0 \exp \left[ -1/(V_{\text{inter}} \sqrt{N_h N_e}) \right].$$

(5)

To calculate the experimental data of $\Delta C$ versus $T_c$ for a Fe-122 compound with a series of doping, we need a modeling of doping. First, we notice that the undoped parent compound such as BaFe$_2$As$_2$ is a compensated metal, hence has the same number of electrons and holes, i.e. $n_h = n_e$. Therefore it is a reasonable approximation to take $N_{h1} = N_{h2}$ at no doping and then the doping of holes (K, Na, etc) or electrons (Co, Ni, etc) is simulated by varying $N_{h2}$ and $N_e$ while keeping $N_{h1} + N_{h2} = N_{\text{tot}} = \text{const}$. We have several remarks on this modeling of doping: (1) the assumption $N_{\text{tot}} = \text{const}$ is only for convenience. The sensitive parameters of our model are the relative values between $N_e$ and $N_h$ but not the total DOS $N_{\text{tot}}$. Therefore, we use normalized parameters such as $N_{b(i)e} = N_{b(i)e}/N_{\text{tot}}$ and dimensionless coupling constants $V_{\text{inter/intra}} = N_{\text{tot}} \cdot V_{\text{inter/intra}}$ in our calculations. (2) We do not literally mean $n_{b(i)e} = N_{b(i)e}$. The actual change of DOS $N_{b(i)e}$ with doping ‘$x’$ (holes or electrons) should be complicated and also nonlinear. What our model assumes is: $N_{h1} \approx N_h$ at no doping and the difference of DOSs $\Delta N_h = N_h - N_{h1}$ increases with doping. This assumption is consistent with the angle-resolved-photo-emission-spectroscopy measurements of (Ba$_{1-x}$K$_x$)$_2$Fe$_2$As$_2$ [22] and Ba (Fe$_{1-x}$Co$_x$)$_2$As$_2$ [23] which show the systematic changes of hole (electron) FS sizes with dopings. For the rest of

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7 This thermodynamic average formula is consistent with the experimental gap values. For example, in the optimal doped Ba$_{1-x}$K$_x$Fe$_2$As$_2$ [20], the gap values $\Delta_{h1} = 12.3$ meV, $\Delta_{h2} = 5.8$ meV for the hole bands, combined with an estimate of the relative DOSs from the sizes of the FSs $N_{h1}/N_{h2} \sim 2$ gives $\Delta_{h1}^e \approx 8$ meV, and for the electron band gaps $\Delta_{e1} = 12$ meV, $\Delta_{e2} = 11.4$ meV with $N_{e1}/N_{e2} \sim 1$ gives $\Delta_{e1}^e \approx 12$ meV. The obtained values $\Delta_{h1}^e/\Delta_{h2}^e \approx 2/3$ and $N_{h1} = (N_{h2} + N_{h1})/N_{h1} = (N_{e1} + N_{e2})/2 \approx 3/2$ are then consistent with the inverse relation of our two band model ($N_{h1} \approx N_{h2}$ as $T \to 0$, and $\sqrt{N_{h1}/N_{h2}} \approx \sqrt{N_{e1}/N_{e2}}$ as $T \to T_c$).

8 As we mentioned in footnote 4, $N_{e1}$ can change by a factor 3 with dopings in real compounds. In our two band model, changing the value $N_{e1}$ would change the results of $\Delta C$ and $T_c$. However, when we plot $\Delta C$ versus $T_c$, the effect of varying $N_{e1}$ is mostly cancelled in the relation of $\Delta C$ versus $T_c$.

9 For the undoped parent compound BaFe$_2$As$_2$, our model assumes $N_{e1} = N_{h1} \approx 0.5$. For electron doping in Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$, hole pocket (s) disappears ($N_{h1} = 0$) around $x \approx 0.15$. For the hole doping cases, electron pockets (s) disappear ($N_{e1} = 0$) in (Ba$_{1-x}$K$_x$)Fe$_2$As$_2$, when $x > 0.7$ but in (Ba$_{1-x}$Na$_x$)Fe$_2$As$_2$, the electron pocket still remains when $x \approx 1$. Therefore, the actual doping ‘$x’$ and our model doping parameter $N_{e1}$ should be properly rescaled according to the $T_c$ variation versus doping.
this paper, it is convenient to use the normalized DOSs as \( \bar{N}_{h,e} = N_{h,e}/N_{\text{tot}} \) and define the dimensionless coupling constants as \( V_{\text{intra/inter}} = N_{\text{tot}} \cdot V_{\text{intra/inter}} \).

Expanding the gap equation (2) near \( T_c \) and using equation (4), we obtain \( \Delta_{h,e}(T) \) near \( T_c \) as

\[
\Delta_{h}^2(T) \approx \frac{2}{1 + N_h/N_e} \Delta_{\text{BCS}}^2(T), \\
\Delta_{e}^2(T) \approx \frac{2}{1 + N_e/N_h} \Delta_{\text{BCS}}^2(T)
\]

(6)

with \( \Delta_{\text{BCS}}^2(T) = \pi^2 \frac{\hbar^2}{2m(1)} T_c^2 (1 - T/T_c) \). Combining the results of equations (4) and (6), equation (1) provides

\[
\frac{\Delta C}{T_c} \approx 4 \times (3.06)^2 N_{\text{tot}} \cdot (\bar{N}_h \bar{N}_e).
\]

(7)

This is our key result of this paper. In contrast to the one band BCS superconductor, equation (7) clearly shows that \( \Delta C/T_c \) can have a strong \( T_c \) dependence through \( \bar{N}_h \bar{N}_e \) even with a constant \( N_{\text{tot}} \) (see equation (5)). With doping in a given FePn/Ch compound, \( \bar{N}_h \) and \( \bar{N}_e (=1 - \bar{N}_h) \) varies over the range of [0, 1] (see footnote 8). As such if \( (\bar{N}_h \bar{N}_e) \sim T_c^2 \) at least for some region of \( \bar{N}_{h,e} \) we would obtain the BNC scaling for that region.

Having analyzed the simple case \( V_{\text{intra}} = 0 \), in the next section we numerically study more realistic cases with \( V_{\text{intra}} \neq 0 \) and including the impurity scatterings. We solve the coupled gap equation (2) for \( \Delta_{h,e}(T) \) near \( T_c \) and directly calculate \( \Delta C \) using equation (1). We find that the non-pair-breaking impurity scattering plays a crucial role in order to explain the ideal BNC scaling \( \Delta C/T_c \sim T_c^2 \) in BaFe\(_{1-x}\)TM\(_x\)As\(_2\) (TM = Co, Ni) as well as a strong deviation in Ba\(_{1-x}\)K\(_x\)Fe\(_2\)As\(_2\))\(_{10}\).

3. Numerical results

In figure 1(A), we calculated \( T_c \) versus \( \bar{N}_h \) of the two band model equation (2) for \( V_{\text{inter}} = 1.0 \) and 2.0, respectively, with \( V_{\text{intra}} = 0 \) for both cases. Indeed, the calculated \( T_c \) shows a strong dependence on \( \bar{N}_h \), symmetric with respect to \( \bar{N}_h = 0.5 \). We plot the same data as \( \bar{N}_h \cdot \bar{N}_e \) versus \( T_c \) in figure 1(B). In the case of \( V_{\text{inter}} = 2.0 \), we find \( \bar{N}_h \cdot \bar{N}_e \sim T_c^2 \) near the maximum \( T_c \) region which is the necessary condition for the BNC scaling from equation (7). It also shows that the overall power of the relation \( \bar{N}_h \cdot \bar{N}_e \sim T_c^2 \) becomes weaker with the weaker pairing potential \( V_{\text{inter}} \). Now we calculate \( \Delta C(\bar{N}_h) \) and \( T_c(\bar{N}_h) \) from equations (1) and (2). \( \Delta C(\bar{N}_h) \) and \( T_c(\bar{N}_h) \) are implicitly related through \( \bar{N}_h \in [0, 1] \). In figure 1(C), we plot \( \Delta C/T_c \) versus \( T_c \) in log–
log scale, for different pairing potentials $V_{\text{inter}} = 1.0, 1.5, 2.0, 3.0$ and $5.0$, respectively, with $V_{\text{intra}} = 0.0$ for all cases. First, as seen in figure 1(C), we can see the general trend that the region where the BNC scaling $\Delta C/T_c \sim T_c^{\delta}$ holds becomes widened near the maximum $T_c$ region with increasing the pairing potential strength $V_{\text{inter}}$. With extensive numerical experiments, we found: (1) $\Delta C/T_c$ becomes $\sim T_c^{\delta}$ for the whole range if $V_{\text{inter}} > 5.0$, however, this strength of pairing potential might be unrealistically strong. (2) Including $V_{\text{intra}} = 0.0$ does not change the general behavior shown in figure 1(C) as long as $V_{\text{intra}} < V_{\text{inter}}/2$. (3) Finally, as $T_c$ approaches its maximum value (as $N_{\text{intra}} \rightarrow 0.5$), $\Delta C/T_c$ approaches the BCS limit ($9.36N_{\text{BCS}}$) for weak coupling ($V_{\text{inter}} < 1.0$) and exceeds it for strong coupling ($V_{\text{inter}} > 1.0$). This shows that our results—although our model is a mean field theory—partially capture a strong coupling effect by full numerical calculations of $\Delta(T)|_{\mu}$.

Although it is not completely successful to produce the ideal BNC scaling behavior, the results of the generic two band model in figure 1(C) is remarkably non-BCS and very encouraging in that it shows that $\Delta C/T_c$ has changed more than one order of magnitude with $N_{\text{inter}} = \text{const.}$ for all calculations. However, the BNC scaling behavior is still limited in a region near the higher $T_c$ region (where $\Delta N = |N_{\text{intra}} - N_{\text{inter}}|$ is small) and we need an extra mechanism to extend the power law scaling behavior at lower temperatures. We remind the fact that the jump $\Delta C$ occurs at $T_c$ (a finite temperature) and the impurity scattering effect will be increasingly effective at lower temperatures. In particular, if the impurity scattering should efficiently reduce $\Delta C$ but not so much affect $T_c$, then the slope of $\Delta C/T_c$ versus $T_c$ would become steeper in this region and the region of the BNC scaling would be widened even with a moderate strength of $V_{\text{intra}}$.

Phenomenologically we can consider two kind of impurity scattering in the two band model: $\Gamma_h$ (intra-band scattering) and $\Gamma_c$ (inter-band scattering)\textsuperscript{10}. As we assumed the $S_{\text{BCS}}$-wave state, $\Gamma_c$ causes strong pair-breaking effect (e.g. suppression of $T_c$ and reduction of $\Delta_{\text{BCS}}$), while $\Gamma_h$ does not affect the superconductivity itself\textsuperscript{[24]}. For example, the pair-breaking scattering $\Gamma_c$ enters the pair-susceptibility $\chi_{h_c}(\Sigma) = T_c^{2} \sum_{\nu} \int_{-\infty}^{\infty} \frac{d\nu}{2\pi} \chi_{\nu}^{h_c}(\Sigma) \chi_{\nu}^{h_c}(\Sigma)$ of equation (3) replacing as $\omega_{\nu} \rightarrow \omega_{\nu} + \Gamma_c$. As a result, $\Gamma_c$ directly affects both $T_c$ and $\left(-\frac{d\Delta_c}{dt}\right)$. However, we have already discussed in the Introduction that increasing $\Gamma_c$ does not help to produce the BNC scaling (see footnote 4). On the other hand, there is another effect of the impurity scattering which does not directly affect the superconductivity, namely the quasiparticle broadening. This quasiparticle broadening is determined by the total scattering rate $\Gamma_{\text{tot}} = \Gamma_h + \Gamma_c$ and the SH jump of $\Delta C$ of equation (1) should take into account of this quasiparticle broadening as follows\textsuperscript{[25]},

$$\Delta C = \sum_{\nu = h,c} N_{\nu} \left( -\frac{d\Delta_c}{dt} \right) \left| L_{\nu} \int_{0}^{\infty} \frac{dx}{2} \frac{1}{\cosh^{2} \left( \frac{x}{2} \right)} \frac{x^{\delta}}{x^{\delta} + \lambda^{\nu}_{\text{BCS}}}, \right. (8)$$

where $x = \omega/T_c$. Compared to equation (1), the additional integration part in the above equation contains the thermal average effect including the quasiparticle broadening $\Gamma_{\text{tot}}$. And it shows that the non-pair-breaking scattering rate $\Gamma_h$ entering the thermal average part can strongly reduce $\Delta C$ without affecting $T_c$.

In figure 2, we show the numerical results of $\Delta C/T_c$ versus $T_c$ in log–log scale with a choice of a moderate strength of the pairing potentials, $V_{\text{inter}} = 2.0$ and $V_{\text{intra}} = 0.5$\textsuperscript{11} and varied the impurity scattering rates $\Gamma_h$ and $\Gamma_c$. First, all cases, with and without impurity scattering, show a strong deviation from the standard BCS limit (the horizontal dashed line). This behavior is the generic feature of the multiband superconductors as we explained in the previous section. The case without impurity scattering (red ‘×’ symbols, $\Gamma_h = \Gamma_c = 0$), $\Delta C/T_c$ shows the $T_c^{2}$ scaling only for the limited region near the maximum $T_c$ and it quickly becomes flatterened and slower than $\sim T_c^{1}$. Interestingly, this behavior looks very similar to the experimental data of Ba$_{1-x}$K$_x$Fe$_2$As$_2$\textsuperscript{[10]}. Therefore, we speculate that Ba$_{1-x}$K$_x$Fe$_2$As$_2$ system belongs to the clean limit superconductor. This is understandable since K and Ba ions are out of the Fe–As planes and hence the doped K ions would introduce much weaker impurity potentials for the superconductivity. Next, only a small increase of impurity scattering (green ‘+’ symbols, $\Gamma_h = 0.02$ in unit of $\lambda_{\text{BCS}}$) immediately changes $\Delta C/T_c$ versus $T_c$ steeper such as $\Delta C/T_c \sim T_c^{1.5}$ over the whole $T_c$ range. Further increasing the impurity scattering rate the case with $\Gamma_h = 0.1$ and $\Gamma_c = 0.05$ (pink ‘◆’ symbols) displays an ideal BNC scaling $\Delta C/T_c \sim T_c^{2}$ for the entire range of $T_c$. For the demonstration purposes, we also calculated the case with unrealistically large impurity scattering rates, $\Gamma_h = 0.5$ and $\Gamma_c = 0.05$ (dark yellow ‘+’ symbols), which displays $\Delta C \sim T_c^{4}$, a super-strong scaling.

\textsuperscript{10}In general, the impurity potential is a momentum dependent function $\Gamma(q)$. For the $S_{\text{BCS}}$-wave pairing state, a large momentum $g \sim |q| \sim |q|$, scattering part acts as a pair-breaking component $\Gamma_h$ and the small momentum $|q| \ll |q|$, scattering part acts as a non-pair-breaking component $\Gamma_c$.

\textsuperscript{11}As can be seen in figure 1(c), any choice of values in between $1.5 < V_{\text{intra}} < 3.0$ would yield qualitatively similar results. Also the dimensionless interaction $V_{\text{inter}} = V_{\text{intra}} \cdot N_{\text{inter}}$ defined in our paper should be compared to a more conventional dimensionless interaction, defined in the $T_c$-equation (see equation (5)), $\tilde{\lambda}_{\text{inter}} = V_{\text{intra}} \cdot N_{\text{inter}} \sqrt{N_{\text{intra}}/N_{\text{BCS}}}$. This means that the typical dimensionless coupling strength can be $0.75 < \tilde{\lambda}_{\text{inter}} < 1.5$. 

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Although it is not our main interest in this paper, we have a remark on the absolute magnitude of $\Delta C / T_c$ which is traditionally compared to the Sommerfeld coefficient

$$\gamma_{\text{normal}} = \frac{2\pi T_c^3}{3} N(0).$$

The BCS value $R = \Delta C / T_c = 1.43$ is a common criterion to indicate the strong coupling superconductors (if $R > 1.43$). However, reliable measurement of $\gamma_{\text{normal}}$ is difficult in most of cases and that was the original reason why Canfield and coworkers [1] plotted $\Delta C / T_c$ versus $T_c$ instead of the conventional plotting of $\Delta C / T_c$ versus $\gamma_{\text{normal}}$. In figure 2, the values of $\Delta C / T_c$ in clean limit ($\Gamma_0 = 0, \Gamma_x = 0$) have a maximum value slightly above the BCS limit ($1.43 \gamma_{\text{BCS}} = 9.36 N(0)$) and other cases with finite impurity scatterings have the reduced values of $\Delta C / T_c$ because the SH jump becomes broadened by the impurity scatterings—both by $\Gamma_0$ and $\Gamma_x$. These values and the trend are not inconsistent with most of experiments. Among the data collected in [12], it is notable that the Co-doped $\text{Ba(Fe}_{1-x}\text{Co}_x)_{2}\text{As}_2$ compounds have uniformly smaller value of $R < 1.43$ while the K-doped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ compounds have values $R$ from slightly to moderately larger than $R_{\text{BCS}} = 1.43$. As discussed in the next section, this different trend can be understood from the fact that the K-doping in $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ does not introduce strong impurity scattering while the Co-doping in $\text{Ba(Fe}_{1-x}\text{Co}_x)_{2}\text{As}_2$ does introduce strong impurity scattering. And in general the magnitude of $\Delta C / T_c$ increases with increasing the strength of the pairing interaction ($V_{\text{int}}$) due to a strong coupling effect as shown in figure 1(C).

4. BNC scaling and its deviation

The main message of the numerical calculations in figures 1 and 2 is: (1) the strong non-BCS relation (see footnote 3) of $\Delta C \sim T_c^{\alpha}$ with a power $\alpha$ larger than $\alpha = 1$(BCS limit) is a generic feature of the multiband superconductors, and this is due to a pure kinematic constraint of equation (4); (2) however, the system needs some amount of impurity scattering (for example, $\Gamma_0/T_c^0 \approx 1/3$, the pink $\diamond$ symbols in figure 2) to have the

$$R_{\text{BCS}} = \frac{\Delta C}{T_c}$$

Figure 2. Numerical calculations of $\Delta C / T_c$ versus $T_c$ with $V_{\text{int}} = 2.0$ and $V_{\text{intra}} = 0.5$, for different impurity scattering strengths of $\Gamma_0$ and $\Gamma_x$ (in unit of $\Lambda_0$). Horizontal dashed line is the BCS limit of $9.36 N(0)$ and the dotted lines of $\sim T_c^0$ (BNC scaling) and $\sim T_c^3$ (super-strong scaling) are guides for the eyes.

$\text{Ba(Fe}_{0.925}\text{Co}_{0.075})_2\text{As}_2$ 1.26 [26]
$\text{Ba(Fe}_{0.92}\text{Co}_{0.08})_2\text{As}_2$ 1.2 [27]
$\text{Ba}_{0.65}\text{Na}_{0.35}\text{Fe}_2\text{As}_2$ 1.26 [28]
$\text{Ba}_{0.68}\text{K}_{0.8}\text{Fe}_2\text{As}_2$ 1.55–2.0 [29, 30]
$\text{Ba}_{0.64}\text{K}_{0.32}\text{Fe}_2\text{As}_2$ 2.4 [31]
$\text{KFe}_2\text{As}_2$ 0.3 [32]
$\text{LiFeAs}$ 1.24 [33]
$\text{FeSe, FeTe}_{0.57}\text{Se}_{0.43}$ 1.65, 2.11 [34, 35]

References
observed BNC scaling. If the impurity scattering strength is weaker, a deviation from the BNC scaling becomes stronger, in particular in the low $T_c$ region. These theoretical features can consistently explain why a majority of the Fe-based pnictides [1–9] follow the BNC scaling but some systems [10, 11] show a deviation from it.

We note that most of data which best fit the BNC scaling are from the electron doped compounds Ba(Fe₁₋ₓTMₓ)$_2$As₂ (TM transition metals such as Co, Ni). Electron doping ions, replacing Fe sites, directly enters onto the Fe–As plane so that they introduce more efficient scattering centers (pair-breaking and non-pair-breaking (see footnote 9)). Therefore, the electron doped systems will have a sufficient strength of impurity scattering to produce an ideal BNC scaling as shown in figure 2. On the other hand, in the case of the hole doped systems such as (Ba₁₋ₓKₓ)Fe₂As₂[10], (K₁₋ₓNaₓ)Fe₂As₂[8, 11], and (Ba₁₋ₓNaₓ)Fe₂As₂[8], etc the doped ions enters in between the Fe–As planes so that they will introduce relatively weak scattering centers. Therefore, the hole doped systems would have more chance to be in the weak impurity scattering limit, hence would have more chance to deviate from the ideal BNC scaling. In fact, the case of (Ba₁₋ₓKₓ)Fe₂As₂[10] shows a very strong deviation from the BNC scaling and the case of (K₁₋ₓNaₓ)Fe₂As₂[8, 11] shows a moderate deviation as $\Delta C \sim T^2_c$ (although this power law has a large uncertainty because it has a very limited data distribution). On the other hand, another hole doped system (Ba₁₋ₓNaₓ)Fe₂As₂[8] displays a perfect BNC scaling. According to our theory, we should conclude that Na ions substituting Ba ions should create relatively strong scattering centers although they enter in between the Fe–As planes. This speculation is quite reasonable because the difference of the ion sizes between Na$^{+}$ (period 3) and Ba$^{2+}$ (period 6) is the largest compared to the other cases where the combinations are between K$^{+}$ (period 4) and Ba$^{2+}$ (period 6), and between Na$^{+}$ (period 3) and K$^{+}$ (period 4).

All these behaviors tell us that the BNC scaling is indeed a reflection of the specific features of the Fe-based superconductors. Namely, the slope of $\Delta C$ versus $T_c$ in the Fe-based superconductors is universally much steeper than the BCS limit due to the generic feature of the multiband superconductors. Then doping inevitably provides a sufficient strength of impurity scattering (in particular, the electron doped cases) which makes the already steep slope of $\Delta C$ versus $T_c$ into a BNC power law $\Delta C \sim T^2_c$. When the impurity scattering is not sufficiently strong (mostly, hole doped systems), a varying degrees of deviation from the ideal BNC scaling would occur.

5. Coexistence region with the magnetic and SC orders

Experiments showed that the BNC scaling continues to be valid even when the spin density wave (SDW) order coexists with the SC order in the underdoped regime [5]. Therefore we would like to extend our model including the magnetic order in the underdoped regime. We consider only the hole doped region $N_h \in [0.5, 1]$, because our model is symmetric with respect to the hole or electron dopings. We took a simple phenomenological approach ignoring the self-consistent calculation of the magnetic and the SC orders. We arbitrarily chose the coexistence region for $0.5 < N_h < 0.7$ (this is the underdoped regime; $N_h = 0.5$ means no doping in our model), just for the sake of demonstration, and introduced the magnetic order $M (N_h)$ for this region by hand. This negligence of the self-consistency is a posteriori well justified by the result we found that the BNC scaling relation $\Delta C / T_c \sim T^2_c$ is insensitive to the details of $M (N_h)$.

We assumed that the magnetic OP $M (N_h)$ linearly grows from zero at $N_h = 0.7$ to a maximum value $M_{\text{max}}$ at $N_h = 0.5$ as shown in figure 3(A). When a finite $M$ exists, it affects the superconductivity in two important ways: (1) it weakens the SC pair susceptibility and we take the simplest approximation as $M_{\text{eff}} (M) = T_c \sum_{\text{f}} \sum_{\text{oc}} \frac{\delta^f}{2 \pi^2 \varepsilon^2_f + \Delta^2}$ [15]; (2) the presence of SDW order $M$ also removes a part of the FSs. Phenomenologically, we take this effect into account by linearly reducing the total DOS $N_{\text{tot}}$ starting from $N_{\text{tot}} = 0.7$ to a maximum reduction at $N_h = 0.5$ as $N_{\text{tot}} (N_h) = N_{\text{tot}}^0 \left[1 - a \frac{M (N_h)}{N_h^0}ight] (a = 0.5$ was chosen for calculations in figure 3; for example, $N_{\text{tot}}$ reduced to $\frac{1}{2} N_{\text{tot}}^0$ at $N_h = 0.5$ with $\frac{M_{\text{max}} (N_h = 0.5)}{N_h^0} = 1.0$). With these phenomenological ansätze, we solved the $T_c$ equations from equation (2) with fixed pairing interactions and impurity scattering rates ($\tilde{V}_{\text{inter}} = 2.0$, $\tilde{V}_{\text{intra}} = 0.5$; and $\Gamma_h = 0.10$, $\Gamma_c = 0.05$) for three different strengths of $M (N_h)$ in figure 3(A). The results qualitatively simulate the experimental phase diagram: $T_c$ starts decreasing when $M (N_h)$ starts growing from $N_h = 0.7$ to a maximum value $M_{\text{max}}$ at $N_h = 0.5$ and the reduction of $T_c$ is faster with a stronger magnetic order. For the region where $M = 0$ for $N_h > 0.7$, the calculations of $T_c$ and $\Delta C$ are the same as the results in figure 2.

In figure 3(B), $\Delta C / T_c$ versus $T_c$ is calculated for the corresponding three cases of figure 3(A). The data with dark yellow ‘o’ symbols, displaying the $\Delta C \sim T^2_c$ BNC scaling, is the same calculation as in figure 2 with $\Gamma_h = 0.10$ and $\Gamma_c = 0.05$ but only over the region $N_h \in [0.7, 1]$ where $M = 0$. Then the three solid symbols are the calculation results for the region of $N_h \in [0.5, 0.7]$ with three different strengths of magnetic order $M (N_h)$ of figure 3(A). The results of figure 3(B) reveal an interesting behavior. Namely, while it is more natural to expect that the relation between $\Delta C$ and $T_c$ should dramatically change with and without a magnetic order [15], the
calculations of figure 3(B) with the coexisting magnetic and SC orders show that the BNC scaling is robustly obeyed even with widely different strengths of M. We trace the origin of this surprising result to the fact that the underdoped region (i.e. where $N_{h} / N_{tot} = 0.7, 1$) where $M(N_{h}) = 0$, $T_{c}$ are all the same for three cases. Open symbols are the magnitudes of the corresponding magnetic order $M(N_{h})$. The pairing interactions and the impurity scattering rates are chosen $V_{inter} = 2.0$, $V_{intra} = 0.5$, and $\gamma = 0.10$, $\gamma = 0.05$, respectively. (B) Calculated $\Delta C / T_{c}$ versus $T_{c}$ for the corresponding three cases of (A). The results for the region $N_{h} \notin [0.7, 1]$ where $M(N_{h}) = 0$ are the same for all three cases and displayed with dark yellow ‘+’ symbols.

Figure 3. (A) Numerical calculations of $T_{c}$ (solid symbols) versus $N_{h}$ with coexisting magnetic order $M(N_{h})$ of three different strengths of $M_{max}$ ($N_{h} = 0.5, N_{h} = 1.0, N_{h} = 0.6$) in (blue), (red), and (green) (in unit of $\Lambda_{hh}$). For the region $N_{h} \notin [0.7, 1]$ where $M(N_{h}) = 0$, $T_{c}$ are all the same for three cases. Open symbols are the magnitudes of the corresponding magnetic order $M(N_{h})$. The pairing interactions and the impurity scattering rates are chosen $V_{inter} = 2.0$, $V_{intra} = 0.5$, and $\gamma = 0.10$, $\gamma = 0.05$, respectively. (B) Calculated $\Delta C / T_{c}$ versus $T_{c}$ for the corresponding three cases of (A). The results for the region $N_{h} \notin [0.7, 1]$ where $M(N_{h}) = 0$ are the same for all three cases and displayed with dark yellow ‘+’ symbols.

6. Summary and conclusions

We have shown that the puzzling BNC scaling relation $\Delta C / T_{c} \sim T_{c}^{2}$ observed in a wide range of the FePt/Ch SC compounds [1–9] is a manifestation of the generic property of the multiband superconductor paired by a dominant inter-band pairing potential $V_{inter} \gg V_{intra}$. While each of $\Delta C(N_{h}, V_{c}, M)$ and $T_{c}(N_{h}, V_{c}, M)$ have non-trivial and non-universal dependencies on the material specific parameters such as the DOSs ($N_{h}$), pairing potentials ($V_{c}$), competition with SDW ($M$), etc, these non-universal dependencies are largely cancelled in the plot of $\Delta C / T_{c}$ versus $T_{c}$ because $N_{h}$, $V_{c}$, $M$, etc are implicit variables in this plot. As such, the $\Delta C / T_{c}$ plot filters out these material specific details and only reveals the universal and generic features of the Fe-based superconductors.
In this sense, the BNC plotting of $\Delta C$ versus $T_c$ was an ingenious idea—although it was originally done reluctantly in this way instead of the standard plotting of $\Delta C/C_N^{\text{ele}}$ versus $C_N^{\text{ele}}/T_c$ because of the lack of the reliable data of $C_N^{\text{ele}}$ (the normal state electronic SH). In a similar spirit, but in theory, our minimal two band model is a maximally simplified model only to capture the origin of this universal behavior by filtering out (in fact ignoring) the numerous details of the real materials. Using this minimal model, we were able to identify the origin of this universal behavior: the presence of one single parameter $N_0$ which governs both $\Delta C$ and $T_c$ (see equations (5) and (7)) and the kinematic constraint $\Delta e_c / \Delta e_n \sim (\Delta e_n / N_0)$ near $T_c$. Then a consideration of the non-pair-breaking impurity effect which broadens the quasiparticle spectra near $T_c$ explains the systematic evolution from the ideal BNC scaling \cite{1-9} to its deviations as found in Ba$_{1-x}$K$_x$Fe$_2$As$_2$\cite{10} and K$_{1-x}$Na$_x$Fe$_2$As$_2$\cite{11}. In essence, the BNC scaling and its varying degree of deviations reconfirm the fact that the Fe-based superconductors are the multiband superconductors paired by a dominant interband interaction.

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