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Magnetic field dependence of vortex core size in clean superconductors

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The problem of transformation of the quasiclassical Eilenberger theory to the one-parameter London model is considered for the mixed state of clean type-II superconductors. Numerical computations demonstrate that introduction of a field dependent coherence length $\xi_h(B)$ is enough for description of the magnetic field distribution in the vortex core of a superconductor. It is found that the shape of $\xi_h(B)$ has strong temperature dependence. The comparison between *s*- and *d*-wave pairing symmetry is done. Different behavior of $\xi_h(B)$ in triangular and square vortex lattices is found.

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For type-II superconductors it has long been realized that the low-lying quasiparticle excitations are confined to vortex cores with size matching with the coherence length ξ_h of the superconductor. This means that the vortex core behaves like a cylinder of normal metal with radius ξ_h. According to the picture of a rigid normal core, one can easily distinguish the *s*-wave superconductors from the others which have nodal gaps. For example, in this picture, the magnetic field dependence of the specific heat coefficient γ should behave like $\gamma \propto B$ because the vortex number is proportional to the field in the mixed state. This is different from the relation $\gamma \propto \sqrt{B}$ expected from nodal pairing symmetry.[1] However, several investigations of the density of states (DOS) in the mixed state show the existence of a considerable sublinear part in field dependence of DOS in contradiction with the model of a rigid vortex core in *s*-wave superconductors.[2–4] This is caused by delocalization of quasiparticles bound to the vortex core in the flux line lattice (FLL) and the field dependent Kramer-Pesch effect.[5,6] From the microscopical point of view this effect is connected with the changing of the DOS from U shape to V shape in the mixed state of *s*-wave superconductors.[4] The presence of magnetic field dependence $\xi_h(B)$ is also important for interpretation of results of muon spin rotation (μSR) and small-angle neutron scattering (SANS) measurements[7–9] which often show decreasing $\xi_h(B)$ close to $1/\sqrt{\mathrm{B}}$.

When analyzing experimental data with the help of the London model[7] it is usually assumed that the penetration depth should be field dependent. This approach is well founded on the base of Eilenberger equations introducing an anisotropic tensor L_{ij},[10–14] used for calculation of the second moment of the magnetic field distribution and the $\lambda(B)$ dependence.[14] This method is useful for the discussion of μSR and SANS measurements.[7] Anyhow, this method requires embedding an additional fitting parameter in the cutoff function[15–18] resulting in a two-parameter fitting of the magnetic field distribution.

Recently it has been suggested that the magnetic properties of FLL can be explained with a field dependent effective coherence length $\xi_h(B)$,[19,20] and a method to extract $\xi_h(B)$ from the magnetization data and transport measurements using only one fitting parameter was proposed.[19] The Helfand-Werthamer's linearization technique[21] for the calculation of the vortex core size is applied there. This one parameter fitting method allows us to connect the results of magnetic and STM[4] experiments. Within this approach, the quasiclassical Eilenberger equations for the order parameter near the vortex center are reduced to a linear form predicting monotonously decreasing $\xi_h(B)$. This form of $\xi_h(B)$ agrees with experimental observation for superconductors with complicated band structure such as YNi_2B_2C, $LuNi_2B_2C$, and $NbSe_2$ and also corresponds to μSR and SANS measurements.[7] However, it fails for V_3Si [monotonously increasing $\xi_h(B)$] where this theory is supposed to work.

As noted,[19,20] a number of questions should be addressed theoretically: (i) It is not clear whether or not the linearized model is compatible with the Pesch and Kramer prediction[22] that the core size of an isolated vortex goes to zero at $T \to 0$. (ii) The solution in the Ginzburg-Landau (GL) regime at high temperatures should be fulfilled. (iii) The cutoff size extracted from magnetization data is not necessarily the same as the core size ξ_Δ defined as being proportional to the slope of the order parameter at the vortex axis. Approaching the core from the outside to determine the cutoff is not the same as examining the core structure starting from the core center.[23] To emphasize the difference between the characteristic lengths of the order parameters and the magnetic field distributions we define the notations of ξ_Δ and ξ_h, respectively, in this paper.

We consider a clean superconductor, because there is no complete understanding even in this case yet, and show using numerical calculations that the Eilenberger theory can be simplified to get the London equation with only the field dependent parameter $\xi_h(B)$. It is found that at low temperatures ξ_h grows monotonously with the field, but at higher temperatures a minimum in $\xi_h(B)$ appears. This result agrees with the Hao-Clem solution of the GL model.[15] The cases of *s*- and *d*-pairing symmetry are also compared. The numerically obtained results can be used for the explanation of the experimental results for V_3Si.[19]

We solve the quasiclassical Eilenberger equations for the *s*- and *d*-wave pairing potential $\Delta(\mathbf{r})=\bar{\Delta}(\mathbf{r})\exp(i\phi)$ with $\exp(i\phi)=(x+iy)/r$. To simplify the comparison between the *s*- and *d*-wave superconductors we assume the same cylindrical Fermi surface in both cases that is suitable for high-T_c and organic superconductors. Throughout this paper, the energy, the temperature, and the length are measured in units of T_c and the coherence length $\xi_0=\xi_{BCS}\pi\Delta_0/T_c=v_F/T_c$. The magnetic field $\mathbf{h}$ is given in units of $\phi_0/2\pi\xi_0^2$. In computations the ratio $\kappa=\lambda_0/\xi_0=10$ between the penetration depth and the coherence length at zero temperature in clean superconductors is used in all the plots but Fig. 5. The method of Riccati transformation of the Eilenberger equations is used.[16,17,24,25] In this method the quasiclassical Green functions are parametrized via

$$\bar{f}=\frac{2\bar{a}}{1+\bar{a}\bar{b}},\quad \bar{f}^{\dagger}=\frac{2\bar{b}}{1+\bar{a}\bar{b}},\quad g=\frac{1-\bar{a}\bar{b}}{1+\bar{a}\bar{b}}, \tag{1}$$

where the anomalous Green functions $\bar{f}$ and $\bar{f}^{\dagger}$ are related to the usual notations as $f=\bar{f}\exp(i\phi)$ and $f^{\dagger}=\bar{f}^{\dagger}\exp(-i\phi)$. The functions $\bar{a}$ and $\bar{b}$ satisfy the independent nonlinear Riccati equations

$$\partial_{\parallel}\bar{a}(\omega_n,\theta,\mathbf{r})=\bar{\Delta}(\mathbf{r})-[2\omega_n+i(\partial_{\parallel}\phi-\mathbf{A}_{\parallel}) + \bar{\Delta}^{*}(\mathbf{r})\bar{a}(\omega_n,\theta,\mathbf{r})]\bar{a}(\omega_n,\theta,\mathbf{r}), \tag{2}$$

$$\partial_{\parallel}\bar{b}(\omega_n,\theta,\mathbf{r})=-\bar{\Delta}^{*}(\mathbf{r})+[2\omega_n+i(\partial_{\parallel}\phi-\mathbf{A}_{\parallel}) + \bar{\Delta}(\mathbf{r})\bar{b}(\omega_n,\theta,\mathbf{r})]\bar{b}(\omega_n,\theta,\mathbf{r}), \tag{3}$$

where $\omega_n=(2n+1)\pi T$ is the fermionic Matsubara frequency, $\partial_{\parallel}=d/dr_{\parallel}$ and $\partial_{\parallel}\phi=-r_{\perp}/r^2$. Here we use the coordinate system $\hat{\mathbf{u}}=\cos\theta\hat{\mathbf{x}}+\sin\theta\hat{\mathbf{y}}$, $\hat{\mathbf{v}}=-\sin\theta\hat{\mathbf{x}}+\cos\theta\hat{\mathbf{y}}$. Thus a point $\mathbf{r}=x\hat{\mathbf{x}}+y\hat{\mathbf{y}}$ denoted as $\mathbf{r}=r_{\parallel}\hat{\mathbf{u}}+r_{\perp}\hat{\mathbf{v}}$, $\Delta(\mathbf{r})$ is obtained self-consistently from BCS relations, and the supercurrent $\mathbf{J}(\mathbf{r})$ is given in terms of $g(\omega_n,\theta,\mathbf{r})$.[25]

The local magnetic field $\mathbf{h}(\mathbf{r})$ can be split into a constant part, the magnetic induction $\mathbf{B}$ and a periodic part $\mathbf{B}'(\mathbf{r})$ with zero average over the vortex lattice cell. Similarly, the vector potential can be split into two parts,

$$\mathbf{h}(\mathbf{r})=\mathbf{B}+\mathbf{B}'(\mathbf{r})=\nabla\times\bar{\mathbf{A}}+\nabla\times\mathbf{A}', \tag{4}$$

where $\mathbf{A}'(\mathbf{r})$ is periodic with a condition $\nabla\cdot\mathbf{A}'=0$.

Assuming the periodical FLL, the self-consistent Eilenberger equations (2) and (3) are solved numerically by iteration using the fast Fourier transform method[25] for a given vector potential $\mathbf{A}'$ and the gap function Δ. The iteration procedure starts with $\mathbf{A}'=0$ and $\Delta=$const. The functions a and b are then used to calculate new values of $\mathbf{A}'$ and Δ, and the whole process is repeated until self-consistency is achieved.

The nonlocal microscopical Eilenberger theory can be reduced to a one-parameter model with effective coherence length $\xi_h(B)$.[19,20,26] In this approach the London penetration depth $\lambda(T)$ is field independent and has the same value as in the Meissner state, but the field dependence of $\xi_h(B,T)$ is enough for an explanation of the magnetization experiments.

We define the coherent length ξ_h using the standard London model. The magnetic field distribution is given by the equation

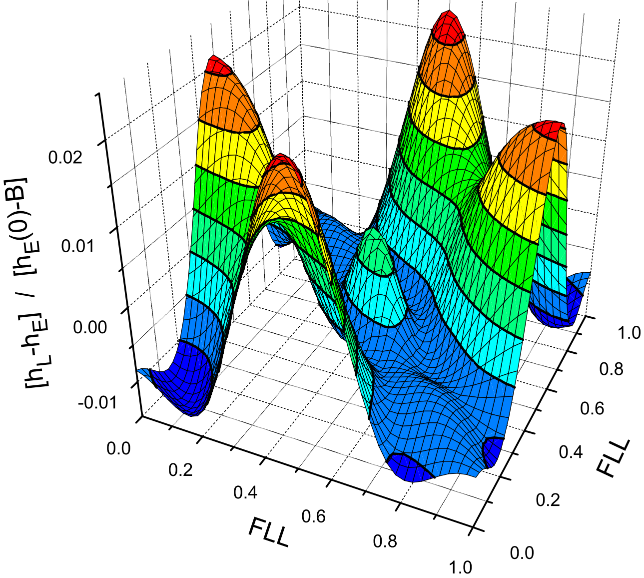

FIG. 1. (Color online) Normalized differences between the fields calculated with the London model and with the Eilenberger equation for $B=5$, $T/T_c=0.5$ and the triangular FLL. The scales of the lengths are those of the flux line lattice unit vectors. The bold lines are the level curves.

$$h(\mathbf{r})=\frac{\phi_0}{S}\sum_{\mathbf{G}}\frac{F(G)e^{i\mathbf{G}\mathbf{r}}}{1+\lambda^2G^2}, \tag{5}$$

where $F(\mathbf{G})=uK_1(u)$, $K_1(u)$ is the modified Bessel function, $u=\sqrt{2}\xi_hG$, $\mathbf{G}$ is a reciprocal lattice vector, and S is the surface of the vortex lattice unit cell. At temperatures near T_c the cutoff function $F(\mathbf{G})$ coincides with solution of the GL equations.[15,18] To find ξ_h we fit the field distribution from Eq. (5) to the solution of the Eilenberger equations. The quality of the fitting can be seen from Fig. 1, where the normalized difference between the fields h_L calculated with the one-parameter London model and with the Eilenberger equation h_E for s-wave superconductors at $B=5$, $T=0.5$ is shown. The accuracy of the fitting is better than 2%.

Figure 2 demonstrates the calculated field and temperature dependence of ξ_h for s-wave superconductors. A strong decrease of the core size with decreasing temperature is clearly observed. It is connected with the Kramer-Pesch effect.[22] The most interesting feature of the obtained results is the nonmonotonous field dependence of ξ_h. The clear minimum of ξ_h/ξ_0 at high temperatures becomes weaker at low temperatures. A minimum was found also in the order parameter coherence length: $1/\xi_\Delta=[\partial|\Delta(r)|/\partial r]_{r=0}/|\Delta_{NN}|$, where $|\Delta_{NN}|$ is the maximum value of the order parameter along the nearest-neighbor direction, which is also the direction of taking the derivative.[23] This reflects an interconnection between the magnetic coherence length $\xi_h(B)$ and the order parameter distribution. Numerical calculations of $\xi_\Delta(B)$ show that embedding impurities results in suppression of the minimum of ξ_h and eventually leads to a monotonically decreasing function.[23] Similar behavior is often observed in experiments,[7] too. The presence of impurities can explain the

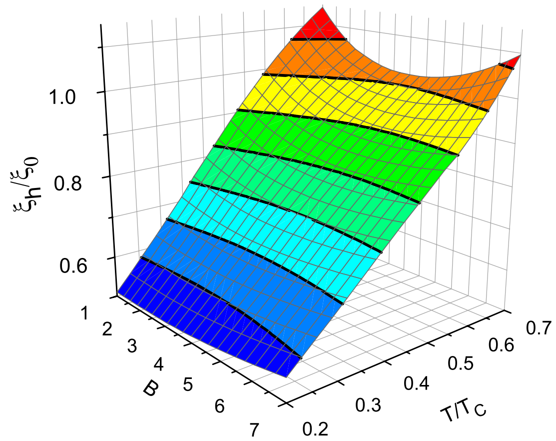

FIG. 2. (Color online) Field and temperature dependences of the coherence length $\xi_h(B,T)$ for s-wave superconductors and the triangular FLL.

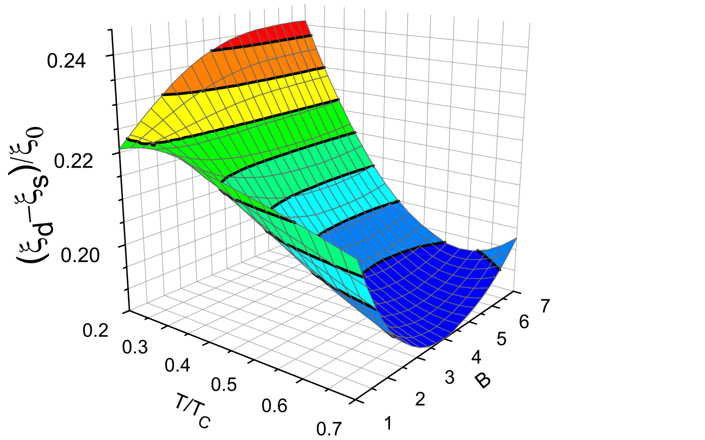

FIG. 4. (Color online) Magnetic field and temperature dependences of the difference between the coherent lengths for s- and d-wave superconductors in triangular FLL.

absence of the minimum in $\xi_h(B)$ in V_3Si and other materials. A second band with small gap can also change the field dependence $\xi_h(B)$ in $NbSe_2$, MgB_2, and probably in boron carbides YNi_2B_2C, $LuNi_2B_2C$ as well.

We also inverstigated the effect of magnetic field on pairing symmetry. The results for s- and d-wave superconductors at different temperatures are presented in Fig. 3. The shapes of the ξ_h/ξ_0 dependences on B are similar in these two cases and differ only by a numerical value. Figure 4 demonstrates that the difference between the coherence lengths for s- and d-wave superconductors has field and temperature dependence less than 10%. This can be explained by the V shape of the low energy density of the states $N(E)=N_0(H)+\alpha|E|$ for all clean superconductors in the vortex state, irrespective of the underlying gap structure. The V shape has been obtained by microscopic calculations for the isotropic gap as well as for the line and the point-node gaps.[4,6] The singular DOS with V shape is universally independent of the underlying original gap structure. Scanning tunneling spectroscopy experiments on $NbSe_2$, YNi_2B_2C support the existence of the V shape.[4]

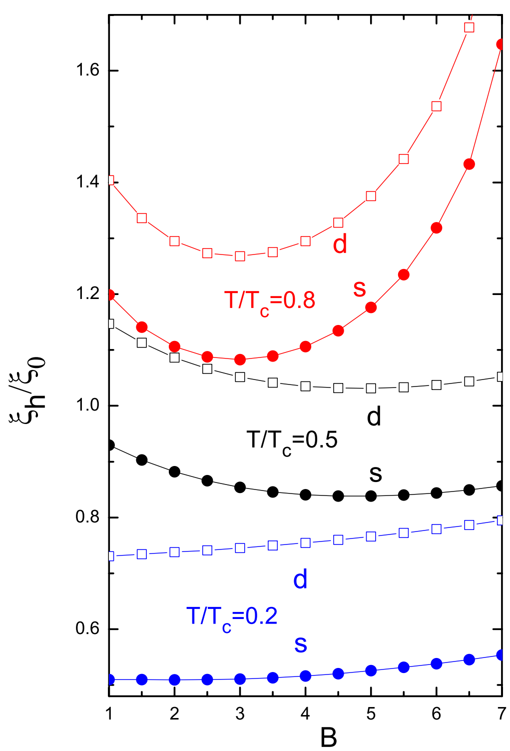

FIG. 3. (Color online) Magnetic field dependences of the coherent length ξ_h in the triangular FLL normalized against the zero field value for s- and d-wave superconductors at different temperatures.

As observed by the SANS technique, in field directions close to perpendicular to the CuO_2 planes of YBCO single crystal, the FLL structure changes smoothly from a distorted triangular symmetry to a nearly perfect square around $B=11$ T.[27] This behavior is expected from d-wave theories.[28] For this reason we compare $\xi_h(B)$ for triangular and square

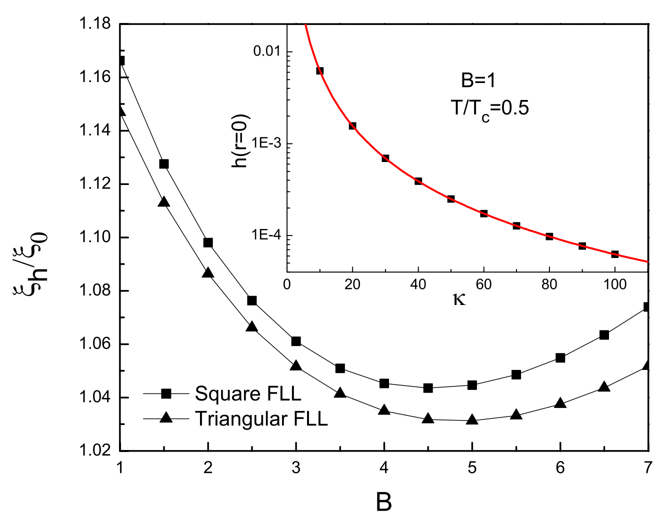

FIG. 5. (Color online) Dependence of the effective coherence length on magnetic induction for triangular and square flux line lattices. The inset shows the dependence of the magnetic field in the vortex center on $\kappa=\lambda_0/\xi_0$ at $T/T_c=0.5$ and $B=1$ in units of $\phi_0/2\pi\xi_0^2$.

lattices. As can be seen from Fig. 5, $\xi_h(B)$ is slightly longer in the square lattice. Considering these two lattices[29] a similar behavior has been found in the Abrikosov coefficient β_A increasing from 1.16 to 1.18. The parameter $\kappa = \lambda_0/\xi_0$ affects only the magnetic field amplitude as shown in the inset to Fig. 5, but does not affect the magnetic field distribution shape, so the coherence length remains independent of κ. The similar κ independent magnetic field distribution was observed for single vortexes.[17] The dependences of magnetic field in the vortex center are well fitted by a power law $h(r=0)=1/(1.266\kappa)^2$. This type of dependence can be explained by GL theory where $h(r=0) \propto 1/\lambda^2$ and taking into account the normalization of the equations.[11]

To conclude, we have solved numerically the quasiclassical Eilenberger equations for clean type-II superconductors in the mixed state. It is found that these equations can be reduced to the London model with only one parameter, $\xi_h(B)$. The shape of the $\xi_h(B)$ function depends on temperature, being nonmonotonic with a minimum at high temperatures and a monotonously increasing function at low temperatures. We believe that this behavior is connected with the characteristic length of the order parameter ξ_Δ.[23] For quantitative comparison of our theory with experiments, including the appearance of the minimum in the $\xi_h(B)$ dependence, samples with high purity are required. The resemblance of the shape of $\xi_h(B,T)$ between s- and d-wave superconductors is connected with the V-shaped DOS in the mixed state in both cases. Comparison between triangular and square FLL is done, and dependence of the magnetic field in the vortex center on screening properties of the superconductors is investigated.

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