Elastic theory for the vortex-lattice melting in iron-based high-\(T_c\) superconductors

Q-H Chen\textsuperscript{1,2,5}, Q-M Nie\textsuperscript{3}, J-P Lv\textsuperscript{1,2} and T-C Au Yeung\textsuperscript{1,4}

\textsuperscript{1} Center for Statistical and Theoretical Condensed Matter Physics, Zhejiang Normal University, Jinhua 321004, People’s Republic of China
\textsuperscript{2} Department of Physics, Zhejiang University, Hangzhou 310027, People’s Republic of China
\textsuperscript{3} Department of Applied Physics, Zhejiang University of Technology, Hangzhou 310 023, People’s Republic of China
\textsuperscript{4} School of Electric and Electronic Engineering, Nanyang Technological University, Singapore 639798, Singapore
E-mail: qhchen@zju.edu.cn

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\textbf{Abstract.} The vortex-lattice melting transitions in two typical iron-based high-\(T_c\) superconductors Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\) (122-type) and Nd(O\(_{1-x}\)F\(_x\))FeAs (1111-type) for magnetic fields parallel and perpendicular to the anisotropy axis are studied within the elastic theory. Using the parameters from experiments, the vortex-lattice melting lines in the \(H–T\) diagram are located systematically by various groups of Lindemann numbers. It is observed that the theoretical results for the vortex melting on both superconductors Ba(Fe\(_{1-x}\)Co\(_x\))\(_2\)As\(_2\) and Nd(O\(_{1-x}\)F\(_x\))FeAs for parallel fields agree well with the recent experimental data. The future experimental results for the vortex melting can be compared with the present theoretical prediction by tuning reasonable Lindemann numbers.

\textsuperscript{5} Author to whom any correspondence should be addressed.
1. Introduction

Recently, some newly discovered iron-based superconductors have attracted considerable scientific interest both experimentally [1]–[17] and theoretically [18]–[23]. First, a novel superconductivity in 1111 phase FeAs superconductors was reported experimentally, giving a new path towards high-temperature superconductivity. LaOFeAs doped with F\(^-\) ions at the O\(^2-\) sites was found to exhibit superconductivity with \(T_c = 26\) K [1], and the superconductivity was also observed with hole doping [2]. Then \(T_c\) was surprisingly increased above 40 K when La in LaO\(_{1-x}\)F\(_x\)FeAs was substituted by other rare earth elements [3, 4]. It was observed later that \(T_c\) is about 55 K in SmO\(_{1-x}\)F\(_x\)FeAs [5, 6] and Gd\(_{1-x}\)Th\(_x\)OFeAs [7]. They were the first non-copper-based superconductors in which the maximum critical temperature is much higher than the theoretical value predicted from the Bardeen, Cooper and Schrieffer (BCS) theory [24]. On the other hand, the 122 phase iron-based superconductor BaFe\(_2\)As\(_2\) was discovered more recently [8], and its superconducting critical temperature was found to be as high as 38 K by hole doping. It has been observed that the electron doping of this compound by Co [9] and Ni [10] also induces superconductivity. Although there are some theoretical studies on iron-based superconductors, the type-II superconductivity as well as the mechanism of superconductivity is not well understood to date.

The vortex-lattice solid (glass with random pinning) state with zero linear resistivity is crucial for the application of high-\(T_c\) superconductors; thus the melting of the vortex lattice in bulk type-II superconductors is of great significance [25]–[29]. The main aspects of the Lindemann criterion suggest that the lattice melts when the root mean square thermal displacements of the components of a lattice reach a certain fraction of the equilibrium lattice spacing; such a criterion was first adopted to study the vortex-lattice melting transition in type-II superconductors with a magnetic field parallel to the anisotropic axis; then this approach was used to draw the melting lines in the case of magnetic field perpendicular to the anisotropic axis [30]–[33]. Since the upper critical field is also high [12, 13] in iron-based high-\(T_c\) superconductors, the thermal fluctuation may drive the vortex lattice to a vortex liquid in a field far below the upper critical field [30] through vortex melting. We will extend the elastic theory to study the vortex melting in these newly discovered superconductors.
In the present paper, using parameters measured in recent experiments, we study the vortex-lattice melting transitions for two typical iron-based layered superconductors \( \text{Ba(Fe}_{1-x}\text{Co}_x\text{)}_2\text{As}_2 \) (122-type) with low anisotropy \([9, 12]\) and \( \text{Nd(O}_{1-x}\text{F}_x\text{)FeAs} \) (1111-type) with high anisotropy \([4, 13]\), in the framework of the elastic theory. The melting lines for magnetic fields parallel and perpendicular to the anisotropic axis are systematically located with different groups of the Lindemann numbers. A comparison with current experimental findings is made. The present paper is organized as follows. In section 2, we introduce the theoretical method used in this work, in section 3 we present the main results, and finally, we give a short summary.

2. Elastic theory

We will consider the fields \( B \) parallel and perpendicular to the anisotropy axis (i.e. the \( c \)-axis in this paper), and the elastic theories in both cases will be presented.

2.1. Thermal fluctuations

Whether the field is parallel or perpendicular to the \( c \)-axis, for the ideal triangular vortex-line lattice, the free energy in elastic theory can be expressed in an unified way with quadratic terms of the deviation vector \( \mathbf{u} = (u_x, u_y) \) describing the fluctuations of vortices from their equilibrium positions \([25, 26], [30]–[33]\)

\[
F = \frac{1}{2} \int \frac{d^3 \mathbf{k}}{(2\pi)^3} \mathbf{u} \cdot \mathbf{C} \cdot \mathbf{u}. \tag{1}
\]

The matrix \( \mathbf{C} \) for fields parallel to the \( c \)-axis is different from that for fields perpendicular to it. We denote by \( \mathbf{C}^c \) and \( \mathbf{C}^{ab} \) the elastic matrix for the fields parallel and perpendicular to the \( c \)-axis, respectively, and they are given as follows:

\[
\mathbf{C}^c = \begin{pmatrix}
  c_L k_x^2 + c_{66} k_x^2 + c_{44} k_z^2 & c_L k_x k_y \\
  c_L k_x k_y & c_L k_y^2 + c_{66} k_y^2 + c_{44} k_z^2
\end{pmatrix} \tag{2}
\]

and

\[
\mathbf{C}^{ab} = \begin{pmatrix}
  c_{11} k_x^2 + c_{66} k_y^2 + c_{44} k_z^2 & c_{11} k_x k_y \\
  c_{11} k_x k_y & c_{11} k_y^2 + c_{66} k_y^2 + c_{44} k_z^2
\end{pmatrix}. \tag{3}
\]

In the matrix \( \mathbf{C}^c \), \( k_x^2 = k_x^2 + k_y^2, c_{66}, c_{11} \) and \( c_{44} \) are the wave-vector-dependent shear, bulk and tilt elastic moduli \([26, 34, 35]\), respectively, which are determined as follows:

\[
c_{44}(\mathbf{k}) = \frac{B^2}{4\pi} \left[ \frac{M}{M_z} \right] \frac{1 - b}{2b\kappa^2} \left[ \frac{1}{k_x^2 + (M/M_z)(k_y^2 + m^2_e)} + 1 \right] \tag{4}
\]

and

\[
c_{11}(\mathbf{k}) = \frac{B^2}{4\pi} \frac{1 - b}{2b\kappa^2} \left[ \frac{k_x^2 + (M/M_z)m^2_e}{(k_y^2 + m^2_e)(k_x^2 + (M/M_z)(k_y^2 + m^2_e))} - \frac{1}{k_x^2 + (M/M_z)k_y^2 + m^2_e} \right], \tag{5}
\]
where we have defined \( m_2^2 = \frac{1 - b}{2a^2} \) and \( m_3^2 = \frac{1 - b}{b} \), \( M \) is a quasi-particle effective mass in the \( xy \)-plane, \( M_2 \) is described along the \( c \)-axis, \( b = B / B_c2 \) with \( B_c2 \) being the upper critical field, and \( \kappa = \lambda / k_\perp \). The bulk modulus is \( \kappa = \kappa_1 - \kappa_6 \) with shear modulus \( \kappa_6 = \frac{B_{c2}^2 b(1 - b)^2}{8\kappa_2^2} \).

The matrix \( \hat{C}^{ab} \) also contains some elastic moduli. Since the anisotropy exists here, tilt and shear moduli are not isotropic anymore. For example, \( c_{44}^b(k) (c_{44}^b(k)) \) is the tilt modulus along (perpendicular to) the \( c \)-axis. Similarly, \( c_{66}^b (c_{66}^b) \) represents the shear modulus parallel to (perpendicular to) the anisotropy axis \( c \). For the detailed expressions for elastic moduli, refer to [33].

The thermal fluctuations of the vortices are given by inverting the kernel \( \hat{C}(k) \) as follows:

\[
\langle u^2 \rangle = \frac{k_B T}{(2\pi)^3} \int dk [\hat{C}^{\alpha\beta}_{\alpha\beta}]^{-1}(k), \quad \alpha = x, y, \quad \beta = c, ab.
\]

The integrations in equation (7) are over \( 0 < k_z < \infty \) and within the first Brillouin zone (BZ) for \( k_z \) and \( k_y \). To be specific, we consider a lattice structure as the low-temperature equilibrium state as shown in figure 1 of [33], where the lattice spacings are \( a_x = a \) and \( a_y = a\sqrt{3}/2 \) for fields parallel to the \( c \)-axis, \( a_z = a/\sqrt{3} \) with \( \hat{z} \parallel \hat{c} \) and \( a_y = a\sqrt{3}/2 \) for fields perpendicular to the \( c \)-axis with \( y^2 = m_z / m_{ab} \) and \( a = \sqrt{2}\Phi_0 / \sqrt{3}B \).

For parallel fields, we consider the mean-square displacement of a vortex lattice from the equilibrium \( d^2(T) = u_x^2 + u_y^2 \), which can be written as

\[
d^2(T) = \frac{k_B T}{(2\pi)^3} \int dk \left[ \frac{1}{c_{66}k_\perp^2 + c_{44}k_z^2} + \frac{1}{c_{11}k_\perp^2 + c_{44}k_z^2} \right].
\]

For convenience, we introduce the dimensionless wave vector \( \mathbf{q} = (k_x / \Lambda_x, k_y / \Lambda_y, k_z / \Lambda) \), where \( \Lambda_{x,y} \) are the wave numbers at the edges of the first BZ. Explicitly, they are given as \( \Lambda_x = 4\pi / 3a \) and \( \Lambda_y = 2\pi / a\sqrt{3} \) for fields parallel to the \( c \)-axis and \( \Lambda_x = 4\pi / \sqrt{3}a \) and \( \Lambda_y = 2\pi / a\sqrt{3}a \) for fields perpendicular to the \( c \)-axis. The unit of wave number in the \( k_z \)-direction is taken as \( \Lambda = \sqrt{4\pi B/\Phi_0} = \sqrt{8\pi / \sqrt{3}a^2} \). The thermal fluctuations are then expressed as

\[
d^2(T) = \frac{\Lambda}{B^2} \frac{k_B T}{(2\pi)^3} \int dq \tilde{C}_{\alpha\alpha}^{-1}(q) \equiv \frac{\Lambda}{B^2} \frac{k_B T}{(2\pi)^3} I_{dd}, \quad \text{for } B \parallel c
\]

and

\[
\langle u^2 \rangle = \frac{\Lambda}{B^2} \frac{k_B T}{(2\pi)^3} \int dq \tilde{C}_{\alpha\alpha}^{-1}(q) \equiv \frac{\Lambda}{B^2} \frac{k_B T}{(2\pi)^3} I_{aa}, \quad \alpha = x, y, \quad \text{for } B \perp c
\]

with the normalized matrix \( \tilde{\hat{C}}(q) \equiv \hat{C}(q) / B^2 \Lambda_x \Lambda_y \).

2.2. The Lindemann criterion

The Lindemann criterion presumes that the lattice melts when the root mean square thermal displacements of the components of a lattice reach some fraction of the equilibrium lattice spacing. For two cases, we write the usual isotropic Lindemann criterion for parallel fields,

\[
\langle d^2 \rangle < c^2 a^2.
\]
and the anisotropic one for perpendicular fields,

\[ \langle u_x^2 \rangle = c_x^2 a_x^2, \quad \langle u_y^2 \rangle = c_y^2 a_y^2 \]  \hfill (12)

with \( c_x \) and \( c_y \) being two Lindemann numbers for two transverse directions. Combining the Lindemann criterion and the elastic theory, we can get the melting equations for two cases,

\[ \frac{t}{\sqrt{1 - t}} = c_a^2 \frac{32 \pi^4 k^2 \sqrt{b}}{\sqrt{3 \varepsilon_d}} \frac{\sqrt{b}}{I_{dd}}, \quad \text{for } B \parallel c \]  \hfill (13)

and

\[ \frac{t_a}{\sqrt{1 - t_a}} = \left( \frac{a_a}{a} \right)^2 c_a^2 \frac{32 \pi^4 k^2 \sqrt{b_a}}{\sqrt{5 \varepsilon}} \frac{\sqrt{b_a}}{I_{aa}}, \quad \alpha = x, y, \quad \text{for } B \perp c \]  \hfill (14)

with \( \varepsilon \) being the Ginzburg parameter \( \varepsilon_d = 16 \pi^3 k^4 (k_B T_c)^2 / \Phi_0^3 H_{c2}^2 (0) \) and \( \varepsilon = 16 \pi^3 k^4 (k_B T_c)^2 / \Phi_0^3 H_{c2}^2 (0) \).

2.3. Layer pinning effect

When the field is perpendicular to the \( c \)-axis, the effect of layer pinning reduces fluctuations in both the directions and induces an additional momentum-independent term to the elastic matrix in equation (3) such that

\[ C_{ab}^{\text{lp}} = \begin{pmatrix} c_{11} k_x^2 + c_{66} k_y^2 + c_{44} k_z^2 + \Theta & c_{11} k_x k_y \\ c_{11} k_x k_y & c_{11} k_y^2 + c_{66} k_x^2 + c_{44} k_z^2 \end{pmatrix}, \]  \hfill (15)

where

\[ \frac{\Theta}{\Lambda^2 B^2} = \frac{4 \sqrt{\pi}}{\beta_A k^2 \gamma} \left( \frac{\xi_c^0}{s} \right)^3 \frac{1 - b}{b^2} \frac{1}{(1 - t)^{3/2}} e^{-[8/(1-t)](\xi_c^0/s)^2} \]  \hfill (16)

is proportional to the critical depinning current [36], with \( \xi_c^0 \equiv \xi_c (T = 0) \), \( \beta_A \approx 1.16 \) and \( s \) is the layer separation.

3. Results

3.1. Vortex melting in Ba(Fe\(_{1-x}\)Co\(_{x}\))\(_2\)As\(_2\)

We study the vortex melting in Ba(Fe\(_{1-x}\)Co\(_{x}\))\(_2\)As\(_2\) (\( x = 0.1 \)) as a representative of 122-type iron-based superconductors [11]. Parameters measured from a very recent experiment [12] gives \( T_c = 22 \text{ K}, \lambda_\perp = 160 \text{ nm}, \xi_\perp = 2.44 \text{ nm}, H_{c2}^\perp (T = 0) = 50 \text{ T}, H_{c2}^{ab} (T = 0) = 70 \text{ T} \) and \( s = 23 \text{ A} \). The anisotropic parameter \( \gamma \) falls from 2.0 to 1.5 with a decrease of temperature. In our calculation, we observe that the melting lines determined in the framework of elastic theory only change slightly with the variation of \( \gamma \) (in the range of 1.5–2.0). So we have set \( \gamma = 2 \) in our calculations.

We first calculate the melting line for the parallel fields with various Lindemann numbers. It is interesting to note in figure 1 that the vortex melting line for Ba(Fe\(_{1-x}\)Co\(_{x}\))\(_2\)As\(_2\) obtained in this paper is in good agreement with the irreversible line measured experimentally [12] with the Lindemann number \( c = 0.2 \). The irreversibility line in a superconductor is usually regarded as the melting line [30].

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Figure 1. Comparison of vortex-lattice melting lines for Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ with the experimental results of [12] for magnetic fields parallel to the c-axis.

Figure 2. Vortex-lattice melting lines for Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ with magnetic field perpendicular to the c-axis (without intrinsic layer pinning). From left to right, $C_x = 0.05$, $C_y = 0.05$, $C_y = 0.0375$; $C_x = 0.1$, $C_y = 0.1$, $C_y = 0.075$; $C_x = 0.2$, $C_y = 0.2$, $C_y = 0.15$.

Then we study the vortex melting for perpendicular fields. Due to the lack of experimental data until now, three groups of Lindemann numbers are selected to calculate the melting lines ($C_x = 0.05$, $C_y = 0.05$, $C_y = 0.0375$; $C_x = 0.1$, $C_y = 0.1$, $C_y = 0.075$; $C_x = 0.2$, $C_y = 0.2$, $C_y = 0.15$). The obtained melting curves are shown in figure 2. Future experimental results can be inserted into this figure, and can be compared with the interpolation values obtained here.

Setting $C_x = C_y$, we obtain two curves as shown in figures 2(a)–(c), as in [31]. As pointed out in [32], to interpret these two curves as two ‘melting lines’ and thus reach a conclusion of an intermediate phase has no physical basis, since the elastic theory can give at best one melting line. Imposing the same Lindemann number along the two directions has no physical basis. In order to achieve a single melting line, one can tune the Lindemann numbers in the two directions. A good collapse of the melting lines in two directions can be achieved by setting the ratio $c_x/c_y \approx 1.33$. It is interesting to note that this ratio is very close to the 1.37 observed in [33] using the parameters for cuprate superconductors.

The vortex melting for fields perpendicular to the c-axis is also influenced by the layer pinning. In order to study this intrinsic layer pinning effect, the matrix (15) is used to calculate
the thermal fluctuations along two transverse directions. The melting lines for two groups of Lindemann numbers ($C_x = 0.1, C_y = 0.1, C_y = 0.075; C_x = 0.2, C_y = 0.2, C_y = 0.15$) are collected in figure 3. A good collapse can also be obtained by setting the same ratio $c_x/c_y \approx 1.33$. Future experimental data can also be compared with these values.

3.2. Vortex melting in Nd(O$_{1-x}$F$_x$)FeAs

We now turn to another typical iron-based layered superconductor Nd(O$_{1-x}$F$_x$)FeAs (1111-type) [13]–[16]. We take parameters from [15]. $T_c = 49$ K, $\lambda_\perp = 200$ nm, $\xi_\perp = 2.3$ nm, $H_{c2}^1 (T = 0) = 95$ T, $H_{c2}^{ab} (T = 0) = 220$ T and $\gamma^2 = 25$. The separation between the FeAs planes is given by twice the lattice parameter $s = 2c \approx 17$ Å [1, 14, 22].

Similarly, we first calculate the melting lines for the fields parallel to the $c$-axis, as shown in figure 4. Since the melting line has not been explicitly reported, the data for which the resistance reaches a small percentage (0.5%) of the normal-state resistance in [15] are regarded as the approximated melting line here, which are also shown in figure 4. Interestingly, the
Figure 5. Vortex-lattice melting lines for Nd(O$_{1-x}$F$_x$)FeAs with magnetic field perpendicular to the $c$-axis (without intrinsic layer pinning). From left to right, $C_x = 0.1$, $C_y = 0.1$, $C_y = 0.075$; $C_x = 0.2$, $C_y = 0.2$, $C_y = 0.15$; $C_x = 0.3$, $C_y = 0.3$, $C_y = 0.225$.

Figure 6. Vortex-lattice melting lines for Nd(O$_{1-x}$F$_x$)FeAs with magnetic field perpendicular to the $c$-axis (with intrinsic layer pinning).

Theoretical melting line with $c = 0.18$ is consistent with the experimental data in a considerably wide temperature range. The discrepancy between experiment and theory becomes larger at high magnetic fields and low temperatures. A trend of temperature-independent melting data is shown at high magnetic fields in experiments, implying that the dimensional crossover occurs in this regime. If the vortex system is of two-dimensional nature at high magnetic fields, the melting line is almost independent of the temperature [30].

Next, we calculate the melting lines when the fields are perpendicular to the $c$-axis, which are shown in figure 5. For perpendicular fields, three different groups of Lindeman numbers ($C_x = 0.1$, $C_y = 0.1$, $C_y = 0.075$; $C_x = 0.2$, $C_y = 0.2$, $C_y = 0.15$; $C_x = 0.3$, $C_y = 0.3$, $C_y = 0.225$) are used to locate the melting lines. A good collapse of the melting lines in two directions can also be achieved by setting the ratio $c_x/c_y \approx 1.33$, almost the same as that in the 122 type.

We also investigate the effect of the intrinsic layer pinning on the vortex melting in a Nd(O$_{1-x}$F$_x$)FeAs sample. The results are exhibited in figure 6. Surprisingly, we observe an intersection between two melting lines with two transverse directions for typical Lindemann numbers, which is not shown in the above 122 type. Obviously, a collapse of these two
curves could not be achieved by setting any ratio $c_x/c_y$. It is implied that the intermediate smectic phase $[31]–[33]$ may exist in Nd(O$_{1-x}$F$_x$)FeAs. However, its identification is beyond the phenomenological Lindemann theory. It is interesting to note that, when the exponentially weak intrinsic pinning was taken into account for weakly anisotropic Ba$_{(1-x)Co_x}^2$As$_2$, the vortex melting behavior is changed only slightly, but for the strongly anisotropic Nd(O$_{1-x}$F$_x$)FeAs, the intrinsic pinning would play a much more significant role.

4. Summary

In terms of the elastic theory, we have studied the thermal fluctuations in two typical iron-based superconductors Ba$_{(1-x)Co_x}^2$As$_2$ and Nd(O$_{1-x}$F$_x$)FeAs for magnetic fields parallel and perpendicular to the anisotropy axis. Using the parameters of these superconductors from experiments, the melting lines with various Lindemann numbers are composed. Interestingly, we can derive the melting line observed in both Ba$_{(1-x)Co_x}^2$As$_2$ [12] and Nd(O$_{1-x}$F$_x$)FeAs [15] for magnetic field parallel to the $c$-axis. Neglecting the layer pinning effect, it is found that thermal fluctuations normalized by vortex separations in the two transverse directions for the parallel field are proportional to each other, similar to those observed in cuprate superconductors [32, 33]. Interestingly, the intrinsic layer pinnings play a much more important role in the vortex melting in Nd(O$_{1-x}$F$_x$)FeAs than in Ba$_{(1-x)Co_x}^2$As$_2$. More experimental work is necessary to confirm our prediction by comparing the melting data with the interpolation values presented here. The present prediction may in turn provide a guide or reference to locate the melting line in future experiments.

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