

Pair breaking in iron pnictides

V. G. Kogan

Ames Laboratory and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA
(Received 19 October 2009; revised manuscript received 26 November 2009; published 28 December 2009)

The puzzling features of the slopes of the upper critical field at the critical temperature T_c , $H'_{c2}(T_c) \propto T_c$, and of the specific heat jump $\Delta C \propto T_c^3$ of iron-pnictides are interpreted as caused by a strong pair-breaking.

DOI: [10.1103/PhysRevB.80.214532](https://doi.org/10.1103/PhysRevB.80.214532)

PACS number(s): 74.20.-z, 74.25.Bt, 74.25.Ha

I. INTRODUCTION

Iron-pnictide superconductors have a number of uncommon properties. The subject of this paper are two such properties. (a) The specific heat jump ΔC is proportional to T_c^3 as demonstrated on “122” series of $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ and $\text{Ba}(\text{Fe}_{1-x}\text{Ni}_x)_2\text{As}_2$.¹ This behavior, according to Ref. 2, cannot be explained within the “realm of conventional Bardeen-Cooper-Schrieffer (BCS) theory.” Similar behavior is recorded in 122 crystals with Ba substituted partially with K and with Fe substituted with Pd, Rh,³ and Co-Cu. (b) Slopes of the upper critical field dH_{c2}/dT at T_c are approximately proportional to T_c across both 1111 and 122 series.

It is shown below that both scalings can be understood within the weak-coupling BCS model provided a strong pair-breaking is present in these materials. In fact, these features should also be present in conventional superconductors with magnetic impurities as discussed by Abrikosov and Gor'kov (AG) in the seminal work on the pair-breaking for the nearly critical concentration of these impurities when $T_c \ll T_{c0}$, the critical temperature of clean material.⁴ AG had considered isotropic materials with a spherical Fermi surface and the s -wave order parameter constant along this surface. The symmetry of the order parameter in multiband pnictides is not yet determined with certainty; however, many favor the $\pm s$ structure.^{5,6} The critical temperature in materials with a strongly anisotropic order parameter is suppressed not only by scattering breaking the time reversal symmetry (e.g., the spin-flip); in fact, any scattering reduces T_c . The term “pair-breaking” is used here in a broad sense for any process suppressing T_c . It is shown in this work that both features, $dH_{c2}/dT \propto T_c$ and $\Delta C \propto T_c^3$, follow from the assumption that the “pair-breaking in a broad sense” is strong.

Below, the linearized Ginzburg-Landau (GL) equation and the energy near T_c are derived within the weak coupling scheme (that allows one to evaluate dH_{c2}/dT and ΔC at T_c) for an arbitrary anisotropy of the order parameter Δ and of the Fermi surface in the presence of pair-breaking. The text is focused on the situation when the average $\langle \Delta \rangle$ over the F surface is close to zero that presumably is the case of pnictides.^{5,6} Comparison with the data available concludes the paper.

Perhaps, the simplest for our purpose is the Eilenberger quasiclassical version of Gor'kov's theory that holds for a general anisotropic F surface and for any gap symmetry⁷

$$\mathbf{v}\mathbf{\Pi}f = 2\Delta g - 2\omega f + \frac{g}{\tau_-}\langle f \rangle - \frac{f}{\tau_+}\langle g \rangle, \quad (1)$$

$$-\mathbf{v}\mathbf{\Pi}^*f^+ = 2\Delta^*g - 2\omega f^+ + \frac{g}{\tau_-}\langle f^+ \rangle - \frac{f^+}{\tau_+}\langle g \rangle, \quad (2)$$

$$g^2 = 1 - ff^+, \quad (3)$$

$$\Delta(\mathbf{r}, \mathbf{k}_F) = 2\pi TN(0) \sum_{\omega > 0}^{\omega_D} \langle V(\mathbf{k}_F, \mathbf{k}'_F) f(\mathbf{k}'_F, \mathbf{r}, \omega) \rangle_{\mathbf{k}'_F}. \quad (4)$$

Here, \mathbf{v} is the Fermi velocity, $\mathbf{\Pi} = \nabla + 2\pi i \mathbf{A} / \phi_0$, ϕ_0 is the flux quantum. $\Delta(\mathbf{r}, \mathbf{k}_F)$ is the order parameter that in general depends on the position \mathbf{k}_F at the F surface of other than the isotropic s -wave symmetry. The functions $f(\mathbf{r}, \mathbf{k}_F, \omega)$, f^+ , and g originate from Gor'kov's Green's functions integrated over the energy variable near the F surface. Further, $N(0)$ is the total density of states at the Fermi level per one spin; the Matsubara frequencies are $\omega = \pi T(2n+1)$ with an integer n and $\hbar = k_B = 1$. The averages over the F surface are shown as $\langle \dots \rangle$.

The scattering in the Born approximation is characterized by two scattering times, the transport time τ responsible for conductivity in the normal state, and τ_m for spin-flip processes

$$\frac{1}{\tau_{\pm}} = \frac{1}{\tau} \pm \frac{1}{\tau_m}. \quad (5)$$

The strong scattering in unitary limit is not considered here. Commonly, two dimensionless scattering parameters are employed

$$\rho = \frac{1}{2\pi T_c \tau} \quad \text{and} \quad \rho_m = \frac{1}{2\pi T_c \tau_m}, \quad (6)$$

or equivalently, $\rho_{\pm} = \rho \pm \rho_m$. This is of course a simplification; for multiband F surfaces one may need more parameters for various intra- and interband processes. This and other simplifying assumptions notwithstanding, the model employed is amenable for analytic work and may prove useful.

Long experience in dealing with pair-breaking effects has shown that the formal AG scheme applies to various situations with different causes for the pair-breaking, not necessarily the AG spin-flip scattering.⁸ In each particular situation, the parameter ρ_m must be properly defined. Without specifying the pair-breaking mechanism in materials of interest here, we apply below the AG approach to show that the

pair-breaking accounts for experimental data on slopes of H_{c2} at T_c and for quite unusual dependence of the specific heat jump on T_c .

Commonly, the effective coupling V is assumed factorizable, $V(\mathbf{k}_F, \mathbf{k}'_F) = V_0 \Omega(\mathbf{k}_F) \Omega(\mathbf{k}'_F)$,⁹ this assumption is not necessary but it simplifies the algebra considerably. One then looks for the order parameter in the form

$$\Delta(\mathbf{r}, T; \mathbf{k}_F) = \Psi(\mathbf{r}, T) \Omega(\mathbf{k}_F). \quad (7)$$

Our notation is motivated by the fact that so defined $\Psi(\mathbf{r}, T)$ enters the Ginzburg-Landau theory near T_c . The function $\Omega(\mathbf{k}_F)$, which describes the variation of Δ along the F surface, is conveniently normalized

$$\langle \Omega^2 \rangle = 1. \quad (8)$$

Then, the self-consistency Eq. (4) takes the form

$$\Psi(\mathbf{r}, T) = 2\pi T N(0) V_0 \sum_{\omega > 0}^{\omega_D} \langle \Omega(\mathbf{k}_F) f(\mathbf{k}_F, \mathbf{r}, \omega) \rangle. \quad (9)$$

The assumption of a factorizable potential is quite restrictive as far as complicated F surfaces and interactions are concerned, e.g., within two-band schemes with four coupling constants V_{ij} , the factorizable model implies $V_{11}V_{22} - V_{12}V_{21} = 0$.

Instead of dealing with the effective microscopic electron-electron interaction V_0 and with the energy scale ω_D , one can use within the weak coupling scheme the critical temperature T_{c0} (of the hypothetic clean material) utilizing the identity

$$\frac{1}{N(0)V_0} = \ln \frac{T}{T_{c0}} + 2\pi T \sum_{\omega > 0}^{\omega_D} \frac{1}{\omega}, \quad (10)$$

which is equivalent to the BCS relation $\Delta_0(0) = \pi T_{c0} e^{-\gamma} = 2\omega_D \exp(-1/N(0)V_0)$; γ is the Euler constant. Substitute Eq. (10) in Eq. (9) and replace ω_D with infinity due to fast convergence

$$\frac{\Psi}{2\pi T} \ln \frac{T_{c0}}{T} = \sum_{\omega > 0}^{\infty} \left(\frac{\Psi}{\omega} - \langle \Omega f \rangle \right). \quad (11)$$

II. GL DOMAIN AND $T_c(\tau, \tau_m)$

Near T_c , $f \ll 1$, $g = 1 - ff^*/2$ and Eq. (1) reads

$$\frac{1}{2} \mathbf{v} \Pi f = \Delta - \omega_+ f + \frac{\langle f \rangle}{2\tau_-} - \frac{ff^*}{2} \left(\Delta + \frac{\langle f \rangle}{2\tau_-} \right) + \frac{f \langle ff^* \rangle}{4\tau_+}. \quad (12)$$

Here,

$$\omega_+ = \omega + 1/2\tau_+, \quad (13)$$

and the terms on the right-hand side (RHS) are arranged according to their order in powers of $\delta t = 1 - T/T_c$: the first three terms are of the order $\delta t^{1/2}$ whereas the rest $\sim \delta t^{3/2}$. Note that on the left-hand side (LHS), $\Pi f \sim f/\xi \sim \delta t$.

We look for the solution $f = f_1 + f_2 + \dots$ where $f_1 \sim \delta t^{1/2}$, $f_2 \sim \delta t$, etc. Hence, we have in the lowest order

$$0 = \Delta - \omega^+ f_1 + \frac{\langle f_1 \rangle}{2\tau_-}. \quad (14)$$

Taking the average over the Fermi surface, we obtain

$$\langle f_1 \rangle = \langle \Delta \rangle / \omega_m, \quad \omega_m = \omega + 1/\tau_m \quad (15)$$

(note the difference in definitions of ω_+ and ω_m). Hence,

$$f_1 = \frac{1}{\omega^+} \left(\Delta + \frac{\langle \Delta \rangle}{2\tau_- \omega_m} \right). \quad (16)$$

Comparing terms of the order δt , we get

$$\langle f_2 \rangle = - \frac{\langle \mathbf{v} \Pi f_1 \rangle}{2\omega_m} = 0, \quad (17)$$

and

$$f_2 = - \frac{1}{2\omega_+^2} \mathbf{v} \Pi \left(\Delta + \frac{\langle \Delta \rangle}{2\tau_- \omega_m} \right). \quad (18)$$

Evaluation of higher order corrections for arbitrary Δ anisotropy is increasingly cumbersome unlike the case $\langle \Delta \rangle = 0$ for which one finds for the uniform state:

$$f_3 = - \frac{\Delta}{2\omega_+^3} \left(\Delta^2 - \frac{\langle \Delta^2 \rangle}{2\tau_+ \omega^+} \right). \quad (19)$$

The critical temperature of materials with anisotropic order parameter is suppressed by scattering. In zero field, all quantities are coordinate independent; besides, as $T \rightarrow T_c$, $g \rightarrow 1$. Therefore, we can utilize f of Eq. (16) in the lowest order to obtain for T_c

$$\frac{1}{2\pi T_c} \ln \frac{T_{c0}}{T_c} = \sum_{\omega > 0}^{\infty} \left(\frac{1}{\omega_c} - \frac{1}{\omega_c^+} - \frac{\langle \Omega \rangle^2}{2\omega_c^m \omega_c^+ \tau_-} \right), \quad (20)$$

where the subscript c is to denote that ω 's are taken at T_c . The sums here are expressed in terms of di-gamma functions

$$\begin{aligned} \ln \frac{T_{c0}}{T_c} &= \psi \left(\frac{1 + \rho_+}{2} \right) - \psi \left(\frac{1}{2} \right) \\ &\quad - \langle \Omega \rangle^2 \left[\psi \left(\frac{1 + \rho_+}{2} \right) - \psi \left(\frac{1}{2} + \rho_m \right) \right]. \end{aligned} \quad (21)$$

Within a two-band scheme, generalization of the well-known AG result for the T_c suppression for any (Born) scattering and for an arbitrary symmetry on the order parameter has been given by Golubov and Mazin,¹⁰ in the form (21) it is due to Openov.¹¹

If $T_c \rightarrow 0$, one can use asymptotic expansion $\psi(z) = \ln z - 1/2z$ for large arguments since $\rho, \rho_m \rightarrow \infty$. The leading term then gives that $T_c = 0$ when scattering times satisfy the relation

$$\frac{1}{\tau_m} \left(\frac{\tau_m}{2\tau_+} \right)^{1 - \langle \Omega \rangle^2} = \frac{\Delta_0(0)}{2}. \quad (22)$$

Here, $\Delta_0(0) = \pi T_{c0} e^{-\gamma}$ is the zero temperature gap of the (hypothetic) scattering-free material. Clearly, this reduces to the AG critical rate $1/\tau_m = \Delta_0(0)/2$ for isotropic order param-

eters. If $\langle \Omega \rangle = 0$ (e.g., for the d wave), we have the critical combined rate: $1/\tau_+ = \Delta_0(0)$.

For a general anisotropy $\langle \Omega \rangle \neq 0, 1$ in the absence of spin-flip scattering ($\tau_m \rightarrow \infty$) the LHS is zero and Eq. (22) has no solutions for τ , i.e., T_c does not turn zero for any τ . However, a finite τ at which $T_c = 0$ does exist for any finite τ_m . One can show that near the critical value $\tau_{+, \text{crit}}^{(\Omega)^2-1} = \Delta_0(0)(\tau_m/2)^{\langle \Omega \rangle^2}$, the critical temperature behaves similarly to the AG gapless case, $T_c \propto (\tau_+ - \tau_{+, \text{crit}}^+)^{1/2}$.

Combining Eqs. (11) and (20), one excludes the unphysical T_{c0}

$$\frac{\Psi}{2\pi T} \ln \frac{T_c}{T} = \sum_{\omega>0} \left(\frac{\Psi}{t\omega_c^+} + \frac{\Psi \langle \Omega \rangle^2}{2t\omega_c^m \omega_c^+ \tau_-} - \langle \Omega f \rangle \right), \quad (23)$$

where $t = T/T_c$.

III. CASE $T_c \ll T_{c0}$

Situations of interest here are of T_c strongly suppressed relative to T_{c0} (similar to the gapless superconductivity of AG, but not necessarily the same). It is convenient for this purpose to rearrange Eq. (23) by adding and subtracting Ψ/ω_+ under the sum. We transform

$$\begin{aligned} & 2\pi T \sum_{\omega>0} \left(\frac{1}{t\omega_c^+} - \frac{1}{\omega^+} \right) \\ &= \sum_{n=0}^{\infty} \left(\frac{1}{n+1/2+\rho_+/2} - \frac{1}{n+1/2+\rho_+/2t} \right) \\ &= \psi\left(\frac{\rho_+}{2t} + \frac{1}{2}\right) - \psi\left(\frac{\rho_+}{2} + \frac{1}{2}\right) \approx -\ln t - \frac{1-t^2}{6\rho_+^2}. \end{aligned} \quad (24)$$

The parameter ρ_+ is large if $T_c \rightarrow 0$ and one can use large arguments asymptotics of the di-gamma functions. Combining Eqs. (23) and (24), we obtain the self-consistency equation in the form

$$\frac{\Psi(1-t^2)}{12\pi T \rho_+^2} = \sum_{\omega>0} \left(\frac{\Psi}{\omega_+} + \frac{\Psi \langle \Omega \rangle^2}{2t\omega_c^m \omega_c^+ \tau_-} - \langle \Omega f \rangle \right). \quad (25)$$

A. Linearized GL equation and the coherence length

The GL equations are obtained by utilizing smallness of Δ/ω and of $\mathbf{v}\Pi\Delta/\omega^2$ near T_c . Hence, one can use Eqs. (16), (18), and (19) for f and the self-consistency Eq. (25). For the case of exclusively transport scattering ($\tau_m = \infty$), the GL equations have been derived in Ref. 12. It is done below for a finite τ_m .

To write the self consistency Eq. (25) near T_c one has to express $\langle \Omega f \rangle$ with the help of Eq. (12). To this end, one applies $\langle \Omega/\omega_+ \dots \rangle$ to (12) keeping terms up to the order δt

$$\langle \Omega f \rangle = \frac{\Psi}{\omega_+} + \frac{\langle \Omega \rangle \langle f \rangle}{2\tau_- \omega_+} - \left\langle \frac{\Omega}{2\omega_+} \mathbf{v}\Pi f \right\rangle, \quad (26)$$

and substitutes the result to Eq. (25)

$$\frac{\Psi \delta t}{6\pi T \rho_+^2} = \sum_{\omega>0} \left[\frac{\Psi \langle \Omega \rangle^2}{2t\omega_{mc} \omega_c^+ \tau_-} - \frac{\langle \Omega \rangle \langle f \rangle}{2\omega_+ \tau_-} + \left\langle \frac{\Omega}{2\omega_+} \mathbf{v}\Pi f \right\rangle \right]. \quad (27)$$

Since we are expanding in powers of $\sqrt{\delta t}$, the distinction between, e.g., ω_c and $\omega = \omega_c(1 - \delta t)$, is relevant.

When substituting here $f = f_1 + f_2$ of Eqs. (16) and (18) note that $\langle \Omega \mathbf{v}\Pi\Delta \rangle = 0$ because the angular dependence of Ω (the symmetry of Δ) has nothing to do with that of the vector $\Pi\Delta$. We then obtain

$$\begin{aligned} \frac{\Psi \delta t}{6\pi T \rho_+^2} &= \sum_{\omega>0} \left[\frac{\Psi \langle \Omega \rangle^2}{2\tau_- \omega_+^2} \left(\frac{\omega_+^2}{t\omega_c^m \omega_c^+} - 1 - \frac{1}{2\tau_- \omega_m} \right) \right. \\ &\quad \left. - \frac{1}{4\omega_{c+}^3} \left\langle (\mathbf{v}\Pi)^2 \Psi \left(\Omega^2 + \frac{\Omega \langle \Omega \rangle}{2\omega_{cm} \tau_-} \right) \right\rangle \right]. \end{aligned} \quad (28)$$

Note that the LHS and the term in the lower line of this equation are on the order $\delta t^{3/2}$; for this reason all ω 's in this term are taken at T_c . Besides, the parentheses in the upper line of the RHS are easily shown to turn to zero at $t=1$. Expanding the bracketed expression in powers of δt and keeping only the first term one obtains

$$A \Psi \delta t = -B_{ik} \Pi_i \Pi_k \Psi \quad (29)$$

with

$$A = \frac{1}{6\pi T_c \rho_+^2} - \frac{\langle \Omega \rangle^2}{2\tau_-} \sum_{\omega>0} \left[\frac{\omega_+^2 - 2\omega\omega_m}{\omega_m \omega_+^3} - \frac{(2\omega_m + \omega_+)\omega}{2\tau_- \omega_m^2 \omega_+^3} \right], \quad (30)$$

$$B_{ik} = \frac{1}{4} \sum_{\omega>0} \frac{1}{\omega_+^3} \left\langle v_i v_k \left(\Omega^2 + \frac{\Omega \langle \Omega \rangle}{2\omega_m \tau_-} \right) \right\rangle, \quad (31)$$

where all ω 's are at T_c and the subscript c is omitted. This is in fact, the linearized anisotropic GL equation

$$-(\xi^2)_{ik} \Pi_i \Pi_k \Psi = \Psi \quad (32)$$

with the anisotropic coherence length given by

$$(\xi^2)_{ik} = B_{ik}/A \delta t. \quad (33)$$

All sums in Eqs. (30) and (31) are expressed in terms of poly-gamma functions of large parameters ρ_{\pm} . Keeping the leading terms we obtain

$$A = \frac{1}{6\pi T_c \rho_+^2} - \frac{\langle \Omega \rangle^2 (2\rho_+ - \rho_-)}{\pi T_c \rho_-} \ln \frac{\rho_+}{2\rho_m}, \quad (34)$$

$$B_{ik} = \frac{\langle \Omega^2 v_i v_k \rangle \tau_+^2}{2\pi T_c} + \frac{\langle \Omega \rangle \langle \Omega v_i v_k \rangle \tau_-^2}{2\pi T_c} \left[\ln \frac{\rho_+}{2\rho_m} - \frac{\rho_-(2\rho_+ + \rho_-)}{2\rho_+^2} \right]. \quad (35)$$

B. Materials with $\langle \Omega \rangle = 0$ near T_c

This corresponds, e.g., to the d -wave symmetry. Within a two-band model for iron-pnictides the order parameter has a $\pm s$ structure, so that $\langle \Delta \rangle \ll |\Delta_{\text{max}}|$.⁶ One then expects the

model with $\langle\Omega\rangle=0$ to hold, at least qualitatively, for iron-pnictides.

If $\langle\Omega\rangle=0$, A and B are simplified

$$A = \frac{1}{6\pi T_c \rho_+^2}, \quad B_{ik} = \frac{\langle\Omega^2 v_i v_k\rangle \tau_+^2}{2\pi T_c}, \quad (36)$$

and

$$(\xi^2)_{ik} = \frac{3\langle\Omega^2 v_i v_k\rangle}{8\pi^2 T_c^2 \delta t}. \quad (37)$$

For the d -wave order parameter and isotropic two-dimensional Fermi surface, $\Omega = \sqrt{2} \cos 2\varphi$ and $\langle\Omega^2 v_x^2\rangle = v^2/2$

$$\xi^2 = \frac{3\hbar^2 v^2}{16\pi^2 T_c^2 \delta t}. \quad (38)$$

This result has been obtained in Ref. 13 for a clean d wave with a strongly suppressed T_c .

For a uniaxial material, the slope of the upper critical field along the c direction near T_c is given by

$$\frac{dH_{c2,c}}{dT} = -\frac{4\pi\phi_0 k_B^2}{3\hbar^2 \langle\Omega^2 v_a^2\rangle} T_c \quad (39)$$

(in common units). Although the pair-breaking parameters do not enter this result explicitly, they affect $H_{c2,c}$ and its slope via $T_c(\rho_+)$. One readily obtains for the other principal direction

$$\frac{dH_{c2,ab}}{dT} = -\frac{4\pi\phi_0 k_B^2}{3\hbar^2 \sqrt{\langle\Omega^2 v_a^2\rangle \langle\Omega^2 v_c^2\rangle}} T_c. \quad (40)$$

It is worth recalling that in isotropic materials with the standard s -wave order parameter the slope $H'_{c2} \propto T_c$ in the clean limit (because $H_{c2} \propto 1/\xi^2 \propto T_c^2$), whereas for the dirty case H'_{c2} is T_c independent ($H_{c2} \propto 1/\xi \ell \propto T_c$, ℓ is the mean-free path). The proportionality H'_{c2} to T_c is a property of the AG gapless state. In our case, the result (39) is obtained for a strong pair-breaking in materials with anisotropic order parameter.

Note also that even without magnetic scatterers, in materials with $\langle\Omega\rangle=0$ and $\rho \gg 1$, the superconductivity becomes “gapless” in a sense that the *total* density of states at the Fermi level is not zero. As in the AG case, if $T_c \rightarrow 0$, the superconductivity is weak at all temperatures, i.e., $f \ll 1$ and $g = 1 - f^2/2 = 1 - \Delta^2/2\omega_+^2$ in the whole domain $0 < T < T_c$. Then the energy dependence of the total density of states $N(\epsilon) = N(0) \text{Re } g(\omega \rightarrow i\epsilon)$ reads

$$\frac{N(\epsilon)}{N(0)} = 1 - 2\Delta^2 \tau_+^2 \frac{1 - \eta^2}{(1 + \eta^2)^2}, \quad \eta = 2\tau_+ \epsilon. \quad (41)$$

Hence, at zero energy, $N(\epsilon)$ has a nonzero minimum, whereas the maximum of $N(\epsilon)$ is reached at $\epsilon_m = \sqrt{3}/2\tau_+$ (not at Δ). Therefore, the ratio of the “apparent gap” ϵ_m to T_c should vary as $1/T_c$. Since only the total density of states is nonzero, this does not exclude possibility to have gapped and gapless patches on the F surface.

IV. SPECIFIC HEAT JUMP

Eilenberger equations (1) and (11) in zero field can be obtained minimizing the functional⁷

$$\mathcal{F} = N(0) \left[\Psi^2 \ln \frac{T}{T_{c0}} + 2\pi T \sum_{\omega>0} \left(\frac{\Psi^2}{\hbar\omega} - \langle I \rangle \right) \right], \quad (42)$$

$$I = 2\Delta f + 2\omega(g-1) + \frac{f\langle f \rangle}{2\tau^-} + \frac{g\langle g \rangle - 1}{2\tau^+}. \quad (43)$$

The function g here is an abbreviation for $\sqrt{1-f^2}$. Taking account of the self-consistency Eq. (11), we obtain the energy difference between the normal and superconducting states

$$-\frac{F_s - F_n}{2\pi TN(0)} = \sum_{\omega>0} \left\langle \Delta f + 2\omega(g-1) + \frac{f\langle f \rangle}{2\tau^-} + \frac{g\langle g \rangle - 1}{2\tau^+} \right\rangle. \quad (44)$$

One can check that this reduces to the known result for isotropic s -wave cases with or without pair-breaking.⁸ This offers a straightforward way to calculate the specific heat near T_c . The calculation, in general, is tedious because one has to keep track of terms up to $\Delta^4 \propto \delta t^2$. We consider only the case $\langle\Delta\rangle=0$.

Up to the fourth order in Δ , we have, with the help of Eqs. (16) and (19),

$$f = \frac{\Delta}{\omega_+} + \frac{\Delta}{2\omega_+^3} \left(\frac{\langle\Delta^2\rangle}{2\tau_+ \omega_+} - \Delta^2 \right), \quad (45)$$

$$g = 1 - \frac{\Delta^2}{2\omega_+^2} + \frac{3\Delta^4}{8\omega_+^4} - \frac{\Delta^2 \langle\Delta^2\rangle}{4\tau_+ \omega_+^5}, \quad (46)$$

where all ω 's are taken at T_c . Substituting these in the energy difference, we obtain

$$-\frac{F_s - F_n}{2\pi TN(0)} = \frac{\Psi^4}{4} \sum \left(\frac{\langle\Omega^4\rangle}{\omega_+^3} - \frac{1}{2\tau_+ \omega_+^4} \right). \quad (47)$$

For large ρ_+ , one finds

$$\sum \left(\frac{\langle\Omega^4\rangle}{\omega_+^3} - \frac{1}{2\tau_+ \omega_+^4} \right) \approx \frac{(3\langle\Omega^4\rangle - 2)\tau_+^2}{3\pi T}. \quad (48)$$

To complete the energy evaluation one needs $\Psi(T)$, which is obtained with the help of the self-consistency Eq. (27) and expression (45) for f

$$\Psi^2 = \frac{4\pi^2 T_c^2 (1-t)}{3\langle\Omega^4\rangle - 2}. \quad (49)$$

Thus, the energy difference between the normal and superconducting states reads

$$F_n - F_s = \frac{8\pi^4 N(0) \tau_+^2}{3\hbar^2 (3\langle\Omega^4\rangle - 2)} k_B^4 T_c^2 (T_c - T)^2 \quad (50)$$

in common units. The specific heat jump at T_c follows:

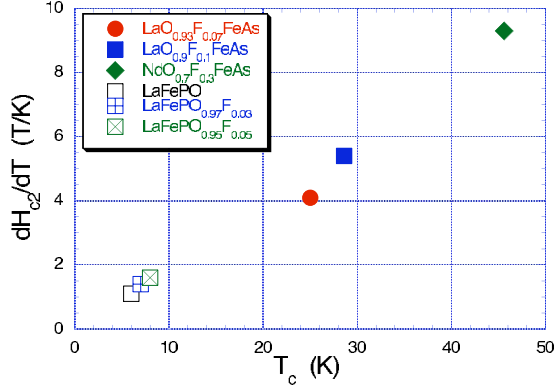


FIG. 1. (Color online) The slopes of $H_{c2}(T)$ near T_c (the absolute values) for a few 1111 compounds. The data for the first three compounds in the legend are taken from Ref. 15; the remaining three points are taken from Ref. 16. The two right-most points are for $H'_{c2,ab}$ of crystalline samples; the rest are for polycrystals, so that all points, in fact, reflect $H'_{c2,ab}$.

$$\Delta C = C_s - C_n = \frac{16\pi^4 k_B^4 N(0) \tau_+^2}{3\hbar^2 (3\langle\Omega^4\rangle - 2)} T_c^3. \quad (51)$$

Within a weak coupling scheme, this result in a more general form has been obtained in Ref. 14.

For the d -wave state on a cylindrical Fermi surface $\Omega = \sqrt{2} \cos^2 2\phi$ and $\langle\Omega^4\rangle = 3/2$ this gives

$$\Delta C = \frac{32\pi^4 k_B^4 N(0) \tau_+^2}{15\hbar^2} T_c^3. \quad (52)$$

V. DISCUSSION

Figure 1 is a compilation of data on the slopes H'_{c2} for 1111 compounds with various dopants and, therefore, with various T_c 's. An approximate scaling $H'_{c2} \propto T_c$ is evident despite the fact that the compounds examined have T_c 's varying from 6 to 46 K. From this data one estimates the slope of dH'_{c2}/dT_c as ≈ 0.2 T/K². Then, the order of magnitude of the Fermi velocity follows from $|dH'_{c2}/dT_c| \sim \pi\phi_0 k_B^2 / \hbar^2 v^2$ as $v \sim 10^7$ cm/s, a reasonable order that can be taken as yet another argument in favor of the picture presented.

In Fig. 2, the data for the 122 family are collected. The same approximate scaling is seen albeit with a considerable scatter. The latter might be caused by variety of reasons: different criteria in extracting H_{c2} from resistivity data, unavoidable uncertainties rooted in sample inhomogeneities in determination of T_c and the slopes of $H_{c2}(T)$ near T_c , possible differences in Fermi velocities and the order parameter anisotropies, to name a few. Moreover, the model employing only two scattering parameters for multiband iron-pnictides is a far-reaching simplification, so that one can expect the model to work qualitatively at best. Nevertheless, the observed scaling seems robust. One can take this as evidence in favor of a strong pair-breaking present in all compounds examined. It should be stressed again that for strongly anisotropic order parameters, $\langle\Delta\rangle \approx 0$, the T_c suppression (or the pair-breaking, which is the same) is caused by the combined

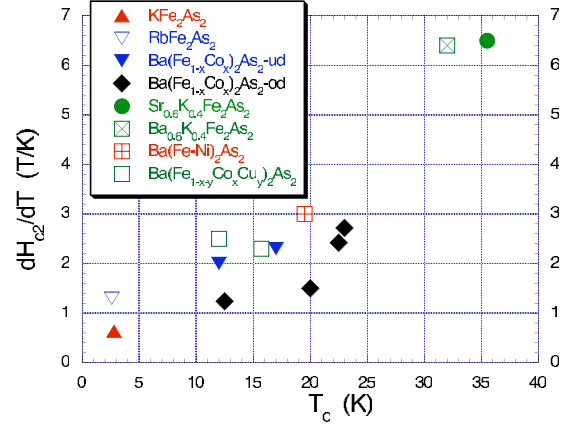


FIG. 2. (Color online) The slopes $H_{c2,c}(T)$ near T_c for a few 122 iron-pnictides. The data are taken from: RbFe₂As₂ (Ref. 17), KFe₂As₂ (Ref. 18), Ba_{0.55}K_{0.45}Fe₂As₂ (Ref. 19), the underdoped (ud) and overdoped (od) Ba(Fe_{1-x}Co_x)₂Fe₂As₂ (Ref. 3), Ba_{0.6}K_{0.4}Fe₂As₂ (Ref. 20), Sr_{0.6}K_{0.4}Fe₂As₂ (Ref. 21), Ba(Fe-Ni)₂Fe₂As₂, and Ba(Fe_{1-x-y}Co_xCu_y)₂Fe₂As₂ (Ref. 22).

effect of the transport and the spin-flip scattering.

We note also that in well-studied MgB₂ with two s -type gaps of the same sign, the slopes of H_{c2} do not show a similar behavior: one can suppress T_c by neutron irradiation leaving the slopes H'_{c2} nearly unchanged.²³ Moreover, carbon doping enhances $H'_{c2}(T_c)$ without causing a substantial reduction of T_c .²⁴

Figure 3 shows the specific heat jump measured in a number of compounds and reported in Ref. 1. The scaling $\Delta C \propto T_c^3$ suggested by Bud'ko, Ni, and Canfield is evident (see also Ref. 26). Again, it is worth noting that only the combined rate ρ_+ enters the coefficient in front of T_c^3 of Eq. (51), so that the source of T_c suppression is not necessarily the spin-flip AG pair-breaking. The ever present transport scattering suppresses T_c as well, provided the order parameter is

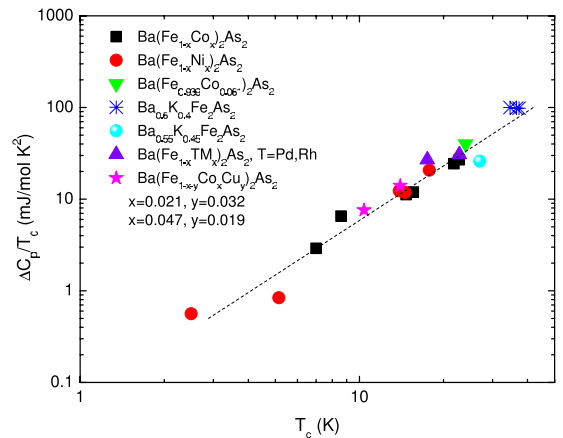


FIG. 3. (Color online) The specific heat jump versus T_c for a few 122 compounds shown on a log-log plot. The dashed line corresponds to $\Delta C \propto T_c^3$. Most of the data are from Ref. 1; the new data points for mixed Co-Cu doping are shown by stars and taken by the same group, but have not been included in the original publication. The data point for Ba(Fe_{0.939}Co_{0.061})₂Fe₂As₂ is from Ref. 25 and that for Ba_{0.6}K_{0.4}Fe₂As₂ from Ref. 19.

strongly anisotropic. This is presumably the case of iron pnictides.

One may wonder why the scaling $H'_{c2} \propto T_c$ and $\Delta C \propto T_c^3$ seem to work across the whole class of iron pnictides for compounds with different couplings, F surfaces, etc. Clearly, the source of this scaling should be universal across the pnictide family of materials. The pair-breaking is offered here as such a universal source.

As for the apparent simplicity of the model used, one should have in mind the often overlooked strength of the weak-coupling scheme: the model is formulated in terms of the *measured* critical temperature T_c , in which the coupling constants and energy scales of the “glue bosons” are incorporated.

One should also bear in mind that a literal interpretation of the model proposed here as implying that all iron pnictides have the same electronic structure and differ only in scattering times τ_+ would, of course, be incorrect. Suffices it to mention that, e.g., BaFe₂As₂ superconducts only being doped, so that dopands play much more important role than just to provide extra scattering. Hence, for each compound listed in Fig. 3, the material characteristics entering Eq. (51) [$N(0)$, τ_+ , the anisotropy parameter $\langle\Omega^4\rangle$] differ. On the other hand, the scaling shown in this figure implies that the combination $N(0)\tau_+^2/(3\langle\Omega^4\rangle-2)$ in all these compounds is roughly the same. This might be rationalized by notions that (a) in all of them the carriers are supplied by Fe, and (b) that in the gapless state with $T_c \ll T_{c0}$ in which all of them presumably reside, the pair-breaking parameter τ_+ is close to the critical value where $T_c=0$.

Having succeeded in describing the scalings just discussed, one can venture to a prediction: according to Eq. (41), tunneling experiments are likely to show the ratio of the apparent gap ϵ_m [where the total density of states $N(\epsilon)$ is

maximum] to T_c varying as $1/T_c$ across the family of iron pnictides.

ACKNOWLEDGMENTS

Numerous discussions and help of my colleagues S. Bud'ko, Ni Ni, P. Canfield, J. Schmalian, Junhua Zhang, R. Prozorov, M. Tanatar, R. Mints, and J. Clem are appreciated. The work was supported by the U.S. Department of Energy, Office of Basic Energy Sciences.

APPENDIX: MATERIALS WITH $\langle\Omega\rangle \neq 0$ NEAR T_c

Interestingly enough, the behavior of the H_{c2} slopes as functions of T_c turns out different if $\langle\Omega\rangle \neq 0$. To see this, consider the coefficient A of Eq. (34). In terms of scattering times, it reads

$$A = \frac{2\pi T_c \tau_+^2}{3} - \frac{\langle\Omega\rangle^2}{\pi T_c} \left(\frac{2\tau_-}{\tau_+} - 1 \right) \ln \frac{\tau_-}{2\tau_+}. \quad (\text{A1})$$

Since all τ 's are finite near the critical point where $T_c \rightarrow 0$, the term $\propto \langle\Omega\rangle^2$ is leading. Consider, e.g., a usual situation $\tau \ll \tau_m$

$$A \approx \frac{\langle\Omega\rangle^2 \ln 2}{\pi T_c}. \quad (\text{A2})$$

After simple algebra, one obtains the slope of $H_{c2,c}$ at T_c

$$\frac{dH_{c2,c}}{dT} = - \frac{\phi_0}{2\pi\tau^2 T_c} \frac{\langle\Omega\rangle^2 \ln 4}{\langle v_d^2 \Omega^2 \rangle + \langle\Omega\rangle \langle v_d^2 \Omega \rangle \ln(2\tau_m/\tau e^{3/2})}. \quad (\text{A3})$$

Thus, the slopes $H'_{c2} \propto 1/T_c$, the dependence opposite to that of the case $\langle\Omega\rangle=0$.

-
- ¹S. L. Bud'ko, Ni Ni, and P. C. Canfield, Phys. Rev. B **79**, 220516(R) (2009).
²J. Zaanen, Phys. Rev. B **80**, 212502 (2009).
³N. Ni, M. E. Tillman, J.-Q. Yan, A. Kracher, S. T. Hannahs, S. L. Budko, and P. C. Canfield, Phys. Rev. B **78**, 214515 (2008).
⁴A. A. Abrikosov and L. P. Gor'kov, Zh. Eksp. Teor. Fiz. **39**, 1781 (1960) [Sov. Phys. JETP **12**, 1243 (1961)].
⁵I. I. Mazin and J. Schmalian, Phys. C: Supercond. **469**, 614 (2009).
⁶Junhua Zhang, R. Sknepnek, R. M. Fernandes, and J. Schmalian, Phys. Rev. B **79**, 220502 (2009).
⁷G. Eilenberger, Z. Phys. **214**, 195 (1968).
⁸K. Maki, in *Superconductivity*, edited by R. D. Parks (Marcel Dekker, New York, 1969), Vol. 2, p. 1035.
⁹D. Markowitz and L. P. Kadanoff, Phys. Rev. **131**, 563 (1963).
¹⁰A. A. Golubov and I. I. Mazin, Phys. Rev. B **55**, 15146 (1997).
¹¹L. A. Openov, JETP Lett. **66**, 661 (1997).
¹²S. V. Pokrovsky and V. L. Pokrovsky, Phys. Rev. B **54**, 13275 (1996).
¹³V. G. Kogan, R. Prozorov, and C. Petrovic, J. Phys.: Condens. Matter **21**, 102204 (2009).
¹⁴L. A. Openov, Phys. Rev. B **69**, 224516 (2004).
¹⁵G. Fuchs, S.-L. Drechsler, N. Kozlova, M. Bartkowiak, J. E. Hamann-Borrero, G. Behr, K. Nenkov, H.-H. Klauss, H. Maeter, A. Amato, H. Luetkens, A. Kwadrin, R. Khasanov, J. Freudenberger, A. Koehler, M. Knupfer, E. Arushanov, H. Rosner, B. Buechner, and L. Schultz, New J. Phys. **11**, 075007 (2009).
¹⁶S. Suzuki, S. Miyasaka, S. Tajima, T. Kida, and M. Hagiwara, arXiv:0910.1711 (unpublished).
¹⁷Z. Bukowski, S. Weyeneth, R. Puzniak, J. Karpinski, and B. Batlogg, arXiv:0909.2740 (unpublished).
¹⁸T. Terashima, M. Kimata, H. Satsukawa, A. Harada, K. Hazama, S. Uji, H. Harima, Gen-Fe Chen, Jian-Jin Luo, and Nan-Lin Wang, J. Phys. Soc. Jpn. **78**, 063702 (2009).
¹⁹U. Welp, G. Mub, R. Xie, A. E. Koshelev, W. K. Kwok, H. Q. Luo, Z. S. Wang, P. Cheng, L. Fang, C. Ren, and H.-H. Wen, Physica C **469**, 575 (2009).
²⁰G. F. Chen, Z. Li, J. Dong, G. Li, W. Z. Hu, X. D. Zhang, X. H. Song, P. Zheng, N. L. Wang, and J. L. Luo, Phys. Rev. B **78**, 224512 (2008).
²¹Ni Ni (private communication).

- ²²R. T. H. Wilke, S. L. Bud'ko, P. C. Canfield, D. K. Finnemore, R. J. Suplinskas, and S. T. Hannahs, *Phys. Rev. Lett.* **92**, 217003 (2004).
- ²³R. T. H. Wilke, S. L. Bud'ko, P. C. Canfield, J. Farmer, and S. T. Hannahs, *Phys. Rev. B* **73**, 134512 (2006).
- ²⁴Jiun-Haw Chu, J. G. Analytis, C. Kucharczyk, and I. R. Fisher, *Phys. Rev. B* **79**, 014506 (2009).
- ²⁵M. M. Altarawneh, K. Collar, C. H. Mielke, N. Ni, S. L. Bud'ko, and P. C. Canfield, *Phys. Rev. B* **78**, 220505(R) (2008).
- ²⁶Gang Mu, Bin Zeng, Peng Cheng, Zhaosheng Wang, Lei Fang, Bing Shen, Lei Shan, Cong Ren, and Hai-Hu Wen, arXiv:0906.4513 (unpublished).