LETTERS TO THE EDITORS

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Inhomogeneous superconducting states in ferromagnetic metal/superconductor structures

(Reply to the comment by Ya V Fominov, M Yu Kupriyanov,

and M V Feigel'man on the review

"Competition between superconductivity and magnetism

in ferromagnet/superconductor heterostructures"

by Yu A Izyumov, Yu N Proshin, and M G Khusainov)

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In our recent review [1], we studied the proximity effect in layered FM/S structures, where FM stands for a ferromagnetic metal, and S for a superconductor. In their ensuing comment on this review, Fominov, Kupriyanov, and Feĭgel'man [2] made two basic remarks which, for some reason, were addressed to the review but not to the original papers [3–9] having provided the basis for the work [1]. The first remark relates to the three-dimensional (3D) boundary conditions we imposed on the anomalous Gor'kov function in an FM/S junction. These conditions immediately lead to the appearance of new 3D Larkin–Ovchinnikov–Fulde–Ferrell (LOFF) states [10, 11]. The second remark concerns the imaginary correction to the diffusion coefficient D_f in a ferromagnetic metal. In what follows, we give brief replies to these remarks.

1. Boundary conditions and the 3D LOFF states

Unfortunately, the authors of the comment [2] constantly demonstrate a misunderstanding of two rather simple facts. First, a ferromagnetic metal is essentially different from an ordinary normal metal (NM), as LOFF demonstrated in their classical works [10, 11]. Second, the Kupriyanov–Lukichev (KL) boundary conditions [12] are not universal. They are valid only for NM/S junctions and, generally speaking, cannot be applied to FM/S structures, as we have demonstrated in Refs [6, 7].

In particular, the authors of the comment [2] assert that our assumption about the existence of 3D LOFF states

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Received 15 October 2003 Uspekhi Fizicheskikh Nauk **173** (12) 1385–1386 (2003) Translated by M V Chekhova; edited by A Radzig follows from our erroneous interpretation of the KL boundary conditions [12]. However, this assertion is very erroneous. In developing our theory we never proceeded from the KL boundary conditions, which are valid only for an NM/S junction in the dirty limit. For the case of FM/S junctions considered in review [1], we derived more general boundary conditions for the Gor'kov–Usadel functions F_s and F_f [7]. These new boundary conditions, in the notations of review [1], have the form

$$\frac{4D_{\rm s}}{\sigma_{\rm s}v_{\rm s}} \frac{\partial F_{\rm s}(\mathbf{\rho}, z, \omega)}{\partial z} \bigg|_{z=+0} = \frac{4D_{\rm f}}{\sigma_{\rm f}v_{\rm f}} \frac{\partial F_{\rm f}(\mathbf{\rho}, z, \omega) \exp\left(-\mathrm{i}\mathbf{g}\mathbf{\rho}\right)}{\partial z} \bigg|_{z=-0}$$
$$= F_{\rm s}(\mathbf{\rho}, +0, \omega) - F_{\rm f}(\mathbf{\rho}, -0, \omega) \exp\left(-\mathrm{i}\mathbf{g}\mathbf{\rho}\right), \qquad (1)$$

where \mathbf{g} is a two-dimensional (2D) reciprocal lattice vector of LOFF surface states in the plane of the FM/S junction, with $g = |\mathbf{g}| \sim (I/D_{\rm f})^{1/2}$. The boundary conditions (1) are essentially different from the KL conditions and coincide with them only at g = I = 0. From the first equality in formula (1), it follows that the flux of BCS pairs from the S layer to the FM layer is equal to the backflux of LOFF pairs giving up their excess 2D momentum g to the lattice and being converted into BCS pairs. At the same time, the second equality indicates that both fluxes are determined by the density drop of such pairs on the S/FM boundary. Multiplying both parts of Eqn (1) by exp(igp), we arrive at the second boundary condition which shows that the flux of LOFF pairs through the FM/S interface is equal, in its turn, to the return flux of BCS pairs that acquire the missing momentum g from the lattice and transform into LOFF pairs. Thus, transport processes and mutual transformations between BCS and LOFF pairs can be interpreted as umklapp processes. As a result of these latter, the 2D momentum g of LOFF pairs becomes confined in the FM layer.

Taking the Fourier transform of Eqn (1) with respect to the 2D radius vector $\mathbf{\rho}$, we obtain

$$\frac{4D_{s}}{\sigma_{s}v_{s}} \frac{\partial F_{s}(\mathbf{q}_{s}, z, \omega)}{\partial z} \bigg|_{z=+0} = \frac{4D_{f}}{\sigma_{f}v_{f}} \frac{\partial F_{f}(\mathbf{q}_{f}, z, \omega)}{\partial z} \bigg|_{z=-0}$$
$$= F_{s}(\mathbf{q}_{s}, +0, \omega) - F_{f}(\mathbf{q}_{f}, -0, \omega), \qquad (2)$$

where $\mathbf{q}_{f} = \mathbf{q}_{s} + \mathbf{g}$. Actually, these are the boundary conditions (3.23) given in our review [1]. As it was pointed out in

Ref. [7], these 3D boundary conditions can be derived the same way as our 1D conditions (a detailed derivation of the latter can be found in Ref. [5]). Similarly to the corresponding differential equations (3.22) in $F_{s(f)}(\mathbf{q}_{s(f)}, z, \omega)$, the boundary conditions (2) admit two types of solutions. First, there are add solutions with $\alpha = \alpha$ and $\alpha = 0$ (the momentum of a pair

old solutions with $\mathbf{q}_{\rm f} = \mathbf{q}_{\rm s}$ and $\mathbf{g} = 0$ (the momentum of a pair can be flipped along the normal to the FM/S boundary). Second, new 3D solutions with $\mathbf{q}_{\rm f} = \mathbf{q}_{\rm s} + \mathbf{g}$ and $\mathbf{g} \neq 0$ appear (the momentum of a pair can also be flipped along the FM/S boundary). From the condition that the free energy is minimal and, hence, $T_{\rm c}$ is maximal, it follows that $\mathbf{q}_{\rm s}$ is equal strictly to zero. This is not surprising since, for BCS type pairing in the S layer, the pair amplitude $F_{\rm s}(\mathbf{p}, z, \omega)$ should be of constant signs. At the same time, pairing in the FM layer proceeds according to the LOFF mechanism, with nonzero 3D coherent pair momentum $\mathbf{k} = (\mathbf{q}_{\rm f}, k_{\rm f})$ and the oscillating pair amplitude $F_{\rm f}(\mathbf{p}, z, \omega)$. From Eqns (3.25)–(3.27) derived in Ref. [1], it follows that the 2D momentum $q_{\rm f} = g$ of LOFF pairs, which is so far arbitrary, should be determined through optimization, i.e., from the $T_{\rm c}$ maximum condition.

Contrary to the statement made in the comment [2], the boundary conditions (1), (2) remain valid even in the case of an ideally transparent boundary, i.e., for $\sigma_s, \sigma_f \rightarrow \infty$. In this limit, from Eqn (1) follows the continuity condition for the pair amplitude on the FM/S interface:

$$F_{\rm s}(\mathbf{\rho}, +0, \omega) = F_{\rm f}(\mathbf{\rho}, -0, \omega) \exp\left(-\mathrm{i}\mathbf{g}\mathbf{\rho}\right). \tag{3}$$

Taking into account that $F_{s}(\mathbf{p}, z, \omega) = F_{s}(z, \omega)$ and

$$F_{\rm f}(\mathbf{\rho}, z, \omega) = F_{\rm f}(z, \omega) \exp\left(\mathrm{i}\mathbf{g}\mathbf{\rho}\right),$$

we see that, in reality, there is no anomalous Green function discontinuity with the size varying along the FM/S boundary. One should take into account that in the framework of the diffusion description, which is based on equations (3.22) from Ref. [1] and the boundary conditions (1) and (2), the Gor'kov functions $F_{f(s)}(\mathbf{\rho}, z, \omega)$ are asymptotically smoothed. The diffusion description of the function behavior is only valid on scales comparable with the coherence lengths $\xi_{\rm f} = (D_{\rm f}/I)^{1/2}$ and $\xi_{\rm s} = (D_{\rm s}/2\pi T)^{1/2}$, which are much larger than the mean free paths $l_{\rm f}$ and $l_{\rm s}$. This approach does not reveal the real behavior of the functions $F_{f(s)}(\mathbf{p}, z, \omega)$ in the vicinity of the interface z = 0, since it does not embrace peculiar LOFF+BCS surface states confined in a layer of about $(l_f + l_s)$ in thickness on the FM/S boundary. It is in this surface layer that the LOFF and BCS wave functions should be matched on the basis of the quantum-mechanical continuity condition: $\psi_s(\mathbf{\rho}, +0, \omega) = \psi_f(\mathbf{\rho}, -0, \omega)$. However, the surface layer thickness $(l_f + l_s)$ is negligibly small if we proceed from the typical scales in the rough diffusion approach to the proximity effect. Therefore, surface effects can be described as above, i.e., in terms of a 2D lattice of LOFF pairs and umklapp processes with the asymptotic matching condition (3) for a transparent FM/S interface.

Thus, the boundary conditions (3.23) from review [1] can be used for a correct and adequate (to the physical grounds) description of layered FM/S systems. From these conditions, the competition between the old 1D states ($\mathbf{q}_f = \mathbf{q}_s = \mathbf{g} = 0$) and new 3D LOFF states ($\mathbf{q}_s = 0$; $\mathbf{q}_f = \mathbf{g} \neq 0$) follows, which, in its turn, causes a cascade of 3D-1D-3D phase transitions and nonmonotone behavior of T_c with a pronounced minimum or a single peak [1], in agreement with the results of most experiments. The foregoing proves that the proximity effect in FM/S structures should be described faithfully in the framework of a three-dimensional theory. Unfortunately, this fact is often ignored, and one-dimensional theory is used as before in many publications for the description of the proximity effect, which leads to results that are valid only in particular cases or that are even wrong. Evidently, such results should be reconsidered in the light of the 3D boundary conditions similar to Eqns (1), (2) and properly corrected.

2. Diffusion coefficient

Certain remarks should be made in connection with the complex diffusion coefficient. First, we have indeed shown that in the dirty limit (in particular, for $2I\tau_f \ll 1$), the diffusion coefficient $D_f(I)$ is complex [3–9], viz.

$$D_{\rm f}(I) = \frac{D_{\rm f}}{1 + 2\mathrm{i}I\tau_{\rm f}} \,. \tag{4}$$

The small imaginary correction of the order of $2I\tau_f$ appears since quasi-particles, in addition to their diffusion motion, can also wave-like propagate in the strong exchange field (with energy *I*) of the ferromagnet. This is another demonstration of the difference between FM/S junctions and NM/S systems that makes the KL boundary conditions with a real coefficient D_f invalid even for the case of 1D LOFF states.

Second, in June 2001, when our review was submitted to *Physics – Uspekhi*, it was indeed supposed that the diffusion coefficient $D_{\rm f}(I)$ had the form (4), and nobody argued against this statement. Numerical corrections [13] consisting of the replacement of $2I\tau_{\rm f}$ by $2I\tau_{\rm f}/5$ appeared only in a year's time and, naturally, could not be mentioned in our review. To find those corrections, one should abandon the diffusion approximation, which requires, generally speaking, a separate study. Indeed, to make the replacement of $2I\tau_{\rm f}$ by $2I\tau_{\rm f}/5$, the authors of Ref. [13] simply reduce the homogeneous fourth-order differential equation for $F_{\rm f}$ to a second-order equation, instead of renormalizing $D_{\rm f}$ according to the microscopic theory. The easiest way of verifying this is to expand the exact characteristic equation

$$\frac{kl_{\rm f}}{\arctan\left[kl_{\rm f}/(1+2iI\tau_{\rm f})\right]} - 1 = 0, \qquad (5)$$

obtained in Ref. [5], in a power series of $kl_f/(1+2iI\tau_f)$. The above equation is equivalent to the homogeneous equation in $F_{\rm f}(\mathbf{k}, \omega)$, where $k^2 = q_{\rm f}^2 + k_{\rm f}^2$. By the way, one can easily see from Eqn (5) that each term of the expansion will contain the renormalized mean free path $l_f/(1 + 2iI\tau_f)$ which, in turn, will lead to the renormalization (4) in the expansion coefficient of k^2 . Strictly speaking, the diffusion coefficient of the second derivative of the Gor'kov-Usadel function will still have the form (4) since, in reality, the equations in $F_{\rm f}(\mathbf{p}, z, \omega)$ are not homogeneous (see formulas (3.12) and (3.22) in Ref. [1]). The correction to the solution of the characteristic equation (5) in the diffusion approximation can only be obtained by neglecting the right-hand sides of Eqns (3.12) and (3.22), i.e., by setting $\Delta_f = 0$ and taking into account terms proportional to k^4 in expression (5). However, we stress once again that this has no relation to the renormalization of the diffusion coefficient.

On the other hand, taking into consideration higher-order derivatives of $F_{\rm f}$, one can arrive at the appropriate 'correction' of the boundary conditions (1), (2), too. In this case,

passing to effective diffusion boundary conditions, as in Ref. [13], results in an alternative renormalization of $D_{\rm f}$ that is already different from $2I\tau_{\rm f}/5$. Therefore, in the dirty limit for $2I\tau_{\rm f} \ll 1$ one should either omit the imaginary correction to $D_{\rm f}$ or apply a purely diffusion approximation with the renormalization (4), which has the same form both for equations and boundary conditions.

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