The problem of raising T_c for superconductors: an approach based on surface effects

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It is possible to approach the problem of computing T_c for complex compounds by starting with spatially inhomogeneous systems: first, consider a structure made up of macroscopic blocks of size $L \gg a$ (where a is the interatomic spacing), and then make the extrapolation $L \to a$. A general theorem for the Gor'kov equation implies that when T_c is computed for such a block structure, neglect of transitional behavior of all physical quantities at boundaries results in a value of T_c which cannot exceed the largest value of T_c for the constituent materials of the structure. However, this bound is removed when we take into account surface effects, a fact that makes them important for problems of high-temperature superconductivity. In this paper, we use general expressions obtained in Refs. 6 and 7 to investigate surface contributions to T_c for a periodic structure consisting of alternating layers of two metals 0 and 1 with quadratic spectra. We discuss three possible differences between the spectra of metals 0 and 1: (a) different energies for the bottoms of the conduction band, (b) different longitudinal masses, and (c) different transverse masses. All these differences lead to nontrivial oscillatory behavior of T_c as we vary the thickness d of the layers of material 1. Based on this dependence $T_c(d)$, we predict the maximum value of T_c, discuss its dependence on the parameters of metals 0 and 1, and identify factors that favor or hinder increasing this value. At the same time, the contents of this paper may be regarded as a systematic theory of the effect of quantum oscillations in T_c first discussed by Kagan and Dubovskii.[14]

1. INTRODUCTION

An ideal theory of superconductivity should make it possible to calculate the transition temperature T_c for an arbitrary material. In principle, there is a well-known algorithm for performing this calculation "from first principles," i.e., starting only from knowledge of the atoms entering into the compound and their positions in space (see, e.g., Ref. 1); however, it requires tedious numerical calculations for each specific material. Therefore, the search for compounds with high T_c is reduced to systematic trials, as in an experimental investigation. For this reason, a need has arisen for a cruder method whose use could yield some sort of qualitative pattern.

It is possible to approach the problem of calculating T_c for complex compounds by starting with spatially inhomogeneous systems. For example, we replace a lattice made of alternating A and B atoms (Fig. 1a) with a system made up of macroscopic blocks of bulk materials A and B (Fig. 1b), assuming that the size L of a block is large compared to the interatomic spacing a. We then extrapolate down to $L \sim a$ at the end of the calculation, which marks the limit of the region of applicability of the latter. For $L \gg a$ we may use information about the bulk properties of materials A and B, which leads to a great saving in computation (it is known that in first-principles calculations most of the computer time is expended not in calculating T_c but in "constructing" the solid out of atoms).

In order to obtain nontrivial results in this approach, we require a systematic analysis of surface effects. The point is that when the transitional behavior of all physical quantities is neglected at the boundaries for any block structure of type Fig. 1b (independent of the number of materials or the shape of the blocks that make up the structure), the value of $T_c \equiv T_c^{\text{vol}}$ obtained will lie in the interval

$$T_{\min} \leqslant T_c^{\text{vol}} \leqslant T_{\max}, \tag{1}$$

i.e., between the minimum and maximum bulk transition temperatures of the materials that make up the structure. In particular, T_c^{vol} may not exceed $T_{\max}$. This result clearly follows from the intuitive picture of superconductivity in a spatially inhomogeneous system in which the effective interaction constant λ that enters into the BCS formula $T_c \sim \omega_0 \exp(-1/\lambda)$ arises from some type of volume averaging. Specific recipes for averaging have been obtained in special cases by Cooper,[2] De Gennes,[3] Kirzhnits and Maksimov,[4] and one of the authors;[5] in fact, the inequality (1) is a consequence of a general theorem for the Gor'kov equation[1)] (see Sec. 2).

Surface effects may be taken into account heuristically by assuming that there is a layer of thickness $\sim a$ at the boundary between materials A and B (Fig. 1b), made of a third material. Then averaging of λ over the system volume[2)] gives the following expression for T_c:

$$T_c = T_c^{\text{vol}} + T_s \frac{a}{L}. \tag{2}$$

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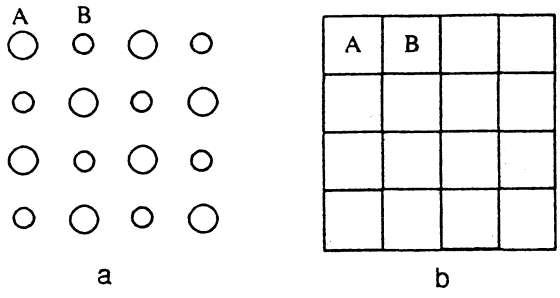

FIG. 1. We may replace a lattice made up of atoms A and B (a) by a system made up of macroscopic blocks of materials A and B (b), taking at the end of the calculation the extrapolation $L \to a$.

Taking the limit $L \to a$ gives $T_c - T_c^{vol} \sim T_s$, so that once we know the value of T_s, we can decide how good our chances are of increasing T_c for the system above T_{max}. Of course, it is impossible to predict T_c with any serious degree of accuracy in this approach; however, we can separate out the promising situations (large positive T_s) from the non-promising ones, and thereby determine a direction to search in.

In what follows, we will discuss systems with spatial variation mogeneity in one direction, which are simpler to investigate both theoretically and experimentally. That is, we introduce thin layers of material 1 into a bulk superconductor 0, layers with thickness d and a distance L between them; we assume $d \ll L \ll \xi_0$, where ξ_0 is the coherence length. Let superconductor 0 be a high-temperature material in which $T_c = T_{c0}$; the question we will pose is whether it is possible to increase T_c by introducing layers of a very "bad" material 1, i.e., under the conditions

$$V_1 N_1 \leqslant V_0 N_0, \tag{3}$$

where V_0, V_1 and N_0, N_1 are constants for the four-fermion interaction and density of states of materials 0 and 1. For $d \ll L$ we can investigate surface effects by using the expressions obtained in Refs. 6 and 7 for T_c, which follow from the Gor'kov equations without any assumptions except smallness of the parameter d/L. These expressions have been used previously to investigate localization of the order parameter,[6,7] coherent interaction between planar defects,[6] and enhancement of the singularities in T_c over and above the singularities in the density of states.[9]

As to investigating how T_c for a compound depends functionally on the characteristics of the elements that make it up, this problem has not been posed seriously in the literature due to its obvious complexity and the absence of constructive concepts. The approach we propose here allows significant progress to be made in this direction, which we will demonstrate below for the example of a model in which the spectra of materials 0 and 1 are quadratic:

$$\varepsilon_0(k_\parallel, k_z) = \frac{k_\parallel^2}{2M} + \frac{k_z^2}{2m}, \quad \varepsilon_1(k_\parallel, k_z) = U + \frac{k_\parallel^2}{2M_1} + \frac{k_z^2}{2m_1}, \quad k_\parallel = (k_x, k_y) \tag{4}$$

(we distinguish the longitudinal (M, M_1) and transverse (m, m_1) masses because they enter into the equations in different ways); the boundary conditions for the wave function $\varphi(z)$ of the transverse motion that arises after separation of variables $[\Psi(r) = \exp(ik_\parallel r_\parallel)\varphi(z),\ r_\parallel = (x,y)]$ has the form

$$\varphi'(+0) - \varphi'(-0)\frac{m}{m_1} = \kappa\varphi(0), \quad \varphi(+0) = \varphi(-0) \tag{5}$$

(if materials 0 and 1 are in the regions $z > 0$ and $z < 0$ respectively); the parameter κ describes the surface potential at the boundary, which is approximated by a δ function.

If material 1 is a metal, then T_c of the system will be an oscillatory function of d; this quantum-oscillations effect, which is observed on films with coatings,[10-12] sandwiches,[10] and superlattices,[13] was discussed theoretically by Kagan and Dubovskii.[14] We recently showed[15] that the qualitative picture that follows from Ref. 14 requires a radical reexamination, and that the experiments of Refs. 10–12 should be interpreted based on two physical mechanisms—interference between de Broglie waves reflected from the two surfaces of the defect[3)] (Ref. 8), and interference at one defect determined by the jump in the order parameter at the other.[15] A critique of the quantitative aspects of Ref. 14 was given previously in Ref. 7; here we note only that when the proximity effect is ignored in an uncontrolled way, terms $\sim d/L$ are lost when we are investigating effects that are $\sim a/L$. In this paper we will attempt a systematic description of the quantum-oscillation effect. In particular, we will show that these oscillations may arise from any difference in the spectra of materials 0 and 1, viz., differences in (a) positions of the bottom of the bands $(U \neq 0)$, (b) transverse mass $(m \neq m_1)$ or (c) longitudinal mass $(M \neq M_1)$, just like the presence of a δ-function-like potential (d) at the boundary $(\kappa \neq 0)$. For simplicity and clarity we will discuss the role of each of these factors individually: cases (a)–(c) are treated in Secs. 4–6. Case (d) was already discussed previously in Ref. 8. Interest in the effect of quantum oscillations for this problem stems from the fact that the position of the first maximum in the oscillations and the value of T_c at this maximum are convenient measures of the surface contribution to T_c, and as such can indicate whether or not it is possible to increase T_c (Sec. 7).

2. AN INEQUALITY FOR T_c^{vol}

If we incorporate into our description of spatially inhomogeneous superconductors assumptions that are characteristic of the BCS theory (e.g., a pointlike interaction with a high-frequency cutoff), then T_c is determined by the conditions for the occurrence of a nontrivial solution to the Gor'kov equation:[17]

$$\Delta(\mathbf{r}) = V(\mathbf{r}) \int K(\mathbf{r}, \mathbf{r}')\Delta(\mathbf{r}')d\mathbf{r}', \tag{6}$$

where $\Delta(\mathbf{r})$ is the superconducting order parameter, $V(\mathbf{r})$ is the coordinate-dependent constant of the four-fermion interaction, and $K(\mathbf{r},\mathbf{r}')$ is the superconducting kernel, which in the absence of magnetic effects is positive and symmetric, and also satisfies the sum rule:[3,17]

$$\int d\mathbf{r}' K(\mathbf{r},\mathbf{r}') = N(\mathbf{r}) \ln \frac{1.14\omega_0}{T}, \tag{7}$$

where $N(\mathbf{r})$ is the local density of states:

$$N(\varepsilon,\mathbf{r}) = \sum_n |\Psi_n(\mathbf{r})|^2 \delta(\varepsilon - \varepsilon_n) \tag{8}$$

at the Fermi level; $\Psi_n(\mathbf{r})$ and ε_n are the single-particle eigenstates and eigenvalues. If a dimensionless interaction constant is introduced through the relation $\lambda(\mathbf{r}) = V(\mathbf{r})N(\mathbf{r})$, then for T_c the BCS expression $T_c = 1.14\omega_0 \exp(-1/\lambda_{\text{eff}})$ is valid with a constant λ_{eff} that satisfies the inequality

$$\min \lambda(\mathbf{r}) \leqslant \lambda_{\text{eff}} \leqslant \max \lambda(\mathbf{r}). \tag{9}$$

In order to prove (9) we make the system discrete, dividing it into small blocks with volume Ω and assigning to the indices i and j values that refer to the ith and jth blocks. Setting

$$K_{ij} = L_{ij} \ln \frac{1.14\omega_0}{T}, \qquad \frac{1}{\lambda} = \ln \frac{1.14\omega_0}{T}, \tag{10}$$

we rewrite (6) in the form

$$\lambda \Delta_i = V_i \Omega \sum_j L_{ij} \Delta_j. \tag{11}$$

It is not difficult to see that λ_{eff} equals the maximum eigenvalue of the Eq. (11). Let us consider two cases individually.

(a) If $V(\mathbf{r}) \geqslant 0$ for all $\mathbf{r}$, then λ_{eff} is the maximum eigenvalue of a positive matrix and lies in the interval between the minimum and maximum of the row-by-row sums:[18]

$$\min \Omega V_i \sum_j L_{ij} \leqslant \lambda_{\text{eff}} \leqslant \max \Omega V_i \sum_j L_{ij}. \tag{12}$$

Returning to the continuous variables and taking (7) into account, we obtain (9).

(b) Let $V(\mathbf{r})$ be an indefinite function. We make use of a theorem for generalized eigenvalue problems $\hat{A}y = \lambda \hat{B}y$ (see Ref. 19, pp. 439, 442): if $\hat{A}$ and $\hat{B}$ are hermitian operators, and $\hat{B}$ is positive definite, then addition to $\hat{A}$ of a positive definite hermitian operator cannot decrease even one of the eigenvalues. Using the replacement $y_i = \Sigma_j L_{ij} \Delta_j$, we reduce (11) to this form; then the operators $\hat{A}$ and $\hat{B}$ are determined by the matrices $\|\Omega V_i \delta_{ij}\|$ and $\|L_{ij}^{-1}\|$. We set $\tilde{V}_i = \max(V_i, 0)$; then for the problem (11) with $\tilde{V}_i$ in place of V_i, the maximum eigenvalue lies in the interval from 0 to $\max \tilde{V}_i N_i = \max \lambda_i$; however, this eigenvalue cannot decrease in passing from V_i to $\tilde{V}_i$, so $\lambda_{\text{eff}} \leqslant \max \lambda_i$. A lower-bound estimate for λ_{eff} is not of interest in this case, because the minimum possible value $T_c = 0$ is admissible in view of the admissibility of $\lambda_{\text{eff}} = 0$.

For the block structure of Sec. 1, when we neglect transitional behavior near the boundaries the function $\lambda(\mathbf{r})$ takes on only discrete values λ_i, which equal the bulk values for the materials that make up the structure; therefore, λ_{eff} lies between the minimum and maximum values of λ_i and inequality (1) for T_c is valid.

3. EXPRESSIONS FOR THE SURFACE CONTRIBUTION TO T_c

By treating the layers of material 1 as planar defects, we can use the results of Refs. 6 and 7. In the absence of bound states near a planar defect, the following expression for T_c is valid:

$$\frac{\delta T_c}{T_{c0}} = \frac{T_c - T_{c0}}{T_{c0}} = \frac{1}{\lambda_0^3 L} \int dz V_0 N(z) [V(z)N(z) - V_0 N_0], \tag{13}$$

where $\lambda_0 = V_0 N_0$, and $V(z)$ and $N(z)$ are the functions $V(\mathbf{r})$ and $N(\mathbf{r})$ introduced above, which depend only on z due to the one-dimensional geometry; the integration is carried out over the region that contains one planar defect.[6,7]

When m bound states are present near the planar defect (for fixed $k_\parallel$), T_c is determined by the condition for solvability of the system of $m+1$ equations (see Eqs. (4) and (5) of Ref. 8). If all the bound states are extended along material 1, i.e., they belong to the quasidiscrete spectrum, then we can obtain the following explicit expression for T_c:[7]

$$\frac{\delta T_c}{T_{c0}} = \frac{1}{\lambda_0^3 L} \left\{ \lambda_{cc} d + \frac{\lambda_1 - \lambda^*}{\lambda_0 - \lambda^*} \left(\lambda_{cq} d + \frac{V_0}{V_1} \lambda_{qc} a \right) + \left(\frac{\lambda_1 - \lambda^*}{\lambda_0 - \lambda^*} \right)^2 \frac{V_0}{V_1} \lambda_{qq} a \right\}, \tag{14}$$

where the parameters λ_{cc}, λ_{cq}, λ_{qc}, and λ_{qq} (see Eq. (29) of Ref. 7) are defined by the functions $N_c(z)$ and $N_{ql}(z)$ that enter into the decomposition

$$N(z) = N_c(z) + N_{ql}(z), \tag{15}$$

which in turn is defined by Eq. (8), which contains only states of the continuous or quasidiscrete spectrum respectively. The functions $N_c(z)$ and $N_{ql}(z)$ have the values N_0 and 0 in material 0, while in material 1 they have the values N^{**} and N^* (here $N_1 = N^* + N^{**}$) and change at the boundary on scales a_c and a_{ql} respectively: $\lambda_1 = V_1 N_1$, $\lambda^* = V_1 N^*$. Equation (14) becomes incorrect for $\lambda_0 \approx \lambda^*$, due to the "Anderson transition" mentioned in Ref. 5, in which localization of the order parameter takes place in layers of material 1, so that for $\lambda^* > \lambda_0$ we have (Ref. 7)

$$T_c = T^* \left(1 + \frac{\lambda_{qq} a}{\lambda^{*3} d} \right), \tag{16}$$

where $T^* = 1.14\omega_0 \exp(-1/\lambda^*)$. Analysis shows that Eq. (16) remains valid for $\lambda^* < \lambda_0$ if the expression on the right side exceeds T_{c0} by an amount $\sim \sqrt{d/L}$; Eq. (14) holds if we have $d \gg a_c, a_{ql}$ and the right side of (16) is smaller than T_{c0} by an amount $\sim \sqrt{d/L}$. For the case $a_c \gg a_{ql}$, in order to describe the region $a_{ql} \ll d < a_c$ we must replace (14) by a more general expression

$$\frac{\delta T_c}{T_{c0}}=\frac{1}{\lambda_0^3 L}\left\{\lambda_{cc}d+\frac{\bar{\lambda}_c}{\lambda_0-\lambda^*}\lambda_{cq}d+\left(\frac{\bar{\lambda}_c}{\lambda_0-\lambda^*}\right)^2\frac{V_0}{V_1}\lambda_{qq}a\right\},\tag{17}$$

which we obtain by analogy with (14), and which is valid for $d\gg a_{ql}$. The quantity

$$\bar{\lambda}_c=\lambda_0(\lambda^*)^{-1}\int dz V_1 K_{ql}(0,z)V(z)N_c(z)$$

is not solely a function of $N_{ql}(z)$ and $N_c(z)$ ($K_{ql}(z,z')$ is a kernel constructed from states of the quasidiscrete spectrum[7]), although usually the following result is sufficient:

$$K_{ql}(0,z)=N_{ql}(z)\ /d\ \ln(1.14\omega_0/T)+O(a_{ql}/d),$$

which follows from the sum rule (7).

In Eqs. (13) and (14) we can identify the general term that is linear in d/L, which corresponds to the quantity T_c^{vol} introduced above and which coincides with the results of Ref. 5; the remaining contribution $\sim a/L$ is a surface effect, and is the subject of investigation of the present paper.

The functions $N_c(z)$ and $N_{ql}(z)$ need only be known in the vicinity of the planar defects; therefore, it is sufficient to consider a sandwich containing material 1 for $|z|<d/2$ and material 0 for $d/2<|z|<L/2$, with zero boundary conditions at the points[4] $z=\pm L/2$, and boundary conditions of type (5) at the points $z=\pm d/2$, after which the computations are analogous to Ref. 8. We will consider the quantity $V(z)$ to be piece-wise-constant, taking on the value V_1 for $|z|<d/2$ and V_0 for $|z|>d/2$, assuming that V_1 satisfies the inequality (3); since an increase in V_1 for fixed distribution of electronic states leads to an increase[5] in T_c, the maximum T_c is attained for $N_1V_1=N_0V_0$, i.e., $\lambda_1=\lambda_0$, for which the bulk effect is absent and δT_c is determined purely by the surface contribution. Therefore, in illustrating the results graphically we will pay special attention to the case $\lambda_1=\lambda_0$.

In the usual formulations, T_s is determined by the redistribution of electron density: this is quite natural since just such a redistribution takes place when chemical bonds are formed. In fact, our approach in this paper is a peculiar way to describe chemical bonding.

4. SURFACE EFFECTS ASSOCIATED WITH DIFFERENT POSITIONS OF THE BOTTOM OF THE BAND ($U\neq 0$, $m=m_1$, $M=M_1$, $\kappa=0$)

In this paper we limit ourselves to discussing metallic layers. In what follows, ε_F is understood to mean the Fermi energy measured from the bottom of the band of material 0, while k_F and q_F are the transverse Fermi wave vectors of materials 0 and 1.

4.1. The case $\varepsilon_F-U\ll\varepsilon_F$

For $U>0$ the single-particle wave functions either extend throughout the system (A), or extend into material 0 but decay toward the interior of material 1 (B); in accordance with this, it is convenient to decompose $N(z)$ as follows:

$$N(z)=N_A(z)+N_B(z),\tag{18}$$

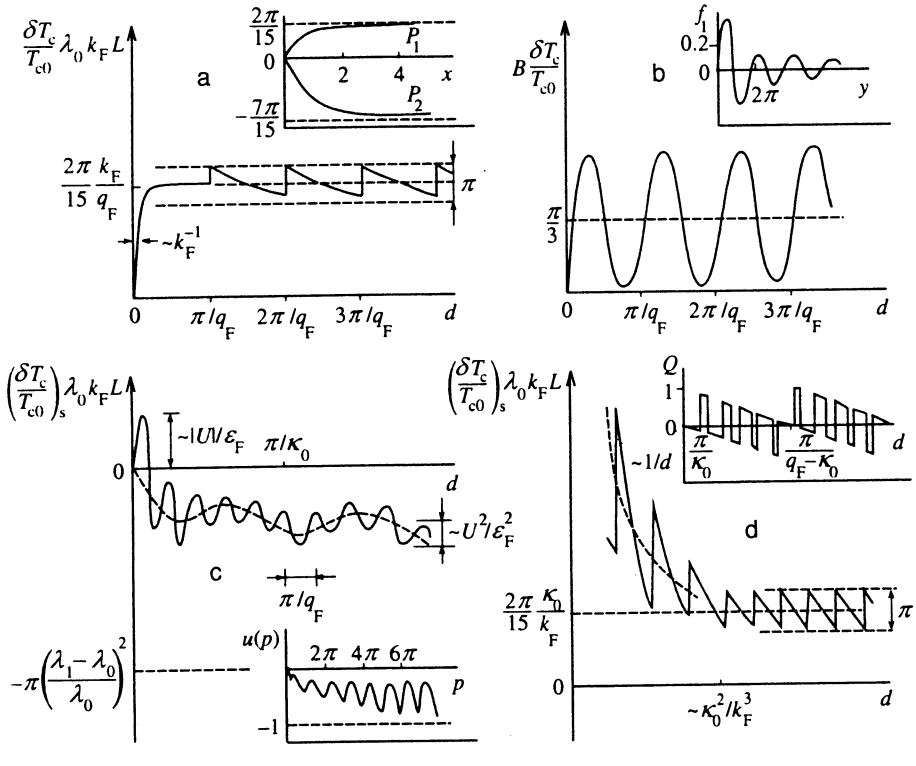

FIG. 2. Dependence of T_c on d for materials 0 and 1 that differ by the position of the band minimum for the following cases: (a) $\varepsilon_F-U\ll\varepsilon_F$, $\lambda_1=\lambda_0$; (b) $0<U\ll\varepsilon_F$, $\lambda_1=\lambda_0$; $\beta=16\varepsilon_F^2U^{-2}\lambda_0k_FL$; (c) $U<0$, $|U|\ll\varepsilon_F$, $\lambda_1<\lambda_0$; and (d) $U<0$, $|U|\ll\varepsilon_F$, $\lambda_1=\lambda_0$. In the insets we show the functions $P_1(x)$, $P_2(x)$, $f_1(y)$, $u(p)$, and $Q(d)$ entering into Eqs. (24), (32), (43), (47), and (48).

where $N_A(z)$ and $N_B(z)$ are determined by the expressions

$$N_A(z)=\frac{M}{(2\pi)^2}\int_0^{q_F}dq\,\frac{q}{k}\,H(k,q,z)|_{k=\sqrt{k_0^2+q^2}}, \tag{19}$$

$$N_B(z)=\frac{M}{(2\pi)^2}\int_0^{k_0}dq\,\frac{q}{k}\,H(k,iq,z)|_{k=\sqrt{k_0^2-q^2}}, \tag{20}$$

here

$$k_0=\sqrt{2mU},\quad q_F=\sqrt{k_F^2-k_0^2},\quad k_F=\sqrt{2m\varepsilon_F}, \tag{21}$$

while the function $H(k,q,z)$ has the form

$$H(k,q,z)=\begin{cases}2k^2\left(\dfrac{\cos^2(qz)}{u^+(k,q)}+\dfrac{\sin^2(qz)}{v^+(k,q)}\right), & |z|<d/2,\\ 2+\cos(2kz')\left[\dfrac{u^-(k,q)}{u^+(k,q)}+\dfrac{v^-(k,q)}{v^+(k,q)}\right]\\ +kq\sin(2kz')\sin(qd)\left[-\dfrac{1}{u^+(k,q)}+\dfrac{1}{v^+(k,q)}\right], & z'=|z|-d/2>0,\end{cases}$$

$$u^{\pm}(k,q)=k^2\cos^2(qd/2)\pm q^2\sin^2(qd/2),$$

$$v^{\pm}(k,q)=k^2\sin^2(qd/2)\pm q^2\cos^2(qd/2). \tag{22}$$

In the case $\varepsilon_F-U\ll\varepsilon_F$, the parameter q_F/k_0 is small and the expression for $N_A(z)$ in the integrand is localized near the point $q_s=\pi s/d$ [in these computations it is convenient to combine the fractions in (22)] and can be approximated by a set of δ functions; to lowest order in q_F/k_0 we obtain

$$N_A(z)=\begin{cases}N_0\dfrac{\pi}{k_Fd}\displaystyle\sum_{s=1}^{Q}[1-(-1)^s\cos(2q_sz)], & |z|<d/2\\ 0, & |z|>d/2\end{cases}, \tag{23}$$

where $Q=[q_Fd/\pi]$, and [...] is the integer part of a number. Substituting the decomposition (18) into Eq. (13), we obtain integrals that are linear and bilinear combinations of $N_A(z)$ and $N_B(z)$. The integrals involving only $N_A(z)$ and $N_B^2(z)$ are computed by using (23): the integral involving $N_A(z)N_B(z)$ is small over the range $|z|<d/2$ (because $N_A(z)$ reduces to zero at $z=\pm d/2$ and increases toward the interior of material 1 to a value $\sim N_0q_Fd/k_0$ over a scale q_F^{-1}, while $N_B(z)$ decreases from a value $\sim N_0$ at $z=\pm d/2$ to zero over a scale k_0^{-1}), and in the range $|z|>d/2$ it reduces to zero by virtue of (23). The integrals involving $N_B(z)$ and $N_B^2(z)^2$ can be made dimensionless and computed numerically. As a result we obtain for T_c

$$\frac{\delta T_c}{T_{c0}}=\frac{1}{\lambda_0k_FL}\left\{\left(\frac{\lambda_1}{\lambda_0}-1\right)q_Fd+f(q_Fd/\pi)+\frac{V_1}{V_0}P_1(k_0d)+P_2(k_0d)\right\}, \tag{24}$$

where the term linear in d agrees with Ref. 5, and

$$f(x)=\pi\{x\}+\pi\frac{\lambda_1}{\lambda_0}\left(\frac{1}{2}-2\{x\}+\frac{2\{x\}-1}{2x}\{x\}\right) \tag{25}$$

(here {...} is the fractional part of a number); the functions $P_1(x)$ and $P_2(x)$, which are shown in the inset to Fig. 2a, have the asymptotic forms

$$P_1(x)=\begin{cases}x, & x\ll1\\ 2\pi/15, & x\gg1\end{cases}\qquad P_2(x)=\begin{cases}-3x/2, & x\ll1\\ -7\pi/15, & x\gg1\end{cases}. \tag{26}$$

Thus, the dependence of T_c on d contains: (a) a contribution that is linear in d; (b) oscillations with period πq_F^{-1} that have a sawtooth shape due to the smallness of the transmission coefficient of the boundary (see Ref. 8); and (c) transitional behavior over a scale $k_0^{-1}\approx k_F^{-1}$. For $\lambda_1=\lambda_0$ we have $V_0/V_1=k_F/q_F\gg1$; hence, the transitional behavior is determined by the function $P_1(x)$, and the amplitude of the oscillations is small compared to the constant contribution (Fig. 2a). To leading order, the maximum value of T_c equals

$$\left(\frac{\delta T_c}{T_{c0}}\right)_{\max}=\frac{1}{\lambda_0k_FL}\frac{2\pi}{15}\sqrt{\frac{\varepsilon_F}{\varepsilon_F-U}} \tag{27}$$

and is attained over the entire region $d\gtrsim k_F^{-1}$.

4.2. The case $0<U\ll\varepsilon_F$

As in the previous section, the local density of states is determined by Eqs. (18)–(22), only now we have $k_0\ll k_F\ll q_F$. Let us decompose $N_A(z)$ as follows:

$$N_A(z)=\begin{cases}2q_FM/(2\pi)^2+F(z)+G(z), & |z|<d/2\\ (2k_F-2k_0)M/(2\pi)^2+F(z)+G(z), & |z|>d/2\end{cases}, \tag{28}$$

where

$$F(z)=\begin{cases}\dfrac{M}{(2\pi)^2}\displaystyle\int_0^{\infty}dq\left[\frac{q}{k}H(k,q,z)-2\right]_{k=\sqrt{k_0^2+q^2}} & |z|<d/2\\ \dfrac{M}{(2\pi)^2}\displaystyle\int_0^{\infty}dq\,\frac{q}{k}[H(k,q,z)-2]_{k=\sqrt{k_0^2+q^2}} & |z|>d/2\end{cases}, \tag{29}$$

and $G(z)$ is defined by analogous expressions with opposite signs and integration from q_F to ∞. By the methods of contour integration we can show (see the Appendix) that

$$F(z)=\begin{cases}-N_B(z), & |z|<d/2\\ 2k_0M/(2\pi)^2-N_B(z), & |z|>d/2,\end{cases} \tag{30}$$

so that

$$N(z)=\begin{cases}N_1+G(z), & |z|<d/2\\ N_0+G(z), & |z|>d/2.\end{cases} \tag{31}$$

In the expression for $G(z)$ we can also expand with respect to k_0/q over the entire range of integration $q\gg k_0$; substituting (42) into (21) (in this case $G^2(z)$ is written in the form of a double integral) and integrating over z, we obtain for T_c

$$\frac{\delta T_c}{T_{c0}}=\frac{1}{\lambda_0 k_F L}\left\{\left(\frac{\lambda_1}{\lambda_0}-1\right)q_F d+\left(\frac{\lambda_1}{\lambda_0}-1\right)\frac{U}{2\varepsilon_F}f_1(2q_Fd)+\frac{U^2}{16\varepsilon_F^2}f_2(2q_Fd)\right\}, \tag{32}$$

where the functions $f_1(y)$ and $f_2(y)$ are defined by the expressions

$$f_1(y)=y^2\int_y^\infty \frac{\sin x}{x^3}\,dx,$$

$$f_2(y)=\left(\frac{2\lambda_1}{\lambda_0}-1\right)\sin y+\frac{\pi}{3}+\frac{4\cos y}{y}-(12y^2+\pi y^3)\int_y^\infty\frac{\cos x}{x^4}\,dx+2y^3\int_y^\infty\frac{\sin x}{x^4}\ln\frac{x-y}{x+y}\,dx \tag{33}$$

and have asymptotic forms

$$f_1(y)=\begin{cases}y, & y\ll 1\\ \dfrac{\cos y}{y}, & y\gg 1\end{cases}$$

$$f_2(y)=\begin{cases}(2\lambda_1/\lambda_0+1)y, & y\ll 1\\ \dfrac{\pi}{3}+\left(\dfrac{2\lambda_1}{\lambda_0}-1\right)\sin y, & y\gg 1.\end{cases} \tag{34}$$

The dependence of T_c on d contains a linear term in accordance with Ref. 5, decaying oscillations $\sim U/\varepsilon_F$, and nondecaying oscillations $\sim(U/\varepsilon_F)^2$. When λ_1 and λ_0 differ significantly, the function $f_2(y)$ can be replaced by its asymptotic form for $y\gg 1$, while for $\lambda_1\approx\lambda_0$ we may set $\lambda_1=\lambda_0$ in the latter.[6] The dependence of T_c on d for $\lambda_1=\lambda_0$ determined by the functions $f_2(y)$, and the function $f_1(y)$, are shown in Fig. 2b; in the case $\lambda_1=\lambda_0$, the first maximum occurs for $d=1.1q_F^{-1}$, and the value of T_c in this case is

$$\left(\frac{\delta T_c}{T_{c0}}\right)_{\max}=0.13\,\frac{1}{\lambda_0 k_F L}\left(\frac{U}{\varepsilon_F}\right)^2. \tag{35}$$

4.3. The case $U<0$, $|U|\ll\varepsilon_F$

For $U<0$ the spectrum contains both continuum and quasi-discrete states; therefore, decomposition (15) of $N(z)$ is correct, where

$$N_c(z)=\frac{M}{(2\pi)^2}\int_{\kappa_0}^{q_F}dq\,\frac{q}{k}\,H(k,q,z)\Big|_{k=\sqrt{q^2-\kappa_0^2}} \tag{36}$$

with $\kappa_0=\sqrt{2m|U|}$ and $q_F=\sqrt{k_F^2+\kappa_0^2}$; for $N_{ql}(z)$ we have

$$N_{ql}(z)=\sum_s N_{2D}^s\,\frac{k_s}{k_s d+2}\times\begin{cases}[1-(-1)^s\cos(2q_sz)], & |z|<d/2\\ \dfrac{2q_s^2}{k_s^2+q_s^2}\exp(-2k_sz'), & z'=|z|-d/2>0,\end{cases} \tag{37}$$

where q_s is a root of the equation

$$\tan\left[\frac{q_sd}{2}+\frac{\pi(s+1)}{2}\right]=\frac{k_s}{q_s},\quad k_s=\sqrt{\kappa_0^2-q_s^2} \tag{38}$$

lying in the interval from zero to κ_0, and N_{2D}^s is the density of states at the Fermi level of the sth two-dimensional band, which in the present case equals $M/2\pi$. As in the previous case, we set

$$N_c(z)=\begin{cases}N_1-N^*+F(z)+G(z), & |z|<d/2\\ N_0+F(z)+G(z), & |z|>d/2,\end{cases} \tag{39}$$

where the function $F(z)$ is defined by expressions of type (29) with integration from κ_0 to ∞ and $k=\sqrt{q^2-\kappa_0^2}$, and $G(z)$ is defined by analogous expressions with the opposite sign and integration from q_F to ∞. By the methods of contour integration we can prove (see the Appendix) that

$$F(z)=\begin{cases}N^*-N_{ql}(z), & |z|<d/2\\ -N_{ql}(z), & |z|>d/2,\end{cases} \tag{40}$$

and the result (31) for $N(z)$ is correct as before.

The computation of T_c is carried out using Eqs. (4) and (5) of Ref. 8, in which $\lambda_{00}\sim\lambda_{0s}\sim\lambda_{s0}\sim 1$, and $\lambda_{ss'}\sim a/r_0$ for $s,s'\neq 0$, because the eigenfunctions $\varphi_s(z)$ are localized on a scale $r_0\sim\max(d,\kappa_0^{-1})$. By expanding with respect to T_c-T_{c0} and neglecting $\lambda_{ss'}$ for $s,s'\neq 0$, we obtain

$$\frac{\delta T_c}{T_{c0}}=\frac{1}{L}\left\{\frac{1}{\lambda_0^3}\int dz V_0N(z)[V(z)N(z)-V_0N_0]+\sum_{s=1}^m V_0N_{2D}^s\,\frac{\lambda_{s0}^2}{\lambda_0^4}\right\}. \tag{41}$$

The function $G(z)$ in (31) is the same as in the case $U>0$, and the first term in the curly brackets of (41) gives the result (32). For λ_{s0} we obtain to leading order in κ_0/k_F

$$\lambda_{s0}=(\lambda_1-\lambda_0)\int_{-d/2}^{d/2}dz|\varphi_s(z)|^2 \tag{42}$$

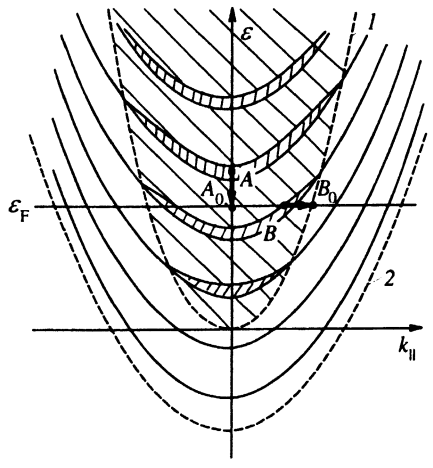

FIG. 3. The region $\varepsilon > k_\parallel^2/2M$ above curve *1* (crosshatched) corresponds to the continuous spectrum of material 0. The spectrum of material 1 lies in the region $\varepsilon > U + k_\parallel^2/2M_1$ above curve *2*, and consists of two-dimensional bands, i.e., size-quantized levels that depend on $k_\parallel$; these levels are true bound states below curve *1*, and are broadened levels above it. The two periods of oscillation correspond to passage of the point A through A_0 and the point B through B_0 for successive two-dimensional bands.

(we can neglect the function $G(z)$ in view of its localization near $z = \pm d/2$ over a scale k_F^{-1}). Substituting the expressions for $\varphi_s(z)$, after isolating the term linear in d we obtain for the surface contribution to T_c

$$\left(\frac{\delta T_c}{T_{c0}}\right)_s = \frac{1}{\lambda_0 k_F L}\left\{\left(\frac{\lambda_1}{\lambda_0}-1\right)\frac{U}{2\varepsilon_F} f_1(2q_F d) + \frac{U^2}{16\varepsilon_F^2} f_2(2q_F d) + \left(\frac{\lambda_1}{\lambda_0}-1\right)^2 \pi u\left(\frac{\kappa_0 d}{2}\right)\right\}, \tag{43}$$

where the functions $f_1(y)$ and $f_2(y)$ are the same as in (32); the function $u(p)$ (see the inset to Fig. 2c) is defined as follows:

$$u(p) = -\frac{2p}{\pi} + \sum_s \left(\frac{py_s + y_s^2}{1+py_s}\right)^2, \tag{44}$$

where $y_s = \sqrt{1-x_s^0}$, $x_s = q_s/\kappa_0$, and has the asymptotic form

$$u(p) = \begin{cases} -2p/\pi + O(p^4), & p \ll 1 \\ -\{2p/\pi\}, & p \gg 1 \end{cases}. \tag{45}$$

From (43) and Fig. 2c it is clear that, in contrast to the previous case, in addition to the oscillations with period π/q_F there is an oscillatory component with period π/κ_0. The origin of the two periods of oscillations is revealed in Fig. 3. The crosshatched region $\varepsilon > k_\parallel^2/2M$ corresponds to the continuous spectrum of material 0. The spectrum of material 1 lies in the region $\varepsilon > U + k_\parallel^2/2M_1$, and for small d it consists of two-dimensional bands, i.e., size-quantized levels that depend on $k_\parallel$; these levels are truly bound below the region of the continuous spectrum and are broadened within it. As d increases, the size-quantized levels are "squeezed out": the period π/q_F corresponds to the passage of successive broadened levels through the Fermi energy (passage of point A through A_0). The second period (which equals π/κ_0 for $M = M_1$) corresponds to the conversion of successive broadened (quasibound) levels into truly bound levels for $\varepsilon = \varepsilon_F$, i.e., to the passage of point B through B_0.

For $\lambda_1 = \lambda_0$, the dependence of T_c on d is found to be the same as in the previous case; accordingly, the result (35) for the maximum value of T_c remains valid.

4.4. The case $U<0$, $|U| \gg \varepsilon_F$

In this case we have $N^* - N_1 \ll N_1$, so that $T^* \approx T_{c1}$. Because λ_{qq} is positive (see below), for small d there is a region where Eq. (16) is applicable when $T_{c1} < T_{c0}$. In this case, an interesting situation arises: the order parameter "exits" the high-temperature superconductor 0 and passes into the "bad" superconductor 1. The reason for this is that states localized in material 1 behave like a sheet in a dielectric medium. Because of the large density of states $N^* = N_0\kappa_0/k_F \gg N_0$ and the small constant V_1, electrons can tunnel into material 0, where the high V_0 increases the effective transition temperature of the "film" above T_{c0}. This, in turn, is the condition for localization of the order parameter, which occurs for $d \gtrsim d_c \sim k_F^{-1}(\lambda_0 - \lambda^*)^{-1}$. Equation (16) applies when $d \lesssim d_c$, while for $d \gg d_c$ Eq. (14) must be used; in the range $d \sim d_c$, the oscillatory behavior of λ_{qq} causes alternating localization and delocalization of the order parameter as d varies.

It follows from Eqs. (15), (36), (37) that the scale on which $N_{ql}(z)$ changes near the boundary from 0 to N^* is κ_0^{-1}. The behavior of the function $N_c(z)$ is more complicated: as $|z|$ decreases, it changes from N_0 to $N_c(d/2)$ on a scale k_F^{-1}, and then from $N_c(d/2)$ to $N^{**} \approx N_0 k_F/2\kappa_0$ on a scale κ_0/k_F^2. The quantity $N_c(d/2)$ is of order N^{**} for $d \gtrsim \kappa_0/k_F^2$, and oscillates from 0 to $\min\{N_0, N^*/\kappa_0 d\}$ for $d \lesssim \kappa_0/k_F^2$. We will consider the case $\lambda_1 \sim \lambda_0$, i.e., $V_0/V_1 \sim \kappa_0/k_F$.

In order to compute λ_{qq}, we substitute (37) into Eq. (29) of Ref. 7, writing $N_{ql}(z)^2$ in the form of a double sum. The contribution that is $\sim n$ (where n is the number of quasilocal levels) must be separated out exactly, as it gives the oscillatory sawtooth dependence. In order to calculate the remaining part of (37), which is $O(n^0)$ for $d \gg a_{ql} \sim \kappa_0^{-1}$, we may convert the summation to an integration. Then

$$\lambda_{qq} a = \pi\lambda^{*2}\frac{V_1}{V_0}\left[\frac{2}{15} - \frac{V_1}{V_0}\left\{\frac{\kappa_0 d}{\pi}\right\}\right]\kappa_0^{-1}. \tag{46}$$

Keeping in mind the properties of $N_c(z)$ and $N_{ql}(z)$, we can determine the parameters λ_{cq}, λ_{qc}, and λ_{cc} for $k_F d \gg 1$ from the integral

$$\int_{|z|<d/2} dz[N_c(z) - N^{**}] = N_0 \pi k_F^{-1} Q(d),$$

$$Q(d) = \left\{\frac{\kappa_0 d}{\pi}\right\} - \left\{\frac{q_F d}{\pi}\right\}. \tag{47}$$

In order to calculate this integral, we note that for $\kappa_0 \gg k_F$ the limits of integration in (36) are found to be close to one another, and we can expand all the functions except the trigo-

nometric ones with respect to $q-\kappa_0$. The localization of the expression under the integral sign near the point $q_s=\pi s/d$ allows us to approximate it by a set of δ functions. When T_c lies in the region $d\leqslant d_c$, we obtain (16) with λ_{qq} given by (46), while in the region $d\gg d_c$ we obtain the result

$$\left(\frac{\delta T_c}{T_{c0}}\right)_s=\frac{\pi}{\lambda_0 k_F L}\left[\left(\frac{\lambda_1-\lambda^*}{\lambda_0-\lambda^*}\right)^2\left(\frac{2}{15}\frac{\kappa_0}{k_F}-\frac{\lambda_1}{\lambda_0}\left\{\frac{\kappa_0 d}{\pi}\right\}\right)+\left(2\frac{\lambda_1-\lambda^*}{\lambda_0-\lambda^*}-1\right)Q(d)\right]. \quad (48)$$

From $\lambda_1-\lambda^*\sim k_F^2/\kappa_0^2$ it follows that the complete formula (48) must be used only for $\lambda_0\approx\lambda_1$; for $\lambda_0-\lambda_1\sim 1$ it simplifies to the form

$$\left(\frac{\delta T_c}{T_{c0}}\right)_s=\frac{1}{\lambda_0 k_F L}[-\pi Q(d)],\quad d\gg d_c. \quad (49)$$

For $\lambda_0\gtrsim\lambda_1\sim k_F/\kappa_0$ we have $d_c\lesssim a_c\sim\kappa_0/k_F^2$, and we must discuss the region $d_c\lesssim d\lesssim a_c$, where Eq. (14) does not apply. Use of the more general formula (17) leads to the same result (49), because $\lambda_c\sim(\kappa_0 d)^{-1}$ implies that we need save only the term with λ_{c0} in (17).

In Fig. 2d we show the dependence of T_c on d for $\lambda_1=\lambda_0$. The inset shows the function $Q(d)$, which determines $T_c(d)$ when $\lambda_0-\lambda_1\sim 1$. For large d and $\lambda_1\neq\lambda_0$, the oscillations of T_c consist of a sum of two periodic functions with periods π/q_F and π/κ_0, in accordance with the qualitative considerations of the previous section. Because these periods are so close together, a characteristic beating behavior is observed. For $\lambda_1=\lambda_0$, the oscillatory component with period π/κ_0 disappears [see (48)]. When $d\lesssim k_F^{-1}$, we find from (16), (46) that $T_c-T_{c0}\gtrsim T_{c0}$, implying that the expressions we have introduced are inapplicable. Physical considerations dictate that T_c increase over a scale $d\sim\kappa_0^{-1}$.

5. SURFACE EFFECTS CONNECTED WITH A DIFFERENCE IN THE TRANSVERSE MASSES ($U=0$, $m\neq m_1$, $M=M_1$, $\kappa=0$)

In this case all the single-particle states extend throughout the entire system, and the following expression holds for $N(z)$:

$$N(z)=\frac{2M\sqrt{\beta}}{(2\pi)^2}\int_0^{q_F}dq\begin{cases}2\dfrac{(\beta+1)+(\beta-1)\cos(qd)\cos(2qz)}{(\beta+1)^2-(\beta-1)^2\cos^2 qd}, & |z|<d/2\\ 1+\dfrac{(1-\beta^2)\sin^2(qd)\cos(2q\tilde{z})-\sqrt{\beta}(\beta-1)\sin(2qd)\sin(2q\tilde{z})}{(\beta+1)^2-(\beta-1)^2\cos^2(qd)}, & \tilde{z}=\sqrt{\beta}(|z|-d/2)\end{cases} \quad (50)$$

where $q_F=\sqrt{2m_1\varepsilon_F}$, and the notation $\beta=m/m_1$ is used.

5.1. The case $m\gg m_1$

For $\beta\gg 1$ the expression in the integrand of (50) is localized near the point $q_s=\pi s/d$; by approximating it with a set of δ functions and substituting into (13), we obtain for T_c

$$\frac{\delta T_c}{T_{c0}}=\frac{1}{\lambda_0 k_F L}\left\{\left(\frac{\lambda_1}{\lambda_0}-1\right)q_F d+g(q_F d/\pi)\right\}, \quad (51)$$

in which the linear term agrees with Ref. 5, while the function $g(x)$ equals

$$g(x)=\pi\{x\}+\pi\frac{\lambda_1}{\lambda_0}\left(-2\{x\}+\frac{5}{2}+\frac{\{x\}^2-5\{x\}/2+1}{x}\right)-\pi. \quad (52)$$

For $0<x<1$ the we have $g(x)\propto 1/x$, which diverges as $x\to 0$. In order to eliminate the divergence we need a more accurate treatment of the region $q_F d\ll 1$. For this we expand the integrand in qd without using the δ-function approximation; as a result we obtain

$$g(x)=\frac{\lambda_1}{\lambda_0}\frac{4}{\pi}\frac{1}{x}\left[\arctan\left(\frac{\pi\sqrt{\beta}}{2}x\right)\right]^2,\quad x\ll 1. \quad (53)$$

The dependence of T_c on d for $\lambda_1=\lambda_0$ is shown in Fig. 4a: it is sawtooth-shaped because of the smallness of the transmission coefficient of the boundaries.[8] The maximum value of T_c is reached for $d=2.8k_F^{-1}$, and equals

$$\left(\frac{\delta T_c}{T_{c0}}\right)_{max}=\frac{0.4}{\lambda_0 k_F L}\sqrt{\frac{m}{m_1}}. \quad (54)$$

5.2. The case $|m-m_1|\ll m$

Expanding (50) with respect to $\beta-1$ and substituting into (13), we obtain

$$\frac{\delta T_c}{T_{c0}}=\frac{1}{\lambda_0 k_F L}\left\{\left(\frac{\lambda_1}{\lambda_0}-1\right)q_F d+\frac{\beta-1}{2}\left(\frac{\lambda_1}{\lambda_0}-1\right)\mathrm{Si}(2q_F d)+\left(\frac{\beta-1}{4}\right)^2 g_1(2q_F d)\right\}, \quad (55)$$

where the function $g_1(x)$ is defined as

$$g_1(x)=\pi+(2\lambda_1/\lambda_0-1)\sin x+\frac{\sin x}{x}[-\pi+2\mathrm{Si}(2x)]-\frac{\cos x}{x}2S_1(2x) \quad (56)$$

(with $S_1(x)=\ln x+\mathrm{Ci}(x)$; $\mathrm{Si}(x)$ and $\mathrm{Ci}(x)$ are the sine and cosine integrals, and C is Euler's constant; see Ref. 19, pp. 732, 733). This function has the asymptotic form

$$g(x)=\begin{cases}(2\lambda_1/\lambda_0+1)x, & x\ll 1\\ \pi+(2\lambda_1/\lambda_0-1)\sin x, & x\gg 1\end{cases}. \tag{57}$$

Besides the usual linear term, the dependence of T_c on d contains decaying oscillations that are $\sim(\beta-1)$ and nondecaying oscillations that are $\sim(\beta-1)^2$. When λ_1 and λ_0 differ significantly, we may replace the function $g_1(x)$ by its asymptotic form for $x\gg 1$, while for $\lambda_1\approx\lambda_0$ we evaluate it for $\lambda_1=\lambda_0$. When $\lambda_1=\lambda_0$, the behavior of T_c as a function of d is determined by the function $g_1(x)$ and is shown in Fig. 4b; the maximum value of T_c is reached for $d=1.2k_F^{-1}$ and equals

$$\left(\frac{\delta T_c}{T_{c0}}\right)_{\max}=\frac{0.33}{\lambda_0 k_F L}\left(\frac{m-m_1}{m}\right)^2. \tag{58}$$

5.3. The case $m\ll m_1$

For $\beta\ll 1$ the expression under the integral sign is localized near the point $q_s=\pi s/d$; after approximating it with a set of δ functions and substituting into (13), we obtain

$$\frac{\delta T_c}{T_{c0}}=\frac{1}{\lambda_0 k_F L}\left\{\left(\frac{\lambda_1}{\lambda_0}-1\right)q_F d+g_2(q_F d/\pi)\right\}, \tag{59}$$

where

$$g_2(x)=\pi\left[\frac{\lambda_1}{\lambda_0}\left(\frac{\{x\}-1/2}{x}\{x\}-2\{x\}+1/2\right)+\{x\}+1\right]. \tag{60}$$

Expression (60) cannot be used in the region of small x (i.e., when $q_F d\ll 1$). This region must be discussed separately, by expanding the expression in (50) with respect to qd and not using the δ-function approximation; as a result, we obtain

$$g_2(x)=\arctan(x/\varepsilon)+\frac{\pi}{2}\frac{x-\varepsilon\ \arctan(x/\varepsilon)}{x},$$

$$\varepsilon=\frac{2\sqrt{\beta}}{\pi},\quad x\ll 1. \tag{61}$$

For $\lambda_1=\lambda_0$ the dependence of T_c on d is determined by the function $g_2(x)$ and is shown in Fig. 4c; the maximum value of T_c equals

$$\left(\frac{\delta T_c}{T_{c0}}\right)_{\max}=\frac{1}{\lambda_0 k_F L}\frac{3\pi}{2} \tag{62}$$

which is valid at the points $d=\pi s/q_F$ $(s=1,2,...)$.

6. SURFACE EFFECTS CONNECTED WITH DIFFERENT PARALLEL MASSES ($U=0$, $m=m_1$, $M\neq M_1$, $\kappa=0$)

6.1. The case $M\gg M_1$

For $M>M_1$ the longitudinal Fermi momentum in material 0 is larger than it is in material 1, and some of the states do not extend from material 0 into material 1 due to the impossibility of conserving longitudinal momentum; therefore, the decomposition (18) is valid for $N(z)$, where

$$N_A(z)=\frac{M}{(2\pi)^2}\frac{1}{\gamma}\int_0^{q_F}dq\,\frac{q}{k}H(k,q,z)\Big|_{k=\sqrt{(k_0^2+q^2)/\gamma}} \tag{63a}$$

$$N_B(z)=\frac{M}{(2\pi)^2}\frac{1}{\gamma}\int_0^{k_0}dq\,\frac{q}{k}H(k,iq,z)\Big|_{k=\sqrt{(k_0^2-q^2)/\gamma}} \tag{63b}$$

and the following notation is used:

$$\gamma=M/M_1,\quad k_0=k_F\sqrt{\gamma-1},\quad k_F=q_F=\sqrt{2m\varepsilon_F}.$$

For $M\gg M_1$, i.e., $\gamma\gg 1$, little simplication of (63) is possible—we can only set $k\approx k_F$ in (63a). Therefore, we immediately substitute (18), (63) into Eq. (13), representing the bi-linear combinations of $N_A(z)$ and $N_B(z)$ in the form of double integrals. These integrals are computed in the following way:

1) In the integrals that involve $N_B(z)$ and $N_B^2(z)$, we discuss in order of occurrence the three terms that result from integrating with respect to z. For $k_F d\gg 1$ the leading term in the integral (63b) arises from the region $q\sim k_F$, which allows us to take the limit $qd\to\infty$ in the hyperbolic functions entering into $H(k,iq,z)$. When $\gamma^{-1}\ll k_F d\ll 1$, the leading term in the integral (63b) comes from the region $q\sim d^{-1}\gamma^{-1/2}$, and the hyperbolic functions can be expanded as series in which we keep only the leading order in qd. When $k_F d\ll\gamma^{-1}$ the entire region of integration in the integral (63b) is important; after expanding the hyperbolic functions in series, we must carefully distinguish the contributions from the neighborhood of the upper limit of integration.

2) The integral involving $N_A(z)N_B(z)$ is small compared to the integrals that involve $N_B(z)$, $N_B(z)^2$ in the region $k_F d\lesssim 1$; in the region $k_F d\gtrsim 1$ it determines the oscillatory part of T_c. After integrating with respect to z we calculate this quantity to logarithmic accuracy, including the contribution $\sim\ln\gamma/\gamma$ that arises from the region $|z|>d/2$, but discarding terms $\sim 1/\gamma$.

3) The surface portion of the integrals involving $N_A(z)$ and $N_A^2(z)$ are estimated from above by a quantity $\sim 1/\gamma$, and so we may neglect them. This becomes obvious for the integral involving $N_A(z)-N_A(\infty)$ after the integration with respect to z over the region $|z|>d/2$. The remaining integrals are estimated by taking into account the behavior of the function $N_A(z)$, which far from the boundary enters in with a value $N_A(\infty)=N_0/\gamma$ over a scale γk_F^{-1} in material 0 and with a value $N_A(0)=N_0/\gamma$ over a scale k_F^{-1} in material 1.

As a result, we obtain for the surface contribution to T_c

$$\left(\frac{\delta T_c}{T_{c0}}\right)_s = \frac{1}{\lambda_0 k_F L} \times \begin{cases} \left(\frac{\lambda_1}{\lambda_0}-1\right)\gamma k_F d + \frac{\pi}{2}\left(-\frac{\lambda_1}{\lambda_0}+\frac{5}{6}\right)(\gamma k_F d)^2, & k_F d \ll \gamma^{-1}, \\ -\frac{[\ln(\gamma k_F d)]^2}{2\gamma k_F d}, & \gamma^{-1} \ll k_F d \ll 1, \\ \frac{\ln\gamma}{\gamma}\left[\pi + \frac{\sin(2k_F d)}{8(k_F d)^2}\right], & k_F d \gg 1. \end{cases} \tag{64}$$

The dependence of T_c on d for $\lambda_1=\lambda_0$ is shown in Fig. 5a; the maximum value of T_c is reached for $d\sim k_F^{-1}$ and is of the same order as the quantity

$$\left(\frac{\delta T_c}{T_{c0}}\right)_{max} \sim \frac{1}{\lambda_0 k_F L}\frac{\ln\gamma}{\gamma}. \tag{65}$$

6.2. The case $0<M-M_1\ll M$

As before, the expressions (18), (63) are valid for $N(z)$. In complete analogy with Sec. 4.2 we can establish the result (31), with the function $G(z)$ defined by integrals from q_F to ∞. For $\gamma-1\ll 1$ we have $k_0\ll k_F$ and $k-q\ll q$ over the entire range of integration; expanding with respect to $(k-q)/q$ and substituting (31) into Eq. (13), we obtain[7)] for the surface contribution to T_c:

$$\left(\frac{\delta T_c}{T_{c0}}\right)_s = \frac{1}{\lambda_0 k_F L}\left\{\left(\frac{\lambda_1}{\lambda_0}-1\right)(\gamma-1)h_1(2q_F d) + (\gamma-1)^2 h_2(2q_F d)\right\}, \tag{66}$$

where $h_1(p)$ and $h_2(p)$ are defined as follows:

$$h_1(p) = \frac{\pi}{4} + \frac{1}{2}\int_1^\infty dx\left(\frac{1}{x^3}-\frac{1}{x}\right)\sin(px)$$

$$h_2(p) = \frac{\pi}{12} - \frac{\pi}{4}\frac{1}{p}\int_1^\infty dp\,\frac{\sin(px)}{x^5} + \frac{1}{8}\int_1^\infty \frac{\sin(px)}{x^2}\frac{x^2-1}{x^2}\ln\frac{x+1}{x-1}\,dx - \frac{1}{8}\int_0^1 \sin(px)\frac{x^2-1}{x^2}\ln\frac{x+1}{x-1}\,dx \tag{67}$$

and have the asymptotic forms

$$h_1(p) = \begin{cases} p, & p\ll 1 \\ \frac{\pi}{4}+\sin p/p^2, & p\gg 1 \end{cases}$$

$$h_2(p) = \begin{cases} -\frac{\pi}{48}, & p\ll 1 \\ -\frac{\pi}{24}-\frac{\pi}{4}\cos p/p^2, & p\gg 1 \end{cases}. \tag{68}$$

When λ_1 and λ_0 differ significantly, the dependence of T_c on d is determined by the function $h_1(p)$, while for $\lambda_1=\lambda_0$ it is determined by $h_2(p)$; the behavior of these functions is shown in Fig. 5b. For $\lambda_1=\lambda_0$ the quantity δT_c is negative for all d; the first maximum of the oscillations occurs for $d=3.6q_F^{-1}$, and the value of T_c at this point is

$$\left(\frac{\delta T_c}{T_{c0}}\right)_{max} = -\frac{0.24}{\lambda_0 k_F L}\left(\frac{M-M_1}{M}\right)^2. \tag{69}$$

6.3. The case $0<M_1-M\ll M$

For $M<M_1$ the decomposition (15) is valid in view of the presence of the quasidiscrete spectrum for $N(z)$, where

$$N_c(z) = \frac{M}{(2\pi)^2}\frac{1}{\gamma}\int_{\kappa_0}^{q_F} dq\,\frac{q}{k}H(k,q,z)\Big|_{k=\sqrt{(q^2-\kappa_0^2)/\gamma}},$$

$$\kappa_0 = k_F\sqrt{1-\gamma}, \tag{70}$$

while $N_{ql}(z)$ is defined by Eq. (37) with N_{2D}^s of the form

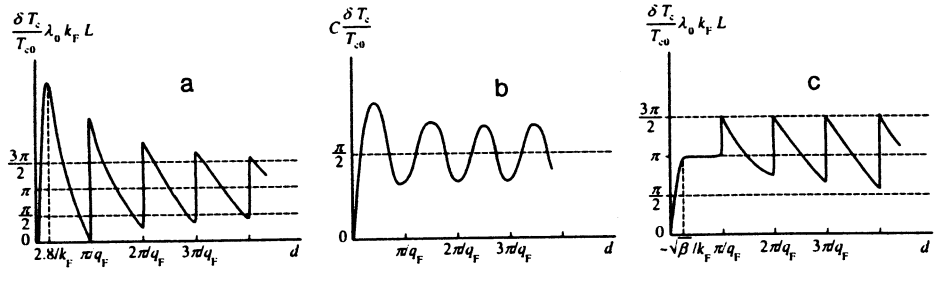

FIG. 4. The dependence of T_c on d for materials 0 and 1 that differ in their transverse masses for $\lambda_1=\lambda_0$: (a) $m\gg m_1$; (b) $|m-m_1|\ll m$; and (c) $m\gg m_1$. We have used the notation $C=16(\beta-1)^{-2}\lambda k_F L$.

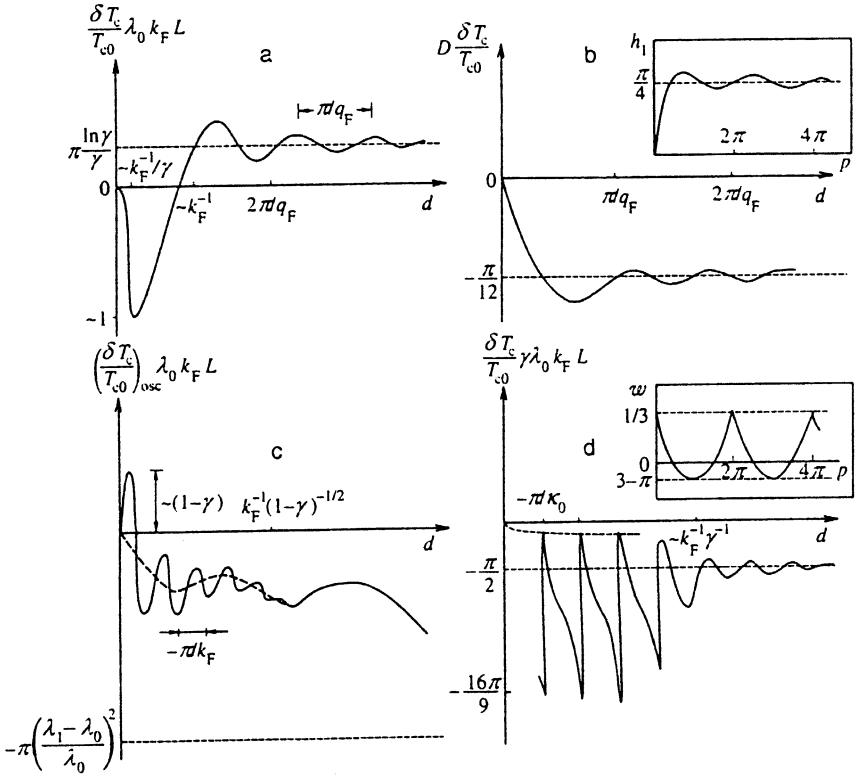

FIG. 5. The dependence of T_c on d for materials 0 and 1 that differ in their parallel masses: (a) $M \gg M_1$, $\lambda_1=\lambda_0$; (b) $0<M-M_1 \ll M$, $\lambda_1=\lambda_0$; (c) $0<M_1-M \ll M$, $\lambda_1<\lambda_0$; and (d) $M \ll M_1$, $\lambda_1=\lambda_0$. In the insets we show the functions $h_1(p)$ and $w(p)$ entering into Eqs. (66) and (76); we have used the notation $D=\lambda_0 k_F L(\gamma-1)^{-2}$.

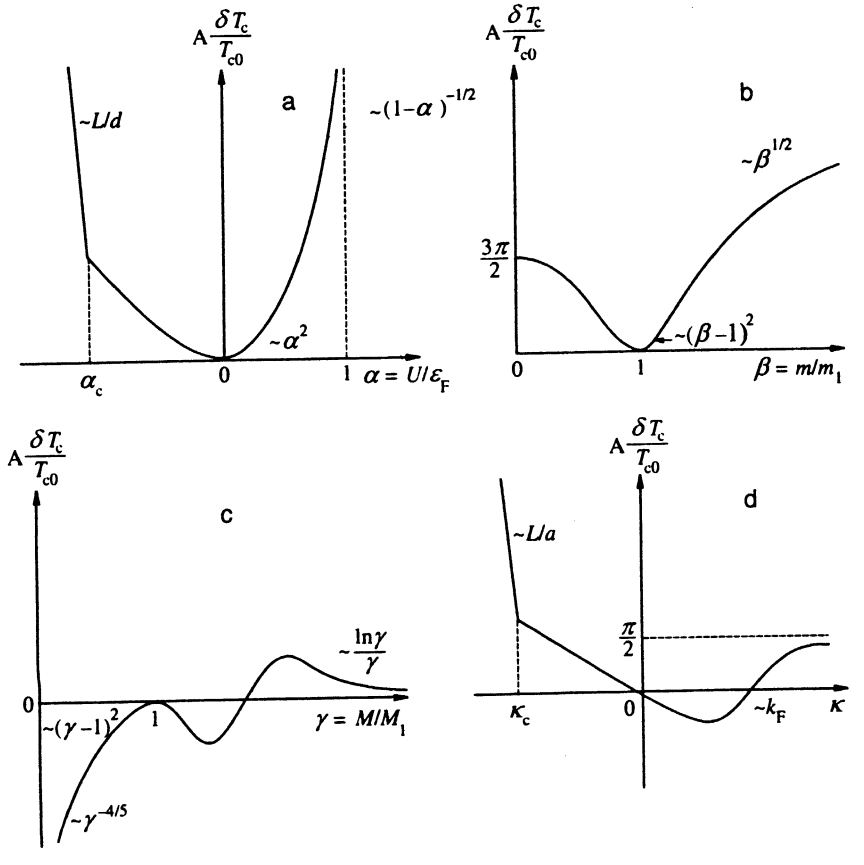

FIG. 6. The dependence of the value of T_c at the first maximum of the quantum oscillations on the parameters of the model for $\lambda_0=\lambda_1$ in the following cases: (a) $U\neq 0$, $m=m_1$, $M=M_1$, $\kappa=0$; (b) $U=0$, $m\neq m_1$, $M=M_1$, $\kappa=0$; (c) $U=0$, $m=m_1$, $M\neq M_1$, $\kappa=0$; and (d) $U=0$, $m=m_1$, $M=M_1$, $\kappa\neq 0$. We have used the notation $A=\lambda_0 k_F L$.

$$N_{2D}^{s}=\frac{M_1}{2\pi}(k_s d+2)\left(k_s d+2+\frac{1-\gamma}{\gamma}\frac{2q_s^2}{k_s^2+q_s^2}\right)^{-1}$$
$$\times\theta(\kappa_0-q_s)\theta(q_s), \tag{71}$$

where $k_s=\sqrt{(\kappa_0^2-q_s^2)/\gamma}$ *and* q_s is a root of Eq. (38). By analogy to Sec. 4.3, we establish the result (31) with the same function $G(z)$ as we used in Sec. 6.2. For $1-\gamma\ll 1$, Eq. (41) is valid for T_c with λ_{s0} taken from (42), which leads to the following result for the surface contribution to T_c:

$$\left(\frac{\delta T_c}{T_{c0}}\right)_s=\frac{1}{\lambda_0 k_F L}\left\{\left(\frac{\lambda_1}{\lambda_0}-1\right)(\gamma-1)h_1(2q_F d)\right.$$
$$\left.+(\gamma-1)^2 h_2(2q_F d)+\left(\frac{\lambda_1}{\lambda_0}-1\right)^2\pi u\left(\frac{\kappa_0 d}{2}\right)\right\}; \tag{72}$$

the functions $h_1(p)$ and $h_2(p)$ are defined in (84), and the function $u(p)$ is the same as in (43) to lowest order in $1-\gamma$. The dependence of T_c on d for $\lambda_1\neq\lambda_0$ is shown in Fig. 5c; for $\lambda_1=\lambda_0$ it is determined by the function $h_2(p)$ and is found to be the same as in the previous case.

6.4. The case $M\ll M_1$

From (70) it is not difficult to sort out the behavior of the functions $N_{ql}(z)$ and $N_c(z)$ for $\gamma\ll 1$: the function $N_{ql}(z)$ changes near the boundary from 0 to $N^*\approx N_0/\gamma$ over a scale k_F^{-1}, reaching a value $\sim N_0$ at the boundary, whereas the function $N_c(z)$ changes from N_0 to $N_c(d/2)\sim N_0$ as $|z|$ decreases on a scale k_F^{-1}, and then from $N_c(d/2)$ to $N^*=N_0/2$ on a scale k_F^{-1}/γ. Thus, we have $a_{ql}\sim k_F^{-1}$, $a_c\sim k_F^{-1}/\gamma$; in the region $k_F d\gg 1/\gamma$ we make use of Eq. (14), while in the region $1\ll k_F d\lesssim 1/\gamma$ we use the more general formula (17); because we have $\lambda_{qq}<0$ (see below), there is no quasi-phase transition (see Ref. 5). Taking into account that for $\lambda_1\sim\lambda_0$ we have $V_0/V_1\sim 1/\gamma$, we find that the parameters λ_{qc}, λ_{cq}, λ_{cc} are determined by the integral

$$\int_{|z|<d/2}dz[N_c(z)-N^{**}]$$
$$=\begin{cases}\frac{1}{2}N_0 d w(q_F d/2), & \gamma k_F d\ll 1\\ \frac{N_0}{\gamma k_F}\left[\pi\left\{\frac{\kappa_0 d}{\pi}\right\}-\frac{\pi}{2}-\frac{\sin(2k_F d)}{8(\gamma k_F d)^2}\right], & \gamma k_F d\gg 1\end{cases}, \tag{73}$$

which can be computed in two limiting cases: for $\gamma k_F d\ll 1$ we set $q\approx\kappa_0$ in (70), while for $\gamma k_F d\gg 1$ we can expand in a Fourier series with respect to qd by analogy with (A2), and use the asymptotic form of the integrals with rapidly oscillating exponentials.[20] The terms in (73) with periods π/κ_0 and π/q_F are computed to lowest order in $1/d$, and the function $w(p)$ equals (see the inset to Fig. 5d):

$$w(p)=\bar{w}(p)+\bar{w}(p+\pi/2)-1,$$
$$\bar{w}(p)=\frac{\cos p-\pi\, p(1/2-\{p/\pi\})\sin}{\cos^2 p}. \tag{74}$$

In calculating λ_{qq}, we have identified the contribution $\sim n$, as we did in Sec. 4.4. The remaining part $O(n^0)$ is computed in two limiting cases: for $\gamma k_F d\gg 1$, by passing from a summation to an integration, and for $\gamma k_F d\ll 1$, by using the asymptotic form of q_s as $\gamma\to 0$ ($q_s=\pi s/d$, $s=1,...,n-1$, $q_n=\kappa_0$) and the fact that the leading terms come from q_n and q_{n-1}. As a result we have

$$\lambda_{qq}a=\frac{\pi\lambda_1\lambda^*}{k_F}\begin{cases}-\{\kappa_0 d/\pi\}, & \gamma k_F d\gg 1\\ \sigma(\kappa_0 d/\pi), & \gamma k_F d\ll 1\end{cases},$$
$$\sigma(x)=-\{x\}-\frac{\varepsilon}{\{x\}^{3/2}+\varepsilon},\quad \varepsilon=\frac{2\sqrt{\gamma k_F d}}{(2\pi)^{3/2}}. \tag{75}$$

Calculating T_c based on (14), (17) gives

$$\left(\frac{\delta T_c}{T_{c0}}\right)_s=\frac{1}{\lambda_0 k_F L}\frac{1}{\gamma}\begin{cases}-\pi\left(\frac{\lambda_1-\lambda^*}{\lambda_0-\lambda^*}\right)^2\left\{\frac{\kappa_0 d}{\pi}\right\}+\left(1-2\frac{\lambda_1-\lambda^*}{\lambda_0-\lambda^*}\right)\left[\frac{\pi}{2}+\frac{\sin(2q_F d)}{8(\gamma k_F d)^2}\right], & \gamma k_F d\gg 1\\ -w(q_F d/2)\frac{\gamma k_F d}{2}+\pi\left(\frac{\lambda_1-\lambda^*}{\lambda_0-\lambda^*}\right)^2[w(q_F d/2)+1]^2\sigma(\kappa_0 d/\pi), & \gamma k_F d\ll 1\end{cases}. \tag{76}$$

For large d the oscillatory contribution comes from the sum of two periodic functions with periods π/q_F and π/κ_0, analogous to the previous case. For $\lambda_1=\lambda_0$ the quantity δT_c is negative for all d (Fig. 5d): its value at the first maxima of the quantum oscillations ($k_F d\sim 1$) is of order

$$\left(\frac{\delta T_c}{T_{c0}}\right)_{max}\sim-\frac{1}{\lambda_0 k_F L}\left(\frac{M_1}{M}\right)^{4/5}. \tag{77}$$

7. DISCUSSION OF RESULTS

In order that the bulk contribution to T_c be small, we must use the smallest possible d. If we examine the curves shown in Figs. 2, 4 and 5 with this in mind, it is not difficult to verify that in all cases the first maximum of the quantum oscillations is a measure of whether or not it is feasible to increase T_c. The value of T_c at this maximum gives a convenient estimate of the surface contribution to T_c: its dependence on the parameters of the model for $\lambda_1=\lambda_0$ is shown in Fig. 6 (Fig. 6d was plotted using the results of Ref. 8). It is

not difficult to see that a difference in the positions of the band bottoms ($U\neq 0$) and a difference in the transverse masses ($m\neq m_1$) will always favor an increase in T_c, whereas a difference in the parallel masses ($M\neq M_1$) will hinder it in most cases. The presence of a δ-function-like potential at the boundary ($\kappa\neq 0$) acts to prevent T_c from increasing when $0<\kappa\lesssim k_F$, but aids it in the other cases. A qualitative representation of the combined action of all the factors can be obtained by superposing the curves in Fig. 6a–6d.

Physically, the increase in T_c for $\kappa\gtrsim k_F$ (Fig. 6) is associated with interference of plane waves reflected from the two boundaries,[8] and takes place only when d is commensurate with some multiple of the wavelength (for which the variation of T_c averaged over the oscillations is close to zero). For $\kappa<0$ the reason for an increase in T_c is an increase in the local density of states at the boundary, which is caused by the surface potential having the form of a potential well; for $\kappa<\kappa_c$ this leads to localization of the order parameter at the boundary.[6,7] These effects are partially present in the other cases as well (Figs. 6a–6c); now, however, it is the transfer of electrons from the material with high density of states and low value of V to the material with high V that plays the primary role. The qualitative manifestation of this effect depends on the specific situation: for $\alpha<\alpha_c$ it causes localization of the order parameter in the layers of material 1, whereas for $\gamma\ll 1$ it is not "triggered" in general.

The picture we have presented may require some correction, because in a real experiment factors may be present that are not included in the model we have discussed here. Therefore, it is desirable to carry out a systematic experimental investigation of the dependence of T_c on d in layered systems. Contemporary technology allows us to create superlattices with thicknesses of a few angstroms (see, e.g., Ref. 21); however, most experiments are carried out on long-period systems, in which these surface effects are unimportant.[22,23]

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APPENDIX

The Transformation of $F(z)$

For $U>0$ we rewrite $F(z)$ in the form

$$F(z)=\frac{1}{2}\frac{M}{(2\pi)^2}\lim_{\delta\to\infty}\int_{-\infty}^{\infty}dq\,\frac{\delta^2}{q^2+\delta^2}\left[\frac{|q|}{k}H(k,q,z)-2\right] \tag{A1}$$

for $|z|<d/2$, and analogously for $|z|>d/2$. Let us expand the functions u^+,v^+ entering into $H(k,q;z)$ in Fourier series with respect to qd:

$$\frac{1}{u^+(k,q)}=\sum_{n=-\infty}^{\infty}\frac{1}{k|q|}\left(\frac{|q|-k}{|q|+k}\right)^{|n|}e^{inqd},$$

$$\frac{1}{v^+(k,q)}=\sum_{n=-\infty}^{\infty}\frac{1}{k|q|}\left(\frac{k-|q|}{k+|q|}\right)^{|n|}e^{inqd}. \tag{A2}$$

By making the replacement $n\to -n$, $q\to -q$ where necessary, we can write the result in the form of a sum that contains the exponents $\exp(icq)$ with positive c only; for $|z|>d/2$ we also expand the functions $\cos(2kz')$ and $\sin(2kz')$ in power series. The integrand is analytic in the complex q plane except for the combination

$$|q|k=\sqrt{q^2+\varepsilon^2}\sqrt{q^2+k_0^2},\quad \varepsilon\to 0, \tag{A3}$$

which we regularize by making the cuts $(i\varepsilon,ik_0)$ and $(-ik_0,-i\varepsilon)$. Shifting the contour of integration upward, we obtain an integral over the cut $(i\varepsilon,ik_0)$ (the contribution of the pole $i\delta$ disappears as $\delta\to\infty$), leading to the expression (30).

For $U<0$ the cut is made from ε to κ_0 and from $-\kappa_0$ to $-\varepsilon$. The integrand has no singularities in the upper half-plane, and $F(z)$ reduces to an integral over the upper side of the cut $(-\kappa_0,\kappa_0)$. On this cut there are poles that correspond to levels of the quasidiscrete spectrum. We write the integral in the form of a principal value and the sum of half-residues from the poles: then the principal value gives the constant N^* for $|z|<d/2$ and 0 for $|z|>d/2$, and the sum is found to be $-N_{ql}(z)$.

[1)]We are neglecting the spatial dependence of the cutoff frequency ω_0, which is valid in the weak-coupling approximation.

[2)]Note that the surface contribution to T_c may not contain any portion $\sim a/L$ if localization of the superconducting order parameter occurs at the boundaries;[6,7] when this happens, regions that are far from the boundary enter into the average of the quantity λ with zero weight.

[3)]Recently, the existence of this mechanism has been confirmed experimentally.[16]

[4)]The form of the boundary conditions at the points $z=\pm L/2$ is important only for the behavior of $N(z)$ in the vicinity of these points.

[5)]The formal proof that T_c increases when $V(\mathbf{r})$ is replaced by $V(\mathbf{r})+\Delta V(\mathbf{r})$ with $\Delta V(\mathbf{r})\geq 0$ is clear from Sec. 2.

[6)]In connection with this, the difference between λ_1 and λ_0 appears in (33) only in the unattenuated portion of $f_2(y)$; in what follows we set $\lambda_1=\lambda_0$ in terms that are important only for $\lambda_1\approx\lambda_0$, without mentioning explicitly that we have done so.

[7)]Due to the conditional convergence of the integrals, the expressions for $G(z)$ are inapplicable within an infinitesimally small neighborhood of the points $z=\pm d/2$, where unphysical δ-function-like singularities arise whose contribution should not be included in the integration over z.

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