Phase diagram of superconducting-normal-metal superlattices

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The transition temperatures and the perpendicular upper critical fields of superconductingnormal-metal superlattices are calculated by solving exactly the Usadel equations. For thin films our results differ substantially from previous approximate results.

There have been several attempts to account for the critical temperatures and fields of superconducting proximity systems.¹ One approach, first proposed by de Gennes and Guyon² and recently generalized by Takahashi and Tachiki,³ and Auvil and co-workers⁴ starts from a linearized integral self-consistency equation for the "pair potential" $\Delta(\mathbf{r})$. An alternative way of treating such systems was given by Biagi et al.⁵ who used Usadel's dirty-limit quasiclassical theory⁶ to calculate for all temperatures the perpendicular upper critical fields $H_{c2\perp}$ of superlattices made of superconducting (S) and normal (N) layers. These authors used a simple method to solve the coupled system of linearized Usadel's equations in both metals. However, the solutions obtained satisfy the boundary conditions only approximately. As a result their method works well only for thick layers. We solve the Usadel equations *exactly* for *any* layer thickness; in particular, we give correct thin-layers-limit expressions for T_c and $H_{c2\perp}$.

Consider an infinite stack of alternating S and N layers, parallel to the x-y plane, with thicknesses d_S and d_N , respectively. The coordinates are chosen so that z = 0 defines the middle of an S layer. Near the second-order phase transition we take a uniform magnetic field $\mathbf{H} = H\hat{z}$ throughout the sample, with the gauge $\mathbf{A} = (0, H\mathbf{x}, 0)$.

The linearized Usadel equations for the averaged Gorkov's Green's function, $F_{\omega}(\mathbf{r})$, for each metal separately are^{5,6}

$$-\frac{\hbar D_S}{2} \mathbf{\Pi}^2 F^S_{\omega}(\mathbf{r}) = \Delta^S(\mathbf{r}) - \hbar |\omega| F^S_{\omega}(\mathbf{r}) , \qquad (1)$$

$$\Delta^{S}(\mathbf{r}) = \pi k_{B} T \lambda_{S} \sum_{\omega} F_{\omega}^{S}(\mathbf{r}) , \qquad (2)$$

for S, and

$$\frac{\hbar D_N}{2} \mathbf{\Pi}^2 F^N_{\omega}(\mathbf{r}) = \hbar |\omega| F^N_{\omega}(\mathbf{r}) , \qquad (3)$$

for N. Here

$$\Pi = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y} + \frac{2\pi i H x}{\Phi_0}, \frac{\partial}{\partial z}\right)$$

is the gauge-invariant gradient, $D_{S,N}$ are the diffusion coefficients, $\hbar \omega = \pi k_B T(2l+1)$, $l = 0, \pm 1, \pm 2, \ldots$, and the coupling constant

$$\lambda_S = \left(\pi k_B T_{cS} \sum_{\omega(T_{cS})} \frac{1}{\hbar |\omega|} \right)^{-1}.$$

The summations are cut off at $\omega_D = k_B \Theta_D / \hbar$, Θ_D being the Debye temperature and T_{cS} the bulk transition temperature of the S metal. For $\Theta_D \gg T_{cS}$

$$\lambda_S = \left(\ln \frac{1.134\Theta_D}{T_{cS}}\right)^{-1}$$

For the N metal we set $\lambda_N = 0$ ($T_{cN} = 0$), implying $\Delta^N(\mathbf{r}) = 0$.

The function $F_{\omega}(\mathbf{r})$ is subject to standard boundary conditions^{5,7} at S-N interfaces:

$$F_{\omega}^{S} = F_{\omega}^{N} \quad \text{and} \quad \frac{\partial F_{\omega}^{S}}{\partial z} = \eta \frac{\partial F_{\omega}^{N}}{\partial z} \quad ,$$
 (4)

where, for the specular scattering, $\eta = \sigma_N / \sigma_S$, with $\sigma_{S,N}$ being the normal conductivities.

In what follows we assume the separation of variables

$$F^{S,N}_{\omega}(\mathbf{r}) = f(x,y)g^{S,N}_{\omega}(z) \quad , \tag{5}$$

since one expects that in the plane perpendicular to the external field (x-y plane) an Abrikosov vortex lattice is formed, as in an infinite bulk superconductor. Hence, f(x, y) is metal and ω independent.

For N, from Eqs. (5) and (3), one obtains

$$\frac{d^2 g_{\omega}^N(z)}{dz^2} = q_N^2 g_{\omega}^N(z) , \qquad (6)$$

$$-\left[\frac{\partial^2}{\partial x^2} + \left(\frac{\partial}{\partial y} + \frac{2\pi i H x}{\Phi_0}\right)^2\right] f(x,y)$$
$$= \left(q_N^2 - \frac{2|\omega|}{D_N}\right) f(x,y), \quad (7)$$

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where the separation constant q_N^2 has been introduced. Exactly as in a bulk superconductor, the requirement that f(x, y) is finite in the whole x-y plane implies

$$q_N^2 - \frac{2|\omega|}{D_N} = \frac{2\pi H_{c2\perp}}{\Phi_0} ,$$
 (8)

which is the lowest eigenvalue of Eq. (7), giving the highest $H = H_{c2\perp}$.

We look for the ground-state solution, which is periodic in z direction with the period $d_S + d_N$ and is symmetric with respect to the middle of each film. This gives the following solution for Eq. (6):

$$g^{N}(z) = C_{N} \cosh\left[q_{N}\left(\frac{d_{S}+d_{N}}{2}-|z|\right)\right]$$

for $\frac{d_{S}}{2} \le |z| \le d_{N} + \frac{d_{S}}{2}$. (9)

For S, combining Eqs. (5), (7), and (8) with Eq. (1) we get

$$-\frac{\hbar D_S}{2} \left(\frac{\partial^2}{\partial z^2} - \frac{2\pi H_{c2\perp}}{\Phi_0} \right) F_{\omega}^S(\mathbf{r}) = \Delta^S(\mathbf{r}) - \hbar |\omega| F_{\omega}^S(\mathbf{r}) \,.$$
(10)

Using Eqs. (4) and (9), the boundary conditions for $F_{\omega}^{S}(\mathbf{r})$ in Eqs. (2) and (10) become

$$\frac{\partial F_{\omega}^{S}/\partial z}{F_{\omega}^{S}}\Big|_{z=\pm d_{S}/2} = \pm \zeta_{\omega} \quad , \tag{11}$$

where

$$\zeta_{\omega} = \eta q_N \tanh \frac{q_N d_N}{2}$$

and q_N is obtained from Eq. (8).

$$F_{\omega}^{S}(\mathbf{r}) = \sum_{m=-\infty}^{+\infty} F_{\omega}^{S}(Q_{m}) \cos(Q_{m}z) , \qquad (12)$$

where

$$F_{\omega}^{S}(Q_{m}) = \frac{1}{d_{S}} \int_{-d_{S}/2}^{d_{S}/2} dz \, \cos(Q_{m}z) F_{\omega}^{S}(\mathbf{r})$$
(13)

is the Fourier amplitude that depends on x and y, and $Q_m = 2\pi m/d_s$, with the similar expressions for $\Delta^S(\mathbf{r})$ and $\Delta^S(Q_m)$. Putting these expansions into Eq. (10), and applying boundary conditions (11), we obtain

$$\sum_{m'=-\infty}^{+\infty} F_{\omega}^{S}(Q_{m'}) \left\{ \left[\hbar |\omega| + \frac{\hbar D_{S}}{2} \left(Q_{m}^{2} + \frac{2\pi H_{c2\perp}}{\Phi_{0}} \right) \right] \delta_{mm'} + \frac{\hbar D_{S} \zeta_{\omega}}{d_{S}} (-1)^{m+m'} \right\} = \Delta^{S}(Q_{m}).$$

$$(14)$$

Similarly, from Eq. (2), one obtains

$$\Delta^{S}(Q_{m}) = \pi k_{B} T \lambda_{S} \sum_{\omega} F_{\omega}^{S}(Q_{m}) \quad .$$
(15)

Now we solve Eq. (14) analytically for the amplitudes $F^{S}_{\omega}(Q_m)$ and from Eq. (15) we obtain an infinite system of homogeneous linear equations for the amplitudes $\Delta^{S}(Q_m)$:

$$\sum_{m'=-\infty}^{+\infty} A_{mm'} \Delta^S(Q_{m'}) = 0 \quad , \tag{16}$$

where

$$A_{mm'} = \left(1 - \pi k_B T \lambda_S \sum_{\omega} \frac{1}{\hbar |\omega| + (\hbar D_S/2) \left(Q_m^2 + 2\pi H_{c2\perp}/\Phi_0\right)}\right) \delta_{mm'} + \pi k_B T \lambda_S \sum_{\omega} \frac{(-1)^{m+m'}}{\left[\hbar |\omega| + (\hbar D_S/2) \left(Q_m^2 + 2\pi H_{c2\perp}/\Phi_0\right)\right] \left[\hbar |\omega| + (\hbar D_S/2) \left(Q_{m'}^2 + 2\pi H_{c2\perp}/\Phi_0\right)\right] \left[d_S/\hbar D_S \zeta_{\omega} + \alpha_{\omega}\right)}$$
(17)

and

$$\alpha_{\omega} \equiv \sum_{m=-\infty}^{+\infty} \frac{1}{\hbar |\omega| + (\hbar D_S/2) \left(Q_m^2 + 2\pi H_{c2\perp}/\Phi_0\right)} = \frac{d_S}{\hbar D_S \sqrt{2|\omega|/D_S + 2\pi H_{c2\perp}/\Phi_0}} \coth\left(\frac{d_S}{2} \sqrt{\frac{2|\omega|}{D_S} + \frac{2\pi H_{c2\perp}}{\Phi_0}}\right)$$
(18)

The condition for a nontrivial solution of the system (16)

$$\det \underline{A} = 0 \tag{19}$$

gives $H_{c2\perp}$ for a given T. The transition temperature T_c is obtained by putting $H_{c2\perp} = 0$. Note that, although

the matrix <u>A</u> is infinite, for the calculation of the determinant in Eq. (19) it is sufficient to take a finite number of elements around A_{00} since $A_{mm'} \rightarrow \delta_{mm'}$ when $m, m' \rightarrow \pm \infty$.

In Figs. 1 and 2 the curves for T_c and $H_{c2\perp}$ both from our and the approximate (Ref. 5) calculation are shown.



FIG. 1. Reduced transition temperature $t_c = T_c/T_{cS}$ vs d_N/ξ_N for $d_S/d_N = 2$, $\eta = 1$, $\xi_S/\xi_N = 1$, and $\Theta_D/T_{cS} = 200$. Exact solution — solid curve, $A_{00} = 0$ approximation — dotted curve, and the solution from Ref. 5 — dashed curve.

For convenience, all results are expressed in terms of the quantities t, h, Θ_D/T_{cS} , d_S/ξ_S , d_N/ξ_N , ξ_S/ξ_N , and η , where

$$t = \frac{T}{T_{cS}} , \quad h_{c2\perp} = \frac{2\pi\xi_S^2 H_{c2\perp}}{\Phi_0} ,$$

$$\xi_S = \left(\frac{\hbar D_S}{2\pi k_B T_{cS}}\right)^{1/2} , \quad \xi_N = \left(\frac{\hbar D_N}{2\pi k_B T_{cS}}\right)^{1/2}$$



FIG. 2. Reduced perpendicular upper critical field $h_{c2\perp}(0)$ at zero temperature vs d_N/ξ_N . The notation of the curves and the parameters are the same as in Fig. 1.

It is seen that the results of Biagi *et al.*⁵ are qualitatively the same as the exact ones. However, the quantitative discrepancy is large for thin layers. The reason for this is that with the ansatz $F_{\omega}^{S}(\mathbf{r}) = \Delta^{S}(\mathbf{r})/[\hbar\omega + \pi T y(t)]$ used in Ref. 5 to solve Eq. (1) [y(t) defined by Eq. (2) of Ref. 5], one cannot satisfy the boundary conditions, Eq. (4), for all ω . The ansatz is strictly valid only for an infinite superconductor, or for vacuum-superconductor interfaces. One of the consequences of the ansatz is that $F_{\omega}^{S}(\mathbf{r})$ becomes an eigenfunction of the operator Π^{2} . As we have shown in this paper, such an approach, used in numerous previous papers,² is not valid in general and in fact fails for short-period superlattices. In addition, our solution comprises the parameter Θ_{D}/T_{cS} , which is absent in the previous calculations.^{2,5}

In the calculation of T_c and $H_{c2\perp}(T)$, for almost any choice of parameters, it is sufficient to take only a 3×3 matrix with $m, m' = -1, 0, 1.^8$ Moreover, as can be seen from Figs. 1 and 2, if only the A_{00} element is taken, one obtains excellent agreement with the exact results for thin layers (not only in the saturation region but for slightly thicker layers as well).

In the thin layers limit $(d_S, d_N \to 0)$, the matrix <u>A</u> in Eq. (16) becomes diagonal, with all diagonal elements except A_{00} tending to 1. Then, the condition (19) becomes simply

$$A_{00} = 0 \quad . \tag{20}$$

After some purely algebraic transformations this gives a transcendental equation for $H_{c2\perp}(T)$ in the thin layers limit:

$$\ln \frac{t_c^{\text{Cooper}}}{t} = \Psi\left(\frac{1}{2} + \frac{\rho}{2t}\right) - \Psi\left(\frac{1}{2}\right) \quad . \tag{21}$$

Here

$$\rho = \frac{1 + \nu (\xi_N / \xi_S)^2}{1 + \nu} h_{c2\perp} \quad ,$$
$$\nu = \frac{d_N / \xi_N}{d_S / \xi_S} \frac{\eta \xi_S}{\xi_N} \quad ,$$

 Ψ is the digamma function, and t_c^{Cooper} is the well-known Cooper's result for the critical temperature in the thin layers limit:

$$t_c^{\text{Cooper}} = \left(\frac{1.134\Theta_D}{T_{cS}}\right)^{-\nu} \quad . \tag{22}$$

Note that Eq. (21) was also obtained by the de Gennes correlation function method.⁹

Equation (21) can be solved analytically at zero temperature giving a very simple expression for $h_{c2\perp}(0)$:

$$h_{c2\perp}(0) = 0.28 \frac{1+\nu}{1+\nu(\xi_N/\xi_S)^2} \left(\frac{1.134\Theta_D}{T_{cS}}\right)^{-\nu} \quad .$$
(23)

As can be seen, there is a strong power-law dependence on Θ_D/T_{cS} , in contrast with the result of Biagi *et al.*⁵

To summarize, we have developed a method for the calculation of T_c and $H_{c2\perp}$ of superconductor-normalmetal superlattices, valid for any superlattice period. In the thin-layers limit we have obtained simple Cooper-like results for $H_{c2\perp}$.

ACKNOWLEDGMENTS

We should like to thank John R. Clem and Vladimir G. Kogan for valuable discussions. This work is supported in part by Grant No. JF 898 under the National Science Foundation's U.S.-Yugoslavia Cooperative Research Program.

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