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# Magnetic moment of single vortices in YBCO nano-superconducting particle: Eilenberger approach

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**Abstract.** Temperature dependence of single vortex magnetic moment in nanosize superconducting particles is investigated in the framework of quasiclassical Eilenberger approach. Such nanoparticles can be used for preparation of high-quality superconducting thin films with high critical current density. In contrast to bulk materials where the vortex magnetic moment is totally determined by flux quantum, in nano-sized specimens (with characteristic size, $D$, much less than effective penetration depth, $\lambda_{eff}$) the quantization rule is violated and magnetic moment is proportional to $D^2/\lambda_{eff}^2(T)$. Due to strong repulsion between vortices in nanoparticles only a single vortex can be trapped in them. Because of small size of particles the screening current of the vortex is located near the vortex core where the current is quite high and comparable to depairing currents. Therefore, the superconducting electron density, $n_s$, depends on the current value and the distance from the vortex core. This effect is especially important for superconductors having gap nodes, such as YBCO.

The current dependence of $n_s$ in nanoparticles is analogous to the Volovik effect in flux-line lattice in bulk samples. The magnitude of the effect can be obtained by comparing the temperature dependence of magnetic moment in the vortex and in the Meissner states. In the last case the value of screening current is small and superconducting response to the external field is determined by London penetration depth. Because of importance of nonlinear and nonlocal effects, the quantum mechanical Eilenberger approach is applied for description of the vortex in nanoparticles. The flattening of $1/\lambda_{eff}^2(T)$ dependence has been found. A comparison of the theoretical results with experimental magnetization data in Meissner and mixed states of YBCO nanopowders has been done. The presence of nonlinear and nonlocal effects in vortex current distribution is clearly visible. The obtained results are important for the description of pining in nanostructured high-$T_c$ thin films.

## 1. Introduction

Quasiclassical calculation of the density of states of a single vortex in an anisotropic superconductor was performed in Ref. [1], and it was shown that if the gap itself is not highly anisotropic, the Fermi surface anisotropy dominates, preventing direct observation of superconducting gap features. This serves as a cautionary message for the analysis of scanning tunneling spectroscopy data on the vortex state on Fe-based superconductors, in particular LiFeAs, which was treated explicitly. It was found that Doppler shift (DS) on quasiparticle excitations on extended states (so-called "Volovik effect" [2]) immediately induce zero energy

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excitations proportional to $H$ from a smaller gap band in $s^{\pm}$ symmetry [3]. The structure of a single vortex in a FeAs superconductor was studied in Ref. [4] in the framework of two formulations of superconductivity for the recently proposed sign-reversed $s$-wave ($s^{\pm}$) scenario: (i) a continuum model taking into account the existence of an electron and a hole band, with a repulsive local interaction between the two; (ii) a lattice tight-binding model with two orbitals per unit cell and a next-nearest-neighbour attractive interaction. An impurity located outside the vortex core has little effect on the local density of states peak, but an impurity close to the vortex core can almost suppress it and modify its position. In Ref. [5] a linear regime at higher fields and a limiting square root $H$ behavior at very low fields were found. The crossover from a Volovik-like $\sqrt{H}$ to a linear field dependence can be understood from a multiband calculation in the quasiclassical approximation assuming gaps with different momentum dependence on the hole- and electron-like Fermi surface sheets.

In a direct scanning tunneling spectroscopy experiment the problem of the quantum vortex phases in strongly confined superconductors was addressed [6]. The strong confinement regime is achieved in grown ultrathin single nanocrystals of Pb by tuning their lateral size (diameter $\approx 140$ nm and height $\approx 2.8$ nm) to a few coherence lengths. Cren *et. al.* [6] used the phenomenological Ginzburg-Landau theory for explanation of obtained results. However, the aim of our paper is to apply microscopical Eilenberger approach to high-$T_c$ nanoparticles. The asymptotical behaviour of the amplitude and the phase of the pairing potential is obtained. The Eilenberger equations can be obtained from a full quantum mechanical approach (the Bogoliubov-de Gennes equations) using an expansion in terms of $\alpha^{-1}$, where $\alpha = v_F/v_\Delta$ is the Dirac cone anisotropy, $v_F$ is the Fermi velocity, and $v_\Delta$ is the quasiparticle velocity tangential to the Fermi surface at the node. This expansion is quite reasonable for the description of high-$T_c$ superconductors, where $\alpha = 14$ for YBaCuO and 20 for BiSrCaCuO [7]. The Eilenberger equations have been solved previously [8] in the vortex core region. Here, we find the behaviour of the amplitude and the phase of the pairing potential $\Delta(r)$ at long distances $r$ from the vortex core. It is found that the DS method works reasonably well at distances $r \geq \xi_0$ at low temperatures. The nonlocal effects are important inside the core and for the description of effects of the fourfold vortex symmetry outside the core. It is also shown that at higher temperatures the DS method should be modified by including a pairing potential $\Delta(r)$ calculated self-consistently.

## 2. Quasiclassical approach

We consider an isolated two-dimensional vortex in a d-wave superconductor. The center of the vortex is taken as the origin. The Fermi surface is assumed to be isotropic and cylindrical. To obtain the quasiclassical Green functions we solve the quasiclassical Eilenberger equations for the pairing potential $\Delta(\theta, r) = \bar{\Delta}(r)\cos(2\theta)\exp(i\phi)$ [8,9], where $\theta$ is the angle between the $\mathbf{k}$ vector and the $a$ axis (or $x$ axis) and $\exp(i\phi) = (x+iy)/r$. It should be noted here that the spatial variation of the supercurrent and the $d$-wave order parameter induce small subdominant $s$ and $d_{xy}$ components in the pairing order parameter [10]. We are not considering these effects because they can be included in a straightforward way in our calculations. Throughout this paper, the energies and the lengths are measured in units of the uniform gap $\Delta_0$ at $T=0$ and the coherence length $\xi_0 = v_F/\Delta_0$, respectively.

For calculation it is convenient to parametrize the quasiclassical Green function via [9]

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

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 Ricatti equations

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

$$\partial_\parallel \bar{b}(\omega_n, \theta, \mathbf{r}) \;=\; -\bar{\Delta}(\theta, \mathbf{r}) + \{2\omega_n + i\partial_\parallel \phi + \bar{\Delta}(\theta, \mathbf{r})\bar{b}(\omega_n, \theta, \mathbf{r})\}\bar{b}(\omega_n, \theta, \mathbf{r}), \tag{3}$$

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 $\mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}}$ is denoted as $\mathbf{r} = r_\parallel\hat{\mathbf{u}} + r_\perp\hat{\mathbf{v}}$. Eqs. (2) and (3) 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 $\partial_\parallel \phi$). Since we consider an isolated vortex in extreme type-II superconductors, the vector potential in Eqs. (2) and (3) can be neglected.

As has been shown [11] the solution of Eqs. (2) and (3) is quite stable: after integration over a length of a few $\xi_0$ it becomes almost independent of the initial values. This solution corresponds to a simple exponential relaxation of the functions $\bar{a}$ and $\bar{b}$ to their local "steady-state" values defined by the local values of the order parameter. Therefore, to find $\bar{\Delta}$ at a given point, one does not need the values of $\bar{\Delta}$ at distances larger than several $\xi_0$ along the trajectory. This peculiarity is used for integration of Eqs. (2) and (3) at long distances. First, we find some approximative solution at the distance of several $\xi_0$ from a given point and consider it as the boundary condition. Next, we make the integration up to the given point by the Runge-Kutta method with a variable step. To find this approximative boundary condition a linear expansion $\bar{a} = a_0 + a_1 r_\parallel$, $\bar{b} = b_0 + b_1 r_\parallel$, and $\bar{\Delta} = \Delta_0 + \Delta_1 r_\parallel$ is used near the given point. Substituting this expansion to Eqs. (2) and (3) and equating the coefficients under the same power of $r_\parallel$ we obtain the set of equations for $a_0$, $a_1$, $b_0$ and $b_1$.

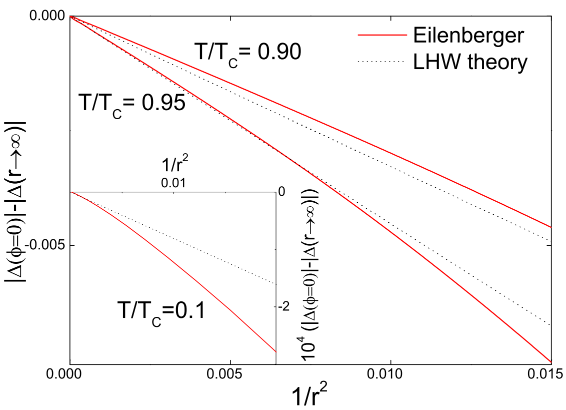


**Figure 1.** Asymptotical behaviour of the amplitude of the pairing potential $|\Delta|$ at long distances for $\phi = 0$ and $T/T_c = 0.9, 0.95$ and at $T/T_c = 0.1$ (solid lines). The dotted lines in the main panel and the inset show the values $|\Delta(T,r)| - |\Delta(T)|$ obtained from Eq. (4) at $T/T_c = 0.9$ and 0.95 and from Eq. (5) at $T/T_c = 0.1$, respectively.

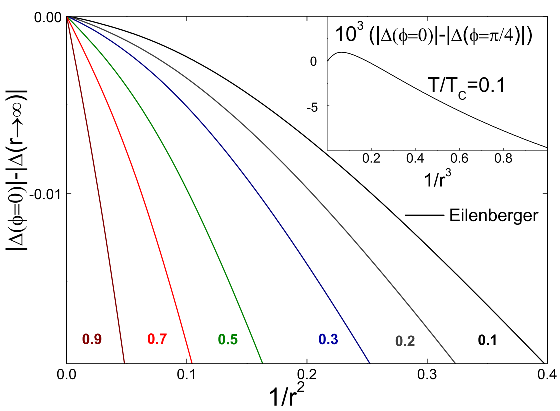


**Figure 2.** Behaviour of the amplitude of the pairing potential at intermediate distances for $\phi = 0$ and six values of $T/T_c$ between $0.1 - 0.9$. The inset depicts the asymptotical behaviour of the difference of the amplitude along 0 and $\pi/4$ directions, $|\Delta(\phi = 0)| - |\Delta(\phi = \pi/4)|$ at $T/T_c = 0.1$.

Figure 1 shows the asymptotical behaviour of the amplitude of the pairing potential at long distances for $\phi = 0$, $T/T_c = 0.9, 0.95$ in the main panel and $T/T_c = 0.1$ in the inset (solid lines), obtained using Eilenberger approach. As can be seen from this figure $|\Delta|$ relaxes to its bulk value ($r \to \infty$) as $1/r^2$ with the power of $r$ being independent of the temperature. The same law of the relaxation has been obtained in the numerical solution of the Bogoliubov-de Gennes equations [12] at $T = 0$ K. This relaxation law is different from the law [8], $|\Delta(r)| \propto \tanh(r)$.

The analytical expansion of the BCS solution near the infinity point has been obtained perturbatively by Li, Hirschfeld and Wölfle (LHW theory) [10]. In Ginsburg-Landau regime near $T_c$ they found

$$|\,\Delta(T,r)\,| - |\,\Delta(T)\,| = -\frac{1}{3/4 + \epsilon_F m v_s^2(\mathbf{r})/\Delta^2(T)} \frac{\epsilon_F m v_s^2(\mathbf{r})}{\Delta^2(T)}, \tag{4}$$

where $\epsilon_F$ is the Fermi energy and $\mathbf{v_s}(\mathbf{r})$ is the superconducting electron velocity. At low temperatures and long distances $mv_s v_F \ll T \ll \Delta(T)$ the solution [10] is

$$|\,\Delta(T,r)\,| \quad - \quad |\,\Delta(T)\,| = -\frac{2\ln 2}{1 - [9\zeta(3)T^3 - 4\ln 2\epsilon_F T m v_s^2(\mathbf{r}]/\Delta^3(T)} \times \frac{\epsilon_F m v_s^2(\mathbf{r})}{\Delta^2(T)} \frac{T}{\Delta(T)}, \tag{5}$$

where $\zeta(3)$ is the Riemann function. The dotted lines in the main panel and the inset of Fig. 1 shows the values $|\,\Delta(T,r)\,| - |\,\Delta(T)\,|$ obtained from Eq. (4) at $T/T_c = 0.9$ and 0.95 and from Eq. (5) at $T/T_c = 0.1$, respectively. As can be seen from this figure the slopes of asymptotics in LHW theory agrees well with those obtained numerically by us (solid lines).

Figure 2 shows the behaviour of the amplitude of the pairing potential at intermediate distances for $\phi = 0$ and six values of $T/T_c$ between $0.1 - 0.9$. The behaviour of $|\,\Delta(\phi = 0)\,| - |\,\Delta(\phi = \pi/4)\,|$ at $T/T_c = 0.1$ and the change of the sign of this quantity is clearly visible in the inset to Fig. 2.

## 3. Conclusions

The quasiclassical Eilenberger equations are solved numerically for an isolated two-dimensional vortex for high-$T_c$ nanoparticles. In the core area our results reproduce those obtained previously [8]. New asymptotical behaviour of the amplitude is obtained. Taking into account the suppression of the pairing potential as in the self-consistent Doppler-shift method, good agreement with the exact calculation is observed over the whole range of the radius. The temperature dependencies of the magnetic moment for superconducting YBaCuO nanoparticles was investigated (i) in the Meissner state and (ii) when the magnetic flux is trapped in the particles. It was found that the ratio $\lambda_{ab}^2(0)/\lambda_{ab}^2(T)$ obeys the power law behaviour with the exponent $n = 2.0 \pm 0.2$ and $n = 2.5 \pm 0.05$ in these two cases, respectively [13]. We connect this behaviour with Volovik effect in nanoparticles.

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