Anomalous Scaling Relations and Pairing Mechanism of the Fe-based Superconductors

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Abstract. The anomalous scaling behavior of the specific heat jump $\Delta C$ vs. $T_c$ ($\Delta C \sim T_{c}^{\alpha}$, $\alpha \approx 3$), first observed by Bud’ko et al[1], has been confirmed with several families of the Fe-based superconducting compounds with various dopings. And more recently, Xing et al[2] have reported that the condensation energy (CE) vs. $T_c$ also follows an anomalous power law ($\Delta E \sim T_{c}^{\alpha}$) with about forty different samples of the Fe-based superconductors. These apparently non-BCS power law relations have strongly hinted at a non-BCS pairing mechanism of the Fe-based superconductors. We have studied a minimal two band BCS model to understand these anomalous scaling behaviors and showed that these non-BCS relations of $\Delta C \sim T_{c}^{3}$ as well as $\Delta E \sim T_{c}^{3.5}$ can be well reproduced by the simple two-band BCS model paired by a dominant interband repulsive interaction ($V_{inter} > V_{intra}$). The origin of these anomalous scaling relations are the kinematic constraint of $\frac{\Delta c}{\hbar} \sim \sqrt{\frac{\Delta e}{\hbar \omega}}$ near $T_c$ of the two band BCS model, as realized in the $s_{\pm}$-wave pairing state. Our results imply that these seemingly non-BCS-like scaling behaviors, on the contrary to the common expectations, are in fact strong experimental evidences that the pairing mechanism of the Fe-based superconductors is genuinely a BCS mechanism, meaning that the Cooper pairs are formed by the itinerant carriers glued by a pairing interaction.

1. Introduction
The pairing mechanism of the Fe-based superconductors (IBS) still remain an open question. It is because there is almost no direct experimental probe for identifying a pairing mechanism while there are numerous experimental probes for identifying the pairing symmetry or gap functions. In this regard, the anomalous scaling behavior of the specific heat jump $\Delta C$ vs. $T_c$ ($\Delta C \sim T_{c}^{\alpha}$), first observed by Bud’ko et al[1] and confirmed by many researchers[3, 4, 5, 6, 7] has stimulated many people to speculate this non-BCS relation as a strong evidence of the quantum critical point (QCP) driven superconductivity in IBS[8]. And more recently, Xiang et al[2] has reported another non-BCS scaling behavior with the condensation energy (CE) $\Delta E$ vs. $T_c$ ($\Delta E \sim T_{c}^{3.5}$) with about forty different samples of the IBS, which therefore reinforced the speculation that the QCP is the underlying reason for these anomalous scaling behaviors and its strong connection to the superconducting (SC) pairing mechanism itself.

While we do not know the microscopic pairing mechanism of the IBS, we noted that the multiband nature itself of the IBS has produced many unusual deviations[9, 10] from a standard single band BCS superconductors. Motivated by this simple idea, we studied a minimal two band BCS...
model with dominant interband repulsive interaction \((V_{\text{inter}} > 0)\) to calculate the \(\Delta C\) vs. \(T_c\) and the CE \(\Delta E\) vs. \(T_c\). To our surprise, we have found that the simple two band BCS model naturally produces both anomalous scaling relations simultaneously. Our results imply that these seemingly non-BCS-like scaling behaviors observed in the thermodynamic quantities, on the contrary to the common expectations, are in fact strong experimental evidences of a BCS pairing mechanism in the IBS. All strong correlation effects, abundantly observed in the normal state of the IBS, should renormalize the effective mass \(m^*\) of quasiparticles, density of states \(N_{h,e}\), the pairing interactions \(V_{\text{inter,intra}}(q)\), etc., but when the system enters the SC transition, the pairing mechanism itself seems to be governed by the BCS mechanism.

2. Minimal two Band model for the SH jump \(\Delta C\) vs. \(T_c\)

2.1. Formalism

We consider a minimal two band model for the IBS\([9]\) consisting of one hole band and one electron band; each band represents a thermodynamic average of a group of hole bands around \(\Gamma\) point and a group of electron bands around \(M\) point in the Brillouin zone (BZ). We assume that the pairing interactions \(V_{ab}(a,b = h,e)\) are all repulsive \((V_{ab} > 0)\) but with a dominant interband repulsion as \(V_{\text{he,eh}} > V_{\text{hh,ee}} > 0\). This is an extremely simplified phenomenological model and defined by the following coupled BCS gap equations.

\[
\begin{align*}
\Delta_h &= -[V_{hh}N_h \chi] \Delta_h - [V_{he}N_e \chi] \Delta_e, \\
\Delta_e &= -[V_{ee}N_e \chi] \Delta_e - [V_{eh}N_h \chi] \Delta_h,
\end{align*}
\]

where \(N_{h,e}\) are the DOS of the hole and electron bands, respectively, and the pair susceptibility \(\chi\) at \(T_c\) is defined as \(\chi(T_c) = T_c \sum_n \int_{-\hbar \omega_n}^{\hbar \omega_n} d\xi \frac{1}{\pi e^2} \approx \ln \left[ \frac{1.14A_0}{T_c} \right]\), with \(\omega_n = \pi T_c(2n+1)\), and \(A_0\) is a pairing energy cut-off. This model produces the \(s\)-gap solution in which the order parameter (OP) \(\Delta_{h,e}\) on each band has opposite sign and different magnitudes, in general\([9]\). In particular, in the limit \(V_{\text{inter}}/V_{\text{intra}} \to 0\), the above gap equations can be analytically solved and provides the following kinematic relation\([9]\)

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

and the critical temperature is also obtained as

\[
T_c \approx 1.14A_0 \exp \left[ -1/(V_{\text{inter}} \sqrt{N_e/N_h}) \right].
\]

And the total SH jump \(\Delta C\) should be a summation of the SH jump contribution of each band as follows

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

Now in order to calculate the experimental data of \(\Delta C\) vs. \(T_c\) for a Fe-122 compound with a series of doping, we need a modelling 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 \(N_h = N_e\) at no doping and then the doping of holes (K, Na, etc.) or electrons (Co, Ni, etc.) is simulated by varying \(N_h\) and \(N_e\) while keeping \(N_e + N_h = N_{\text{tot}} = \text{const.}\) We have several remarks on this modelling 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 \(N_{\text{tot}}\). (2) We do not literally mean \(n_{h(e)} = N_{h(e)}\). The actual change of DOS \(N_{h(e)}\) with
doping “x” (holes or electrons) should be complicated and also non-linear. What our model assumes is: \(N_h \approx N_e\) at no doping and the difference of DOSs \(|N_h - N_e|\) increases with doping. This assumption is consistent with the Angle-Resolved-Photo-Emission-Spectroscopy (ARPES) measurements of \((\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2[11]\) and \((\text{Ba}\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2[12]\) which show the systematic changes of hole (electron) Fermi surface (FS) sizes with dopings. For the rest of this paper, we use the normalized DOSs as \(N_{h,e} = N_{h,e}/N_{tot}\) and accordingly define the dimensionless coupling constants as \(V_{\text{intra/inter}} = N_{tot} \cdot V_{\text{intra/inter}}\).

In the case of \(V_{\text{intra}} = V_{hh,ee} = 0\), we can obtain the analytic solutions \(\Delta_{h,e}(T)\) near \(T_c\) as

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

\[
\Delta_e^2(T) \approx \frac{2}{1 + N_e/N_h} \Delta_{BCS}^2(T)
\]

with \(\Delta_{BCS}^2(T) = \pi^2 \frac{\hbar \xi(3)}{\hbar e^2} T_N^2 (1 - T/T_c)\). Substituting the results of Eq.(5) into Eq.(4) yields

\[
\frac{\Delta C}{T_c} \approx 4 \times (3.06)^2 N_{tot} \cdot (N_h,N_e).
\]

In contrast to the one band BCS superconductor, Eq.(6) clearly shows that \(\Delta C/T_c\) can have a strong \(T_c\) dependence through \(N_h, N_e\) even with a constant \(N_{tot}\). With doping in a given Fe-Pnictide/Chalcogenide (FePn/Ch) compound, \(N_h\) and \(N_e\) (= \(1 - N_h\)) can vary over the range of \(\tilde{N}_h, \tilde{N}_e = [0, 1]\).

In the next section, we will show numerical results for the cases of \(V_{\text{intra}} = 0\) and \(V_{\text{intra}} \neq 0\), and also include the impurity scatterings. We found that the non-pair-breaking impurity scattering plays a crucial role in order to explain the ideal BNC scaling \(\Delta C/T_c \propto T_N^2\) in \((\text{Ba}\text{Fe}_{1-x}\text{TM}_x)_2\text{As}_2\) (TM=Co,Ni) as well as a strong deviation in \((\text{Ba}_{1-x}\text{K}_x)\text{Fe}_2\text{As}_2[13]\).

### 2.2. Numerical results

In Fig.1, we show the numerical results of \(\Delta C(N_h) vs T_c(N_h)\) for the case of \(V_{\text{intra}} = 0.0\) for different inter-band potentials \(V_{\text{inter}} = 1.0, 1.5, 2.0, 3.0,\) and \(5.0\), respectively, where \(\Delta C(N_h)\) and \(T_c(N_h)\) are implicitly related through \(N_h \in [0, 1]\). With extensive numerical experiments, we found: (1) \(\Delta C/T_c\) becomes \(\sim T_N^2\) for the whole region if \(V_{\text{inter}} > 5.0\), however, this strength of pairing potential might be unrealistically strong. (2) Including \(V_{\text{intra}} \neq 0.0\) does not change the general behavior shown in Fig.1 as long as \(V_{\text{intra}} < V_{\text{inter}}/2\).

Although it is not completely successful to reproduce the ideal BNC scaling behavior, the results of the generic two band model in Fig.1 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 \(N_{tot} = \text{const.}\). However, the BNC scaling behavior is still limited in a region near the higher \(T_c\) region (where \(\Delta N = |N_e - N_h|\) is small) and we need an extra mechanism to extend the power law scaling behavior at the lower temperature region. We noticed from the experimental data that the size of jump \(\Delta C\) is more severely reduced by impurity scattering when the jump size is small (low \(T_c\) region in Fig.1) compared to when the jump size is large (higher \(T_c\) region in Fig.1).

Phenomenologically we can consider two kind of impurity scattering in the two band model: \(\Gamma_0\) (intra-band scattering) and \(\Gamma_\pi\) (inter-band scattering)[14]. As we assumed the \(s_\pm\)-wave state, \(\Gamma_\pi\) causes strong pair-breaking effect (e.g. suppression of \(T_c\) and reduction of \(\Delta_{h,e}\)), while \(\Gamma_0\) doesn’t affect the superconductivity itself[15]. Besides the standard impurity effects on \(T_c\) and \(\Delta_{h,e}[14]\), the quasiparticle spectra becomes broadened by the impurity scattering. Therefore the SH jump of \(\Delta C\) of Eq.(4) should be modified with this quasiparticle broadening as follows[16],

\[
\Delta C = \sum_{i=h,e} N_i \left( \frac{-d\Delta_i^2}{dT} \right) \left|_{T_c} \int_0^\infty dx \frac{1}{2\cosh^2\left(\frac{x}{2}\right)} \left( x^2 + \frac{1}{(\frac{T_c}{T})^2} \right) \right.
\]

(7)
where \( x = \omega / T_c \) and the total scattering rate \( \Gamma_{tot} = \Gamma_0 + \Gamma_\pi \). Eq. (7) shows that the non-pair-breaking scattering rate \( \Gamma_0 \) entering the thermal average part can strongly reduce \( \Delta C \) without affecting \( T_c \). In Fig. 2, we show the numerical results of \( \Delta C / T_c \) vs. \( T_c \) with the above impurity scattering included. The calculations were done with moderate strength of the pairing potentials, \( \tilde{V}_{\text{inter}} = 2.0 \) and \( \tilde{V}_{\text{intra}} = 0.5 \), and with the varied impurity scattering rates \( \Gamma_0 \) and \( \Gamma_\pi \). The case without impurity scattering (red \( \times \) symbols, \( \Gamma_0 = \Gamma_\pi = 0 \)), \( \Delta C / T_c \) shows the \( T_c^2 \) scaling only for the limited region near the maximum \( T_c \) and it quickly becomes flattened and slower than \( T_c \). Interestingly, this behavior looks very similar to the experimental data of \( \text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2 \) [13]. Therefore, we speculate that \( \text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2 \) 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, \( \Gamma_0 = \Gamma_\pi = 0.02 \) in unit of \( \Lambda_{hi} \)) immediately changes \( \Delta C / T_c \) vs. \( T_c \) steeper such as \( \Delta C / T_c \sim T_c^{4.5} \) over the whole \( T_c \) range. Further increasing the impurity scattering rate the case with \( \Gamma_0 = 0.1 \) and \( \Gamma_\pi = 0.05 \) (pink \( \bullet \) 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, \( \Gamma_0 = 0.5 \) and \( \Gamma_\pi = 0.05 \) (dark yellow \( \bigcirc \) symbols), which displays \( \Delta C \sim T_c^4 \), a super-strong scaling.

The main message of the numerical calculations in Fig. 1 and Fig. 2 is: (1) the strong non-BCS relation 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 Eq. (2); (2) however, the system needs some amount of non-pair-breaking impurity scattering (for example,
$\Gamma_0/T_c^0 \approx 1/3$, the pink "♦" symbols in Fig.2) to have the 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-pnictide systems[1, 3, 4, 5, 6, 7] follow the BNC scaling but some systems[13, 17] show a deviation from it.

3. Condensation Energy $\Delta E$ vs. $T_c$

3.1. Formalism

Using the exactly same model of the previous section, we can calculate the CE $\Delta E$ that is the zero temperature property. Therefore we need to solve the coupled gap equation Eq.(1) at $T = 0$ which is rewritten as

$$\Delta_h = -\sum_k V_{hh} b_k^h - \sum_k V_{he} b_k^e$$

$$\Delta_e = -\sum_k V_{eh} b_k^h - \sum_k V_{ee} b_k^e$$  \(8\)

with the Cooper pair amplitudes $b_k^h = < h_k^+ h_{-k}^- >$ and $b_k^e = < e_k^+ e_{-k}^- >$, respectively, and at $T = 0$, $b_k^{(e)} = \sum_k b_k^{(e)} = \sum_k \frac{\Delta_{h(e)}}{\sqrt{\Delta_{h(e)}(k) + \Delta_{h(e)}(k)}} = N_{h(e)} \Delta_{h(e)} \log \frac{\Lambda_{h(e)} + \sqrt{\Lambda_{h(e)}^2 + \Delta_{h(e)}^2}}{|\Delta_{h(e)}|}$. In general, the CE consists of the kinetic energy loss (increase) and the potential energy gain (decrease) as $\Delta E \equiv < H >_0 - < H >_n = \Delta K E + \Delta P E$, which are written as the following general expressions

$$\Delta K E = \sum_{a=h,e} \frac{1}{2} N_a \Delta_a^2 + N_i \Delta_i^2 \log \frac{\Lambda_{h(i)} + \sqrt{\Lambda_{h(i)}^2 + \Delta_{h(i)}^2}}{|\Delta_{h(i)}|},$$  \(9\)

$$\Delta P E = V_{hh} b^h b^h + V_{ee} b^e b^e + V_{he} b^h b^e + V_{ke} b^e b^h.$$

The total $\Delta E$ has no further simplification and should be calculated numerically.

3.2. Numerical Results

In Fig.3, we plotted the results of the case of $V_{\text{inter}} = (V_{ee} = 0) = 0$ with varying inter-band potential $V_{\text{inter}} = (V_{ee} = V_{hh}) = 1.0, 2.0, 3.0, 4.0$, and 5.0, respectively. To our surprise, this simple model immediately produces a strongly non-BCS power law scaling $\Delta E \sim T_c^\beta$ ($\beta \approx 3$) for a wide range of $T_c$, and $\Delta E$ varies over three orders of magnitude. This is exactly the key feature of the experimental data[2].

In Fig.4, we studied the effect of the intra-band interaction $V_{\text{intra}} = (V_{ee} = 0) = 0$. We experimented both repulsive ($V_{\text{intra}} > 0$) and attractive ($V_{\text{intra}} < 0$) intra-band interactions while fixing the inter-band interaction $V_{\text{inter}} = 2.0$ at a moderate value. First, adding even very weak attractive ($V_{\text{intra}} < 0$) intra-band interaction (black squares, pink stars), the scaling relation quickly converges to the BCS limit $\Delta E \sim T_c^2$. This result strongly suggests that the intra-band interaction in the Fe-based superconductors should be repulsive ($V_{\text{intra}} > 0$) – at least, not attractive. On the other hand, a repulsive intra-band interaction ($V_{\text{intra}} > 0$) causes the opposite trend although its effect is rather weak, so that we cannot reach the experimental power $\beta \approx 3.5$ with reasonable parameter set.

Finally, in Fig.5, we studied the effect of the pair-breaking impurity scattering (interband impurity scattering) $\Gamma_\pi$. We have also studied the non-pair-breaking impurity scattering (intraband impurity scattering) $\Gamma_0$ and found that it has no effect on the scaling which is understandable with Anderson theorem. The results in Fig.5 shows that a very weak impurity scattering rate $\Gamma_\pi/\Lambda_{hi} = 0.05$ is already sufficient to make the scaling as $\Delta E \sim T_c^{3.5}$ as consistent with the experimental data[2].
4. Summary and Conclusions
We have studied the scaling relations of the $\Delta C$ vs. $T_c$ (BNC scaling) and $\Delta E$ vs. $T_c$ based on the minimal two band BCS model. Despite the extreme simplicity of the model, our results almost
immediately reproduced the two anomalous scaling relations – $\Delta C \sim T^3_c[1]$ and $\Delta E \sim T^{3.5}_c[2]$ – simultaneously. Adding a small amount of impurity scattering effect, our numerical results can perfectly fit all experimental data. Important implication of our study is that the experimentally observed seemingly non-BCS scaling relations of $\Delta C \sim T^3_c$ and $\Delta E \sim T^{3.5}_c[2]$ are in fact strong experimental evidences that the Fe-based superconductors are the BCS superconductors, but with multi-bands, mediated by a dominant repulsive inter-band pairing interaction. Strong correlation effects, abundantly observed in the normal state, should renormalize the effective mass $m^*_{qp}$ of quasiparticles, DOS $N_{h,e}$, the pairing interactions $V_{\text{inter,intra}}(q)$, etc., but when the system enters the SC transition, the pairing mechanism itself seems to be governed by the BCS mechanism. Finally, the results of this paper does not have direct relevance to the FeSe monolayer and related systems where only electron FSs exist[18].

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