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Vortex-induced strain and magnetization in type-II superconductors

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It is argued that the stress caused by vortex cores in the mixed state of superconductors may result in a measurable field-dependent contribution to the free energy and magnetization. For sufficiently strong stress dependence of the critical temperature, $\partial T_c/\partial p$, this contribution may result in the "second peak" in the field dependence of the *reversible* magnetization, the effect often masked by vortex pinning and creep.

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The so-called second peak in the field dependence of the magnetization $M(H)$ in a number of type-II superconductors is a long-standing puzzle. The peak has been observed in magnetization loops having a "fishtail" shape so that the loop width of the irreversible magnetization increases with increasing field in intermediate field range and the critical current rises with H in this domain.[1]

A few explanations based on peculiarities of pinning and flux creep have been offered for this apparently strange phenomenon.[2] These suggestions may well be correct but they do not cover all cases in which the second peak has been observed. Puzzling in particular is the fact that in some systems the second peak has been reported also in the *reversible* $M(H)$; the examples are $NbSe_2$, $La_{1.45}Nd_{0.40}Sr_{0.15}CuO_4$, and $CeCoIn_5$.[3–5]

In this work, the second peak in reversible $M(H)$ is associated with the strain caused by normal vortex cores embedded in the superconducting phase, a "magneto-elastic" effect. The strains arise due to a small difference in densities of the normal and superconducting phases which is related to the stress dependence of the critical temperature $\partial T_c/\partial p$.[6] It turned out recently that this derivative in pnictides, and in $Ca(Fe_{1-x}Co_x)_2As_2$ in particular,[7] by one or two orders of magnitude exceeds values for conventional superconductors making Fe-based pnictides especially favorable for observation of magneto-elastic effects.

Strain caused by a single vortex. Consider vortex nucleation prior to which the superconductor has been strain free. We model the vortex core as a normal (n) cylinder of radius $\rho \sim \xi$, the coherence length, immersed in the superconducting (s) phase with a constant order parameter. This is a London-type approach[8] which suffices for qualitative estimates, although Ref. 9 argues that such an approach underestimates magneto-elastic effects.

Nucleation of the normal core causes stress, since the n phase has a larger specific volume V_n as compared to V_s. The relative volume change ζ is related to the pressure dependence of the condensation energy or of the critical field H_c: [6]

$$\zeta = \frac{V_n - V_s}{V_s} = \frac{H_c}{4\pi}\frac{\partial H_c}{\partial p}. \tag{1}$$

The elastic energy density in isotropic solids reads[10]

$$F = \lambda u_{ll}^2/2 + \mu u_{ij}^2, \tag{2}$$

where u_{ij} is the strain tensor and λ, μ are Lamé coefficients; summation over double indices is implied. The stress tensor $\sigma_{ij} = \partial F/\partial u_{ij} = \lambda u_{ll}\delta_{ij} + 2\mu u_{ij}$, and the equilibrium condition $\partial\sigma_{ij}/\partial x_j \equiv \sigma_{ij,j} = 0$ is given by

$$\lambda u_{ll,i} + 2\mu u_{ij,j} = 0. \tag{3}$$

For brevity, the comma in $u_{ik,j}$ is used to denote derivatives with respect to the coordinate j.

For a single vortex directed along z, the displacement $\mathbf{u} = (u_x, u_y, 0)$ is radial in the plane xy, i.e., curl $\mathbf{u} = 0$ or $\mathbf{u} = \nabla\chi$, and $u_{\alpha\beta} = \chi_{,\alpha\beta}$ where χ is a scalar and α,β acquire only x and y values. The equilibrium condition (3) reads $(\lambda + 2\mu)\chi_{,\alpha\beta\beta} = 0$ with the first integral

$$\chi_{,\beta\beta} \equiv \nabla^2\chi = C = \text{constant}. \tag{4}$$

To fix this constant, we note that $\chi_{,\beta\beta} = u_{\beta\beta}$ describes compression and is related to the hydrostatic pressure within the system. For the problem of the strain caused by a single vortex in otherwise unrestrained crystal, the pressure is zero, and we have to solve $\nabla^2\chi = 0$ under the boundary condition $u \to 0$ at large distances. Hence, the problem is the same as that of a linear charge in electrostatics: $\chi \propto \ln r$, $\boldsymbol{r} = (x,y)$. Hence, we obtain[8]

$$\mathbf{u}_s = \frac{\gamma_s\xi^2\mathbf{r}}{r^2}, \quad u_{\alpha\beta}^{(s)} = \frac{\gamma_s\xi^2}{r^2}\left(\delta_{\alpha\beta} - \frac{2}{r^2}x_\alpha x_\beta\right), \tag{5}$$

where ξ^2 is introduced for convenience and the constant γ_s is given below.

At the core center $\mathbf{u}(0) = 0$; we have

$$\mathbf{u}_n = -\gamma_n\mathbf{r}, \quad u_{\alpha\beta}^{(n)} = -\gamma_n\delta_{\alpha\beta} \tag{6}$$

in the core interior. The constants γ are evaluated by using boundary conditions at the interface:[8]

$$\gamma_n = \frac{\zeta\mu}{2(\lambda + 2\mu)}, \quad \gamma_s = \frac{\zeta(\lambda + \mu)}{2(\lambda + 2\mu)}. \tag{7}$$

The displacement $\boldsymbol{u}_s$ of Eq. (5) is analogous to the electric field of a charge with linear density $\gamma_s\xi^2/2$ situated at the z axis. Hence, the vortex can be considered as the linear source of deformation $\boldsymbol{u}$ outside the core, whereas the scalar potential χ satisfies

$$\nabla^2\chi = 2\pi\gamma_s\xi^2\delta(\boldsymbol{r}). \tag{8}$$

Vortex lattice. Consider now a 2D periodic lattice of vortices at positions $\boldsymbol{a}$ in an infinite sample. At first sight, the potential χ should obey

$$\nabla^2\chi = 2\pi\gamma_s\xi^2\sum_{\boldsymbol{a}}\delta(\boldsymbol{r} - \boldsymbol{a}). \tag{9}$$

The electrostatic analogy, however, shows that this equation cannot have bound solutions, whereas we are interested in periodic $\chi(\boldsymbol{r})$ to describe an infinite vortex lattice. We therefore introduce a uniform background "charge density" of a sign opposite to $\gamma_s\xi^2/2$ to make the system "quasineutral." In other words, the condition for a periodic χ to exist is

$$\int d\boldsymbol{r}\left(2\pi\gamma_s\xi^2\sum_{\boldsymbol{a}}\delta(\boldsymbol{r}-\boldsymbol{a})+C\right)=0. \qquad (10)$$

This translates to $2\pi\gamma_s\xi^2N+CA=0$ where N is the total number of vortices and A is the area of the sample cross section perpendicular to the induction $\boldsymbol{B}$; $N/A=B/\phi_0$ is the density of vortices. Hence, $C=-2\pi\gamma_s\xi^2B/\phi_0$ and we have to look for solutions of

$$\nabla^2\chi=2\pi\gamma_s\xi^2\left[\sum_{\boldsymbol{a}}\delta(\boldsymbol{r}-\boldsymbol{a})-\frac{B}{\phi_0}\right], \qquad (11)$$

an equation consistent with the equilibrium condition $\nabla^2\chi=$ constant.

The general solution of this equation was discussed in Ref. 11. Dealing with periodic solutions, one can consider $\chi(\boldsymbol{r})$ in a single cell under the condition $\partial\chi/\partial\boldsymbol{n}=0$ at the cell boundary ($\boldsymbol{n}$ is the normal to the boundary). The potential within the cell centered at $\boldsymbol{a}=0$ satisfies

$$\nabla^2\chi=2\pi\gamma_s\xi^2\left[\delta(\boldsymbol{r})-\frac{B}{\phi_0}\right]. \qquad (12)$$

The form of the unit cell depends on the vortex lattice structure which is hexagonal (triangular) in isotropic case of interest here. For this lattice, the boundary is a hexagon which—in the Wigner-Zeitz approximation—can be replaced with a circle. The cylindrically symmetric solution satisfying $\chi'(R)=0$ with $\pi R^2=\phi_0/B$ is

$$\chi=\gamma_s\xi^2\left(\ln\frac{r}{r_0}-\frac{\pi B}{2\phi_0}r^2\right); \qquad (13)$$

r_0 is an arbitrary constant irrelevant for the following.

The crystal displacement has only one component:

$$u_r=\gamma_s\xi^2\left(\frac{1}{r}-\frac{\pi B}{\phi_0}r\right). \qquad (14)$$

The strain tensor in cylindrical coordinates[10] has two nonzero components:

$$u_{rr}=\frac{\partial u_r}{\partial r}=-\gamma_s\xi^2\left(\frac{1}{r^2}+\frac{\pi B}{\phi_0}\right),$$
$$u_{\varphi\varphi}=\frac{u_r}{r}=\gamma_s\xi^2\left(\frac{1}{r^2}-\frac{\pi B}{\phi_0}\right). \qquad (15)$$

The elastic energy density averaged over the cell is

$$F_{el}=\frac{B}{\phi_0}\int_\rho^R 2\pi r\,dr\left[\lambda u_{\alpha\alpha}^2(r)/2+\mu u_{\alpha\beta}^2(r)\right], \qquad (16)$$

where the lower integration limit is the core radius on the order of ξ. Within the London approach one cannot determine the radius ρ; we will choose it below as to have the elastic contribution to magnetization to vanish at the upper critical field H_{c2}.

A straightforward evaluation gives

$$F_{el}=\frac{\tilde{\lambda}}{2}\gamma_s^2b^2\left(1-\frac{\rho^2}{2\xi^2}b\right),\quad b=\frac{B}{H_{c2}}, \qquad (17)$$

and

$$\tilde{\lambda}=\lambda+\mu+\mu\frac{2\xi^2}{\rho^2 b} \qquad (18)$$

is a quantity on the order of the elastic constants.

Parameter ζ in terms of $\partial T_c/\partial p$. The stress dependence of the condensation energy $\partial(H_c^2/8\pi)/\partial p$, to which the coefficient γ_s is proportional, can be evaluated only within a detailed microscopic theory to account for evolution of the band structure and of the coupling responsible for superconductivity with pressure. Such a calculation, if possible, would be material specific. Instead, we resort to a qualitative approach to see how the the vortex-induced strain could affect macroscopic properties of type-II superconductors.

First, the derivative in Eq. (1) can be expressed in terms of the measured $\partial T_c/\partial p$:

$$\frac{\partial\left(H_c^2/8\pi\right)}{\partial p}=\frac{\partial\left(H_c^2/8\pi\right)}{\partial T_c}\frac{\partial T_c}{\partial p}. \qquad (19)$$

Unfortunately, there is no simple enough expression for the condensation energy $H_c^2/8\pi=F_n-F_s$ for arbitrary temperatures, fields, and scattering regimes. The exception is the case of a strong pair-breaking considered originally by Abrikosov and Gor'kov,[12] who argued that due to extra suppression of the order parameter by, e.g., spin-flip scattering, the GL energy expansion holds for all temperatures down to 0. This argument has recently been specified for order parameters with zero Fermi surface averages (such as d-wave or $\pm s$ for iron-based pnictides).[13] This scheme will be used below mostly because of its formal simplicity, although the qualitative results obtained have a broader applicability.

The zero-field condensation energy for gapless state is

$$\frac{H_c^2}{8\pi}=A\left(T_c^2-T^2\right)^2,\quad A\sim\frac{N(0)\tau_+^2}{\hbar^2}, \qquad (20)$$

where $N(0)$ is the density of states, and $1/\tau_+=1/\tau+1/\tau_m$ whereas $1/\tau$ and $1/\tau_m$ are the transport and pair-breaking scattering rates. One then finds

$$\frac{\partial H_c^2/8\pi}{\partial T_c}=\frac{H_{c0}^2}{2\pi T_c}(1-t^2),\quad t=T/T_c. \qquad (21)$$

Thus, we estimate

$$\zeta\approx\frac{H_{c0}^2}{2\pi T_c}(1-t^2)\frac{\partial T_c}{\partial p}. \qquad (22)$$

Also, within the gapless state, the upper critical field and the London penetration depth have simple T dependencies used below:

$$H_{c2}=H_{c2,0}(1-t^2),\quad \lambda_L^2=\lambda_{L,0}^2\big/(1-t^2). \qquad (23)$$

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Magnetization. The free energy density of the mixed state is

$$F = F_0 + B^2/8\pi + F_L + F_{el}, \tag{24}$$

where F_0 is the zero-field energy. The London energy of the vortex lattice in intermediate fields is given by

$$F_L \approx \frac{\phi_0 B}{32\pi^2\lambda_L^2} \ln \frac{\eta H_{c2}}{B} \tag{25}$$

with $\eta \sim 1$. The elastic part is obtained with the help of Eqs. (17), (22), and (23):

$$F_{el} \approx \overline{\lambda} \left[\frac{H_{c0}^2}{2\pi T_c} \frac{\partial T_c}{\partial p} \frac{B}{H_{c2,0}} \right]^2 \left(1 - \frac{\rho^2 B}{2\xi^2 H_{c2}} \right). \tag{26}$$

Here, $\overline{\lambda} \sim 10^{12}$ erg/cm^3 is a new combination of λ and μ.

Both F_L and F_{el} are evaluated here within the London approach for $H_{c1} \ll B \ll H_{c2}$ and, therefore, fail near both H_{c2} and H_{c1}. Still, we can force the magnetization to be zero at H_{c2} by setting $\eta = e \approx 2.718$ and $\rho = 2\xi/\sqrt{3}$. We then obtain

$$M = \frac{B - H}{4\pi} = \frac{B}{4\pi} - \frac{\partial F}{\partial B} = M_L + M_{el}, \tag{27}$$

$$M_L = -\frac{\phi_0}{32\pi^2\lambda_L^2} \ln \frac{H_{c2}}{B}, \tag{28}$$

where M_L is the London part. The average penetration length λ_L, that governs the field distribution in the mixed state, depends on B because the average order parameter Δ is suppressed by the field. This dependence is relevant in particular near H_{c2}, since there the averaged order parameter $\overline{\Delta^2} \propto (1 - B/H_{c2})$ which translates to $\lambda_L \propto 1/\sqrt{1 - B/H_{c2}}$.[14] We take this field dependence to characterize qualitatively $M_L(T,B)$.

The elastic contribution to M is

$$M_{el} = -2\overline{\lambda} \left[\frac{H_{c0}^2}{2\pi T_c H_{c2,0}} \frac{\partial T_c}{\partial p} \right]^2 B \left(1 - \frac{B}{H_{c2}} \right). \tag{29}$$

It is worth noting that this contribution is diamagnetic and has a minimum at $B_p = H_{c2}/2$ in a reasonable agreement with data of Refs. 4 and 5. The London part of M shifts the minimum to smaller fields, but the stronger the elastic part relative to M_L, the closer B_p to $H_{c2}/2$.

Taking $\overline{\lambda} \approx 10^{12}$ erg/cm^3, $H_{c2,0} = 5.9$ T, $H_{c0} = 0.35$ T, $\lambda_L(0) \approx 3.5 \times 10^{-5}$ cm, $T_c \approx 10.5$ K, and $\partial T_c/\partial p \approx 3 \times 10^{-9}$ K cm^3/erg $= 30$ K/GPa one obtains $M(B)$ shown in Fig. 1. These numbers roughly correspond to parameters for $La_{1.45}Nd_{0.40}Sr_{0.15}CuO_4$.[4] It should be noted that $\partial T_c/\partial p$ for this particular material was not measured, but the data on a similar crystal, $La_{1.44}Nd_{0.40}Sr_{0.14}CuO_4$,[15] show that $\partial T_c/\partial p|_{p\to 0}$ exceeds 15 K/GPa.

Qualitatively, the calculated $M(B)$ is similar to that recorded by Ostenson *et al.*[4] and shown in Fig. 2. The major features of the data are reproduced by the model remarkably well. One must bear in mind that the London-type isotropic model cannot pretend for quantitative agreement with data near H_{c2} and for $B \to 0$. Besides, in anisotropic materials one cannot use the data on the T_c dependence of hydrostatic pressure p as a fair representation of actual dependence of T_c on the stress in the plane perpendicular to the applied field.[16,17] Moreover, the use of temperature dependencies of quantities

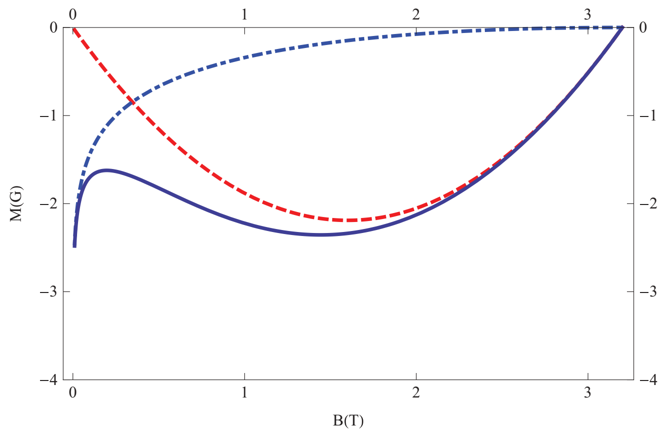

FIG. 1. (Color online) The magnetization M versus B according to Eqs. (27)–(29) for parameters given in the text. The dot-dashed line is the London contribution; the dashed line is the elastic part.

involved, which are characteristic of the gapless situation, was only motivated by formal simplicity. Nevertheless, one may conclude that the evidence for the vortex-induced strain as responsible for the second peak of $M(B)$ in materials with large $\partial T_c/\partial p$ is strong.

Discussion. The elastic contribution to the vortex-vortex interactions has been studied in a number of publications; see Refs. 8, and 9 and references therein. It has been shown that this contribution is responsible for the observed flux-line lattice structures in fields tilted with respect to the c axis of $NbSe_2$. The observed structures cannot be explained by London interactions alone; they in fact correspond to the maximum of the London energy. Vortex lattices are extremely sensitive to a number of factors, among which the nonlocal corrections to London interactions were proven to be important.[18,19] Energy differences between various vortex lattices are exceedingly small. It is shown in this work that the elastic deformations caused by vortices may influence such a quantity as magnetization involving much larger energies.

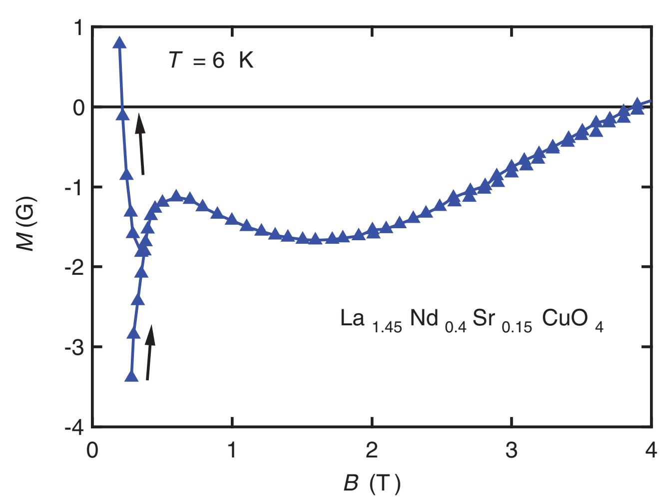

FIG. 2. (Color online) The magnetization $M(B)$ measured in increasing and decreasing fields along the c crystal axis; the data are compiled from Ref. 4. It is seen that $M(B)$ is reversible for $B >$ 0.4 T.

The model suggested here is profoundly qualitative. Materials to which the model is applied are anisotropic for which one needs to know a number of elastic constants.[20] We lumped all this complexity to one number, $\overline{\lambda} \approx 10^{12}$ erg/cm^3. Our estimates of material parameters and in particular of $\partial T_c/\partial p$ needed for evaluation of elastic contribution to magnetization are quite crude. In particular, it is hard to get reliable values of $\partial T_c/\partial p$ for $p \to 0$ since usually people are interested in high pressures.[15]

We model vortices as having normal cores surrounded by a superconductor with an unperturbed order parameter so that the condensation energy is just $H_c^2/8\pi$, which is so only far from H_{c2}; see also Ref. 9. Hence, the model fails in high fields approaching H_{c2}. We have used simplified T dependencies of H_{c2} and λ_L corresponding to the strong pair-breaking situation. Still, simplifications notwithstanding, the model reproduces qualitatively the behavior of $M(B)$ with the second peak.

The interpretation of the second peak in $M(H)$ as an equilibrium thermodynamic property of deformable type-II superconductors is new; it differs from traditional models based on defects-related irreversible material properties. The latter are always present, of course, and make it difficult to extract relatively weak magneto-elastic properties of vortex lattices. It should be noted, however, that well-pronounced second peaks in reversible $M(H)$ must result in similar peaks in irreversible magnetization loops; in other words, the fishtail loops seen in layered materials may also be caused by the vortex induced strain.

The elastic contribution to the vortex line energy may cause enhancement of the low critical field H_{c1}, the problem for a separate study. Near H_{c2}, however, the cores overlap whereas the condensation energy goes as $(H_{c2} - B)^2$ so that one does not expect changes of the phase transition at H_{c2}.

Layered materials having strong stress dependencies of T_c are therefore good candidates not only for unmasking equilibrium magneto-elastic phenomena from the background of strong irreversibilities, but for understanding the irreversible fishtails as well. Recently, the pressure dependence of T_c in $Ca(Fe_{1-x}Co_x)_2As_2$ has been found to reach $\partial T_c/\partial p \approx -60$ K/GPa, which is by a factor of 100 more than in "conventional" superconductors. The present work suggests that magneto-elastic effects should be studied in materials with large $\partial T_c/\partial p$ with an emphasis on macroscopic magnetization, the problem deserving more experimental and theoretical attention.

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