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Comparison of several methods for determining the critical temperature of a superconducting transition in ferromagnet/superconductor heterostructures

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Two methods for calculating the superconducting transition critical temperature of superconductor / ferromagnetic metal heterostructures in the dirty limit are compared. The first method relies on an approximation where the order parameter is assumed to be constant within each superconducting layer. The second method does not use any approximations and involves a numerical iterative process where the critical temperature and the order parameter distribution are jointly searched for in each iteration. Using these methods, we study various heterostructures involving a ferromagnetic and superconducting layers, including case where the ferromagnetic layer is split into domains.

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Dedicated to Professor Boris I. Kochelaev Mentor, Teacher and Friend, on the occasion of his 90th birthday

1. Introduction

Layered structures containing superconducting (S) and ferromagnetic (F) materials allows to observe a wide range of interesting and important phenomena associated with the coexistence of these two types of ordering in the conduction electron subsystem. Compared to conventional magnetic superconductors, these layered S/F structures are not limited to a specific class of compounds, allowing a variety of superconducting and ferromagnetic metals to be used into systems with desired properties for practical applications. The exchange interaction between localized and collectivized electrons leads to the phase rotation of the anomalous Green's function, which describes the state of superconducting electrons penetrating into ferromagnetic layer [1]. This interaction can cause non-linear behavior of the critical temperature and critical Josephson current as the thickness of the ferromagnetic layer is changed [1–3]. These systems can also be used as spin-switch devices. In systems such as F/F/S [4], F/S/F [5,6] and systems with a larger number of layers [7–11], the critical temperature of the system can change depending on the relative orientation of the magnetization of the individual ferromagnetic layers. In systems with two superconducting layers separated by a ferromagnetic layer, the relative phase difference $\Delta\phi$ between the superconducting order parameters may be different from zero. Within a certain range of ferromagnetic layer thicknesses, the phase difference is equal to π [12, 13] and these systems are known as a π junctions.

The contact between a superconductor and an inhomogeneous ferromagnet can significantly expand the range of observable phenomena. The presence of an inhomogeneous magnetization leads to the emergence of triplet correlations, which can be observed through the long-range proximity effect [14]. This effect manifests itself in the deep penetration of triplet pairs into the ferromagnetic metal, and can be traced by the dependence of the Josephson current on the thickness of the ferromagnetic barrier. When a superconductor comes into contact with a ferromagnet split into domains, a significant increase in the intensity of superconducting correlations near domain boundaries occurs. This leads to a local increase in the critical temperature [8,15–17] and critical Josephson current [18]. Another interesting scenario is the contact between a superconductor and a chiral ferromagnet. In particular, the bound state between the skyrmion and the Abrikosov vortex is of great interest to researchers [19,20].

To calculate the superconducting critical temperature in heterostructures, the most convenient and widely used methods are based on solving quasi-classical superconducting equations. Within this framework, a boundary-value problem is formulated and supplemented with self-consistency equation. Despite the fact that the Usadel and Eulenberger equations can be linearized near the critical temperature, the task becomes difficult for complex magnetization configurations in a ferromagnetic layer. To solve the Usadel equations, two types of methods can be identified: approximate methods such as the single-mode approximation [3] and the approximation of a constant order parameter within each layer [21,22], and exact methods such as the multimode method and fundamental solution method [23]. The latter method and its slight modifications have been used in numerous works [1,2,24]. However, they require the existence of an analytic solution to the Usadel equations for a ferromagnetic layer.

This study compares the approximation of a constant order parameter within each layer [21, 22] (we will call it below "Step order parameter method") with the recent iterative numerical method [17]. The accuracy of the latter method does not differ from the fundamental solution method. The advantage of this method lies in its applicability to a wider range of complex systems. We will briefly describe both methods and compare the calculated critical temperature in various ways and order parameter distribution for some superconductor / ferromagnetic heterostructures.

2. Model

In this paper, we consider the layers of a superconductor and a ferromagnet in the dirty limit. This means the coherence length in a superconductor and ferromagnet $\xi_{s(f)}$ is significantly greater than the corresponding free path lengths $l_{s(f)}$ [1,3]. This ratio of parameters is typical for most experimental systems [1,12,25]. In this case we can use the Usadel equations for S and F layers [3] to describe proximity effect in layered system. The field generated by a ferromagnetic layer plays an important role in certain cases [26]. For very thin ferromagnetic films, it is relatively weak and, according to most researchers (see, e.g., work [27] or reviews [1–3]), the critical temperature in the case of good metal contact is affected mainly by the penetration of Cooper pairs into the ferromagnet. We will neglect such fields in this work. The Usadel equations for a ferromagnetic layer with arbitrary magnetization can be written as [28,29]:

$$\frac{D_f}{2}\hat{\nabla}^2\hat{F}_f(\mathbf{r},\omega) - |\omega|\hat{F}_f(\mathbf{r},\omega) - \frac{i}{2}\operatorname{sgn}\omega\left\{(\mathbf{I}\cdot\hat{\boldsymbol{\sigma}}),\hat{F}_f(\mathbf{r},\omega)\right\} = 0, \tag{1}$$

where ω is the Matsubara frequency, $\mathbf{I}$ is the vector of the effective exchange field, $\hat{F}_f(\mathbf{r},\omega)$ and D_f are Usadel matrix functions [28,30] and the diffusion coefficient in ferromagnetic layer, respectively. $\hat{\boldsymbol{\sigma}}$ is a vector composed of Pauli matrices. Here and further, for simplicity, it is assumed that $k_\mathrm{B} = \mu_\mathrm{B} = \hbar = 1$, where k_B is the Boltzmann constant, μ_B is the Bohr magneton. In the superconducting layer, the Usadel equations have the form

$$\frac{D_s}{2}\hat{\nabla}^2\hat{F}_s(\mathbf{r},\omega) - |\omega|\hat{F}_s(\mathbf{r},\omega) = -\Delta(\mathbf{r}), \tag{2}$$

$\Delta(\mathbf{r})$ is the superconducting order parameter, $\hat{F}_s(\mathbf{r},\omega)$ and D_s are the Usadel matrix function and the diffusion coefficient in the superconducting layer, respectively. In this paper, we will consider systems without a supercurrent, and we also do not take into account the existence of electron-electron interaction in the ferromagnetic layer [31]. The boundary conditions at the external boundaries correspond to a lack of Cooper pair flow through them

$$\frac{\partial \hat{F}_{s(f)}(\mathbf{r},\omega)}{\partial x} = 0. \tag{3}$$

Here and further, for simplicity of writing, we assume that the boundaries are parallel to the plane $x = 0$. In general, the partial derivative with respect to x will be replaced by a directional derivative along the normal to the boundary. On the internal S/F borders, we apply the generalized Kupriyanov-Lukichev boundary conditions [3, 32]

$$\begin{aligned} \frac{4D_s}{\sigma_s v_s}\frac{\partial \hat{F}_s(\mathbf{r},\omega)}{\partial x} &= \frac{4D_f}{\sigma_f v_f}\frac{\partial \hat{F}_f(\mathbf{r},\omega)}{\partial x}, \\ \frac{4D_f}{\sigma_f v_f}\frac{\partial \hat{F}_f(\mathbf{r},\omega)}{\partial x} &= \hat{F}_f(\mathbf{r},\omega) - \hat{F}_s(\mathbf{r},\omega), \end{aligned} \tag{4}$$

where $\sigma_s(f)$ are the transparency parameters from superconductor (ferromagnetic metal) side. Taking into account the condition of the detailed balance [33] $N_s(0)\,\sigma_s v_s = N_f(0)\,\sigma_f v_f$ these values are related to each other through a parameter $n_{sf} = N_f(0)v_f/N_s(0)v_s$, where $N_{s(f)}(0)$ is the density of electronic states at the Fermi level, $v_{s(f)}$ is the Fermi velocity. The boundary value problem is accompanied by the self-consistent equation [1]

$$\Delta(\mathbf{r}) \ln \frac{T}{T_{cs}} = \pi T \sum_{\omega>0}^{\omega_{\mathrm{D}}} \mathrm{Sp}\left(\hat{F}_s(\mathbf{r},\omega) - \frac{\Delta(\mathbf{r})}{|\omega|}\right), \tag{5}$$

where T_{cs} is the critical temperature of the bulk superconductor, and ω_{D} is the Debye frequency.

3. Step order parameter method

To solve the boundary value problem described above in conjunction with the self-consistency equation, we can use the following approximation: the order parameters in the Usadel equations and self-consistency equations are replaced with their average values for each S layer. With this approximation, equations (2) and (5) take the forms:

$$\frac{D_s}{2}\hat{\nabla}^2 \hat{F}_{s(k)}(\mathbf{r},\omega) - |\omega|\hat{F}_{s(k)}(\mathbf{r},\omega) = -\Delta_{(k)}, \tag{6}$$

$$\Delta_{(k)} \ln \frac{T}{T_{cs(k)}} = \pi T \sum_{\omega>0}^{\omega_{\mathrm{D}(k)}} \mathrm{Sp}\left(\langle \hat{F}_{s(k)}(\mathbf{r},\omega)\rangle_{(k)} - \frac{\Delta_{(k)}}{|\omega|}\right), \tag{7}$$

where index k lists superconducting layers. The angle brackets indicate averaging within the layer. The system of differential equations (1), (6) together with the boundary conditions (3)-(4) forms a boundary value problem that allows us to obtain an analytical expression for the Usadel functions for fairly simple magnetization configurations. For more complex magnetic textures, a numerical solution of the boundary value problem can be used. The obtained functions $F_{s(k)}$, averaged over the x coordinate within the layer, are substituted into the system of self-consistency equations (7), which allows us to obtain a system of homogeneous linear equations for Δ_k. The nontriviality condition for this system is the equation on the critical temperature of the heterostructure.

For example, we provide the equations for the critical temperature in the case of two superconducting layers with collinear magnetization in the ferromagnetic layers. In this case, it is enough to consider the scalar Usadel function that is responsible for the a zero-spin component of the superconducting condensate. The Usadel function $F_{s(k)}(\mathbf{r}, \omega, \Delta_1, \Delta_2)$ depends linearly on the average order parameters Δ_1 and Δ_2. In this notation, the equation for T_c has the following form

$$\left(\ln\frac{T_c}{T_{cs}} - 2\pi T_c \mathrm{Re}\sum_{\omega>0}^{\omega_\mathrm{D}}\left(\langle F_{s1}(\mathbf{r},\omega,1,0)\rangle_{(1)} - \frac{1}{\omega}\right)\right) \cdot \left(\ln\frac{T_c}{T_{cs}} - 2\pi T_c \mathrm{Re}\sum_{\omega>0}^{\omega_\mathrm{D}}\left(\langle F_{s2}(\mathbf{r},\omega,0,1)\rangle_{(2)} - \frac{1}{\omega}\right)\right) = = (2\pi T_c)^2\,\mathrm{Re}\sum_{\omega>0}^{\omega_\mathrm{D}}\langle F_{s1}(\mathbf{r},\omega,0,1)\rangle_{(1)} \cdot \mathrm{Re}\sum_{\omega>0}^{\omega_\mathrm{D}}\langle F_{s2}(\mathbf{r},\omega,1,0)\rangle_{(2)}. \quad (8)$$

The critical temperature of a system is the largest root of the given equation. In practice, there is usually only one solution.

4. Iterative method

Without resorting to approximations, problem described in the "model" chapter can be solved using the multimode or fundamental solution methods, if it is possible to obtain an analytical solution for the Usadel equation in a ferromagnetic layer. In the more general case, an iterative approach can be used [17], which we will briefly describe in this section (see the algorithm diagram in Figure 1).

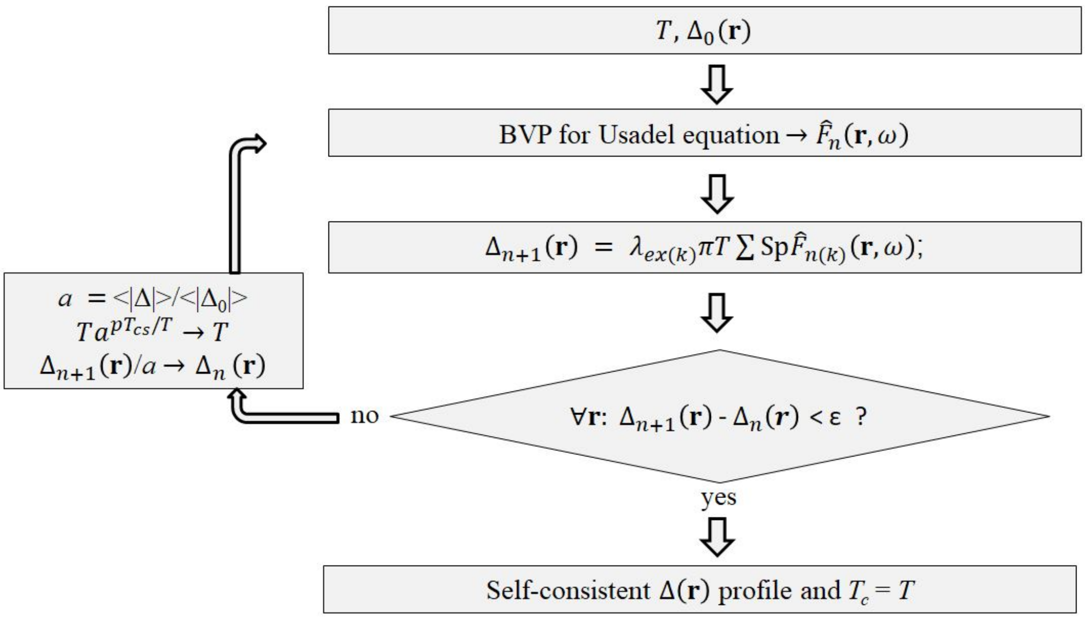

Figure 1. The iterative algorithm's scheme.

1. At the first stage, the starting temperature is selected (less than the maximum of the T_{cs} values for superconducting layers), and the order parameter in one or more layers is defined. A constant order parameter in one of the superconducting layers is often chosen. For more information on choosing the initial configuration of the order parameter for multilayer systems see [17].

2. The boundary value problem described in the model section is then solved using any method. We use the finite-difference method in the current implementation.

3. To calculate the order parameter in each layer during the next iteration, we use a self-consistency equation of the following form:
$$\Delta(\mathbf{r}) = \lambda_{\mathrm{ex}(k)}\pi T_c \sum_{\omega>0}^{\omega_{\mathrm{D}}} \mathrm{Sp}\, \hat{F}_{s(k)}(\mathbf{r},\omega), \tag{9}$$
where $\lambda_{\mathrm{ex}(k)}$ is expressed from the bulk critical temperature
$$\lambda_{\mathrm{ex}(k)} = \left(2\pi T_{cs(k)} \sum_{\omega>0}^{\omega_{\mathrm{D}}} \frac{1}{\omega}\right)^{-1}, \tag{10}$$
where index k lists superconducting layers.

4. Next, we calculate the average value of the order parameter modulus throughout the entire system and define the parameter $a = \langle|\Delta|\rangle/\langle|\Delta_0|\rangle$. This parameter plays a crucial role in analyzing the present state of convergence of the algorithm.

5. The temperature is also adjusted at each iteration. The current implementation utilizes the following formula:
$$T_{c(n+1)} = T_{c(n)} a^{p\left(T_{cs}/T_{c(n)}\right)}, \tag{11}$$
where parameter p ($0.3 < p < 10$ in the current implementation) is adjusted to achieve faster and more stable convergence. In this formula, the largest T_{cs} in the system is selected.

6. When the order parameters in neighboring iterations converge to a given accuracy, we conclude that the self-consistent boundary value problem has been solved. Otherwise the order parameter is normalized by the value of a, and we proceed to calculate the Usadel function (Step 1).

The temperature obtained during the operation of the algorithm can be considered the critical temperature. Strictly speaking, the critical temperature would be the highest temperature at which self-consistency is ensured within the framework of this algorithm. However, in most cases, the algorithm finds a single solution with the accuracy set. A similar situation arises in the context of the possibility of multiple roots in equation on the critical temperature (8). For S/F bilayer with homogeneous ferromagnetic materials, the results obtained using our technique are consistent with the results obtained by the fundamental solution method reported in [23].

5. Methods comparison

Let us first consider the simplest case of a superconductor in contact with a homogenous ferromagnet. The Figure 2 shows the dependence of critical temperature on the thickness of the superconducting layer for different thicknesses of the superconducting layer. The calculations were done using the two methods described above. For example we chose a case of high transparency, where we expect the most significant differences between the results obtained by these methods. In Figures 2-4, the parameters used are close to experimental values for vanadium as a superconductor: $l_s = 77\,\text{Å}$, $\xi_s = 100\,\text{Å}$, $2I\tau_f = 0.3$ (τ_f is the mean free time in the ferromagnet), $n_{sf} = 3$, $I = 500\,\mathrm{K}$, $a_f = 10\,\text{Å}$, $T_{cs} = 5.4$, $\omega_{\mathrm{D}} = 390\,\mathrm{K}$. The results from both methods are quite similar. A significant qualitative difference was observed in a narrow range where the critical temperature is highly sensitive to a set of parameters.

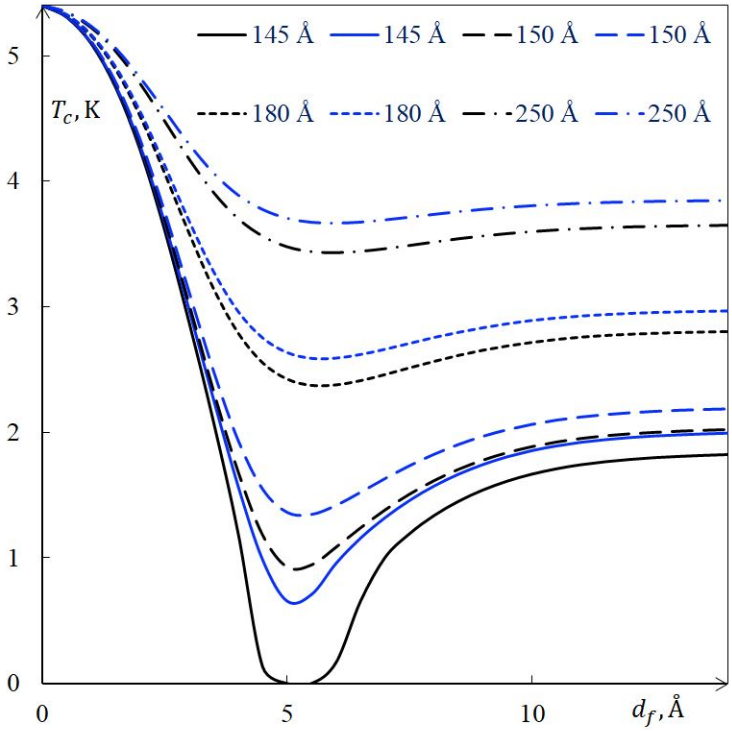

Figure 2. Critical temperature of the S/F structure calculated by various methods. The blue curves correspond to the iterative method, the black ones correspond to step order parameter method. Transparency parameter $\sigma_s = 8$, and S layer thickness $d_s = 145$ Å for solid lines, $d_s = 150$ Å for dashed lines, $d_s = 180$ Å for dotted lines, $d_s = 250$ Å for dash-dotted lines.

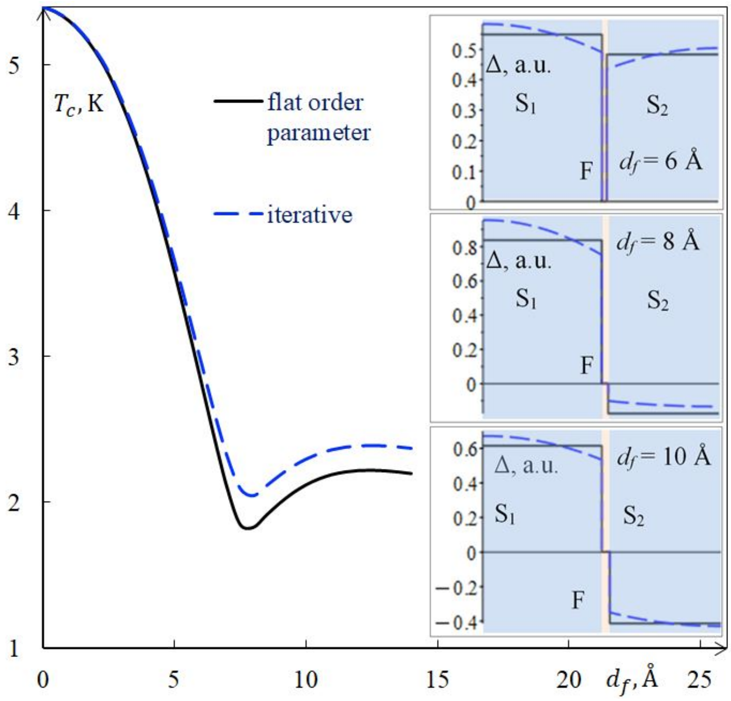

Figure 3. Critical temperature of the S_1/F/S_2 structure calculated by various methods. The blue curve corresponds to the iterative method, the black one corresponds to step order parameter method. Inset shows the distribution of the order parameter within the system for different ferromagnetic layer thickness. Transparency parameter $\sigma_s = 10$, S layer thickness $d_{s1} = 150$ Å, $d_{s2} = 140$ Å.

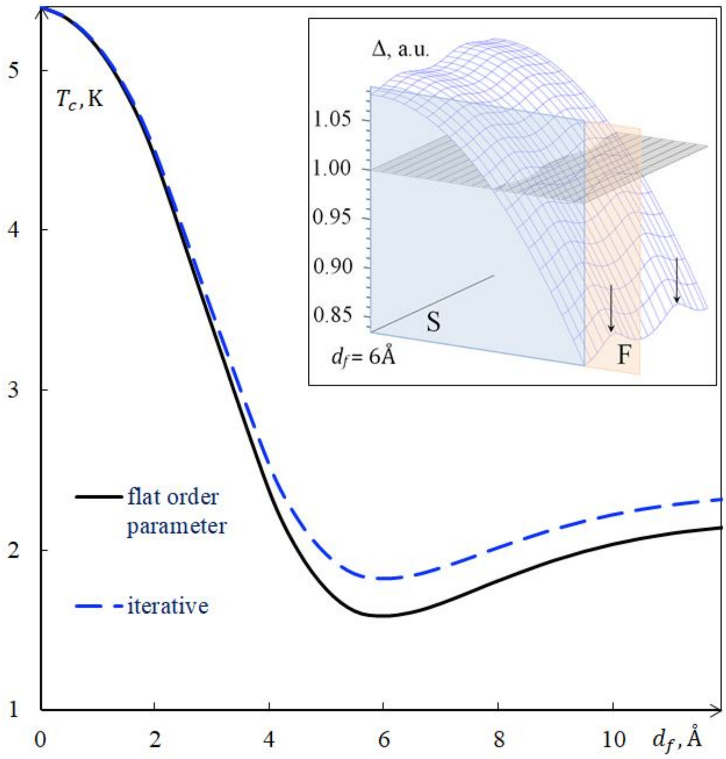

Figure 4. Critical temperature contact of superconductor / ferromagnet split into periodical domains structure calculated by various methods. The blue curve corresponds to the iterative method, the black one corresponds to step order parameter method. Insert shows the distribution of the order parameter within the system. The arrows indicate the positions of the domain walls. Transparency parameter $\sigma_s = 10$, S layer thickness $d_s = 150\,\text{Å}$, period of the domain structure $l_d = 1000\,\text{Å}$, domain wall thickness $l_{dw} = 25\,\text{Å}$.

The Figure 3 shows the dependence of the critical temperature for an asymmetric S/F/S heterostructure as a function of the ferromagnetic layer thickness d_f, calculated by two different methods. The inset shows the distribution of the order parameter as a function of the coordinate perpendicular to the boundaries, for cases of equilibrium phase difference of the order parameter 0 and π. The step order parameter method shows a very rough but qualitatively correct distribution of the order parameter within the system.

The Figure 4 shows the critical temperature for the contact of a superconductor with a ferromagnet split into domains by the two methods presented above. The inset shows the profile of order parameter in superconducting layer using two methods. By definition, approximate method shows constant value throughout entire layer. The domain wall is described by the following dependence of the polar angle on the coordinate [34].

$$\theta = 2 \arctan \exp\left(\frac{y - y_0}{l_{dw}}\right), \tag{12}$$

where y_0 is the position of the domain wall, l_{dw} is taken to be the domain wall thickness. If the azimuthal angle $\varphi = \frac{\pi}{2}$ it is the Neel domain wall and if $\varphi = 0$ it is the Bloch domain wall. If we neglect the magnetic field, then the type of wall does not affect the critical temperature. In this case the qualitative differences between methods are slightly more significant because an approximate method can not take into account the distribution of order parameter across the border.

6. Summary

We have carried out a critical temperature calculation for various heterostructures of a ferromagnetic superconductor using two different methods: step order parameter method and iterative method. In fairly simple cases, it is possible to obtain an analytical solution for boundary value problem. In this instance, only the critical temperature equation needs to be calculated numerically, and step order parameter method turns out to be more computationally efficient than iterative method and the fundamental solution method. The profile of the order parameter appears to be rather rough, but it does allow for accurate determination of the position of the phase transition from the 0 to π state. The calculation of the critical temperature gives satisfactory accuracy in many cases. Application of step order parameter method for superconductor / inhomogeneous ferromagnetic systems is more suitable. Such a method is not able to take into account the change of the order parameter due magnetization inhomogeneity distribution across the boundary. A modified version of this method has been used in previous studies [16, 35] for complex magnetic textures. But in both cases, due to approximations, the problem has been reduced to a set of one-dimensional boundary value problems. However, for the interface between a superconductor and a ferromagnet with helicoidal or conical magnetization [24], the applicability of this method is similar to homogeneous ferromagnetic material after local unitary transformations of the Usadel equation. Iterative method is well suited for calculating the critical temperature and the order parameter distribution for systems where an analytical solution for the Usadel equation in a ferromagnetic layer is not available or for complex system geometries. Such systems are discussed in more detail in [17]. For relatively simple problems, the method may not offer clear advantages over the fundamental solution method, but performs well due to its versatility and ease of use.

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