Quasiclassical approach to nonlocal generalized London equation in mixed state of *s*-wave superconductors

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(Received 4 May 2007; published 30 May 2007)

We extend the Ginsburg-Landau solution for cutoff function in London equation to low temperatures by solving numerically the quasiclassical Eilenberger equations in mixed state of *s*-wave superconductors. As a result the nonlocal generalized London equation (NGLE) is obtained. The magnetic field and temperature dependence of the cutoff function parameter $k_1(B,T)$ are calculated. Due to Kramer-Pesch effect k_1 decreases strongly at low temperatures. It is also found that k_1 has a minimum at a value of magnetic field depending on temperature. We reduce the NGLE model to an effective local model and calculate the value of an effective penetration depth $\lambda_{\mathrm{eff}}(B,T)$. The sublinear field dependence of λ_{eff} is predicted that agrees with experimental μSR results for the penetration depth of magnetic field in the *s*-wave superconductor V_3Si and $NbSe_2$.

DOI: 10.1103/PhysRevB.75.174524 PACS number(s): 74.20.Rp, 74.20.Fg, 74.25.Op

I. INTRODUCTION

Structural and electronic properties of the flux-line lattice (FLL) in type-II superconductors have been extensively studied by microscopic techniques such as scanning tunneling spectroscopy (STS), small-angle neutron scattering (SANS), nuclear magnetic resonance, and muon spin rotation (μSR) experiments. In particular, recent development has made it possible to find details of the spatial field distribution $\mathbf{h}(\mathbf{r})$ of the FLL directly from μSR time spectra.[1,2] Experimental results on the magnetic field distribution in the mixed state of superconductors are usually explained by the modified London equation. In this approach the effect of the vortex core is phenomenologically described by a cutoff function obtained from solution of the Ginzburg-Landau equations (GL) (Refs. 3 and 4) valid at temperatures near T_c.

The supercurrent flowing around the vortex core modifies the superconducting electron density resulting in change of the second moment $\langle \delta h^2 \rangle$ of the field distribution in the vortex lattice.[5] Magnetic properties of clean superconductors at low temperatures are affected by nonlocality of the microscopic current-field relation. A theory taking into account the first order nonlocal correction to the London equation has been elaborated[6] and used for explanation of the structural transitions of FLL observed experimentally.[7,8] The nonlocal generalized London equation (NGLE) including higher-order gradient corrections[9,10] has been used for description of the temperature and field dependences of the penetration depth $\lambda(T,B)$ in the high-T_c *d*-wave superconductor $YBa_2Cu_3O_{6.95}$,[11,12] treating the core effects and nonlinear effects phenomenologically and perturbatively, respectively.

In recent years there has been great interest in measurements of the magnetic penetration depth in *s*-wave superconductors such as V_3Si, MgB_2, $LuNi_2B_2C$, YNi_2B_2C to get information about their vortex state and the underlying physics.[13–20] However, it is not easy to compare the experimental results with the prediction of the GL theory which fails in the region of $T \ll T_c$ and does not take into account nonlocal corrections to the London equation. To avoid these difficulties we bridge in the present paper the phenomenological and microscopical theories by solving the quasiclassical Eilenberger equations[21] and NGLE for the mixed state of *s*-wave superconductors. In this way the nonlocal, the nonlinear and the core effects can be included simultaneously and the parameters of generalized London equation can be obtained.

We construct a model where the vortex core effects and the nonlinear corrections are described by an effective cutoff function. The nonlocal screening effects are included in the model explicitly, i.e., instead of the fitting parameter $\lambda(T,B)$ we use an analytically obtained anisotropic electromagnetic response tensor[9,10] which is the exact solution of the Eilenberger equations neglecting the core effects. As a result a good agreement between the quasiclassical approach and NGLE is obtained and the $k_1(B,T)$ dependence is found. Thus, we do not use a phenomenologically introduced field dependent London penetration depth in NGLE. Instead, field distribution $h(\mathbf{r})$ in the mixed state is described only by the cutoff parameter $k_1(B,T)$ of the order of the normalized vortex core size $\xi(B,T)/\xi_0$. We show that the second moment of the field distribution depends strongly on $k_1(B,T)$.

To make connection with experimental results we reduce NGLE to a local effective London equation (LELE) with field dependent λ_{eff}. The LELE results reasonably explain the experimental μSR data.[13]

II. CUTOFF FUNCTION FOR NGLE

To consider the mixed state of an *s*-wave superconductor we assume that the Fermi surface is isotropic and cylindrical. Then the magnetic field distribution in the NGLE approximation can be given as[9]

$$h(\mathbf{r}) = \frac{\phi_0}{S}\sum_{\mathbf{G}} \frac{F(G)e^{i\mathbf{G}\cdot\mathbf{r}}}{1 + L_{ij}(\mathbf{G})G_iG_j}, \tag{1}$$

where

$$L_{ij}(\mathbf{G}) = \frac{Q_{ij}(\mathbf{G})}{\det\hat{\mathbf{Q}}(\mathbf{G})} \tag{2}$$

and S is the surface of the vortex lattice unit cell. The anisotropic electromagnetic response tensor is defined as

$$Q_{ij}(\mathbf{G}) = \frac{4\pi T}{\lambda_0^2}\sum_{\omega_n>0}\int_0^{2\pi}\frac{d\theta}{2\pi} \times \frac{\bar{\Delta}(\theta)^2\hat{v}_{Fi}\hat{v}_{Fj}}{\sqrt{\omega_n^2+\bar{\Delta}(\theta)^2[\omega_n^2+\bar{\Delta}(\theta)^2+\gamma_{\mathbf{G}}^2]}}, \quad (3)$$

where $\lambda_0=(c^2/4\pi e^2 v_F^2 N_0)^{1/2}$ is the London penetration depth at $T=0$, including the Fermi velocity v_F and the density of states N_0 at the Fermi surface, θ is the angle between the $\mathbf{k}$ vector at the Fermi surface and the x axis, and $\gamma_{\mathbf{G}}=\mathbf{v}_F\cdot\mathbf{G}/2$. In Eq. (3) the term including $\gamma_{\mathbf{p}}$ describes the nonlocal correction to the London equation. With $\gamma_{\mathbf{G}}=0$ we obtain the London result $L_{ij}(\mathbf{p})=\lambda(T)^2\delta_{ij}$.

The cutoff function for NGLE is written in the form of $F(\mathbf{G})=uK_1(u)$, where $K_1(u)$ is the modified Bessel function, $u=k_1\sqrt{2}\xi_{\mathrm{BCS}}G$, $\mathbf{G}$ is a reciprocal lattice vector, $\xi_{\mathrm{BCS}}=v_F/\Delta(T)\pi$, and $\Delta(T)$ is a temperature dependent uniform gap. The cutoff parameter k_1 can be found by comparison of the solution of the Eilenberger equations with NGLE. Our approach follows the previously developed idea to extend the Ginzburg-Landau (GL) theory to low temperatures. Calculations of the parameters $\kappa_1(T)$ and $\kappa_2(T)$ with Eilenberger equations[22] were used to distinguish the temperature dependences of the upper critical field H_{c2} and the initial slope of the magnetization M/H, respectively.[23] At high temperatures these parameters correspond to κ_{GL}. In the same way we extend the GL solution for $h(\mathbf{r})$ at high temperatures[3] by introducing a cutoff parameter $k_1(B,T)$ describing the core size at low temperatures. Therefore the shape of the cutoff function $F(\mathbf{G})$ is taken in the form of analytical GL solution.[3] This method was successfully used for the problem of single vortex[24] and FLL (Ref. 25) in d-wave superconductors. It was shown that a cutoff function with exponential shape leads to a worse agreement between the NGLE and the Eilenberger equations.[24]

To derive the quasiclassical Green functions the quasiclassical Eilenberger equations are solved for the s-wave pairing potential $\Delta(\mathbf{r})=\bar{\Delta}(\mathbf{r})\exp(i\phi)$ with $\exp(i\phi)=(x+iy)/r$. Throughout this paper, the energies, temperatures and the lengths are measured in units of T_c and the coherence length $\xi_0=\xi_{\mathrm{BCS}}\pi T_c\Delta_0=v_F/T_c$, respectively. The magnetic field $\mathbf{h}$ is given in units of $\phi_0/2\pi\xi_0^2$. Taking into account the value of $\xi_{\mathrm{BCS}}=100$ Å we find that the unit of the magnetic field is 0.126 T. We solve the Eilenberger equations by using the Riccati transformation.[26–28] In this method the quasiclassical Green functions are parametrized via

$$\bar{f}=\frac{2\bar{a}}{1+\bar{a}\bar{b}}, \quad \bar{f}^{\dagger}=\frac{2\bar{b}}{1+\bar{a}\bar{b}}, \quad g=\frac{1-\bar{a}\bar{b}}{1+\bar{a}\bar{b}}, \quad (4)$$

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

$$\partial_{\parallel}\bar{a}(\omega_n,\theta,\mathbf{r}) = \bar{\Delta}(\mathbf{r}) - [2\omega_n + i(\partial_{\parallel}\phi - \mathbf{A}_{\parallel}) + \bar{\Delta}^*(\mathbf{r})\bar{a}(\omega_n,\theta,\mathbf{r})]\bar{a}(\omega_n,\theta,\mathbf{r}), \quad (5)$$

$$\partial_{\parallel}\bar{b}(\omega_n,\theta,\mathbf{r}) = -\bar{\Delta}^*(\mathbf{r}) + [2\omega_n + i(\partial_{\parallel}\phi - \mathbf{A}_{\parallel}) + \bar{\Delta}(\mathbf{r})\bar{b}(\omega_n,\theta,\mathbf{r})]\bar{b}(\omega_n,\theta,\mathbf{r}), \quad (6)$$

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 $\mathbf{r}=x\hat{\mathbf{x}}+y\hat{\mathbf{y}}$ is denoted as $\mathbf{r}=r_{\parallel}\hat{\mathbf{u}}+r_{\perp}\hat{\mathbf{v}}$. Equations (5) and (6) include both the nonlocal effects ($\partial_{\parallel}\bar{a}$ and $\partial_{\parallel}\bar{b}$ terms) and the nonlinear effects ($\bar{a}$ and $\bar{b}$ are nonlinear functions of $\partial_{\parallel}\phi$) and $\Delta(\mathbf{r})$ is obtained self-consistently from BCS relations.[26] To take into account the influence of screening, the vector potential $\mathbf{A}(\mathbf{r})$ in Eqs. (5) and (6) is obtained from the equation

$$\nabla\times\nabla\times\mathbf{A}=\frac{4}{\kappa^2}\mathbf{J}, \quad (7)$$

where the supercurrent $\mathbf{J}(\mathbf{r})$ is given in terms of $g(\omega_n,\theta,\mathbf{r})$ by the equation

$$\mathbf{J}(\mathbf{r}) = 2\pi T\sum_{\omega_n>0}\int_0^{2\pi}\frac{d\theta}{2\pi}\frac{\hat{\mathbf{k}}}{i}g(\omega_n,\theta,\mathbf{r}). \quad (8)$$

$\mathbf{A}$ and $\mathbf{J}$ are in units of $\phi_0/2\pi\xi_0$ and $2ev_F N_0 T_c$, respectively, and $\kappa=\lambda(T=0)/\xi_0$. The spatial variation of the internal field $h(\mathbf{r})$ is determined by the Maxwell equation.

For every temperature T and magnetic field B we solve Eqs. (5) and (6) by the fast Fourier transform method for a triangular flux line lattice[25,26] taking the resulting magnetic field distribution as the origin. Then the NGLE is solved with the cutoff parameter k_1 and the detailed magnetic field distribution is compared with that origin. The value of k_1 is found using the criterion of minimum mean-square difference between the magnetic field distributions. The quality of the fitting can be seen from Fig. 1 where the normalized difference between the fields calculated in the NGLE model and the Eilenberger equation at $B=3$, $T=0.5$, and $\kappa=10$ is shown. The accuracy of the fitting is better than 2%.

Temperature dependence of k_1 in units of T_c is depicted in Fig. 2, in the case of $\kappa=10$. The shrinking of the core size and k_1 with decreasing values of T can be attributed to thermal depopulation of the more spatially extended high-energy core states [Kramer-Pesch (KP) effect[29]]. The strong decrease of k_1 with reducing of the temperature, as shown in Fig. 2, is in agreement with recent experimental results.[13] A similar temperature dependence was found for the effective core radius ξ_{eff} determined by the ratio $1/\xi_{\mathrm{eff}}=[\partial|\Delta(r)|/\partial r]_{r=0}/|\Delta_{\mathrm{NN}}|$.[30] Here $|\Delta_{\mathrm{NN}}|$ is the maximum value of the order parameter along the nearest-neighbor direction, which is also the direction of taking the derivative.

As shown in Fig. 3 the $k_1(B)$ dependence has a minimum at a certain value of the magnetic field $B_{\min}$. Three important reasons for existence of $B_{\min}$ can be given.

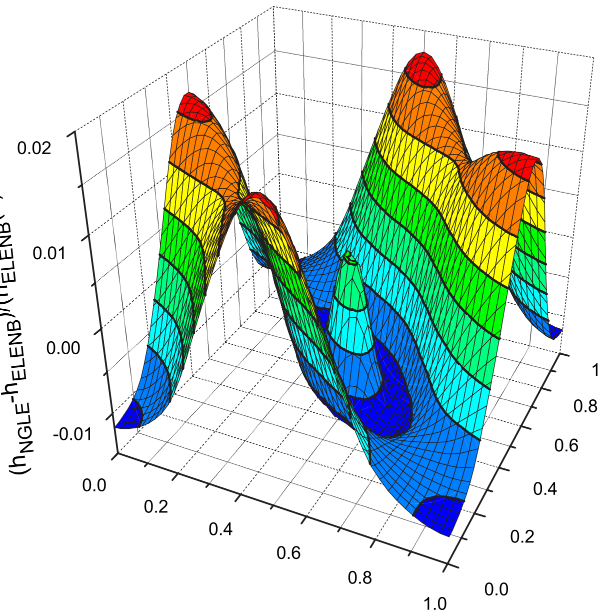

FIG. 1. (Color online) Normalized differences between the fields calculated with the London model (NGLE) and the Eilenberger equation (ELENB) for $B=3$ and $T=0.5$. The scales of lengths are those of the flux line lattice unit vectors.

(i) Nonlinear effects arising due to current in the core area comparable to depairing current: increasing of the magnetic field results in a significant overlap of the currents of nearest-neighbor vortices leading to shrinking of the vortex core.[3]

(ii) Nonlocal effects: solution of linearized Eilenberger equations gives a monotonically decreasing function $\xi(B)$ assuming a uniform magnetic field.[31,32] Both (i) and (ii) can be used to explain the decreasing of k_1 in increasing fields below B_{min}, in agreement with the behavior of the vortex core observed experimentally in different materials.[2]

(iii) Core effect (the nonlinear terms of Δ): at high temperatures in high magnetic fields comparable with the second critical field B_{c2}, the suppression of the superconducting gap by the field becomes important with the result that the coherence length and k_1 are increased for $B>B_{min}$.[3] At low temperatures the KP effect becomes important decreasing strongly the value of k_1 with temperature.

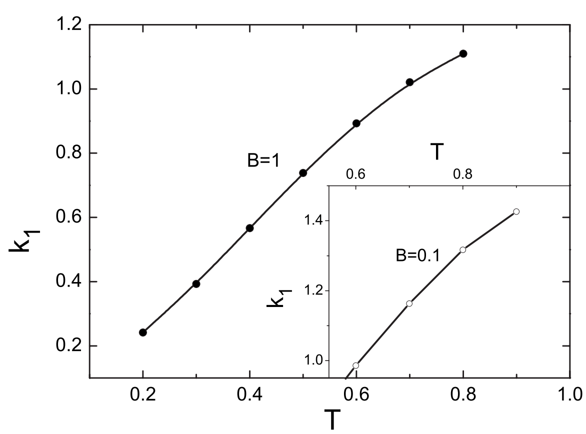

FIG. 2. Temperature dependence of the cutoff parameter $k_1(T)$ for s-wave superconductors obtained at $\kappa=10$ and $B=1$ from fitting to the solution of the Eilenberger equations. The inset demonstrates $k_1(T)$ dependence at $B=0.1$.

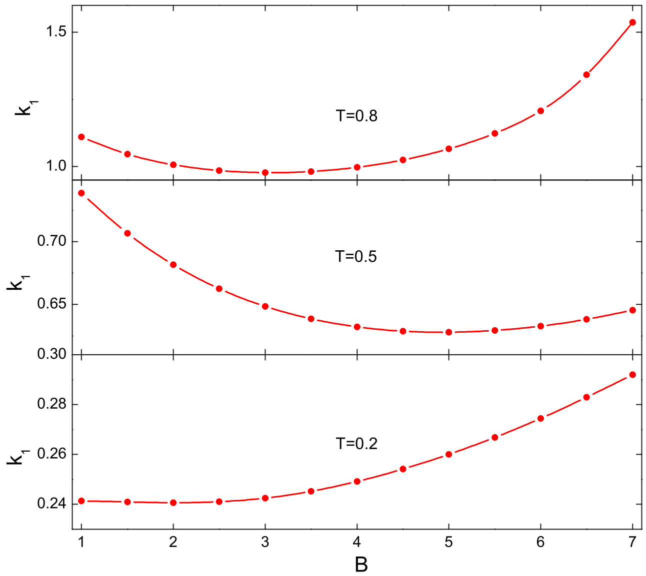

FIG. 3. (Color online) The field dependence of the cutoff parameter k_1 for s-wave superconductors with $\kappa = 10$ and $T = 0.2$, 0.5, and 0.8 from fitting to the solution of the Eilenberger equations.

At high temperatures $T>0.5$ the tendency of the dependence of B_{min} on T is in agreement with prediction of the local Hao-Clem theory[3] because the nonlocal effects are not important. Then the Abrikosov solution for FLL can be used which gives a minimum in the $k_1(B)$ dependence.[31] In low magnetic fields the solution of the Ginzburg-Landau theory[4] gives the value of $k_1 \approx 3/2$ which is also clearly visible from our results in the inset to Fig. 2 at the limit of $T \to T_c$. The decreasing of B_{min} with increasing temperature, as shown in Fig. 4 at $T>0.5$, is similar to the behavior predicted by the Ginzburg-Landau theory[3] although the applicability of this theory is limited to temperatures near T_c resulting in some quantitative deviation from our calculation. The behavior $k_1(B,T)$ at high temperatures (called the GL regime in Fig. 4)

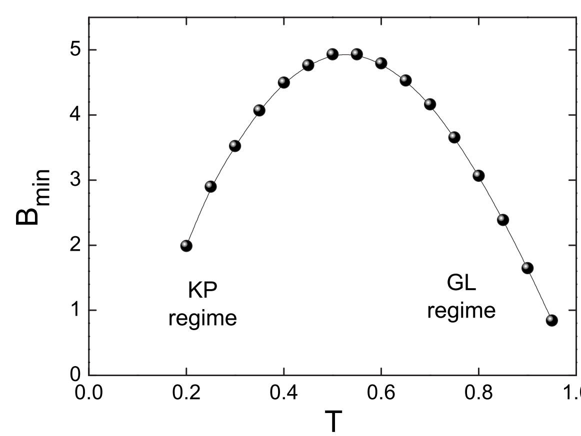

FIG. 4. The temperature dependance of the magnetic field B_{min} at which the cutoff parameter k_1 has the minimum in s-wave superconductors.

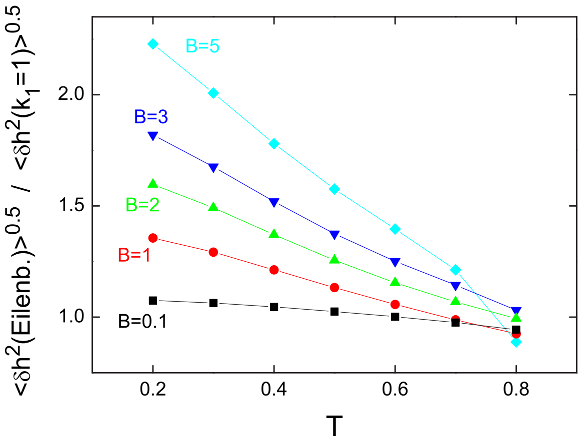

FIG. 5. (Color online) Temperature dependence of the ratio of the second moment of the magnetic field distributions obtained from the solution of the Eilenberger equations to that of the NGLE model with the parameter $k_1=1$.

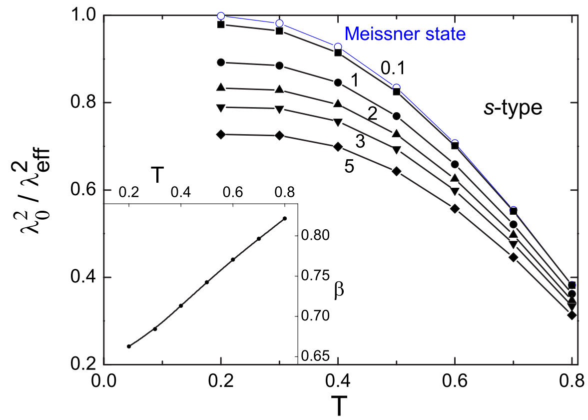

FIG. 6. (Color online) Temperature dependence of the ratio $\lambda_0^2/\lambda_{\text{eff}}^2$ calculated for $B=0-5$. The upmost curve with the open circles shows the values in the Meissner state. The inset shows the coefficient $\beta(T)$ in the field dependence of $\Delta\lambda_{\text{eff}}$.

can be explained by decreasing of B_{c2} and the corresponding increasing of the B/B_{c2} ratio. Therefore, the effect (iii) above prevails the effects (i) and (ii) in smaller fields.

As shown in Fig. 4 the $B_{\min}(T)$ dependence has a maximum at the temperature $T_{\max}\approx 0.5$. The $k_1(B,T)$ dependences at $T<T_{\max}$ resemble the behavior of $\xi_{\text{eff}}(B,T)$ found by solving the Eilenberger equations for dirty superconductors.[33] According to the results in Ref. 33 the value of $B_{\min}$ decreases strongly with increasing of the electron mean-free path l_0. The same effect can be obtained by decreasing the temperature. As can be seen from Fig. 7 in Ref. 33 the position of $B_{\min}$ increases with decreasing of the mean free path l when $0<\xi_0/l\leq 0.5$. This corresponds to the behavior of $k_1(B,T)$ in the KP regime $0<T<0.5$. Because $\xi_{\text{eff}}(B,T)$ is determined by the order parameter behavior in the vortex center it depends strongly on the KP effect at low temperatures (iii). This effect has an opposite influence to the slope of the field dependence $k_1(B)$ than those in (i) and (ii), resulting in appearance of the minimum in $\xi_{\text{eff}}(B)$ and $k_1(B)$. Decreasing of the value of $B_{\min}$ with decreasing temperature at $T<T_{\max}$ is similar to the behavior of $\xi_{\text{eff}}(B,T)$ and can also be explained by the KP effect. We call this regime the KP regime (see Fig. 4).

To show the influence of the magnetic field and temperature dependence of k_1 we calculate the values of $\langle\delta h^2\rangle$ using the field distribution obtained in the NGLE model. Figure 5 shows the temperature dependence of the ratio of $\langle\delta h^2\rangle$ obtained from the solution of the Eilenberger equations to that of the NGLE model with the fixed parameter $k_1=1$. As one can find from the data presented in Fig. 5, this ratio deviates considerably from unity when the temperature is lowered.

III. EFFECTIVE LOCAL PENETRATION DEPTH

A local effective London equation (LELE) with field dependent penetration depth is often used for analysis of the experimental data (μSR, SANS, magnetization, etc.).[13–20] The way of reducing NGLE to LELE was suggested in Refs. 10 and 12:

$$\frac{\lambda_{\text{eff}}}{\lambda}=\left(\frac{\overline{\Delta B_0^2}}{\overline{\Delta B^2}}\right)^{1/4}. \tag{9}$$

Here $\overline{\Delta B_0^2}$ is the mean squared value of the magnetic field $B_0(\mathbf{r})-B_{\text{av}}$ obtained by applying the ordinary London model with the same average field B_{av} and λ. However, the cutoff function was not determined[10,12] which is important for quantitative interpretation of the results.[10,24] We use the proper shape of the cutoff function obtained from the Eilenberger equation in the previous section. The values of λ_{eff} defined in this way are determined by a large scale of the order of the FLL period and is not very sensitive to details of the microscopical core structure and the cutoff parameter.[25]

In Fig. 6 are shown the temperature dependences of $\lambda_0^2/\lambda_{\text{eff}}^2$. The low-field result ($B=0.1$) for λ_{eff} is close to $\lambda(T)$ in the Meissner state.

μSR measurements of λ in different s-wave low-temperature superconductors often show some magnetic field dependence. To demonstrate this for $\lambda_{\text{eff}}(T,B)$ we use an expression $\Delta\lambda_{\text{eff}}=[\lambda_{\text{eff}}(T,B)-\lambda(T,0)]\propto B^{\beta(T)}$, where the values of $\lambda_{\text{eff}}(T,0)$ in zero field are obtained from the BCS theory in the Meissner state. A similar phenomenological expression is often used for fitting experimental results concerning the vortex state.[14,17] Temperature dependence of the exponent $\beta(T)$ is shown in the inset to Fig. 6.

In Fig. 7 the experimental data of the magnetic penetration depth λ obtained for s-wave superconductors V_3Si and $NbSe_2$ are shown.[13] These materials have an anisotropy different from that used in our calculations, V_3Si possesses a simple cubic crystal structure and $NbSe_2$ is an anisotropic two-band superconductor. Nevertheless, these compounds demonstrate clear sublinear field dependence of λ which is quite different from prediction of the mixed state model of a rigid vortex core.[30,34] Similar effects were observed in the field dependences of the quasiparticle DOS (Ref. 34) and specific heat.[35] Our calculations also predict sublinear $\lambda(B,T)$ dependence with power coefficient β shown in the

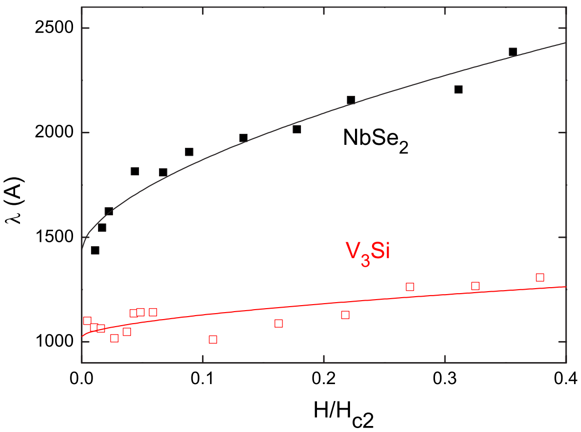

FIG. 7. (Color online) The magnetic field dependence of λ derived from μSR measurements (Ref. 13) for the s-wave superconductors V_3Si (T=0.2) and $NbSe_2$ (T=0.33). The solid lines are fits to $\Delta\lambda_{eff} \propto B^{\beta(T)}$ with β obtained from the inset to Fig. 6.

inset to Fig. 6. As can be seen from Fig. 7 low temperature extrapolation of β to 0.6 (see inset to Fig. 6) describes the shape of the experimental field dependence of λ. The coefficient of proportionality of $\Delta\lambda_{eff}$ is determined by the band structure and is out of scope of our model.

IV. CONCLUSION

To conclude, we have solved numerically the quasiclassical Eilenberger equations in the mixed state of s-wave superconductors by parametrizing them with nonlinear Riccati equations. The obtained magnetic field distribution within the vortex core is fitted by the solution of the NGLE. It is found that the field dependence of k_1 is nonmonotonous and shows a minimum at a field B_{min} which depends on temperature. At high temperatures the behavior of $B_{min}(T)$ agrees with the prediction of the Hao-Clem theory.[3] At low temperatures the Kramer-Pesch effect is important resulting in appearance of a maximum in the $B_{min}(T)$ dependence. We reduce the NGLE model to effective LELE model and calculate $\lambda_{eff}(B,T)$ predicting the sublinear field dependence of λ_{eff}. The obtained dependences $k_1(B,T)$ and $\lambda_{eff}(B,T)$ are quite different from the predictions of a rigid core model. Our results agree with experimental μSR results for the penetration depth of the magnetic field in the s-wave superconductors V_3Si and $NbSe_2$.[13]

ACKNOWLEDGMENTS

This work was supported by the Wihuri Foundation, Finland. Discussions with Professor J. Sonier are acknowledged.

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