Vortex-induced deformation of the superconductor crystal lattice

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Deformation of the superconductor crystal lattice caused by Abrikosov vortices is formulated as a response of the elastic crystal lattice to electrostatic forces. It is shown that the lattice compression is linearly proportional to the electrostatic potential known as the Bernoulli potential. Possible consequences of the crystal lattice deformation on the effective vortex mass are discussed.

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During the transition from a normal to a superconducting state, metals change their specific volumes.[1,2] In a mixed state, would it be the Abrikosov vortex lattice or a structure of lamellae, the superconductivity is locally suppressed and the specific volume is inhomogeneous. The mixed state is thus accompanied by strains and stresses, which enter the balance of total energy.

In general, the energy of strains is much smaller than the energy of the superconducting condensation and the energy of the magnetic field. Its contribution becomes appreciable only under special conditions. For example, experiments on single crystals of Pb alloys[3,4] and Nb alloys[4–6] revealed that the orientation of the vortex lattice is influenced by its angles to the main crystal axes. Since the gap of alloyed samples is quite isotropic, purely electronic models have failed and this effect has been explained with the help of strains induced by vortices.[7]

In the 1990s, a different structural effect has been observed on $NbSe_2$. If the magnetic field is tilted away from the c axes, the Ginzburg-Landau (GL) theory predicts a state in which rows of vortices are aligned with the parallel component of the tilted magnetic field,[8] while experiments[9–12] show them aligned in the perpendicular direction. Again, the interaction of vortices with the crystal strain explains the observed alignment.[13]

Finally, we would like to mention phenomena which are predicted but not yet fully confirmed experimentally. Perhaps, one of the most interesting predictions is a sizable contribution of the lattice deformation to the mass of vortex.[14–17] Besides, there are a number of phenomena due to strains at surfaces which are discussed in Ref. 18. It is also argued that the strain can mediate an attractive long-range interaction between vortices.[19]

As far as we know, all theoretical studies of deformable superconductors use a phenomenological model, which assumes that the superconducting condensate interacts with the lattice density directly via a strain dependence of material parameters. This model dates back to the 1960s, when it was used to describe vortex pinning.[20,21] The strength of the interaction is deduced from changes of the specific volume in the phase transition (see also Ref. 14).

In this Brief Report, we assume that the condensate interacts with the crystal lattice via electrostatic forces created by the so-called Bernoulli potential. We show that this mechanism results in the interaction based on the specific volume. In addition to known theories, we obtain gradient corrections and demonstrate that they are important for the motion of the vortex lattice in niobium.

In an isotropic continuum, the displacement field $\mathbf{u}$ obeys the equation[22]

$$\left(K+\tfrac{4}{3}\mu\right)\nabla(\nabla\cdot\mathbf{u})-\mu\nabla\times\nabla\times\mathbf{u}=\mathbf{F},\qquad(1)$$

where K and μ are the bulk and the shear modulus, and $\mathbf{F}$ is the volume density of force acting on the lattice. Some authors prefer to express the coefficients on the left hand side in terms of the Poisson ratio $\sigma=(3K-2\mu)/(6K+2\mu)$ and the Young modulus $E=3K(1-2\sigma)$. In the basic approximation, K and μ are constants. Their small change in the superconducting state was assumed in Ref. 23.

The inhomogeneous superconductivity results in the force $\mathbf{F}$. The present theory differs from previous approaches in the approximation adopted for $\mathbf{F}$. Let us first outline the approach based on the specific volume. The reader can find more details in Ref. 15.

In the phase transition from the normal to the superconducting state, the system shrinks by a volume difference $\delta V=V_n-V_s=\alpha_T V$. A typical value of α_T is about 10^{-7}. The density of the atomic lattice therefore increases, $\delta n_{lat}=n_{lat}^{s}-n_{lat}^{n}=\alpha_T n$.

The strain coefficient α_T depends on the temperature via the fraction ω of electrons which become superconducting, $\alpha_T=\alpha\omega$. Here, α is the strain coefficient at zero temperature. In the spirit of the GL theory, we express the superconducting fraction in terms of the GL function $\omega=2|\psi|^2/n$, i.e., $\delta n_{lat}=2\alpha|\psi|^2$.

In the region of surface currents and especially in the vortex core, the GL wave function varies in space. As can be seen, e.g., in Fig. 1 of Ref. 24, the superconducting fraction vanishes in the vortex core. The lattice then tends to be inhomogeneous, which causes internal stresses. These stresses lead to a density of force

$$\mathbf{F}_{Sim}=K\alpha\nabla\frac{2|\psi|^2}{n}\qquad(2)$$

proposed by Duan and Šimánek[15] in their study of the vortex mass. The phenomenological formula (2) provides us with a

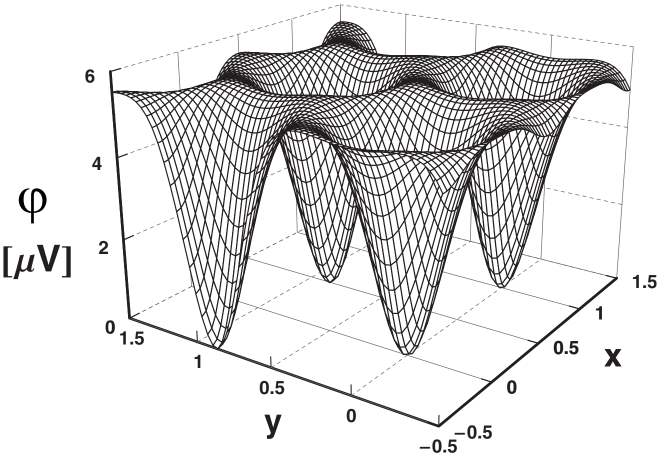

FIG. 1. The electrostatic potential for the triangular Abrikosov vortex lattice. We assume niobium with the GL parameter increased by nonmagnetic impurities to $\kappa=1.5$, the temperature $T=0.7T_c$, and the mean magnetic field $\bar{B}=0.24B_{c2}$.

density of forces irrespective of how the superconducting electrons are coupled to the lattice.

Let us try to express such force on the lattice in a semimicroscopic way. Diamagnetic currents, either flowing along the surface or circulating around the vortex core, always cause inertial and Lorentz forces, which are balanced by an electrostatic field $\mathbf{E}=-\nabla\varphi$ (see Ref. 25). This electric field transfers the Lorentz force from electrons to the lattice; therefore, one can expect that it also causes lattice deformations. Accordingly, we suppose that the electrostatic field force

$$\mathbf{F}=en\nabla\varphi \tag{3}$$

is playing the role of the force $\mathbf{F}$ in Eq. (1). For simplicity of notation, we assume singly ionized atoms, e is the charge of an electron, so that the ionic charge density is $-en$.

The electrostatic potential φ is known as the Bernoulli potential. It has been derived in a number of approximations.[24–27] Here, we will use the formula of Ref. 24,

$$e\varphi=-\frac{1}{2m^*n}\bar{\psi}(-i\hbar\nabla-e^*\mathbf{A})^2\psi+\frac{\partial\varepsilon_{\rm con}}{\partial n}\frac{2|\psi|^2}{n}+\frac{T^2}{2}\frac{\partial\gamma}{\partial n}\left(\sqrt{1-\frac{2|\psi|^2}{n}}-1\right). \tag{4}$$

The space profile of the potential φ is shown in Fig. 1, and the individual terms to the potential are compared in Fig. 2. The first term in Eq. (4) is the quantum kinetic energy and represents the gradient corrections. In the London limit, it reaches the form of the classical Bernoulli law, $\bar{\psi}(-i\hbar\nabla-e^*\mathbf{A})^2\psi/2m^*n\rightarrow e^{*2}A^2\omega/4m^*=\omega mv^2/2$, which gave the name to the entire potential. The superconducting fraction ω multiplying the kinetic energy accounts for the fact that the Lorentz and inertial forces act exclusively on the superelectrons, while the balancing electrostatic force acts on all electrons.[26] This force being proportional to the square of the magnetic field has been used to calculate the shape distortion by flux-pinning-induced magnetostriction.[28]

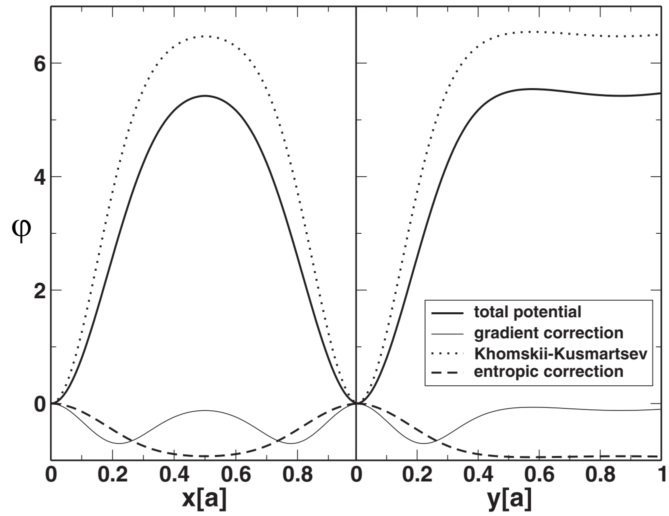

FIG. 2. Cuts through the electrostatic potential from Fig. 1. The thick full line represents the total potential (4), and the dotted line is the Khomskii-Kusmartsev approximation. One can see that the corrections to this approximation are small. The thin full line is the gradient correction given by the "kinetic energy" term of Eq. (4), and the dashed line is the entropic correction given by the last term of Eq. (4).

The second term of the Bernoulli potential (4) is the dominant one and we will focus our discussion on it. This second term is identical to the potential derived by Khomskii and Kusmartsev[27] from the effect of the BCS gap on the local density of electronic states. We call the third term of Eq. (4) the entropic correction.

It is worth noting that Eqs. (4), (3), and (1) resulted from Gibbs variational principle if the free energy used in Ref. 24 is extended by the ionic lattice deformation energy.

Let us link the deformation caused by the electrostatic field with the standard theory of magnetostriction. At zero temperature, the Gibbs energies of the normal and superconducting states differ by the condensation energy,[2] $G_{\rm s}=G_{\rm n}-V\varepsilon_{\rm con}$, where $\varepsilon_{\rm con}=\gamma T_c^2/4=B_c^2/2\mu_0$. Since the pressure derivative of the Gibbs energy determines the sample volume, $V_{\rm s,n}=\partial G_{\rm s,n}/\partial p$, one finds $V_{\rm s}=V_{\rm n}-V\partial\varepsilon_{\rm con}/\partial p$, i.e., $\alpha=\partial\varepsilon_{\rm con}/\partial p$. This relation allows us to show that the force $\mathbf{F}_{\rm Sim}$ from Eq. (2) equals the electrostatic force caused by the second term of the Bernoulli potential (4).

To proceed, we use the fact that the pressure modifies the condensation energy indirectly by an increase of the electron density,

$$\alpha=\frac{\partial\varepsilon_{\rm con}}{\partial p}=\frac{\partial\varepsilon_{\rm con}}{\partial n}\frac{\partial n}{\partial p}=\frac{\partial\varepsilon_{\rm con}}{\partial n}\frac{n}{K}. \tag{5}$$

In the rearrangement, we have employed the definition of the bulk modulus $K=-V/(\partial V/\partial p)=n/(\partial n/\partial p)$. Substituting Eq. (5) into the force (2), one finds

$$\mathbf{F}_{\rm Sim}=n\frac{\partial\varepsilon_{\rm con}}{\partial n}\nabla\frac{2|\psi|^2}{n}. \tag{6}$$

Comparing Eq. (6) with Eq. (3), one can see that the force introduced by Šimánek equals the electrostatic force due to the second term of the Bernoulli potential (4). In this sense, the approximation used within the theory of deformable superconductors is equivalent to the approximation of the electrostatic potential derived by Khomskii and Kusmartsev. The gradient and entropic corrections of the Bernoulli potential (4) provide us with corresponding corrections to the force of Šimánek.

More interesting is the gradient correction. From formula (4), it follows that far from the vortex core, where $\bar{\psi}\psi \to (1-T^4/T_c^4)n/2$, the gradient correction is proportional to the square of the local current. For an isolated vortex, the gradient correction thus decays on the scale of the London penetration depth and so has a long range in high κ materials.

The effect of the gradient correction is traceable also for a conventional material assumed here. To be specific, consider a niobium rod parallel to the magnetic field. The GL coherence length of niobium is reduced by nonmagnetic impurities so that the GL parameter is increased to $\kappa=1.5$, while the other material parameters remain close to the values of pure niobium. All plots are for $T=0.7T_c$ and $\bar{B}=0.24B_{c2}$. In this case, the magnetic field is not split into separated unit fluxes but it is nearly homogeneous with amplitude fluctuations of about 20% around the mean field $\bar{B}$. The vortex cores are well separated, however, as the superconducting fraction ω reaches its nonmagnetic value in the out-of-core region.

Let us analyze the three contributions to the electrostatic potential from the point of view of the forces they cause. According to the position of the inflection point of the Khomskii-Kusmartsev potential seen in Fig. 2, one can estimate that the maximum of the Šimánek force occurs at about $x,y\sim 0.1a$. This is quite close to the center of the vortex core. The gradient correction oscillates rapidly in space, with magnitude much smaller than the Khomskii-Kusmartsev potential. Its gradient, however, is rather comparable to the gradient of the dominant term, which shows that the gradient contribution to the force can appreciably modify the Šimánek force. In the heart of the vortex core, the gradient correction to the force acts against the Šimánek force, while in the skin of the vortex core, it points in the same direction. As a result, the maximum of the total force is shifted outward to $x,y\sim 0.2a$.

Naturally, gradient corrections modify the vortex mass. Figure 3(a) shows how individual regions in the Abrikosov vortex lattice contribute to the vortex mass for the Šimánek force; in Fig. 3(b), the gradient and the entropic corrections are included. The plotted function is the density of kinetic energy of lattice ions driven by vortices moving with velocity V in the x direction,[14]

$$E_{\text{kin}} = \frac{1}{2}V^2 nM\left[\left(\frac{\partial u_x}{\partial x}\right)^2 + \left(\frac{\partial u_y}{\partial x}\right)^2\right], \qquad (7)$$

where M is the mass of a single ion.

In most places of the Abrikosov vortex lattice, the ionic kinetic energy is lowered by the correction terms (see Fig. 3). From the integral over the elementary cell, one obtains the vortex mass per unit length. Keeping both corrections, the

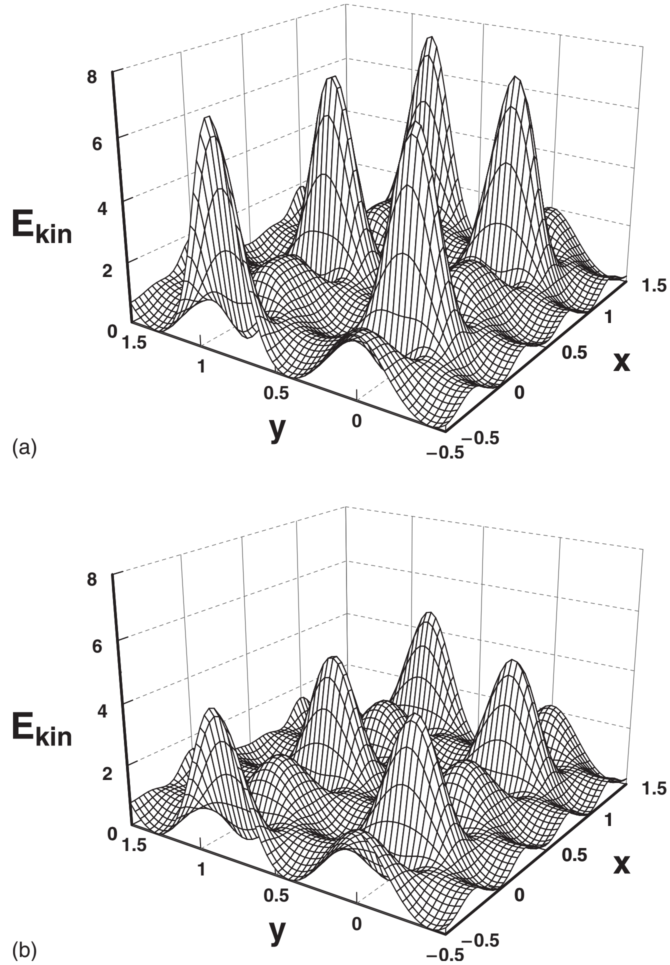

FIG. 3. The density of kinetic energy of lattice ions created by vortices moving in the x direction for the parameters of Fig. 1. The kinetic energy due to (a) the Šimánek force (6) and (b) the electrostatic force (3). The plotted function is proportional to the bracket in Eq. (7).

ion contribution to the vortex mass is reduced by a factor of 0.83 as compared to the Šimánek result. If one neglects the gradient correction keeping only the entropic correction, the reduction factor is 0.70. The gradient correction thus leads to a small enhancement of the vortex mass.

Comparing relative amplitudes of the kinetic energy inside and between the cores, one can see that the corrections have increased the share of the out-of-core region. Since the entropy term merely reduces the amplitude of the Šimánek force, this redistribution of distortions is exclusively due to the gradient correction. According to Cano *et al.*,[19] the out-of-core lattice deformations are important for the strain-mediated interaction of vortices. We suggest that the theory of this interaction should be reexamined with the gradient correction included.

In summary, we have expressed the forces deforming the atomic lattice of a superconductor in terms of the electrostatic force. From experience gained with the theory of the so-called Bernoulli potential, one directly obtains the gradient corrections. We suggest that the value of vortex mass should be reconsidered taking these gradient corrections into account. The vortex mass is of importance for high frequency vortex dynamics, and we expect that with applications in the terahertz frequency region, its fundamental role will be experimentally proven. The present theory is restricted to homogeneous isotropic materials. Its extension to layered materials will be discussed elsewhere.

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