

Upper critical field H_{c3} for a superconducting superlattice

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The transition temperature for a semi-infinite superconducting superlattice composed of alternating layers with different electron diffusion lengths is calculated in the presence of a homogeneous magnetic field aligned parallel to the layers. The effect of the free surface on the discontinuity in the upper critical field H_{c3} that is manifest in such systems, over a certain range of parameters, is examined and the experimental implications of the results obtained are discussed.

I. INTRODUCTION

In recent years there has arisen a considerable theoretical and experimental interest in a new class of superconductivity compounds comprising superconducting superlattices.¹⁻⁵ Much of the interest has been focused on the effect of an externally applied magnetic field on the superconducting transition temperature and a number of intriguing phenomena have been observed.^{4,5} Perhaps one of the more novel effects that can arise in such systems as recently predicted by Takahashi and Tachiki is the discontinuous slope in the upper critical field in superlattices composed of alternating layers composed of metals with differing electron diffusion constants.^{6,7} The existence of such a discontinuity has been confined experimentally in at least two systems.^{4,5}

The origin for the discontinuity in the slope of the upper critical field lies in the effect of the superlattice geometry on the nucleation of the superconductivity. For sufficiently low values of H it is found that the superconductivity nucleates in a clean (N) layer. However for a certain range of parameters the nucleation switches to a dirty (S) layer when the field H exceeds a certain value H^* . It is this translation of the nucleation center that gives rise to the discontinuity in the slope.

It is well known in type-II superconductors that the presence of a free surface allows the superconductivity to nucleate at a higher temperature resulting in an enhancement of the upper critical field.⁸ In this paper we examine the role of a free surface in determining the upper critical field of a metallic superlattice. In particular we wish to examine how the attractive character of the free surface on the nucleation center is modified by the superlattice geometry. The question is of some importance both in providing a better understanding of the present experimental data as well as suggesting some further work.

II. WERTHAMER-DE GENNES THEORY OF THE PROXIMITY EFFECT

Near the critical temperature when the phase transition to the normal state is second order, the self-consistent equation for the superconducting order param-

eter $\Delta(\mathbf{x})$ reduces to the linearized integral equation⁹

$$\Delta(\mathbf{x}) = V \int Q(\mathbf{x}, \mathbf{y}) \Delta(\mathbf{y}) d^3 y, \quad (1)$$

where V denotes the BCS coupling constant and the kernel Q may be written in terms of the one-electron Green's function $g_\omega(\mathbf{x}, \mathbf{y})$. Within the framework of the semiclassical phase integral approximation we can write the kernel Q in the form⁹

$$Q(\mathbf{x}, \mathbf{y}) = e^{2ie\mathbf{A}(\mathbf{x}) \cdot (\mathbf{x} - \mathbf{y})} K(\mathbf{x}, \mathbf{y}). \quad (2)$$

In the Werthamer-de Gennes theory the reduced kernel is evaluated in the single mode approximation and the linearized integral equation, Eq. (1), reduces to

$$\chi \left[-\xi_T^2 \left(\nabla - \frac{2\pi i}{\phi_0} \mathbf{A} \right)^2 \right] \Delta(\mathbf{x}) = \ln \left(\frac{T_c}{T} \right) \Delta(\mathbf{x}), \quad (3)$$

where ϕ_0 denotes the flux quantum, T_c denotes the superconducting transition temperature of the bulk superconductor in zero magnetic field, ξ_T denotes the temperature-dependent coherence length ($= \hbar D / 2\pi k_B T$), and the function χ may be expressed in terms of the digamma function $\psi(z)$ as $\chi(z) = \psi(\frac{1}{2}z + \frac{1}{2}) - \psi(\frac{1}{2})$. Equation (3), together with the boundary conditions at the surface of the superconductor¹⁰

$$\left(\nabla - \frac{2\pi i}{\phi_0} \mathbf{A} \right) \Delta(\mathbf{x}) = 0, \quad (4)$$

permits the determination of the superconducting transition temperature for a particular geometry as a function of the applied magnetic field H .

Within the framework^{11,12} of the Werthamer-de Gennes theory of the proximity effect the order parameter in a system comprising two distinct metals, which we denote by S and N , respectively, separated by a well-defined interface, is also governed by Eq. (3) with ξ_T and T_c appropriately chosen. The resultant equations together with the boundary conditions at the interface

$$\begin{aligned} \frac{D_S}{\Delta_S(\mathbf{x})} \left(\nabla - \frac{2\pi i}{\phi_o} \mathbf{A} \right) \Delta_S(\mathbf{x}) \\ = \frac{D_N}{\Delta_N(\mathbf{x})} \left(\nabla - \frac{2\pi i}{\phi_o} \mathbf{A} \right) \Delta_N(\mathbf{x}) \quad (5) \end{aligned}$$

permits the determination of the superconducting transition temperature for a composite system such as the multilamellar systems that is the subject of this paper.

We wish to apply the above procedure to a semi-infinite superlattice consisting of alternating layers of two superconducting metals. The two metals are assumed to have a common transition temperature T_c in bulk but have different electron diffusion constants which we denote by D_S and D_N for the dirty (S) layers and the clean (N) layers, respectively. In particular we wish to compute the superconducting transition temperature in the presence of a homogeneous magnetic field H aligned parallel to the layers.

Choosing the x axis to be normal to the NS interfaces and the magnetic field to lie along the z direction we choose the magnetic vector potential $\mathbf{A}(\mathbf{x})$ to be of the form

$$\mathbf{A}(\mathbf{x}) = H(0, x, 0). \quad (6)$$

Assuming the order parameter to be of the form

$$\Delta(\mathbf{x}) = \begin{cases} e^{i(2\pi H/\phi_o)x_0 y} f_S(x - x_0), & x \in S, \\ e^{i(2\pi H/\phi_o)x_0 y} f_N(x - x_0), & x \in N, \end{cases} \quad (7)$$

where the parameter x_0 and the functions f_S and f_N are yet to be determined. We define the function g as

$$g(X) \equiv \begin{cases} \rho \frac{d}{dX} \ln f_S\left(\frac{\xi_H}{\sqrt{2}} X\right), & X \in S, \\ \frac{d}{dX} \ln f_N\left(\frac{\xi_H}{\sqrt{2}} X\right), & X \in N, \end{cases} \quad (8)$$

where $X = \sqrt{2}(x - x_0)/\xi_H$ with $\xi_H^{-2} = 2\pi H/\phi_o$, then the Werthamer-de Gennes equations given in Eq. (3) reduce to

$$\frac{dg(X)}{dX} = -\frac{1}{\rho} g^2(X) + \frac{1}{4} \rho X^2 - \frac{1}{2} \lambda, \quad X \in S, \quad (9)$$

$$\frac{dg(X)}{dX} = -g^2(X) + \frac{1}{4} X^2 - \frac{1}{2} \lambda, \quad X \in N, \quad (10)$$

with $\rho = D_S/D_N$. The eigenvalue λ is related to the reduced transition temperature $t = T/T_c$, through the equation

$$\chi \left(\frac{\hbar D_N}{2\pi k_B T} \frac{\lambda}{\xi_H^2} \right) = -\ln t. \quad (11)$$

The boundary conditions at the NS interface given by Eq. (5) reduces to the requirement that the g be continuous across the interface while at the surface of the superconductor $g = 0$. The determination of the observed transition temperature is complicated by the fact that Eqs. (9) and (10) together with the corresponding boundary conditions, has many solutions yielding a set of eigenvalues with the values in the set being dependent upon the particular value of x_0 appearing in the functional form of the order parameter, given by Eq. (7). Since the observed transition temperature corresponds

to the value obtained from the minimum eigenvalue, the calculation of the upper critical field requires that, for each value of x_0 we determine the minimum eigenvalue obtained from Eqs. (9) and (10) subject to the boundary conditions that $g = 0$ at the free surface and is continuous at the NS interfaces. We denote by λ_0 the minimum eigenvalue thus obtained. Since λ_0 depends on x_0 in a nontrivial manner the evaluation of the observed transition temperature requires that we determine the particular value of the x_0 that yields the minimum value of λ_0 . These we denote by x^* and λ^* , respectively. The variable x^* is generally referred to as the nucleation center for the superconducting order parameter, while the eigenvalue λ^* yields the transition temperature by virtue of Eq. (3). This self-consistent determination of the nucleation center x^* considerably complicates the calculation of the upper critical field.

III. THE EVALUATION OF THE UPPER CRITICAL FIELD H_{C3}

The calculation of the superconducting transition temperature as a function of the applied magnetic field separates into two distinct parts. The first part requires the self-consistent determination of the nucleation center x^* and the corresponding eigenvalue λ^* . With λ^* thus determined the second part involves the relatively straightforward evaluation of the superconducting transition temperature T from Eq. (11).

In order to determine λ^* and x^* for a given value of applied external field H we first compute the eigenvalue λ_0 numerically from Eqs. (9) and (10), together with the corresponding boundary conditions, as a function of the parameter x_0 . This yields a family of curves of λ_0 versus x_0 , with each curve corresponding to a different value of H . Four such families of curves are illustrated by the surface plots given in Figs. 1(a), 1(b), 2(a), and 2(b) for various geometries and values of ρ .

The surface plots shown in Figs. 1(a), 1(b), 2(a), and 2(b) share a number of qualitatively similar features. In particular we find that for H sufficiently small (i.e., modulation length $d \ll$ magnetic coherence length ξ_H), the detailed structure of the superlattice does not manifest itself in the functional dependence of the minimum eigenvalue λ_0 on the parameter x_0 . Instead what is observed is a smooth curve with a single minimum. The position of the minimum x^* and the corresponding eigenvalue λ^* can be evaluated in the limit $H \rightarrow 0$ (see the Appendix) as

$$\lim_{h \rightarrow 0} x^* = \left(\frac{0.5091 \sqrt{\rho} (1 + \rho)}{2} \right)^{1/2}, \quad (12)$$

$$\lim_{h \rightarrow 0} \lambda^* = 0.5901 \sqrt{\rho}. \quad (13)$$

This behavior is characteristic of a semi-infinite homogeneous superconductor, with an effective electron diffusion constant $D = \sqrt{D_S D_N}$. The effect of the minima in the functional dependence of λ_0 on x_0 , induced by the presence of the free surface, is to enhance the criti-

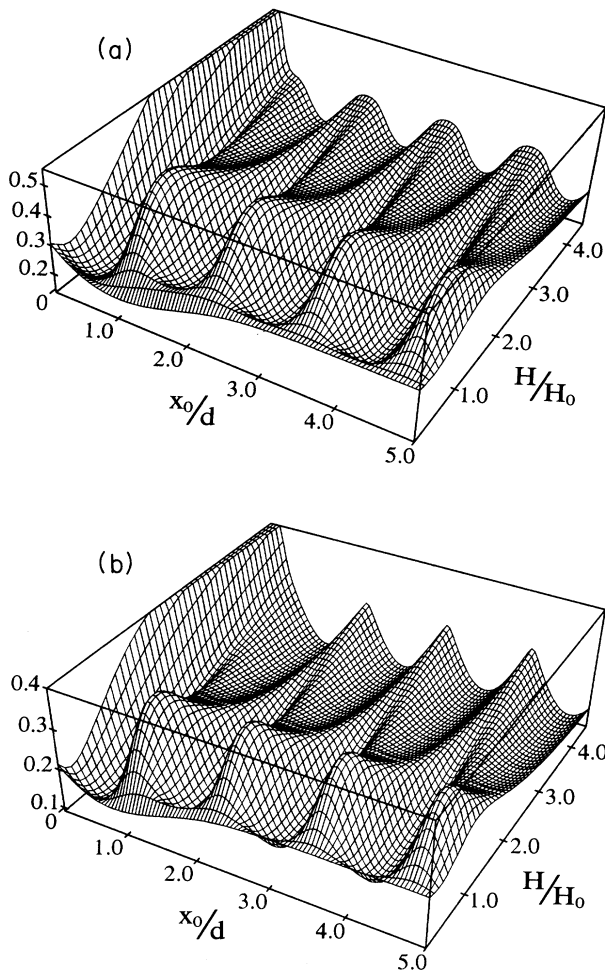


FIG. 1. Plots showing the dependence of the eigenvalue λ_0 on the parameter x_0 as a function of the applied magnetic field for the $(NSN\cdots)$ geometry for (a) $\rho = 0.1$ and (b) $\rho = 0.05$. The parameter $H_o = H_{c2}^N(0)$ and corresponds to the upper critical field of a bulk sample at 0 K with $D = D_N$.

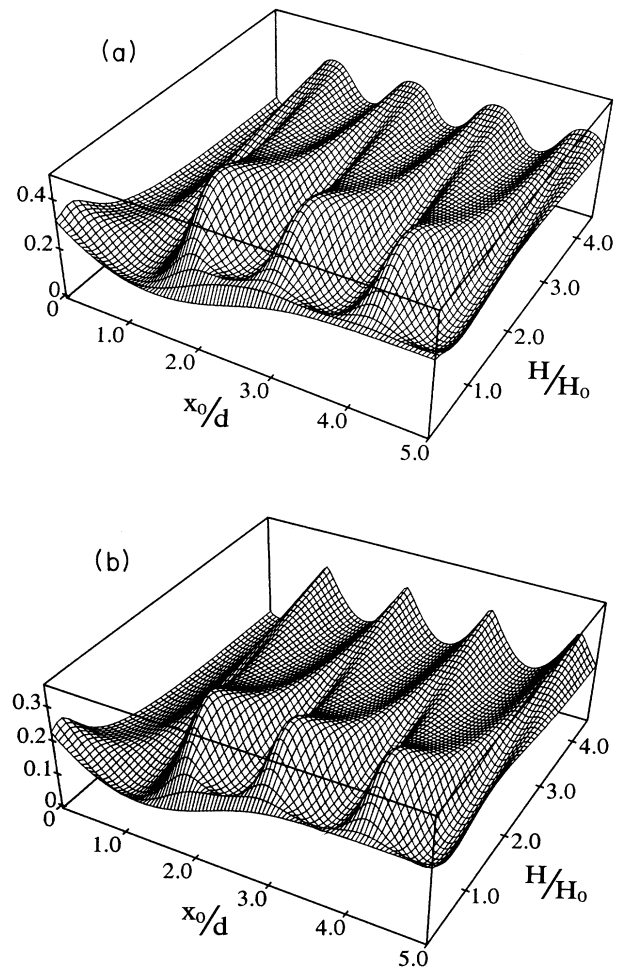


FIG. 2. Plots showing the dependence of the eigenvalue λ_0 on the parameter x_0 as a function of the applied magnetic field for the $(SNS\cdots)$ geometry for (a) $\rho = 0.1$ and (b) $\rho = 0.05$. The parameter $H_o = H_{c2}^N(0)$ and corresponds to the upper critical field of a bulk sample at 0 K with $D = D_N$.

cal field, giving rise to what is commonly referred to as surface superconductivity.⁸ This rather simple behavior disappears, however, as the applied field H is increased and the modulated structure of the superlattice is seen to manifest itself in the functional dependence of λ_0 on x_0 . What we now observe is a curve with multiple minima. For $x_0 \gg \xi_H$, the effect of the free surface on the form of the superconducting order parameter is negligible and we find that the minima occur in either the center of the clean (N) layer, or with increasing magnetic field, in the center of the dirty (S) layers, reflecting the periodic nature of the superlattice. The fact that the nucleation center x^* switches over from the clean (N) layer to the dirty (S) layer with an increasing magnetic field, gives rise to a discontinuous slope in the dependence of λ^* on the applied magnetic field, this may be seen in Figs. 3 and 4. This can result in a discontinuity in the slope of the upper critical field H_{c2} as shown in Fig. 4. This

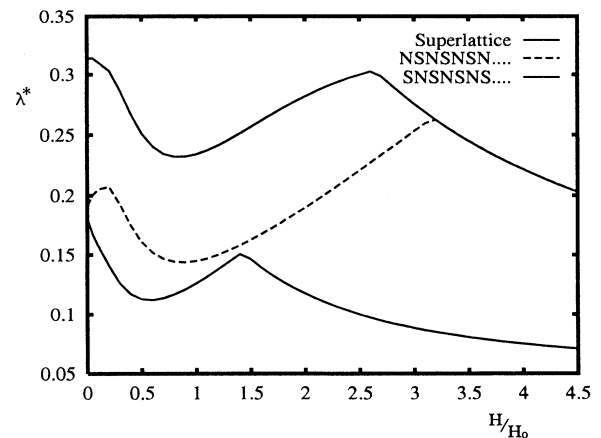


FIG. 3. Plot of the minimum eigenvalue λ^* as a function of the applied magnetic field, for the superlattice and the semi-infinite $(NSN\cdots)$ and $(SNS\cdots)$ geometries for $\rho = 0.1$.

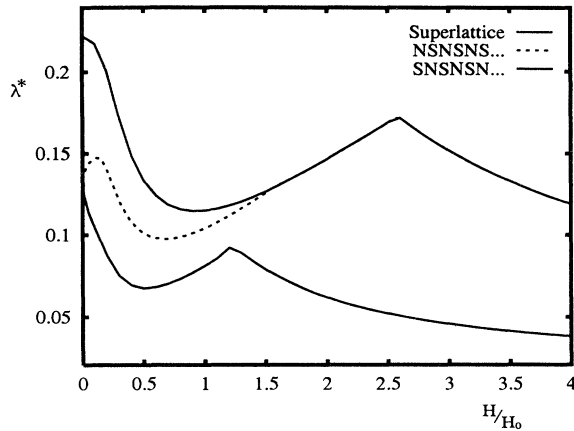


FIG. 4. Plot of the minimum eigenvalue λ^* as a function of the applied magnetic field, for the superlattice and the semi-infinite ($NSN \dots$) and ($SNS \dots$) geometries for $\rho = 0.05$.

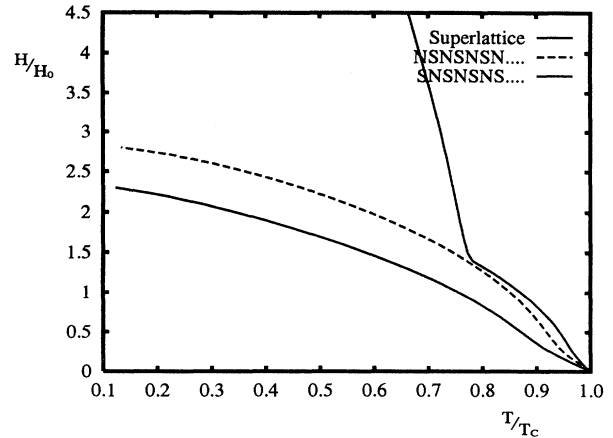


FIG. 5. Upper critical field curves for the superlattice and the semi-infinite ($NSN \dots$) and ($SNS \dots$) geometries for $\rho = 0.1$.

is the basis for the novel crossover behavior predicted by Takahashi and Tachiki⁷ and subsequently confirmed experimentally.^{4,5}

More interestingly, and indeed the substance of this paper is the modification of the functional dependence of the eigenvalue λ_0 on the parameter x_0 due to the presence of the free surface in this particular regime (i.e., modulation length $d \gtrsim$ magnetic coherence length ξ_H) and the corresponding values of x^* and λ^* obtained. In particular we find, not surprisingly, that in the case of the semi-infinite geometry we must distinguish between the case in which the first layer is clean ($NSN \dots$) shown in Fig. 1 and that in which the first layer is dirty ($SNS \dots$) shown in Fig. 2. In the case of the former ($NSN \dots$) the two sets of results ($\rho = 0.05$, $\rho = 0.1$) show some interesting differences. For the case $\rho = 0.1$ we find that as the functional form for λ_0 begins to develop multiple minima, with increasing H , then the nucleation center x^* is located initially in the first N layer but then shifts to the first S layer with increasing magnetic field. This shift in the nucleation center gives rise to the discontinuity in slope of the curve of λ^* with magnetic field H/H_0 , shown in Fig. 3 for the $NSN \dots$ geometry. The resultant critical field curve is shown in Fig. 5 and is seen to correspond closely to the upper critical field curve obtained for the equivalent infinite superlattice also shown in Fig. 5. Note that for both the superlattice and the $NSN \dots$ geometry that for this particular value of ρ the applied field H at which the discontinuity of the eigenvalue λ^* appears in less than the zero temperature upper critical field. Consequently the discontinuous behavior of the eigenvalue λ^* does not manifest itself in the temperature dependence of the upper critical field in either the superlattice or $NSN \dots$ geometries. The results obtained in the $NSN \dots$ geometry for the case $\rho = 0.05$ show a somewhat different behavior. In this instance we find as before that as the functional dependence of λ_0 begins to develop multiple minimum with increasing magnetic field

the nucleation center is located in the first N layer. As the magnetic field H is increased further the nucleation center then shifts to a clean N layer in the center of the sample, thus we observe a crossover from nucleation at the surface to nucleation in the bulk of the sample. This gives rise to the very shallow discontinuity in the slope of the curve λ^* versus H shown in Fig. 4. As the magnetic field is increased further the nucleation center shifts again to the first S layer, giving rise to a second discontinuity in the slope of the curve λ^* versus H . The resultant critical field curve is presented in Fig. 6 and shows the effect of the shifts in the nucleation center. For the particular parameters considered here the first shift in the nucleation center at the crossover from surface nucleation to nucleation in bulk has very little quantitative effect on the calculated upper critical field curve and hence would be very difficult to detect experimentally from measure-

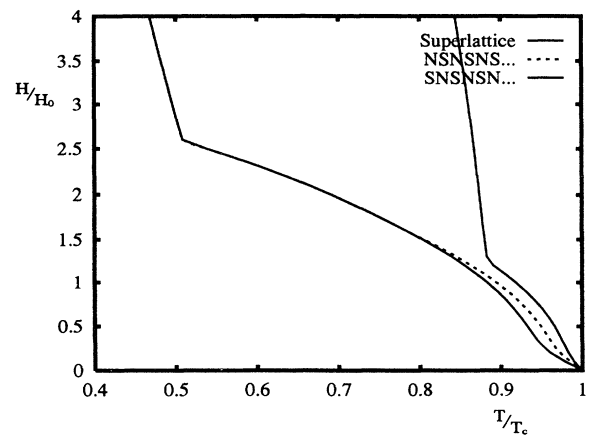


FIG. 6. Upper critical field curves for the superlattice and the semi-infinite ($NSN \dots$) and ($SNS \dots$) geometries for $\rho = 0.05$.

ments of the upper critical field. However it may be that, for a different choice of parameters, the effect is more distinct.

The close correspondence between the upper critical field curve obtained for the $NSN \dots$ geometry and the equivalent infinite superlattice, exhibited by the curves shown in Figs. 5 and 6, is of some importance since it is the $NSN \dots$ geometry that has been examined experimentally and our results support the reasonable assertion that for such geometries the upper critical fields H_{c2} and H_{c3} will differ but little.

In the case of the $(SNS \dots)$ in Fig. 2 geometry we find that, as the functional dependence of λ_0 begins to develop multiple minima with increasing magnetic field H , the nucleation center x^* occurs in the first N layer for both $\rho = 0.1$ and $\rho = 0.05$. As the applied magnetic H field is increased the nucleation center shifts from the first N layer to the first S layer. However due to the attractive character of the free surface the shift in the nucleation center occurs at a much lower value of H than in either the $NSN \dots$ geometry or the infinite superlattice geometry. The resultant critical field curves, for the case $\rho = 0.05$, are shown in Fig. 6 and show that the discontinuity in the upper critical field curve occurs at a much lower value than in the corresponding NSN geometry and the infinite superlattice geometry. The resultant critical field for the case $\rho = 0.1$ is shown in Fig. 5. The presence of the free surface is seen to give rise to a discontinuity in the slope of the upper critical field that does not manifest itself in either the corresponding $NSN \dots$ geometry or the infinite superlattice geometry. Thus we see from the results presented in Figs. 5 and 6, the crossover effect predicted by Takahashi and Tachiki⁷ is considerably enhanced by the presence of the free surface in the case of the $(SNS \dots)$ geometry. Equivalently we can regard this as the enhancement of H_{c3} by the superlattice geometry.

IV. CONCLUSIONS

We have examined the effect of a free boundary on the upper critical field of a superconducting superlattice consisting of alternating layers with different electron diffusion coefficients. For the range of parameters studied we find that in the $(NSN \dots)$ geometry, in which the initial layer is a clean (N) layer, the upper critical field is very close to the value obtained in the case of the infinite superlattice and hence $H_{c2} \sim H_{c3}$. In particular the temperature at which the discontinuity in the slope in the upper critical field occurs is relatively insensitive to the presence of the free surface. This is consistent with

claims made in the literature regarding the interpretation of the experiment data. More interestingly perhaps we find in the case of the $(SNS \dots)$ geometry, in which the initial layer is a dirty (S) layer the upper critical field deviates significantly from the value measured in the case of the infinite superconductor and hence $H_{c3} > H_{c2}$. Moreover the crossover effect predicted by Takahashi and Tachiki⁷ is significantly enhanced and occurs at a much higher temperature and is manifest for a much wider range of parameters. This suggests that some further experimental work comparing the $(NSN \dots)$ geometry and the $(SNS \dots)$ may provide valuable tests of existing theoretical models.

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APPENDIX A

We wish to show how Eqs. (9) and (10) may be solved, subject to the appropriate boundary conditions, in the limit $H \rightarrow 0$ and the minimum eigenvalue λ^* obtained.

In the limit $H \rightarrow 0$ the magnetic coherence length ξ_H goes to infinity hence the reduced thickness of the layers ($\delta = d/\xi_H$), with d being the physical thickness of a layer N or S , becomes vanishingly small. In this limit Eqs. (9) and (10) are well approximated by the linearized difference equations

$$g(x_i) = g(x_{i+1}) - \delta \left[\frac{1}{4} x_{i+1}^2 - \frac{1}{2} \lambda - g^2(x_{i+1}) \right], \quad x \in N, \quad (\text{A1})$$

$$g(x_i) = g(x_{i+1}) - \delta \left(\frac{1}{4} \rho x_{i+1}^2 - \frac{1}{2} \lambda - \frac{1}{\rho} g^2(x_{i+1}) \right), \quad x \in S. \quad (\text{A2})$$

To solve these linearized equations in the limit $\delta \rightarrow 0$ we apply the coarse-graining procedure developed in the analysis of self-similar multilamellar lattice structures.¹³ The technique considers the superlattice as an alternating sequence of S (SNS) and N (NSN) trilayers. Using the continuity of the logarithmic derivative g at the interface between the layers, together with difference equations, Eqs. (A1) and (A2), it is possible to obtain a set of rescaled equations for the superlattice composed of alternating trilayers, namely,

$$g(x_i) = g(x_{i+1}) - D(1) \left(\frac{1}{4} \beta(1) x_{i+1}^2 - \frac{1}{2} \lambda - \frac{\alpha(1)}{\rho} g^2(x_{i+1}) \right), \quad x \in N, \quad (\text{A3})$$

$$g(x_i) = g(x_{i+1}) - D(1) \left(\frac{1}{4} \alpha(1) x_{i+1}^2 - \frac{1}{2} \lambda - \frac{\beta(1)}{\rho} g^2(x_{i+1}) \right), \quad x \in S, \quad (\text{A4})$$

with

$$D(1) = 3\delta,$$

$$\alpha(1) = \frac{1}{3}(2\rho + 1), \quad (\text{A5})$$

$$\beta(1) = \frac{1}{3}(2 + \rho).$$

Repeating the procedure m times yields the equations

$$g(x_L) = g(x_R) - D(m) \left(\frac{1}{4}\beta(m)x_R^2 - \frac{1}{2}\lambda - \frac{\alpha(m)}{\rho}g^2(x_R) \right), \quad x \in N, \quad (\text{A6})$$

$$g(x_L) = g(x_R) - D(m) \left(\frac{1}{4}\alpha(m)x_R^2 - \frac{1}{2}\lambda - \frac{\beta(m)}{\rho}g^2(x_R) \right), \quad x \in S, \quad (\text{A7})$$

with

$$D(m) = 3D(m-1),$$

$$\alpha(m) = \frac{1}{3}[2\alpha(m-1) + \beta(m-1)], \quad (\text{A8})$$

$$\beta(m) = \frac{1}{3}[2\beta(m-1) + \alpha(m-1)].$$

The above equations may be solved and the explicit form for $D(m)$, $\alpha(m)$, and $\beta(m)$ obtained. We find that $\lim_{m \rightarrow \infty} [\alpha(m) - \beta(m)] = 0$ so that the above difference equations reduce to a single difference equation

$$g(x_L) = g(x_R) - D(m) \left(\frac{1}{4}\gamma x_R^2 - \frac{1}{2}\lambda - \frac{\gamma}{\rho}g^2(x_R) \right), \quad x \in N \text{ or } S, \quad (\text{A9})$$

where γ is defined as

$$\gamma = \lim_{m \rightarrow \infty} \alpha(m) = \lim_{m \rightarrow \infty} \beta(m) = \frac{1}{2}(1 + \rho). \quad (\text{A10})$$

Provided $D(m)$ is sufficiently small we can approximate the above difference equation by the differential equation

$$\frac{dg(x)}{dx} = -\frac{\gamma}{\rho}g^2(x) + \frac{1}{4}\gamma x^2 - \frac{1}{2}\lambda. \quad (\text{A11})$$

By defining

$$g_R(x) = \frac{\gamma^{1/2}}{\rho^{3/4}}g(x),$$

$$x_R = \frac{\gamma^{1/2}}{\rho^{1/4}}x, \quad (\text{A12})$$

$$\lambda_R = \rho^{-1/2}\lambda,$$

we can rescale Eq. (A11) as

$$\frac{dg_R(x_R)}{dx_R} = -g_R^2(x_R) + \frac{1}{4}x_R^2 - \frac{1}{2}\lambda_R. \quad (\text{A13})$$

Applying Eq. (A13) to a superlattice geometry yields the result of $\lambda_R = 1$ and thus $\lambda = \sqrt{\rho}$. For the semi-infinite superlattice ($NSN \dots$) or ($SNS \dots$) with the boundary condition at free surface $g_R(0) = 0$, the eigenvalue can be readily calculated to give⁸

$$\begin{cases} x_R = \sqrt{0.59010}, & h \rightarrow 0 \\ \lambda_R = 0.59010, \end{cases} \quad (\text{A14})$$

and hence

$$x = \left(\frac{0.5091\sqrt{\rho}(1+\rho)}{2} \right)^{1/2}, \quad h \rightarrow 0 \quad (\text{A15})$$

while

$$\lambda = 0.59010\sqrt{\rho}, \quad h \rightarrow 0. \quad (\text{A16})$$

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