

Elastic contribution to interaction of vortices in uniaxial superconductors

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The stress caused by vortices in tetragonal superconductors contributes to the intervortex interaction which depends on vortex orientation within the crystal, on elastic moduli, and is attractive within certain angular regions even in fields along the c crystal axis. For sufficiently strong stress dependence of the critical temperature, this contribution may result in distortions of the hexagonal vortex lattice for $\mathbf{H} \parallel c$. In small fields it leads to formation of a square vortex lattice with a fixed H independent spacing. This should be seen in the magnetization $M(H)$ as a discontinuous jump of magnetization at the transition from the Meissner to mixed states.

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The strains in type-II superconductors that arise due to the presence of vortices and defects were considered time ago as a pinning mechanism, see, e.g., Ref. 1 and references therein. Recently, vortex induced strains, their weakness notwithstanding, were shown to cause substantial changes in macroscopic magnetization in materials with strong pressure dependence of the critical temperature T_c , the result of long-range elastic perturbations as opposed to short-range London intervortex interactions.² Here uniaxial materials are considered in fields along principal crystal directions. To calculate the elastic energy, vortices are treated as one-dimensional strain sources in an infinite crystal, so that we deal with a *planar* elasticity problem.³

The value of dT_c/dp (p is the stress or, in particular, the pressure) is an indicator of strength of magnetoelastic effects in the mixed state. It turned out recently that this derivative in pnictides, and in $\text{Ca}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ in particular,⁴ by one or two orders of magnitude exceeds values for conventional superconductors making Fe-based materials favorable for observation of magnetoelastic effects.

It is shown below that elastic intervortex interactions in tetragonal materials are strongly anisotropic even for vortices directed along the c crystal axis. For a particular set of elastic moduli, two vortices situated at [100] or [010] elastically attract each other, whereas being at [110] they are repelled. In large fields the extra interaction removes orientational degeneracy of the standard 60° triangular vortex lattice and should cause distortions of this structure in qualitative agreement with data on KFe_2As_2 .⁵ Possible relevance of the elasticity in hexagonal crystals for low fields vortex arrangement in MgB_2 is discussed.⁶

I. TETRAGONAL CRYSTAL

The general form of elastic energy density is³

$$F = \lambda_{iklm} u_{ik} u_{lm} / 2, \quad (1)$$

where u_{ik} are strains and λ_{iklm} are elastic moduli. For brevity we denote the nonzero components of the elastic tensor in the crystal frame as⁷

$$\begin{aligned} \lambda_{aaaa} = \lambda_{bbbb} = \lambda_1, \quad \lambda_{aabb} = \lambda_2, \quad \lambda_{abab} = \lambda_3, \\ \lambda_{cccc} = \lambda_4, \quad \lambda_{aacc} = \lambda_{bbcc} = \lambda_5, \\ \lambda_{acac} = \lambda_{bcbc} = \lambda_6. \end{aligned} \quad (2)$$

Consider a system of straight parallel vortices along z tilted with respect to the frame (a, b, c) of an infinite tetragonal crystal. Introduce the vortex frame (x, y, z) so that the angle between the vortex axis z and the c axis is θ . Consider the tilt as rotation round the a axis:

$$x = a, \quad y = b \cos \theta - c \sin \theta, \quad z = b \sin \theta + c \cos \theta. \quad (3)$$

Although this is a particular tilt, the resulting physics only weakly depends on this choice.

The elastic perturbation by vortices is caused by a number of reasons among which effects of normal cores and of supercurrents around were discussed, see, e.g., Refs. 8 and 9 and references therein. In this paper, only *planar* deformations are considered, i.e., such that the displacement u_z is zero and all $u_{iz} = 0$.

Components of the stress tensor $\sigma_{ik} = \lambda_{iklm} u_{lm} = \lambda_{ik\alpha\beta} u_{\alpha\beta}$ (hereafter Greek indices take only x, y values) are

$$\sigma_{xx} = \lambda_{xxxx} u_{xx} + \lambda_{xxyy} u_{yy}, \quad (4)$$

$$\sigma_{yy} = \lambda_{yyxx} u_{xx} + \lambda_{yyyy} u_{yy}, \quad (5)$$

$$\sigma_{xy} = 2\lambda_{xyxy} u_{xy}, \quad (6)$$

and

$$\sigma_{zz} = \lambda_{zzxx} u_{xx} + \lambda_{zzyy} u_{yy}. \quad (7)$$

Furthermore,

$$\sigma_{xz} = 2\lambda_{xzyy} u_{xy}, \quad \sigma_{yz} = \lambda_{yzxx} u_{xx} + \lambda_{yzyy} u_{yy}. \quad (8)$$

The needed elastic tensor components in the vortex frame are given in Appendix A.

Given only two independent displacements u_x, u_y in the *planar* problem of our interest, the components of the stress tensor cannot be independent.³ Indeed, express u_{xx} and u_{yy} from Eqs. (4) and (5):

$$u_{xx} d = \lambda_{yyyy} \sigma_{xx} - \lambda_{xxyy} \sigma_{yy}, \quad (9)$$

$$u_{yy} d = \lambda_1 \sigma_{yy} - \lambda_{xxyy} \sigma_{xx}, \quad (10)$$

$$d = \lambda_1 \lambda_{yyyy} - \lambda_{xxyy}^2, \quad (11)$$

and substitute the result in Eq. (7):

$$\sigma_{zz}d = d_1\sigma_{xx} + d_2\sigma_{yy}, \quad (12)$$

$$d_1 = \lambda_{zzxx}\lambda_{yyyy} - \lambda_{zzyy}\lambda_{xxyy}, \quad (13)$$

$$d_2 = \lambda_{zzyy}\lambda_1 - \lambda_{zzxx}\lambda_{xxyy}. \quad (14)$$

The equilibrium conditions $\partial\sigma_{\alpha\beta}/\partial x_\beta = 0$ or

$$\frac{\partial\sigma_{xx}}{\partial x} + \frac{\partial\sigma_{xy}}{\partial y} = 0, \quad \frac{\partial\sigma_{yx}}{\partial x} + \frac{\partial\sigma_{yy}}{\partial y} = 0 \quad (15)$$

are satisfied if one sets

$$\sigma_{xx} = \frac{\partial^2\chi}{\partial y^2}, \quad \sigma_{yy} = \frac{\partial^2\chi}{\partial x^2}, \quad \sigma_{xy} = -\frac{\partial^2\chi}{\partial x\partial y}, \quad (16)$$

with an arbitrary function $\chi(x, y)$.³ Relation (12) then provides an equation for χ :

$$d_1 \frac{\partial^2\chi}{\partial y^2} + d_2 \frac{\partial^2\chi}{\partial x^2} = d\sigma_{zz}. \quad (17)$$

Since $\sigma_{ii} = -3p$ with the pressure p , we have

$$\sigma_{zz} = -3p - \nabla^2\chi. \quad (18)$$

Hence, we obtain

$$D_2 \frac{\partial^2\chi}{\partial x^2} + D_1 \frac{\partial^2\chi}{\partial y^2} = -3pd. \quad (19)$$

$$D_1 = d + d_1, \quad D_2 = d + d_2. \quad (20)$$

The rescaling

$$x_n = x\sqrt{d/D_2}, \quad y_n = y\sqrt{d/D_1} \quad (21)$$

transforms this to a Poisson equation which can be solved for $\chi(x, y)$. Hence, both the stresses $\sigma_{\alpha\beta}$ and strains $u_{\alpha\beta}$ can be found.

At first sight, the problem of elastic perturbation caused by parallel vortices can be considered as planar for any orientation of vortices relative to the crystal. This is, however, not the case. The point is that in general the equilibrium conditions (15) should be complemented by $\partial\sigma_{z\beta}/\partial x_\beta = 0$ with $\sigma_{z\beta}$ given in Eq. (8). However, since the planar solutions $u_{\alpha\beta}$ are already fixed to satisfy (15), there is no room for any extra conditions. The only situation free of this contradiction is when both σ_{zx} and σ_{zy} are zeros. The direct examination of elastic constants involved in $\sigma_{z\beta}$ shows that they are $\propto \sin\theta \cos\theta$, i.e., $\sigma_{z\beta} = 0$ only for $\theta = 0$ and $\theta = \pi/2$. Since the problem is planar indeed for these orientations, they are considered in what follows.

II. SINGLE VORTEX, $\theta = 0$

For $\theta = 0$ we have $\lambda_{yyyy} = \lambda_1$, $\lambda_{xxyy} = \lambda_2$, $\lambda_{xyxy} = \lambda_3$, $\lambda_{xxzz} = \lambda_{yyzz} = \lambda_5$. Furthermore, $d = \lambda_1^2 - \lambda_2^2$, $d_1 = d_2 = \lambda_5(\lambda_1 - \lambda_2)$, and $D_1 = D_2 = D = (\lambda_1 - \lambda_2)(\lambda_1 + \lambda_2 + \lambda_5)$.

For a single vortex in infinite sample the pressure is zero, whereas the stress due to the vortex can be described as due to a δ -function singular source. We have instead of Eq. (19):

$$\nabla^2\chi = 2\pi S(0)\delta(\mathbf{r} - \mathbf{a}), \quad (22)$$

where $d/D \sim 1$ is incorporated in S . Note that no vortex model is used here explicitly; the vortex is described as a δ -function

stress source of a ‘‘strength’’ S which can be estimated by a better-than-London theory. This approach is justified since the elastic perturbation is long range ($\propto 1/r^2$); hence both the effect of the core of a size ξ and of out-of-core region^{9,10} on the order of the London penetration depth can be included in the point source.

The solution is $\chi = S(0)\ln|\mathbf{r} - \mathbf{a}|$ or in the Fourier space

$$\chi(\mathbf{k}) = -\frac{2\pi S(0)}{k^2} e^{i\mathbf{k}\mathbf{a}}. \quad (23)$$

Hence, we have

$$\begin{aligned} \sigma_{xx}(\mathbf{k}) &= \frac{2\pi S(0)k_y^2}{k^2} e^{i\mathbf{k}\mathbf{a}}, & \sigma_{yy}(\mathbf{k}) &= \frac{2\pi S(0)k_x^2}{k^2} e^{i\mathbf{k}\mathbf{a}}, \\ \sigma_{xy}(\mathbf{k}) &= -\frac{2\pi S(0)k_x k_y}{k^2} e^{i\mathbf{k}\mathbf{a}}, \end{aligned} \quad (24)$$

and with the help of Eqs. (9), (10), and (6),

$$u_{xx} = \frac{2\pi S(0)}{d} \frac{\lambda_1 k_y^2 - \lambda_2 k_x^2}{k^2} e^{i\mathbf{k}\mathbf{a}}, \quad (25)$$

$$u_{yy} = \frac{2\pi S(0)}{d} \frac{\lambda_1 k_x^2 - \lambda_2 k_y^2}{k^2} e^{i\mathbf{k}\mathbf{a}}, \quad (26)$$

$$u_{xy} = \frac{\pi S(0)}{\lambda_3} \frac{k_x k_y}{k^2} e^{i\mathbf{k}\mathbf{a}}. \quad (27)$$

III. ELASTIC INTERACTION OF VORTICES, $\theta = 0$

Let a vortex be at the origin and another one at \mathbf{a} . The elastic energy $\mathcal{E} = \int d\mathbf{r} \sigma_{\alpha\beta} u_{\alpha\beta}/2$ contains the self-energies of each one of them and the interaction energy:

$$\mathcal{E}_{\text{int}} = \int d\mathbf{r} \sigma(0)_{\alpha\beta} u_{\alpha\beta}(\mathbf{a}) = \int \frac{d\mathbf{k}}{4\pi^2} \sigma_{\alpha\beta}(0, \mathbf{k}) u_{\alpha\beta}(\mathbf{a}, -\mathbf{k}). \quad (28)$$

After straightforward algebra one obtains for $\theta = 0$:

$$\frac{\mathcal{E}_{\text{int}}}{S^2(0)} = \frac{d}{D^2} \left[\lambda_1(I_1 + I_2) + \frac{d - 2\lambda_2\lambda_3}{\lambda_3} I_3 \right], \quad (29)$$

where

$$\begin{aligned} I_1 &= \int d\mathbf{k} \frac{k_x^4}{k^4} e^{-i\mathbf{k}\mathbf{a}}, & I_2 &= \int d\mathbf{k} \frac{k_y^4}{k^4} e^{-i\mathbf{k}\mathbf{a}}, \\ I_3 &= \int d\mathbf{k} \frac{k_x^2 k_y^2}{k^4} e^{-i\mathbf{k}\mathbf{a}}. \end{aligned} \quad (30)$$

One easily verifies that $I_1 + I_2 = -2I_3$ if $\mathbf{a} \neq 0$. Thus, for $\theta = 0$ the interaction energy is proportional to $I_3(\mathbf{a})$.

Consider the second vortex in the first quadrant $a_x > 0, a_y > 0$. To evaluate, e.g., I_2 , integrate first over k_x utilizing the pole $k_x = -i|k_y|$ in the lower half of the complex plane k_x :

$$\int_{-\infty}^{\infty} \frac{dk_x e^{-ik_x a_x}}{(k_x^2 + k_y^2)^2} = \frac{\pi}{2k_y^4} e^{-|k_y|a_x} (a_x k_y^2 + |k_y|). \quad (31)$$

Integration over k_y gives

$$I_2 = \pi \frac{3a_x^4 - 6a_x^2 a_y^2 - a_y^4}{a^6}. \quad (32)$$

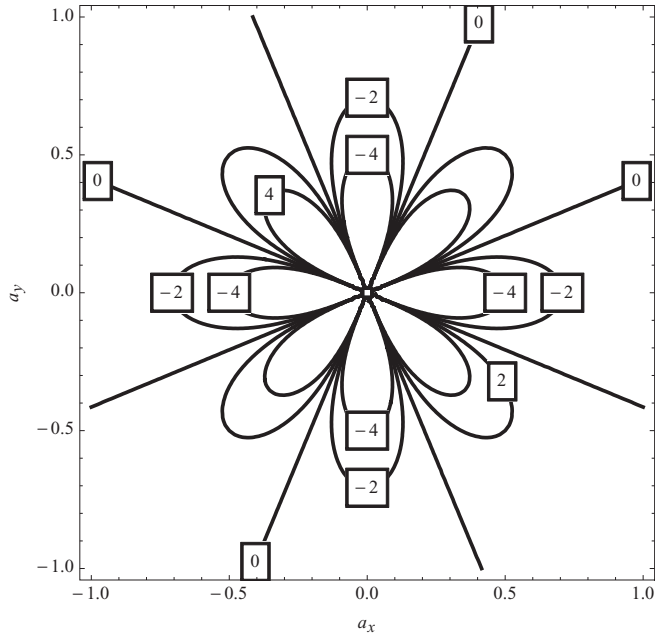


FIG. 1. Contours of constant elastic interaction energy or of $I_3(a_x, a_y)$ corresponding to a vortex at the origin and another one at $\mathbf{a} = (a_x, a_y)$. Both vortices are parallel to the c axis. $\lambda_1 - \lambda_2 - 2\lambda_3$ is assumed positive.

Similarly one obtains

$$I_1 = \pi \frac{3a_y^4 - 6a_x^2 a_y^2 - a_x^4}{a^6}, \quad I_3 = -\pi \frac{a_x^4 - 6a_x^2 a_y^2 + a_y^4}{a^6}. \quad (33)$$

In polar coordinates $a_x = a \cos \varphi$, $a_y = a \sin \varphi$, one has

$$I_3 = -\frac{\pi}{a^2} \cos 4\varphi, \quad I_2 = \frac{\pi}{a^2} (\cos 4\varphi + 2 \cos 2\varphi), \\ I_1 = \frac{\pi}{a^2} (\cos 4\varphi - 2 \cos 2\varphi). \quad (34)$$

Hence, the interaction energy takes the form

$$\frac{\mathcal{E}_{\text{int}}}{S^2(0)} = -\frac{\pi d^3}{D^4 \lambda_3} \frac{(\lambda_1 + \lambda_2)(\lambda_1 - \lambda_2 - 2\lambda_3)}{a^2} \cos 4\varphi. \quad (35)$$

The energy \mathcal{E}_{int} changes sign at $\varphi = \pi/8$ and $3\pi/8$ in the first quadrant. If $\lambda_1 - \lambda_2 - 2\lambda_3 > 0$ and the intervortex vector \mathbf{a} is in the domain $-\pi/8 < \varphi < \pi/8$ adjacent to [100], the elastic contribution to the interaction is attractive, whereas it is repulsive for $\pi/8 < \varphi < 3\pi/8$ near [110]. Figure 1 shows contours of a constant $I_3(a_x, a_y)$. Note that \mathcal{E}_{int} in addition to either attractive or repulsive dependence on the intervortex distance a , depends on the azimuth φ , which for the example shown in the figure means that for a given a the second vortex is pushed toward [100] or [010].

IV. ELASTIC INTERACTION, $\theta = \pi/2$

In this case, examination of elastic moduli, Appendix A, gives $\lambda_{yyyy} = \lambda_4$, $\lambda_{xxyy} = \lambda_5$, $\lambda_{xyxy} = \lambda_6$, $\lambda_{xxzz} = \lambda_2$, $\lambda_{yyzz} = \lambda_5$. Furthermore, $d = \lambda_1 \lambda_4 - \lambda_5^2$, $D_1 = \lambda_4(\lambda_1 + \lambda_2) - 2\lambda_5^2$, and $D_2 = \lambda_1(\lambda_4 + \lambda_5) - \lambda_5(\lambda_5 + \lambda_2)$.

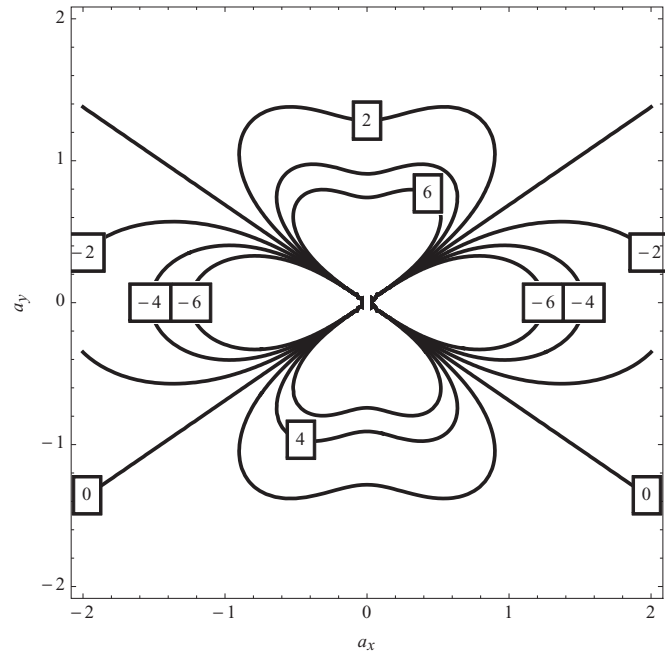


FIG. 2. Contours of constant elastic interaction energy corresponding to a vortex at the origin and another one at a rescaled position (a_x, a_y) . Both vortices are parallel to the b crystal axis. The elastic moduli chosen are $\lambda_1 = 1$, $\lambda_2 = 0.5$, $\lambda_3 = 0.3$, $\lambda_4 = 0.2$, $\lambda_5 = 0.075$, $\lambda_6 = 0.2$.

The same argument which led to derivation of Eq. (22) from Eq. (19) leads again to a Poisson equation but in rescaled coordinates (21) with, however, a new source $S(\pi/2)$. We then obtain the same expressions for $\sigma_{\alpha\beta}(\mathbf{k})$ in properly rescaled \mathbf{k} 's and \mathbf{a} 's. The strains are obtained with the help of Eqs. (9), (10), and (6).

The interaction energy now is a linear combination of I_1 , I_2 , and I_3 with the moduli dependent coefficients. Without going into details, one can write this energy as

$$\mathcal{E}_{\text{int}} = S^2(\pi/2) \frac{A \cos 4\varphi + B \cos 2\varphi}{a^2}, \quad (36)$$

where A, B depend on elastic moduli. The interaction energy may have a structure similar to the case $\theta = 0$ of Fig. 1 but distorted due to the lost symmetry of the 90° rotation. In other words, attractions for \mathbf{a} along [100] and [001] are no longer the same, the attraction domain adjacent to [001] may shrink. For certain choices of moduli, this domain disappears altogether, an example is shown in Fig. 2 where [100] corresponds to attraction, whereas [001] to repulsion.

V. DISCUSSION

The straightforward technique offered above can be applied to a variety of situations for which the elastic moduli are known. There is no point in going to all such possibilities in a general discussion of this paper. It is worth noting, however, that for vortices along the c axis of tetragonal crystals, the generic form of this interaction is that of the geometric factor $I_3(a_x, a_y)$ with the sign and value of the prefactor depending on elastic moduli, i.e., \mathcal{E}_{int} should always be of the form shown in Fig. 1. This implies in particular that the elastic

contribution removes the degeneracy of orientations of the hexagonal vortex lattice for this field orientation. Moreover, since at large distances elastic $1/a^2$ interaction overcomes the exponentially weak London repulsion, one expects low density vortices parallel to c to form a square lattice. In small in-plane oriented fields, $\theta = \pi/2$, one expects to have vortex chains along b or c depending on a particular set of elastic constants.

It is worth noting that the method developed for tetragonal crystals can be applied for the cubic symmetry by setting $\lambda_4 = \lambda_1$, $\lambda_5 = \lambda_2$, and $\lambda_6 = \lambda_3$, see Eqs. (2). It is also easily shown that the elastic energy for the hexagonal symmetry can be obtained from the tetragonal expressions by setting $\lambda_1 = \lambda_2 + 2\lambda_6$, Appendix B. Then Eq. (35) shows that vortices parallel to c of a hexagonal crystal do not interact elastically, the conclusion obtained in Ref. 8.

As was shown above, the elastic field created by parallel vortices can be considered as *planar* only when vortices are oriented along principal crystal directions. This is not so for a general vortex orientation, when the strength S of the stress caused by vortex cores and by the currents around may depend on vortex orientation in a nontrivial manner; enough to mention that in this situation the currents do not flow exclusively in the plane perpendicular to the vortex direction. For arbitrary orientations, one should use a more general approach involving the Green's function of anisotropic elastic media.¹¹ This, in fact, has been done for hexagonal crystals.⁸ This technique is formally more involved while, as far as physics is concerned, the major features of elastic interactions are already seen in the limiting cases of $\theta = 0$ and $\pi/2$.

We now compare the elastic contribution with the standard London repulsion

$$\mathcal{E}_L = \frac{\phi_0^2}{8\pi^2\lambda_L^2} K_0 \left(\frac{a}{\lambda_L} \right), \quad (37)$$

where λ_L is the London penetration depth. Since the a -dependent factors $I_{1,2,3}$ in the elastic interaction (29) go as $1/a^2$, we estimate

$$\mathcal{F}_{el} \sim S^2/\tilde{\lambda}a^2, \quad (38)$$

where $\tilde{\lambda} \sim 10^{12}$ erg/cm³ is the order of magnitude of elastic constants. At large distances the power-law elastic interaction dominates the exponentially weak London repulsion. Hence, \mathcal{E}_{int} positive at short distances may turn negative along the directions where the elastic attraction exceeds the London repulsion, i.e., $\mathcal{E}_{int}(a)$ goes through a minimum at some a_m , and approaches zero being negative as $a \rightarrow \infty$. In other words, in small fields vortices parallel to c will occupy these minima, i.e., form a square lattice in the tetragonal or cubic cases with a fixed field-independent spacing close to a_m .

In Ref. 2 the source term in the equation for *strains*, $\nabla^2\chi_s = 2\pi S_s\delta(\mathbf{r} - \mathbf{a})$, due to the vortex core was estimated as $S_s \sim \zeta\xi^2$, where ξ is the core size and

$$\zeta \approx \frac{H_c^2}{T_c} \frac{dT_c}{dp} \quad (39)$$

is the relative volume change of normal and superconducting phases. It was argued later that this estimate, based on the core solely responsible for the strain, underestimates the vortex induced strain by a factor as large as $(\ln \kappa)^2$ with κ being the Ginzburg-Landau parameter.^{9,10} Hence, the stress source in

our case can be estimated as

$$S \sim \tilde{\lambda}\zeta\xi^2(\ln \kappa)^2. \quad (40)$$

The distance at which the elastic and London interactions are of the same order is estimated by setting $\mathcal{F}_{el} \approx \mathcal{F}_L$:

$$\frac{a^2}{\lambda_L^2} K_0 \left(\frac{a}{\lambda_L} \right) \approx \frac{S^2}{\tilde{\lambda}\phi_0^2} \approx \frac{\tilde{\lambda}\zeta^2\xi^4(\ln \kappa)^4}{\phi_0^2}. \quad (41)$$

Roughly one estimates the right-hand side of this equation as 5×10^{-4} taking a moderate value $dT_c/dp \approx 1$ K/GPa = 10^{-10} K cm³/erg and $H_c \approx 1$ T. Solving Eq. (41) numerically, we get $a/\lambda_L \approx 10$. Taking this distance as a side a_m of the low field square vortex lattice in tetragonal crystals, we obtain the paramagnetic contribution to the magnetization $\Delta M = \phi_0/4\pi a_m^2$. Therefore, at the transition from Meissner to the mixed state at the entry field H_{ent} , $M(H)$ should jump from $-H_{ent}/4\pi$ on the Meissner side to $-H_{ent}/4\pi + \Delta M$. For $\lambda_L \sim 10^{-5}$ cm we estimate $\Delta M \sim 1$ G.

As mentioned, in some Fe-based compounds the derivative dT_c/dp is by an order of magnitude larger,⁴ which results in higher estimates for ΔM . This might be a reason for a very sharp and narrow peak in $M(H)$ at low fields observed in many compounds of this family.^{12,13}

As argued above, in hexagonal crystals the elastic interaction is absent for vortices directed along c . However, a small misalignment of these directions may cause vortex chains to appear with a field independent intrachain spacing. It is of interest to compare our estimates with vortex chains in MgB₂ observed in small fields nominally parallel to c .⁶ In this material $dT_c/dp \approx 1$ K/GPa = 10^{-10} K cm³/erg.¹⁴ Taking $H_c \approx 1$ T, we obtain the same estimate as above: $a/\lambda_L \approx 10$. Reference 6 reports a nearly field-independent intrachain distance as ≈ 2.5 μ m, which is by a factor of 20 larger than $\lambda_L(0) \sim 0.1$ μ m. Since, according to the authors, the actual temperature at which the vortex structure forms might be close to T_c , the relevant λ_L is larger, so one may consider the above estimate as having the correct order. It would be interesting to do the same experiment in a deliberately tilted field and compare the data with calculation based on particular elastic moduli of MgB₂.

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APPENDIX A: ELASTIC MODULI

The tensor components are easily reproduced since tensors transform as products of coordinates. In nonzero λ , index x can appear even number of times, z can come either in even numbers or in combination with y :

$$\begin{aligned} \lambda_{xxxx} &= \lambda_1, \\ \lambda_{yyyy} &= \lambda_1 \cos^4 \theta + \lambda_4 \sin^4 \theta + (\lambda_6 + \lambda_5/2) \sin^2 2\theta, \\ \lambda_{xxyy} &= \lambda_2 \cos^2 \theta + \lambda_5 \sin^2 \theta, \\ \lambda_{xyxy} &= \lambda_3 \cos^2 \theta + \lambda_6 \sin^2 \theta, \end{aligned}$$

$$\begin{aligned}
\lambda_{xxzz} &= \lambda_2 \sin^2 \theta + \lambda_5 \cos^2 \theta, \\
\lambda_{zzyy} &= \lambda_5 (\sin^4 \theta + \cos^4 \theta) + (\lambda_1 + \lambda_4 - 4\lambda_6) \sin^2 \theta \cos^2 \theta, \\
\lambda_{xzxy} &= (\lambda_3 - \lambda_6) \sin \theta \cos \theta, \\
\lambda_{xxyz} &= (\lambda_2 - \lambda_5) \sin \theta \cos \theta, \\
\lambda_{yzzy} &= [(\lambda_1 - \lambda_5) \cos^2 \theta \\
&\quad + (\lambda_5 - \lambda_4) \sin^2 \theta - 2\lambda_6 \cos 2\theta] \sin \theta \cos \theta, \\
\lambda_{yzzz} &= (\lambda_1 \sin^2 \theta + 3\lambda_5 \cos 2\theta - \lambda_4 \cos^2 \theta) \sin \theta \cos \theta.
\end{aligned}$$

Note that the last four entries are zeros for $\theta = 0, \pi/2$.

APPENDIX B: HEXAGONAL CRYSTALS

The elastic energy of hexagonal crystal in the crystal frame is³

$$\begin{aligned}
F_h &= (2\lambda_{\xi\eta\xi\eta} + \lambda_{\xi\xi\eta\eta})(u_{xx}^2 + u_{yy}^2) \\
&\quad + 2(2\lambda_{\xi\eta\xi\eta} - \lambda_{\xi\xi\eta\eta})u_{xx}u_{yy} + 4\lambda_{\xi\xi\eta\eta}u_{xy}^2
\end{aligned}$$

$$\begin{aligned}
&+ \lambda_{zzzz}u_{zz}^2/2 + 2\lambda_{\xi\eta z z}(u_{xx} + u_{yy})u_{zz} \\
&+ 4\lambda_{\xi z \eta z}(u_{xz}^2 + u_{yz}^2). \tag{B1}
\end{aligned}$$

Here $\lambda_{\xi\eta\xi\eta}$, $\lambda_{\xi\xi\eta\eta}$, $\lambda_{\xi\eta z z}$, $\lambda_{\xi z \eta z}$, λ_{zzzz} are five independent elastic constants, $\xi = \eta^* = x + iy$.

Compare this with the energy F_t for the tetragonal case which in the crystal frame and our notation reads

$$\begin{aligned}
F_t &= \lambda_1(u_{xx}^2 + u_{yy}^2)/2 + \lambda_2 u_{xx} u_{yy} + 2\lambda_3 u_{xy}^2 + \lambda_4 u_{zz}^2/2 \\
&\quad + 2\lambda_5(u_{xx} + u_{yy})u_{zz} + 2\lambda_6(u_{xz}^2 + u_{yz}^2). \tag{B2}
\end{aligned}$$

Clearly, $F_h = F_t$ if

$$\begin{aligned}
\lambda_1 &= 2(2\lambda_{\xi\eta\xi\eta} + \lambda_{\xi\xi\eta\eta}), \quad \lambda_2 = 2(2\lambda_{\xi\eta\xi\eta} - \lambda_{\xi\xi\eta\eta}), \\
\lambda_3 &= 2\lambda_{\xi\xi\eta\eta}, \quad \lambda_4 = \lambda_{zzzz}, \quad \lambda_5 = \lambda_{\xi\eta z z}, \quad \lambda_6 = \lambda_{\xi z \eta z}. \tag{B3}
\end{aligned}$$

Hence, we have $\lambda_1 = \lambda_2 + 2\lambda_3$.

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