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# Effect of Born and unitary impurity scattering on the Kramer–Pesch shrinkage of a vortex core in an *s*-wave superconductor

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#### ABSTRACT

We theoretically investigate a non-magnetic impurity effect on the temperature dependence of the vortex core shrinkage (Kramer–Pesch effect) in a single-band *s*-wave superconductor. The Born limit and the unitary limit scattering are compared within the framework of the quasiclassical theory of superconductivity. We find that the impurity effect inside a vortex core in the unitary limit is weaker than in the Born one when a system is in the moderately clean regime, which results in a stronger core shrinkage in the unitary limit than in the Born one.

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#### 1. Introduction

The radius of a vortex core in type-II superconductors is one of the fundamental physical quantities which characterize a property of superconductivity. The temperature and magnetic field dependence of the core radius has been investigated theoretically and experimentally [1–19]. The low-temperature vortex core shrinkage, called the Kramer–Pesch (KP) effect [1], was theoretically investigated under the influence of non-magnetic impurities in the Born limit previously [2]. Impurity effects are characterized by the scattering phase shift related to the impurity potential strength [20–23]. The Born limit corresponds to the limit of weak impurity potential and correspondingly small phase shift. The opposite limit is called the unitary limit, where the impurity potential is infinitely strong and the phase shift is  $\pi/2$ . The difference between these limits plays an important role in, for example, unconventional superconductors [20–22].

In this paper, we theoretically study the KP effect both in the Born and the unitary limit in an *s*-wave superconductor, and compare their results. It is found that the temperature dependence of the core shrinkage is stronger in the unitary limit than in the Born one, in the moderately clean regime where the mean free path is of the order of or larger than the coherence length. Such a difference

\* Corresponding author at: NanoSquare Research Center (N2RC), Osaka Prefecture University, C10 Bldg., 1-2 Gakuen-cho, Naka-ku, Sakai 599-8570, Japan. Tel./ fax: +81 72 254 8203. of the core shrinkage can be investigated experimentally by, e.g., muon spin rotation [3,5,6], scanning tunneling microscopy [24], resistivity [4], and specific heat [11,25] if there is a suitable superconducting material in which different types and densities of impurities can be doped.

#### 2. Formulation

We consider a single vortex in a single-band *s*-wave superconductor. The system is assumed to be an isotropic two-dimensional conduction layer perpendicular to the vorticity along the *z*-axis. In a circular coordinate system within the layer, the real-space position is  $\mathbf{r} = (r\cos \phi, r\sin \phi)$ . The unit vector  $\mathbf{\bar{k}}$  represents the sense of the wave number on a Fermi surface assumed to be circular. The Fermi velocity is  $\mathbf{v}_{\rm F} = v_{\rm F}\mathbf{\bar{k}}$ . The pair potential around the vortex is  $\Delta(\mathbf{r}) = \Delta(r, \phi) = |\Delta(r)| \exp(i\phi)$ . We will consider the temperature *T* dependence of the length  $\xi_1$  that characterizes the vortex core radius [1–3],

$$\frac{1}{\xi_1} = \frac{1}{\varDelta(r \to \infty)} \lim_{r \to 0} \frac{\varDelta(r)}{r}.$$
(1)

This quantity is depicted in Fig. 1. Note that  $\xi_1$  is related to the pair potential slope at the vortex center and scales with the distance at which the vortex current reaches its maximum value [1,3,6,11], while  $|\Delta(r)|$  is restored at a distance of the order of the coherence length ( $\gg \xi_1$  in the clean limit) even at low temperatures [11,26].



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**Fig. 1.** Schematic figure of the pair potential as a function of the distance from the vortex center. It depicts the length  $\xi_1$  that characterizes the vortex core radius [see Eq. (1)].

To obtain  $\xi_1(T)$ , the vortex core structure is calculated by means of the quasiclassical theory of superconductivity as in Ref. [2]. The Eilenberger equation is numerically solved to obtain the quasiclassical Green's function  $\hat{g}(i\omega_n, \mathbf{r}, \mathbf{k})$ . The effect of impurities distributed randomly in the system is taken into account through the impurity self energy  $\hat{\Sigma}(i\omega_n, \mathbf{r}, \mathbf{k})$ . The quasiclassical Green's function, the impurity self energy, and the Eilenberger equation to be solved are, respectively, given as [2,27–31]

$$\hat{g} = -i\pi \begin{pmatrix} g & if \\ -if^{\dagger} & -g \end{pmatrix}, \quad \hat{\Sigma} = \begin{pmatrix} \Sigma_{d} & \Sigma_{12} \\ \Sigma_{21} & -\Sigma_{d} \end{pmatrix},$$
 (2)

$$i\boldsymbol{v}_{\mathrm{F}}\cdot\boldsymbol{\nabla}\hat{\mathbf{g}}+[i\tilde{\omega}_{n}\hat{\tau}_{3}-\widetilde{\widetilde{\Delta}},\hat{\mathbf{g}}]=\mathbf{0}. \tag{3}$$

The equation is supplemented by the normalization condition  $\hat{g}^2 = -\pi^2 \hat{\tau}_0$  [29,32]. Here,  $\hat{\tau}_3$  is the *z* component of the Pauli matrix,  $\hat{\tau}_0$  is the unit matrix, and the brackets denote the commutator  $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ . The Eilenberger equation contains the renormalized Matsubara frequency (pair potential)  $\tilde{\omega}_n$  ( $\hat{A}$ ) defined by

$$i\tilde{\omega}_n = i\omega_n - \Sigma_d,\tag{4}$$

$$\widehat{\widetilde{\Delta}} = \begin{pmatrix} \mathbf{0} & \widetilde{\Delta} \\ -\widetilde{\Delta}^* & \mathbf{0} \end{pmatrix} = \begin{pmatrix} \mathbf{0} & \Delta + \Sigma_{12} \\ -(\Delta^* - \Sigma_{21}) & \mathbf{0} \end{pmatrix}.$$
 (5)

We consider an isolated single vortex in an extreme type-II superconductor (Ginzburg–Landau parameter  $\kappa \gg 1$ ), and therefore the vector potential is neglected in Eq. (3). Throughout the paper, we use units in which  $\hbar = k_B = 1$ .

The Eilenberger equation (3) can be solved by the Riccati parametrization [33–35]. The quasiclassical Green's function is expressed as

$$\hat{g} = -i\pi \frac{\operatorname{sgn}(\omega_n)}{1+ab} \begin{pmatrix} 1-ab & i2a \\ -i2b & -(1-ab) \end{pmatrix}.$$
(6)

Here,  $sgn(\omega_n)$  is the signum (or sign) function. The two quantities  $a(i\omega_n, \mathbf{r}, \mathbf{\bar{k}})$  and  $b(i\omega_n, \mathbf{r}, \mathbf{\bar{k}})$  are independently determined by solving the Riccati equations,

$$\boldsymbol{v}_{\mathrm{F}} \cdot \boldsymbol{\nabla} \boldsymbol{a} + (2\tilde{\omega}_n + \tilde{\varDelta}^* \boldsymbol{a})\boldsymbol{a} - \tilde{\varDelta} = \boldsymbol{0},\tag{7}$$

$$\boldsymbol{v}_{\mathrm{F}} \cdot \boldsymbol{\nabla} b - (2\tilde{\omega}_n + \Delta b)b + \Delta^* = 0. \tag{8}$$

These differential equations are solved along a straight line parallel to  $v_F$  [33,36,37] by using the bulk solutions as initial values [33,38],

$$a_{-\infty} = \frac{-\tilde{\omega}_n + \sqrt{\tilde{\omega}_n^2 + |\tilde{\Delta}|^2}}{\tilde{\Delta}^*} \quad (\omega_n > 0),$$
(9)

$$b_{+\infty} = \frac{-\tilde{\omega}_n + \sqrt{\tilde{\omega}_n^2 + |\tilde{\Delta}|^2}}{\tilde{\Delta}} \quad (\omega_n > 0), \tag{10}$$

and

0

$$u_{+\infty} = \frac{-1}{b_{+\infty}} = \frac{-\tilde{\omega}_n - \sqrt{\tilde{\omega}_n^2 + |\tilde{\Delta}|^2}}{\tilde{\Delta}^*} \quad (\omega_n < \mathbf{0}),$$
(11)

$$b_{-\infty} = \frac{-1}{a_{-\infty}} = \frac{-\tilde{\omega}_n - \sqrt{\tilde{\omega}_n^2 + |\tilde{\Delta}|^2}}{\tilde{\Delta}} \quad (\omega_n < \mathbf{0}).$$
(12)

A stable numerical solution for a(b) is obtained by solving the Riccati equation in forward (backward) direction along the straight line for  $\omega_n > 0$  [33,39]. By contrast, the equation for a(b) is solved in backward (forward) direction for  $\omega_n < 0$ .

Considering an *s*-wave non-magnetic impurity scattering and the *t*-matrix,  $\hat{\Sigma}$  is given by [2,27,40]

$$\widehat{\Sigma}(i\omega_n, \mathbf{r}) = \frac{\Gamma_n}{1 - (\sin^2 \delta_0)(1 - C)} \begin{pmatrix} -i\langle g \rangle & \langle f \rangle \\ -\langle f^{\dagger} \rangle & i\langle g \rangle \end{pmatrix},$$
(13)

where  $C = \langle g \rangle^2 + \langle f \rangle \langle f^{\dagger} \rangle$  with  $\langle \cdots \rangle$  being the average over the Fermi surface with respect to  $\bar{k}$ . The impurity scattering rate in the normal state is  $\Gamma_n$ , which is related to the mean free path  $l = v_F/2\Gamma_n$ . The scattering phase shift is  $\delta_0$ . We set  $\delta_0 = 0$  in the Born limit (keeping  $\Gamma_n$  finite) and  $\delta_0 = \pi/2$  in the unitary limit.

The self-consistency equation for  $\varDelta$ , called the gap equation, is given as

$$\Delta(\mathbf{r}) = \lambda \pi T \sum_{-\omega_{\rm c} < \omega_{\rm n} < \omega_{\rm c}} \langle f(i\omega_{\rm n}, \mathbf{r}, \bar{\mathbf{k}}) \rangle, \tag{14}$$

where  $\omega_c$  is the cutoff energy and the coupling constant  $\lambda$  is given by

$$\frac{1}{\lambda} = \ln\left(\frac{T}{T_c}\right) + \sum_{0 \le n < (\omega_c/\pi T - 1)/2} \frac{2}{2n+1}.$$
(15)

Here,  $T_c$  is the superconducting critical temperature. We set  $\omega_c = 10\Delta_0$  with  $\Delta_0$  being the BCS pair-potential amplitude at zero temperature.

The Eilenberger (Riccati) equation, the impurity self energy, and the gap equation are numerically solved self-consistently. The used boundary conditions for the pair potential and impurity self energy far from the vortex are the same as those discussed in Ref. [2]. See the Appendix A for more details on the calculation procedure. In the next section, we will show results obtained from self-consistent solutions. We define the zero-temperature coherence length  $\xi_0 = v_F / \Delta_0$ .



**Fig. 2.** Spatial profiles of the pair potential amplitude  $|\Delta(r)|$  around the vortex under the influence of impurity scattering in the unitary limit. The horizontal axis *r* is the distance from the vortex center. The scattering rate is  $\Gamma_n/\Delta_0 = 0.1$  (solid lines) and  $\Gamma_n/\Delta_0 = 1$  (dashed lines). For each scattering rate, the temperature is *T*/ $T_c = 0.1 - 0.7$  from top to bottom by 0.2 step.

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