Multi-Band Calculations on the Upper Critical Fields of Iron Pnictide Superconductor $Ba(Fe_{1-x}Ni_x)_2As_2$ ($x = 0.072$)

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Based on two-band Ginzburg–Landau theory, we study the upper critical fields for the overdoped composition of the iron-based superconductor $Ba(Fe_{1-x}Ni_x)_2As_2$ with $x = 0.072$. All the temperature and angular results of this compound are consistent with the experimental data. Thus our analysis strongly suggests that $Ba(Fe_{1-x}Ni_x)_2As_2$ in the overdoped regime is a two-gap superconductor.

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1. Introduction

Since the great discovery of superconductivity in LaFeAs(O,F) with the critical temperature 26 K in 2008 [1], iron pnictides have attracted increasing attention by the scientific community. Up to now, the transition temperature T_c of Fe-based superconductors has been raised to about 55 K [2]. But due to their great variety of structural, electronic and magnetic properties, investigations toward the superconducting nature of iron pnictides, such as the symmetry of the order parameter, the pairing mechanism and their relations to the magnetic properties, are still in progress. Recently systematic measurements of thermal conductivity and magnetic properties have shown that $Ba(Fe_{1-x}Ni_x)_2As_2$ in the strongly overdoped regime exhibits unconventional superconductivity [3, 4]. The Fermi surface of this compound consists of a hole pocket centered at Γ and electron pockets at X points. The critical temperature T_c of $Ba(Fe_{1-x}Ni_x)_2As_2$ ($x = 0.072$) is 7 K, and the upper critical fields are about 6 T in the c-direction and 18 T in the ab-plane [5].

The theory of upper critical field in superconductors was essentially developed right after Abrikosov proposed the type-II superconductivity [6, 7]. It was later recognized that the angular dependence of upper critical field can be used to probe the anisotropy of the superconducting order parameters [8]. As to phenomenological single-band Ginzburg–Landau (GL) theory, the anisotropy of crystal can be simply incorporated by introducing an effective-mass tensor into the kinetic energy term. For a system which may be regarded as uniaxial, the angular dependence of upper critical field has been analytically obtained and characterized by the relation $H_{c2}^{-2} \propto \cos^2\theta$ [9]. Here θ is the angle between the c-axis and the direction of applied magnetic field. Recently based on the resistivity measurements, the dependence of upper critical field on the angle θ has been obtained in a broad temperature range for the overdoped iron-based superconductor $Ba(Fe_{1-x}Ni_x)_2As_2$ with $x = 0.072$. The shape of H_{c2} as a function of θ clearly deviates from the anisotropic GL theory and shows the multi-band signal [5].

We will follow the procedure outlined by Liu and Gan [10] and study angular dependence of upper critical fields for $Ba(Fe_{1-x}Ni_x)_2As_2$ based on two-band GL theory. Our numerical calculations are in agreement with the experimental data. It strongly suggests that $Ba(Fe_{1-x}Ni_x)_2As_2$ in the overdoped regime is a two-gap superconductor.

The paper is organized as follows. In the next section, we discuss the two-band BCS theory and phenomenological two-band GL theory. In Sect. 3, we calculate the temperature and angular dependences of upper critical fields for the iron-based superconductor $Ba(Fe_{1-x}Ni_x)_2As_2$. Finally, Sect. 4 gives the conclusion of the paper.

2. Theoretical methods

Following the work of Zhitomirsky and Dao [11], we write the Hamiltonian of an s-wave two-gap superconductor as

$$\hat{H} = \sum_{i\sigma} C_{i\sigma}^{+}(\boldsymbol{x})\hat{h}(\boldsymbol{x})C_{i\sigma}(\boldsymbol{x}) - \sum_{ii'} g_{ii'} C_{i\uparrow}^{+}(\boldsymbol{x})C_{i\downarrow}^{+}(\boldsymbol{x})C_{i'\downarrow}(\boldsymbol{x})C_{i'\uparrow}(\boldsymbol{x}). \quad (1)$$

Here $i, i' = 1, 2$ are the band indexes. $\hat{h}(\boldsymbol{x})$ is the single-particle Hamiltonian of the normal metal and $g_{ii'}$ is the scattering amplitude.

Introducing two gap functions

$$\Delta_i(\boldsymbol{x}) = -\sum_{i'} g_{ii'} \langle C_{i'\downarrow}(\boldsymbol{x})C_{i'\uparrow}(\boldsymbol{x})\rangle, \quad (2)$$

we can transform the total Hamiltonian into the mean-field form similar to the single-band case. Then in the vicinity of the critical temperature and with an applied magnetic field $\boldsymbol{H}$, we can treat the anomalous term $\Delta_i(\boldsymbol{x})$ as a perturbation and obtain the weak-coupling GL functional for two-gap superconductors as [10–12]:

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$$F = \left(F_1 + F_2 + F_{12} + \boldsymbol{H}^2/8\pi\right) \tag{3}$$

with

$$F_i = \frac{\hbar^2}{2m_i}\left|\left(\boldsymbol{\nabla}_2 - \frac{2\mathrm{i}e\boldsymbol{A}_2}{\hbar c}\right)\Psi_i\right|^2 + \frac{\hbar^2}{2m_{iz}}\left|\left(\nabla_z - \frac{2\mathrm{i}eA_z}{\hbar c}\right)\Psi_i\right|^2 - \alpha_i(T)\left|\Psi_i\right|^2 + \frac{\beta_i}{2}\left|\Psi_i\right|^4 \tag{4}$$

and

$$F_{12} = -R_{12}(\Psi_1^*\Psi_2 + \text{c.c.}). \tag{5}$$

Here F_i is the free energy for each band and F_{12} is the interaction free energy. $\Psi_i \propto \sqrt{N_i}\Delta_i$ with N_i the density of states at the Fermi level is the superconducting order parameter and R_{12} is the Josephson coupling constant. m_i and m_{iz} denote the effective masses in the ab-plane and in the c-direction for band i. Here we assume that the effective mass anisotropy has the uniaxial symmetry appropriate for most layered superconductors. The coefficient α_i is a function of temperature, while β_i is independent of temperature. If the interband interaction is neglected, the functional can be reduced to two independent single-band problems with the corresponding critical temperatures T_{c1} and T_{c2}, respectively. Thus the parameters α_1 and α_2 can be approximately expressed as $\alpha_i = \alpha_{i0}(1 - T/T_{ci})$ with α_{i0} the proportionality constant [13]. The operator $\boldsymbol{\nabla}_2$ is defined as $(\partial/\partial x, \partial/\partial y, 0)$. $\boldsymbol{H} = \boldsymbol{\nabla} \times \boldsymbol{A}$ is the magnetic field and $\boldsymbol{A} = (\boldsymbol{A}_2, A_z) = (A_x, A_y, A_z)$ is the vector potential.

We notice that the free energy is invariant under the scaling transformation $\Psi_i \to \sqrt{l}\Psi_i$, $m_i \to lm_i$, $m_{iz} \to lm_{iz}$, $\alpha_i \to \alpha_i/l$, $\beta_i \to \beta_i/l^2$, $R_{12} \to R_{12}/l$ with l a scaling factor. Therefore we can set $m_2 = m_e$ with m_e the electron mass in the GL theory. From the experience of MgB_2 [14–19], we can reasonably suppose that T_{c1} (or T_{c2}) corresponds to the X-band (or Γ-band) with the larger (or smaller) gap. Then noting that $\ln(T_{c1}/T) \approx 1 - T/T_{c1}$, we can rewrite the microscopic forms of α_1 and α_2 as a linear function of $(1 - T/T_{c1})$ and obtain the relation $\alpha_{10}/\alpha_{20} = T_{c1}/T_{c2}$ [11]. Moreover, with the increase of electron doping to about 0.07, the anisotropy of the Fermi velocities in the Γ-band $(v_{2,x}/v_{2,z})^2$ decreases from 3 to 2.7 [20]. From Ref. [11], we can thus estimate $m_{2z}/m_2 = (v_{2,x}/v_{2,z})^2 \approx 2.7$.

By minimizing the free energy Eq. (3) with Ψ_i^*, we can obtain the two-band GL equation for the description of the two-gap superconductivity

$$\begin{pmatrix} \hat{M}_{11} & \hat{M}_{12} \\ \hat{M}_{21} & \hat{M}_{22} \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = 0 \tag{6}$$

with

$$\hat{M}_{ii} = -\frac{\hbar^2}{2m_i}\left(\boldsymbol{\nabla}_2 - \frac{2\mathrm{i}e\boldsymbol{A}_2}{\hbar c}\right)^2 - \frac{\hbar^2}{2m_{iz}}\left(\nabla_z - \frac{2\mathrm{i}eA_z}{\hbar c}\right)^2 - \alpha_i + \beta_i|\Psi_i|^2 \tag{7}$$

and

$$\hat{M}_{12} = \hat{M}_{21} = -R_{12}. \tag{8}$$

In the absence of the magnetic field and close to the critical temperature, Eq. (6) transforms into

$$\begin{pmatrix} \alpha_1 & R_{12} \\ R_{12} & \alpha_2 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = 0. \tag{9}$$

We then get

$$R_{12}^2 = \alpha_1\alpha_2 \tag{10}$$

at $T = T_c$.

3. Results and discussion

Now let us solve the problem of the nucleation of superconductivity in the presence of a field $\boldsymbol{H}$. Without losing any generalization, we assume that $\boldsymbol{H}$ lies in the bc-plane and takes the form $\boldsymbol{H} = (0, H\sin\theta, H\cos\theta)$. Here θ is the angle of the field from the c-axis. Then the vector potential can be chosen as $\boldsymbol{A} = (0, Hx\cos\theta, -Hx\sin\theta)$. Since the vector potential depends only on x, similar to the single-band anisotropic GL model [21], we can look for solution with the form

$$\Psi_i = \mathrm{e}^{\mathrm{i}ky\cos\theta}\mathrm{e}^{-\mathrm{i}kz\sin\theta}f_i(x). \tag{11}$$

Close to the upper critical field, we can neglect the quartic terms in Eq. (7) and obtain the linearized GL equation. Combining Eq. (6) and Eq. (11), we then obtain

$$\begin{pmatrix} \hat{M}_{11} & \hat{M}_{12} \\ \hat{M}_{21} & \hat{M}_{22} \end{pmatrix}\begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix} = 0 \tag{12}$$

with

$$\hat{M}_{ii} = -\frac{\hbar^2}{2m_i}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}m_i\omega_i^2(x - x_0)^2 - \alpha_i. \tag{13}$$

Here $\omega_i = 2eH\sqrt{\cos^2\theta + (m_i/m_{iz})\sin^2\theta}/m_i c$ and $x_0 = \hbar ck/2eH$. Since inclusion of the factor x_0 only shifts the location of the minimum of the effective potential, it can be neglected. But it will become important when we deal with superconductivity near surfaces of finite samples [22, 23].

At $R_{12} = 0$, we can obtain the solutions to Eq. (12) immediately by noting that, for each band, it is the Schrödinger equation for a particle bound in a harmonic oscillator potential. The resulting harmonic oscillator eigenvalues are

$$E_{i,n} = (n + 1/2)\hbar\omega_i - \alpha_i \quad (n = 0, 1, 2, \ldots). \tag{14}$$

The minimum eigenfunction takes the form of $(\mu_0/\pi)^{1/4}\,\mathrm{e}^{-\mu_0 x^2/2}$ with $\mu_0 = 2\pi H\sqrt{\cos^2\theta + (m_i/m_{iz})\sin^2\theta}/\Phi_0$ and the magnetic flux quantum $\Phi_0 = \pi\hbar c/e$.

If $R_{12} \neq 0$, Eq. (12) describes a system of two coupled oscillators. To obtain the minimum eigenvalue of the coupled oscillators, we follow a variational approach. We look for solution in the form

$$\begin{pmatrix} f_1(x) \\ f_2(x) \end{pmatrix} = \begin{pmatrix} c_1 g_1(x) \\ c_2 g_2(x) \end{pmatrix} = \begin{pmatrix} c_1\left(\frac{\mu_1}{\pi}\right)^{1/4}\mathrm{e}^{-\mu_1 x^2/2} \\ c_2\left(\frac{\mu_2}{\pi}\right)^{1/4}\mathrm{e}^{-\mu_2 x^2/2} \end{pmatrix}, \tag{15}$$

with μ_1 and μ_2 as two variational parameters. Introducing $D_{ij} = \langle g_i|\hat{H}_{ij}|g_j\rangle$, detailed calculations give

$$D_{11} = \frac{\hbar^2\pi^2 H^2}{m_1} \times \left(\frac{\cos^2\theta}{\mu_1 \Phi_0^2} + \frac{m_1}{m_{1z}} \frac{\sin^2\theta}{\mu_1 \Phi_0^2} + \frac{\mu_1}{4\pi^2 H^2} \right) - \alpha_1, \tag{16}$$

$$D_{22} = \frac{\hbar^2\pi^2 H^2}{m_2} \times \left(\frac{\cos^2\theta}{\mu_2 \Phi_0^2} + \frac{m_2}{m_{2z}} \frac{\sin^2\theta}{\mu_2 \Phi_0^2} + \frac{\mu_2}{4\pi^2 H^2} \right) - \alpha_2 \tag{17}$$

and

$$D_{12} = D_{21} = -R_{12} \left[\frac{4\mu_1\mu_2}{(\mu_1+\mu_2)^2} \right]^{1/4}. \tag{18}$$

Then we can transform Eq. (12) into

$$\begin{pmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = 0. \tag{19}$$

By setting the determinant of the D-matrix as zero, we obtain

$$D_{11}D_{22} = D_{12}D_{21}. \tag{20}$$

Furthermore, we notice that with the form of Eq. (15), the free energy per unit area can be written as $D_{11}c_1^2 + D_{22}c_1^2 + 2D_{12}c_1c_2$. By minimizing this free energy with μ_i, we get $(\partial D_{11}/\partial\mu_i)c_1^2 + (\partial D_{22}/\partial\mu_i)c_2^2 + 2(\partial D_{12}/\partial\mu_i)c_1c_2 = 0$. With $c_1/c_2 = -D_{12}/D_{11}$ from Eq. (19), we can solve μ_1 and μ_2 as functions of the magnetic field H. Then after substituting them into Eq. (20), we can obtain the upper critical field H_{c2}.

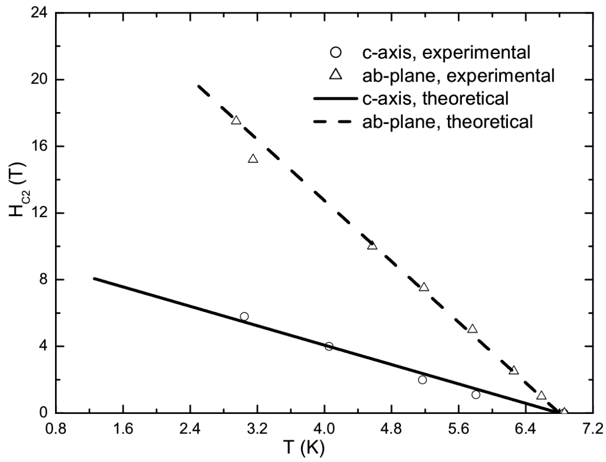

Fig. 1. The temperature dependence of upper critical fields for $\theta = 0^\circ$ and 90°. Circles and triangles are experimental points from Ref. [5] taken with 50% criteria.

We present our numerical results on the temperature dependence of upper critical fields for $Ba(Fe_{1-x}Ni_x)_2As_2$ in Fig. 1. The solid and dashed lines are the upper critical fields in the c-direction ($\theta = 0^\circ$) and in the ab-plane ($\theta = 90^\circ$), respectively. To fit the experimental data, we choose the parameters as following: $m_1 = m_e$, $m_{1z} = 10m_e$, $T_{c1} = 6.6$ K, $T_{c2} = 1.1$ K and $\alpha_{10} = 1.1$ meV. From Eq. (10), we can obtain the interband coupling $R_{12} = 0.26$ meV, which corresponds to a small scale-invariant ratio $R_{12}/\alpha_{10} \approx 0.2$. Moreover, based on the BCS theory, we can roughly estimate the gap ratio $\Delta_1/\Delta_2 \approx T_{c1}/T_{c2} = 6$. Note that the experimental data are almost linear in temperature down to about $0.4T_c$, and our calculations fit the experimental measurements well.

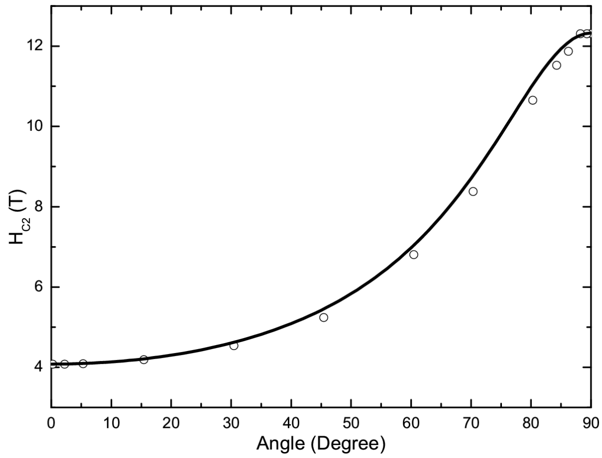

Fig. 2. The angular dependence of upper critical field at $T = 4$ K. The open experimental points are from Ref. [5] taken with 50% criteria.

We also calculate the angular dependence of upper critical field at $T = 4$ K and plot the results in Fig. 2. From Fig. 2, we can see that the upper critical field increases monotonously with the increase of angle θ and our results are in agreement with the experimental data at $T = 4$ K.

4. Conclusion

In summary, we calculate the temperature dependence of upper critical fields for the superconducting compound $Ba(Fe_{1-x}Ni_x)_2As_2$ ($x = 0.072$) and the results fit the experimental data well. Our calculations suggest that $Ba(Fe_{1-x}Ni_x)_2As_2$ has two nodeless superconducting energy gaps and can be well described by the two-band GL theory. The first band exhibits a factor of $m_{1z}/m_1 = 10$ anisotropy between in-plane and out-of-plane direction, which is much larger than that of the other band. But evidence from the penetration depth measurements also suggests that the superconductor $Ba(Fe_{1-x}Ni_x)_2As_2$ in the overdoped regime may develop nodal structure [24], in contrast to the nodeless gaps typical for Fe-based superconductors [25–30]. Based on the experimental investigations up to now, only an upper limit on the gap minimum has been obtained and it is still difficult to be sure whether nodes exist or not. We believe that further experimental studies, such as specific heat at very low temperatures, will be helpful to clarify the nature of superconductivity in the electron-doped $Ba(Fe_{1-x}Ni_x)_2As_2$ compounds.

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