Nonlinear theory of deformable superconductors: Ginzburg-Landau description

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The interaction of the superconducting condensate with deformations of the crystal lattice is formulated assuming the electrostatic potential to be of Bernoulli type and the effect of strain on material parameters. In the isotropic approximation it is shown that within the Ginzburg-Landau theory both contributions can be recast into the local but nonlinear interaction term of the free energy.

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I. INTRODUCTION

When cooled, metals reduce their volume. At the transition from normal to superconducting state, the coefficient of the thermal expansion makes a jump. In most cases, the superconducting systems reduce their volume less than the normal ones. Consequently, inhomogeneities of the superconducting phase cause stresses which are similar to stresses caused by the inhomogeneities due to the temperature.

Since the superconducting condensate affects the specific volume, deformations of the crystal lattice also affect the condensate. Mechanisms of this interaction between the crystal lattice and the condensate can be outlined within the simplest two-fluid free energy of Gorter and Casimir, $f_{GC}=-\frac{1}{4}\gamma T_c^2\omega-\frac{1}{2}\gamma T^2\sqrt{1-\omega}$, where ω is the superconducting fraction, γ is the linear coefficient of the specific heat per unit volume known as the Sommerfeld γ, and T_c is the critical temperature.

Material parameters γ and T_c are not constants. They depend on the electron density n and the deformation of the crystal lattice, which we describe by the lattice density $n_{\rm lat}$. Due to the dependencies $\gamma(n,n_{\rm lat})$ and $T_c(n,n_{\rm lat})$ the crystal lattice interacts with the superconducting condensate.

In literature on deformable superconductors one finds two models of the lattice-condensate (lc) interaction. First, there are various phenomenological theories[1–6] which assume that the density of electrons exactly follows the density of the lattice, $n=n_{\rm lat}$. The perturbation of material parameters due to the deformation, e.g., $\delta\gamma=(\partial\gamma/\partial n)\delta n+(\partial\gamma/\partial n_{\rm lat})\delta n_{\rm lat}$, then can be expressed via the lattice density, $\delta\gamma=[(\partial\gamma/\partial n)+(\partial\gamma/\partial n_{\rm lat})]\delta n_{\rm lat}$. The strength of the lc interaction, thus, depends on the sum of both density derivatives, $(\partial\gamma/\partial n)+(\partial\gamma/\partial n_{\rm lat})$ and $(\partial T_c/\partial n)+(\partial T_c/\partial n_{\rm lat})$.

Second, a model in which the lc interaction is mediated by the electrostatic potential has been discussed.[7,8] Since the theory of the electrostatic potential has been developed under the approximation of a stiff lattice, the lc interaction obtained within this model depends exclusively on the derivatives with respect to the electron density, $\partial\gamma/\partial n$ and $\partial T_c/\partial n$.

The phenomenological approach is more general being applicable to all materials, while the electrostatic approach is limited to cases in which the dependence on the electron density dominates. On the other hand, the electrostatic approach offers a natural picture of the surface, in particular, one can easily see that the electrostatic field of the surface dipole contributes to the forces deforming the crystal lattice.[9] Studies within the phenomenological approach have not noticed the surface tension.

In this paper we derive a phenomenological theory which unifies both approaches. To this end it is necessary to take into account the charge of a deformed lattice in the electrostatic potential and to allow for lc interaction which is not covered by the (mean) electrostatic potential. To avoid lengthy formulas or nontransparent tensor notation with numerous indices, we restrict our attention to the interaction between the lattice compression and the condensate. We neglect the interaction between the condensate anisotropy and shear deformations of the lattice. Interaction of the superconducting condensate with a deformation which can be interpreted as a mutual displacement of sublattices has been discussed in Ref. 10.

A. Origin of two mechanisms

There are various microscopic mechanisms due to which material parameters of the superconductor depend either on the density of electrons or on the deformation of the crystal lattice. Although our discussion is independent of actual microscopic mechanisms, we find it profitable to outline some of these possibilities so that the need to treat perturbations of the electron density and the lattice density independently becomes more apparent.

The Sommerfeld γ is proportional to the single-spin density of states N_0 at the Fermi energy, $\gamma=\frac{2}{3}\pi^2k_B^2N_0$. The density of states naturally depends on the value of the Fermi energy, which itself depends on the electron density. In this way the Sommerfeld γ depends on the electron density.

The density of states also reflects the electron band structure. For example, the saddle points giving a high density of states are quite sensitive to atomic spacing. Moreover, in ionic crystals of high-T_c superconductors the charge transfer between sublattices depends on the lattice deformation. The

Sommerfeld γ thus depends on the lattice deformation via mechanisms which are distinct from changes in the electron density.

The critical temperature is an even more complex quantity. For simplicity we express it within the BCS approximation $T_c=0.85\Theta_D \exp(-1/N_0V)$. Apparently, T_c depends on the electron density and the deformation via the density of states. Besides this, there are additional contributions via the interaction potential V and the Debye temperature Θ_D. For example, a compression of the lattice increases the mass density, which results in a slower velocity of sound. This reduces the Debye temperature Θ_D, leading in some superconductors to a decrease in T_c under an applied pressure.[11]

The above-mentioned mechanisms of the density dependence work in pure materials. Let us mention a mechanism specific for dirty superconductors. In metals doped by paramagnetic impurities the dominant pressure dependence of T_c results from the electron density dependence of the magnetic scattering relaxation time.[12]

B. Plan of the paper

In Sec. II we introduce the free energy which combines the condensation energy of Ginzburg and Landau (GL), the energy of electric and magnetic fields, and the deformation energy. In Sec. III we present the set of equations derived from the Lagrange variational principle. In Secs. IV and V we focus on the electrostatic potential and the strain, respectively. In Sec. VI we write down an effective free energy for deformable superconductors, and Sec. VII is the summary.

II. FREE ENERGY

We start from the free energy and employ the Lagrange variational principle to derive all stability conditions. Following GL, the free energy of the superconducting state

$$f_s = f_n + \alpha|\psi|^2 + \frac{1}{2}\beta|\psi|^4 + \frac{1}{2m^*}|(-i\hbar\nabla - e^*\mathbf{A})\psi|^2 \quad (1)$$

is defined as a biquadratic function of the GL function ψ. The gradient term has a form of the kinetic energy with the Copper pair mass m^* and charge $e^*=2e$.

The GL free energy is added to the free energy of the normal state

$$f_n = f_0 + e\varphi(n - n_{\mathrm{lat}}) - \frac{1}{2}\epsilon|\nabla\varphi|^2 + \frac{1}{2\mu_0}|\nabla\times\mathbf{A}|^2. \quad (2)$$

The normal free energy covers the magnetic energy (last term), the electrostatic energy (second and third terms), and the local free energy f_0.

The local free energy f_0 is a function of the electron density n, deviations of atomic positions $\mathbf{u}$, and temperature T,

$$f_0 = f_0(n,\mathbf{u},T). \quad (3)$$

According to the theory of elasticity,[13] the free energy does not depend directly on the vector $\mathbf{u}$ but only on its derivatives expressed via the strain tensor

$$u_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial r_j} + \frac{\partial u_j}{\partial r_i}\right). \quad (4)$$

There is no term explicitly attributed to the interaction between the deformation $\mathbf{u}$ and the superconducting condensate; however, this interaction has a number of hidden contributions. First, it is mediated by the electrostatic force. Second, the GL parameters α,β,m^* depend on the density of electrons and on the deformation $\mathbf{u}$.

For simplicity we will assume that the GL parameters α, β, and m^* depend on the strain exclusively via the crystal density n_{lat}. In other words we neglect effects of shear deformations which break the isotropy of the system. The reader interested in the anisotropic interaction is referred to papers by Miranović *et al.*[5] or Cano *et al.*[6]

In general, the lattice charge density in deformed crystal is a nontrivial problem since n_{lat} describes the ionic charge and the deformation can change ionicity. We will assume that the ionicity is constant so that the charge is given by the divergence of atomic shifts

$$n_{\mathrm{lat}} = n_0[1 - (\nabla\cdot\mathbf{u})] = n_0(1 - u_{11} - u_{22} - u_{33}). \quad (5)$$

Now all components of the free energy and material dependencies are specified. It remains to derive the equations for the individual fields. To this end we employ the Lagrange variational principle.

III. LAGRANGE VARIATIONAL CONDITIONS

The free energy f_s depends on the following independent variable fields: the vector potential $\mathbf{A}$, the complex GL function ψ, the electrostatic potential φ, the electron density n, and the vector of atomic shifts $\mathbf{u}$. The corresponding variations are well established,[14–16] therefore, we present the resulting equations without derivations. We note that the vector and scalar potentials are in the Coulomb gauge, $(\nabla\cdot\mathbf{A})=0$.

The $\mathbf{A}$ variation yields the Ampere law,

$$\nabla^2\mathbf{A} = -\mu_0\frac{e^*}{m^*}\mathrm{Re}\,\bar{\psi}(-i\hbar\nabla - e^*\mathbf{A})\psi. \quad (6)$$

The $\bar{\psi}$ variation results in the GL equation,

$$(-i\hbar\nabla - e^*\mathbf{A})\frac{1}{2m^*}(-i\hbar\nabla - e^*\mathbf{A})\psi + \alpha\psi + \beta|\psi|^2\psi = 0. \quad (7)$$

The less usual form of the kinetic energy is a Hermitian operator also for an inhomogeneous mass m^*. The dependencies of the material parameters α, β, and m^* on the lattice deformation $\mathbf{u}$, and the electron density n are rather weak but essential for specific problems such as the vortex pinning by the strain around dislocations or for the effect of the elastic energy on the arrangement of vortices.

The φ variation recovers the Poisson equation,

$$-\epsilon\nabla^2\varphi = e(n - n_{\mathrm{lat}}). \quad (8)$$

In deriving this equation we have neglected the ionic contribution to the dielectric function ϵ, i.e., terms proportional to $\partial\epsilon/\partial n_{\mathrm{lat}}$.

The n variation furnishes us with the electrostatic potential known as the Bernoulli potential,

$$e\varphi = -\frac{\partial f_0}{\partial n} - \frac{\partial \alpha}{\partial n}|\psi|^2 - \frac{1}{2}\frac{\partial \beta}{\partial n}|\psi|^4 + \bar{\psi}(-i\hbar\nabla - e^*\mathbf{A}) \times \frac{1}{2m^*}\frac{\partial \ln m^*}{\partial n}\bar{\psi}(-i\hbar\nabla - e^*\mathbf{A})\psi. \quad (9)$$

The density derivative of the local free energy f_0 is nontrivial only if the system is perturbed from the homogenous state. To make $\partial f_0/\partial n$ transparent, it is necessary to expand it in perturbations. This rearrangement is accomplished in Sec. IV.

The $\mathbf{u}$ variation gives the strain equation,

$$\nabla_j \frac{\partial f_0}{\partial u_{ij}} = -\nabla_j \frac{\partial \alpha}{\partial u_{ij}}|\psi|^2 - \frac{1}{2}\nabla_j \frac{\partial \beta}{\partial u_{ij}}|\psi|^4 + \nabla_j e\varphi \frac{\partial n_{\mathrm{lat}}}{\partial u_{ij}} + \nabla_j \bar{\psi}(-i\hbar\nabla - e^*\mathbf{A}) \times \frac{1}{2m^*}\frac{\partial \ln m^*}{\partial u_{ij}}\bar{\psi}(-i\hbar\nabla - e^*\mathbf{A})\psi. \quad (10)$$

We use the Einstein summation rule for doubled indices, e.g., $r_j h_{jm} \equiv \Sigma_{j=1}^{3} r_j h_{jm}$. The strain [Eq. (10)] includes terms which are so far rather symbolic. In Sec. V we express all of them in terms of elastic moduli and forces on the crystal lattice.

IV. BERNOULLI POTENTIAL

We start with a rearrangement of the Bernoulli potential [Eq. (9)]. The first derivative of the local free energy with respect to the electron density is the Fermi energy

$$\frac{\partial f_0}{\partial n} = E_F. \quad (11)$$

The Fermi energy itself depends on the electron density via the Fermi-Dirac statistics and the exchange-correlation potential.[17] Besides, it depends on the lattice deformation via the density of states. Setting the Fermi energy of unperturbed system to zero, to the linear order in perturbations it reads

$$E_F = \frac{\partial E_F}{\partial n}\delta n + \frac{\partial E_F}{\partial u_{ij}}u_{ij}. \quad (12)$$

The Fermi energy E_F depends on the lattice deformation via changes in the electron band structure. Within the isotropic approximation we assume that it is proportional to the perturbation of the lattice density

$$\frac{\partial E_F}{\partial u_{ij}} = \frac{\partial E_F}{\partial n_{\mathrm{lat}}}\frac{\partial n_{\mathrm{lat}}}{\partial u_{ij}} = -\frac{\partial E_F}{\partial n_{\mathrm{lat}}}n_0\delta_{ji}. \quad (13)$$

Using approximation (13) in relation (11) we obtain [$u_{ii} \equiv u_{11}+u_{22}+u_{33}$]

$$\frac{\partial f_0}{\partial n} = \frac{\partial E_F}{\partial n}\delta n - \frac{\partial E_F}{\partial n_{\mathrm{lat}}}n_0 u_{ii}. \quad (14)$$

The first term represents the Thomas-Fermi screening, and the second one results from the charge inhomogeneity of the deformed ionic lattice.

A. Thomas-Fermi screening

Now we express the change of the Fermi energy in terms of the electrostatic potential φ. To this end we use the Poisson equation (8) in the form

$$-\epsilon\nabla^2\varphi = e(\delta n + n_0 u_{ii}). \quad (15)$$

Substituting δn from Eq. (15) in the Fermi energy [Eq. (14)] we arrive at

$$\frac{\partial f_0}{\partial n} = -\frac{\partial E_F}{\partial n}\frac{\epsilon}{e}\nabla^2\varphi - \left(\frac{\partial E_F}{\partial n} + \frac{\partial E_F}{\partial n_{\mathrm{lat}}}\right)n_0 u_{ii}. \quad (16)$$

The first term on the right-hand side can be expressed via the Thomas-Fermi screening length

$$\frac{\partial E_F}{\partial n}\frac{\epsilon}{e^2} = \lambda_{\mathrm{TF}}^2. \quad (17)$$

The Bernoulli potential [Eq. (9)] now reads

$$e\varphi - \lambda_{\mathrm{TF}}^2\nabla^2 e\varphi = \left(\frac{\partial E_F}{\partial n} + \frac{\partial E_F}{\partial n_{\mathrm{lat}}}\right)n_0 u_{ii} - \frac{\partial \alpha}{\partial n}|\psi|^2 - \frac{1}{2}\frac{\partial \beta}{\partial n}|\psi|^4 + \bar{\psi}(-i\hbar\nabla - e^*\mathbf{A})\frac{1}{2m^*}\frac{\partial \ln m^*}{\partial n} \times (-i\hbar\nabla - e^*\mathbf{A})\psi. \quad (18)$$

The electrostatic potential φ resulting from Eq. (18) has two characteristic components, the free and the enforced one. The free solution is nonzero only near the surface decaying into the bulk on the Thomas-Fermi screening length λ_{TF}. This solution is determined by a surface condition. We note that the free solution plays an important role in the surface dipole.[16] Here we focus on the bulk properties, therefore, we ignore the free solution.

Second, there is an electrostatic potential enforced by inhomogeneities in the superconducting density $|\psi|^2$ and the lattice deformation as given by the right-hand side of Eq. (18). We keep the name Bernoulli potential for this component.

Two simplifications of the Bernoulli potential are at hand. First, we can neglect $\lambda_{\mathrm{TF}}^2\nabla^2 e\varphi$. This is because gradients of the GL function and the corresponding potential are on the scale of the GL coherence length or the London penetration, which are both much larger than the Thomas-Fermi screening length λ_{TF}. Second, the logarithmic derivative of the Cooper pair mass m^* is a small quantity and we can neglect its gradient. Therefore,

$$e\varphi = \left(\frac{\partial E_F}{\partial n} + \frac{\partial E_F}{\partial n_{\mathrm{lat}}}\right)n_0 u_{ii} - \frac{\partial \alpha}{\partial n}|\psi|^2 - \frac{1}{2}\frac{\partial \beta}{\partial n}|\psi|^4 + \frac{\partial \ln m^*}{\partial n}\bar{\psi}(-i\hbar\nabla - e^*\mathbf{A})\frac{1}{2m^*}(-i\hbar\nabla - e^*\mathbf{A})\psi. \quad (19)$$

Note that neglecting the term $\nabla^2\varphi$ in the Poisson equation (15) implies the quasineutral approximation $n = n_{\mathrm{lat}}$. In this sense we can work with the nonzero electrostatic potential [Eq. (19)] while using the local charge neutrality for perturbations of material parameters.

The Bernoulli potential [Eq. (19)] extends previous results[16,18] having two additional contributions. First, the charge of the deformed ion lattice is represented by the term $\propto n_0 u_{ii} = n_0(\nabla \cdot \mathbf{u})$. Second, the effect of the charge perturbation on the Cooper pair mass m^* is included.

B. From "nonlocal" to nonlinear corrections

The GL equation (7) multiplied by the conjugate GL function $\bar{\psi}$,

$$\bar{\psi}(-i\hbar\nabla - e^*\mathbf{A})\frac{1}{2m^*}(-i\hbar\nabla - e^*\mathbf{A})\psi = -\alpha|\psi|^2 - \beta|\psi|^4, \tag{20}$$

couples the gradient term on the left-hand side with the nonlinear one $\beta|\psi|^4$. This gives us the freedom to make the Bernoulli potential either a linear or a local function of the superconducting density $|\psi|^2$. We prefer the local but nonlinear form,

$$e\varphi = \left(\frac{\partial E_F}{\partial n} + \frac{\partial E_F}{\partial n_{\mathrm{lat}}}\right) n_0 u_{ii} - \left(\frac{\partial \alpha}{\partial n} + \alpha\frac{\partial \ln m^*}{\partial n}\right)|\psi|^2 - \frac{1}{2}\left(\frac{\partial \beta}{\partial n} + 2\beta\frac{\partial \ln m^*}{\partial n}\right)|\psi|^4. \tag{21}$$

Apparently, there are a number of possible additional rearrangements of the Bernoulli potential. Since we study the interaction between the superconducting condensate and the lattice deformation mediated by the Bernoulli potential, form (21) is optimal as it is expressed in terms of u_{ii} and $|\psi|^2$.

V. STRAIN EQUATION

The strain equation (10) is rather involved as it contains gradients of derivatives with respect to tensor components of the strain. The major simplification follows from the assumption that all material parameters related to the superconducting phase depend on the strain exclusively via the lattice density n_{lat}, i.e.,

$$\frac{\partial \alpha}{\partial u_{ij}} = -\frac{\partial \alpha}{\partial n_{\mathrm{lat}}} n_0 \delta_{ji} \tag{22}$$

and similar for β and m^*. Within this isotropic approximation the strain equation can be rearranged in a manner which in many steps parallels the treatment of the Fermi energy in the previous section.

A. Stress

The stress tensor has a general form of

$$p_{ji} = \Lambda_{jilk} u_{kl}. \tag{23}$$

The moduli matrix Λ has 81 elements, but only 27 of them are independent.[13]

Now we express the moduli tensor Λ in terms of the free energy f. We start with the strain derivative of the local free energy

$$\frac{\partial f_0}{\partial u_{ij}} = \frac{\partial^2 f_0}{\partial u_{ij}\partial u_{kl}} u_{kl} + \frac{\partial^2 f_0}{\partial u_{ij}\partial n}\delta n, \tag{24}$$

which we have expanded in perturbations. The second term of expansion (24) can be expressed with the help of the already specified strain derivative of the Fermi energy

$$\frac{\partial^2 f_0}{\partial u_{ij}\partial n} = \frac{\partial E_F}{\partial u_{ij}} = -\frac{\partial E_F}{\partial n_{\mathrm{lat}}} n_0 \delta_{ji}. \tag{25}$$

Finally we use the Poisson equation (15) to eliminate the perturbation of the electron density δn from the stress,

$$\frac{\partial f_0}{\partial u_{ij}} = \frac{\partial^2 f_0}{\partial u_{ij}\partial u_{kl}} u_{kl} + \delta_{ji} u_{kk} \frac{\partial E_F}{\partial n_{\mathrm{lat}}} n_0^2. \tag{26}$$

We have neglected the term $\delta_{ji}\frac{\partial E_F}{\partial n_{\mathrm{lat}}} n_0 \frac{\epsilon_0}{e}\nabla^2\varphi$ because it is proportional to $\lambda_{\mathrm{TF}}^2\nabla^2\varphi$.

An additional contribution to the stress results from the Coulomb interaction of the ionic lattice with itself. To make it explicit, we have to rearrange the electrostatic term of the strain equation (10) with the help of the Bernoulli potential [Eq. (21)]

$$e\varphi\frac{\partial n_{\mathrm{lat}}}{\partial u_{ij}} = -\delta_{ji} n_0 e\varphi = -\delta_{ji} n_0 \left(\frac{\partial E_F}{\partial n} + \frac{\partial E_F}{\partial n_{\mathrm{lat}}}\right) n_0 u_{ii} + \delta_{ji} n_0 \left(\frac{\partial \alpha}{\partial n} + \alpha\frac{\partial \ln m^*}{\partial n}\right) \times |\psi|^2 + \delta_{ji} n_0 \frac{1}{2}\left(\frac{\partial \beta}{\partial n} + 2\beta\frac{\partial \ln m^*}{\partial n}\right)|\psi|^4. \tag{27}$$

The first term represents the Coulomb interaction of the lattice with itself. Other terms represent the interaction of the lattice with the superconducting condensate.

The stress tensor collects all contributions to the strain equation (10) which are linear in the strain u. The moduli matrix, thus, reads

$$\Lambda_{jilk} = \frac{\partial^2 f_0}{\partial u_{ij}\partial u_{kl}} + \delta_{ji}\delta_{lk}\left(2\frac{\partial E_F}{\partial n_{\mathrm{lat}}} + \frac{\partial E_F}{\partial n}\right) n_0^2. \tag{28}$$

Here the second term arises from the increase in the electron liquid energy under a volume compression.

B. Deforming force

In terms of the stress equation (23) the strain equation (10) reads

$$\nabla_j p_{ji} = F_i, \tag{29}$$

where

$$F_i = \nabla_j\left[\delta_{ji} n_0\left(\frac{\partial \alpha}{\partial n} + \alpha\frac{\partial \ln m^*}{\partial n}\right) - \frac{\partial \alpha}{\partial u_{ij}}\right]|\psi|^2 + \nabla_j\left[\delta_{ji} n_0 \frac{1}{2}\left(\frac{\partial \beta}{\partial n} + 2\beta\frac{\partial \ln m^*}{\partial n}\right) - \frac{1}{2}\frac{\partial \beta}{\partial u_{ij}}\right]|\psi|^4 + \nabla_j\frac{\partial \ln m^*}{\partial u_{ij}}\bar{\psi}(-i\hbar\nabla - e^*\mathbf{A})\frac{1}{2m^*}\bar{\psi}(-i\hbar\nabla - e^*\mathbf{A})\psi \tag{30}$$

is the force (per unit volume) deforming the crystal. We have neglected the gradient of $\partial \ln m^*/\partial u_{ij}$.

In the isotropic approximations (22) the deforming force [Eq. (30)] simplifies to a gradient

$$F_i = -n_0 \nabla_i U \tag{31}$$

of the effective potential

$$U = -\left(\frac{\partial \alpha}{\partial n} + \frac{\partial \alpha}{\partial n_{\rm lat}} + \alpha \frac{\partial \ln m^*}{\partial n} + \alpha \frac{\partial \ln m^*}{\partial n_{\rm lat}}\right)|\psi|^2 - \frac{1}{2}\left(\frac{\partial \beta}{\partial n} + \frac{\partial \beta}{\partial n_{\rm lat}} + 2\beta \frac{\partial \ln m^*}{\partial n} + 2\beta \frac{\partial \ln m^*}{\partial n_{\rm lat}}\right)|\psi|^4. \tag{32}$$

We have used Eq. (20) to replace the gradient term of Eq. (30) by the nonlinear one.

As one can see, the force is given by the biquadratic effective potential with two material parameters,

$$a = \frac{\partial \alpha}{\partial n_{\rm lat}} + \frac{\partial \alpha}{\partial n} + \alpha \frac{\partial \ln m^*}{\partial n_{\rm lat}} + \alpha \frac{\partial \ln m^*}{\partial n},$$

$$b = \frac{\partial \beta}{\partial n_{\rm lat}} + \frac{\partial \beta}{\partial n} + 2\beta \frac{\partial \ln m^*}{\partial n_{\rm lat}} + 2\beta \frac{\partial \ln m^*}{\partial n}. \tag{33}$$

In both terms the derivatives enter in the same way as if one takes the volume or density derivative assuming the strict local charge neutrality. For lead with a constant Cooper pair mass m^*, parameters a and b are derived in the Appendix.

C. Isotropic model

The simplest and mostly used isotropic model uses only two elastic moduli. The bulk modulus K measures changes in the specific volume, and shear modulus μ is the only coefficient of all volume-keeping deformations. For the isotropic system the strain equation (29) simplifies to[13]

$$\left(K + \frac{4}{3}\mu\right) \nabla (\nabla \cdot \mathbf{u}) - \mu \nabla \times \nabla \times \mathbf{u} = \mathbf{F}, \tag{34}$$

where the force acting on a unit volume of the lattice is given by the gradient as

$$\mathbf{F} = a \nabla |\psi|^2 + \frac{1}{2} b \nabla |\psi|^4. \tag{35}$$

Together with Eq. (33) this is our final result for the strain equation.

VI. EFFECTIVE FREE ENERGY

For studies of the lattice deformations it is not necessary to evaluate the electrostatic potential. In this case one can use a simplified free energy

$$f_s' = \alpha|\psi|^2 + \frac{1}{2}\beta|\psi|^4 + \frac{1}{2m^*}|(-i\hbar \nabla - e^*\mathbf{A})\psi|^2 + \frac{1}{2\mu_0}|\nabla \times \mathbf{A}|^2 + \frac{1}{2}\Lambda_{ijkl} u_{ij} u_{kl} - a u_{ii}|\psi|^2 - \frac{1}{2} b u_{ii} |\psi|^4. \tag{36}$$

This free energy depends on the vector potential $\mathbf{A}$, the GL function ψ, and the displacement $\mathbf{u}$. All material parameters α, β, m^*, Λ, a, and b are now constant in space and do not undergo variations.

By the Lagrange variation in the free energy f_s' with respect to the vector potential $\mathbf{A}$ one recovers the Ampere law [Eq. (6)]. The variation in f_s' with respect to the displacement $\mathbf{u}$ yields the strain equation (29) with the force [Eq. (35)].

The effective free energy f_s' is not exactly equivalent to the full free energy f_s, however. By the variation in f_s' with respect to the GL function $\bar{\psi}$ one arrives at the GL equation

$$\frac{1}{2m^*}(-i\hbar \nabla - e^*\mathbf{A})^2 \psi + (\alpha - a u_{ii})\psi + (\beta - b u_{ii})|\psi|^2 \psi = 0. \tag{37}$$

Unlike the full GL equation (7), here the strain effect on the Copper pair mass m^* is absent. It is mimicked by the m^* part of the strain effect on the effective potential [see a and b as given by Eq. (33)].

VII. SUMMARY

Starting from the free energy of the GL type we have derived the force which deforms the crystal lattice in the presence of the inhomogeneous superconducting condensate. Neglecting terms proportional to the square of the small Thomas-Fermi screening length, we have rearranged the deforming force into the gradient of the biquadratic function of the GL function.

Although we took into account perturbations of the charge neutrality and included the electrostatic potential, our result has confirmed that the assumption of the strict local charge neutrality can be applied for the evaluation of the force deforming the lattice.

Based on our results, we have proposed an effective free energy which is simpler in being independent of the electrostatic potential and the density of normal electrons. Moreover, all its field variables are explicit so that there are no hidden interaction mechanisms. In particular, it has no strain effect on the Copper pair mass m^*. Contributions of these eliminated variables and dependencies are covered by the effective local but nonlinear interaction.

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APPENDIX: INTERACTION PARAMETERS

Here we derive the interaction parameters a and b for lead. For simplicity we treat lead as the nearly free-electron

metal; i.e., we assume that the lead band structure does not change with the deformation. This implies that the density of states does not depend on the lattice density; therefore,

$$\frac{\partial \gamma}{\partial n_{\mathrm{lat}}} = 0. \tag{A1}$$

For the free-electron approximation the Sommerfeld γ depends on the electron density as[19]

$$\gamma = \left(\frac{\pi}{3}\right)^{2/3} \frac{k_B^2}{\hbar^2} m n^{1/3}. \tag{A2}$$

In the free-electron approximation and a pure superconductor, the Cooper pair mass is twice the electron mass, $m^* = 2m$; therefore, it is independent of electron and lattice densities

$$\frac{\partial \ln m^*}{\partial \ln n_{\mathrm{lat}}} = \frac{\partial \ln m}{\partial \ln n_{\mathrm{lat}}} = 0 \tag{A3}$$

and

$$\frac{\partial \ln m^*}{\partial \ln n} = \frac{\partial \ln m}{\partial \ln n} = 0. \tag{A4}$$

These derivatives imply that the interaction parameters a and b from Eq. (33) depend exclusively on the density derivatives of GL parameters α and β.

The constant mass m also simplifies the density derivatives of the Sommerfeld γ

$$\frac{\partial \ln \gamma}{\partial \ln n_{\mathrm{lat}}} = 0 \tag{A5}$$

and

$$\frac{\partial \ln \gamma}{\partial \ln n} = \frac{1}{3}. \tag{A6}$$

A simple estimate of GL parameters follows from the Gorter-Casimir two-fluid model as

$$\alpha = \frac{\gamma}{2n}(T^2 - T_c^2) \tag{A7}$$

and

$$\beta = \frac{\gamma T^2}{4n^2}. \tag{A8}$$

We put the actual temperature T equal to the critical temperature T_c after performing derivatives.

From relation (A7) it follows that

$$\frac{\partial \alpha}{\partial n} = -\frac{\gamma T_c^2}{n^2} \frac{\partial \ln T_c}{\partial \ln n} \tag{A9}$$

and

$$\frac{\partial \alpha}{\partial n_{\mathrm{lat}}} = -\frac{\gamma T_c^2}{n^2} \frac{\partial \ln T_c}{\partial \ln n_{\mathrm{lat}}}, \tag{A10}$$

where we have used the neutrality $n = n_{\mathrm{lat}}$, again after performing derivatives. From relation (A8) it follows that

$$\frac{\partial \beta}{\partial n} = -\frac{\gamma T_c^2}{4n^3}\left(2 - \frac{\partial \ln \gamma}{\partial \ln n}\right) = -\frac{5\gamma T_c^2}{12n^3}, \tag{A11}$$

where we have used Eq. (A6). We also see that β does not depend on the lattice density; i.e.,

$$\frac{\partial \beta}{\partial n_{\mathrm{lat}}} = 0. \tag{A12}$$

To complete the estimate we need the density derivatives of the critical temperature. The derivative with respect to the electron density we evaluate from the BCS formula

$$T_c = 0.85\theta_D e^{-1/VN_0}, \tag{A13}$$

where the Debye temperature θ_D and the BCS interaction V are approximately independent from the electron density

$$\frac{\partial \ln T_c}{\partial \ln n} = \frac{1}{VN_0} \frac{\partial \ln N_0}{\partial \ln n} = \frac{1}{3} \ln \frac{0.85\theta_D}{T_c}. \tag{A14}$$

We have used that the Sommerfeld γ is proportional to the density of states N_0 so that $\frac{\partial \ln N_0}{\partial \ln n} = \frac{\partial \ln \gamma}{\partial \ln n} = \frac{1}{3}$.

The change of the critical temperature in lead with compression has been experimentally established by Hake and Mapother[20] from the pressure effect on the critical magnetic field. They provide the change with the volume Ω

$$\frac{\partial \ln T_c}{\partial \ln \Omega} = -\frac{\partial \ln T_c}{\partial \ln n} - \frac{\partial \ln T_c}{\partial \ln n_{\mathrm{lat}}} = 2.89. \tag{A15}$$

The remaining material parameters of lead are $T_c = 7.2$ K, $\theta_D = 105$ K, $\gamma = 163$ Jm^{-3} K^{-2}, and $n = 13.210^{28}$ m^{-3}. From Eq. (A9) we thus obtain

$$n\frac{\partial \alpha}{\partial n} = -3.3510^{-7} \text{ eV}, \tag{A16}$$

while from Eq. (A10) it follows that

$$n\frac{\partial \alpha}{\partial n_{\mathrm{lat}}} = 7.3410^{-7} \text{ eV}. \tag{A17}$$

Finally, Eq. (A11) yields

$$n^2\frac{\partial \beta}{\partial n} = -3.3310^{-7} \text{ eV}. \tag{A18}$$

We have scaled all quantities with the density so that one can compare them with the condensation energy per Cooper pair $\frac{\gamma T_c^2}{2n} = 1.9910^{-7}$ eV. On this scale the resulting interaction parameters are

$$na = 3.9910^{-7} \text{ eV},$$

$$n^2 b = -3.3310^{-7} \text{ eV}. \tag{A19}$$

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