Theory of the π junctions formed in atomic-scale superconductor/ferromagnet superlattices

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Using the Green's-functions method we investigate theoretically a model of atomic-scale superconductor/ferromagnet (S/F) superlattices. In this model the phase of the order parameter changes periodically, and the intrinsic phase difference k in the ground state can be zero or π. Three basic parameters — the transfer integral t between S and F layers, the exchange field h in F, and the pairing constant Λ in S — characterize the system. We find that the critical Josephson current has a nonmonotonic dependence on h, becoming zero at the critical value $h=h_{\rm crit}(T)$, corresponding to the transition between $k=0$ and $k=\pi$ in the ground state. We calculate the densities of states on S and F layers and show that the quasiparticle spectra are strongly influenced by the values of h and t. [S0163-1829(98)01546-X]

I. INTRODUCTION

Recently, the study of so-called π junctions with an intrinsic phase difference $k=\pi$ in the ground state has gained much interest. Many experiments on high-T_c superconducting weak links have been interpreted in terms of π junctions proposed for the superconductors with d-wave pairing.[1]

For the superconductors with s-wave pairing, π junctions have been suggested by Bulaevskii *et al.*[2] to arise in the presence of magnetic impurities in the barrier, in connection with spin-flip-assisted coherent tunneling. Also, the ground state with superconducting order parameter that changes its sign from one superconducting layer to another ($k=\pi$) was predicted theoretically to exist in superconductor-ferromagnet (S/F) multilayers, with layers of finite thickness, by Buzdin and Kupriyanov[3] and by Radović *et al.*,[4] and in the atomic-scale S/F superlattices by Andreev *et al.*[5] In both cases[3–5] a simple model of a constant exchange field in F layers, acting on the electron spins only, was used.

The evidence for π coupling was sought experimentally in several superconductor-ferromagnet[6] and superconductor-spin-glass[7] systems. The characteristic oscillations[3,4] of the superconducting critical temperature T_c with magnetic layer thickness d_F were observed in Nb/Gd (S/F multilayers) by Strunk *et al.*[8] and by Jiang *et al.*[9] and in Nb/CuMn (superconductor/spin-glass multilayers) by Mercaldo *et al.*[7] While the oscillatory T_c behavior was interpreted in terms of $k=\pi$ phase-difference manifestation in Refs. 7 and 9, in Ref. 8 it was attributed to the change from the paramagnetic to the ferromagnetic state with increasing d_F.

In the present paper, we study theoretically other manifestations of π coupling in an atomic-scale S/F superlattice, assuming s-wave pairing in S. This work is based on the microscopic theory of Andreev *et al.*,[5] whose main result is the temperature-exchange field ($T-h$) diagram showing the transition from zero to π phase difference in the ground state for $h>h_{\rm crit}(T)$. We look for manifestations of such ground states in the behavior of supercurrent flowing across the layers. We find that critical current density has a nonmonotonic dependence of h, becoming zero at the transition field $h=h_{\rm crit}(T)$. In this way, we obtain an alternative criterion for the change from $k=0$ to $k=\pi$ phase difference in the ground state, valid beyond the perturbational approach of Ref. 5.

The perpendicular supercurrent is closely related to Andreev reflections,[10] which originate from the multilayered structure: in the case of S/N contacts, where N is a normal metal, it was shown that it flows *via* the bound states in the quasiparticle energy spectrum, resulting from interference between the electronlike and holelike quasiparticles.[11] To investigate the bound states in the S/F case, we calculate the quasiparticles density of states at $T=0$ on S and F layers as a function of the strength of the exchange field h and of the value of the transfer integral t between the layers.

For experimental testing of our results, one should be able to prepare S/F superlattices with thin (of the order of one interatomic length) layers, and with different values of the exchange field in F. Recently, this became possible in superlattices with thicker layers, by taking for F ferromagnetic alloys,[12] e.g., $V_{1-x}Fe_x$, or spin-glass alloys,[7] e.g., $Cu_{1-x}Mn_x$, where h is varied by changing the concentration x of the magnetic ions.[7,12] Due to the progress of methods of multilayer preparation, the fabrication of artificial atomic-scale S/F superlattices could be possible as well. Good candidates for such systems are high-T_c superconductor/colossal magnetoresistance ferromagnet multilayers like $Nd_{2-x}Ce_xCuO_4/La_{1-y}Sr_yMnO_3$ or $Nd_{2-x}Ce_xCuO_4/La_{3-y}Sr_yMnO_7$,[13] where Nd is an s-wave superconductor.

The paper is organized as follows: in Sec. II we present the model and calculate the Green's function of the system. Section III deals with perpendicular supercurrent, and in Sec. IV the quasiparticle density of states is calculated. In Sec. V we discuss our results and the possibility for experimental tests.

II. GENERAL FORMALISM

We adopt the model of Ref. 5 and consider a superlattice with an elementary cell consisting of one superconducting (S) and one ferromagnetic (F) layer, with same dispersion curves $\xi(p)$. Three kinds of basic parameters characterize the system: t which is the transfer energy between the S and F layers, Λ is the pairing constant which is assumed to be nonzero in S layers only, and h is the constant exchange field in the F layers.

The Hamiltonian of the system is

$$H=\sum_{\vec{p},n,i,\sigma}\xi(\vec{p})a^{+}_{ni\sigma}(\vec{p})a_{ni\sigma}(\vec{p})+t(a^{+}_{ni\sigma}(\vec{p})a_{n,-i,\sigma}(\vec{p})+a^{+}_{n+1,-i,\sigma}(\vec{p})a_{ni\sigma}(\vec{p})+\text{H.c.})+H_{\text{int1}}+H_{\text{int2}}, \quad (2.1)$$

$$H_{\text{int1}}=\frac{\Lambda}{2}\sum_{\vec{p}_1,\vec{p}_2,n,\sigma}a^{+}_{n1\sigma}(\vec{p}_1)a^{+}_{n,1,-\sigma}(-\vec{p}_1)a_{n,1,-\sigma}\times(-\vec{p}_2)a_{n1\sigma}(\vec{p}_2), \quad (2.2)$$

$$H_{\text{int2}}=-\sum_{\vec{p},n,\sigma}h\sigma a^{+}_{n,-1,\sigma}(\vec{p})a_{n,-1,\sigma}(\vec{p}), \quad (2.3)$$

where $a^{+}_{ni\sigma}$ is the creation operator of an electron with spin σ in the nth elementary cell and momentum $\vec{p}$ in the layer i, where $i=1$ for the S layer, and $i=-1$ for the F layer.

Corresponding Green's functions are obtained in the standard way,[5,14] assuming that the order parameter changes from cell to cell in the manner $\triangle=|\triangle|e^{ikn}$, and introducing quasimomentum q in the direction perpendicular to the layers.[5]

Note that for two spin orientations we have to deal with Green's functions $G_{\downarrow\downarrow ij}(\vec{p},q+k,\omega)$ and $F^{+}_{\uparrow\downarrow ij}(\vec{p},q,\omega)$ or with $G_{\uparrow\uparrow ij}(\vec{p},q+k,\omega)$ and $F^{+}_{\downarrow\uparrow ij}(\vec{p},q,\omega)$. The latter set is obtained from the former by changing $h\to -h$. Thus, we quote the results for one spin orientation (spin up in G functions) only, omitting the spin indices,

$$F^{+}_{1j}=\frac{|\triangle|\delta_{1j}(\omega_{+}+h)(\omega_{-}+h)+|\triangle|T_{q+k}\delta_{-1,j}(\omega_{+}+h)}{D}, \quad (2.4)$$

where

$$D=|\triangle|^{2}(\omega_{+}+h)(\omega_{-}+h)-[\omega_{-}(\omega_{-}+h)-|T_{q+k}|^{2}]\times[\omega_{+}(\omega_{+}+h)-|T_{q}|^{2}], \quad (2.5)$$

$$F^{+}_{-1j}=\frac{-T^{*}_{q}F^{+}_{1j}}{\omega_{+}+h}, \quad (2.6)$$

$$G_{1j}=\frac{1}{|\triangle|}\frac{|T_{q}|^{2}-\omega_{+}(\omega_{+}+h)}{\omega_{+}+h}F^{+}_{1j}, \quad (2.7)$$

$$G_{-1,j}=\frac{\delta_{-1j}+T^{*}_{k+q}G_{1j}}{\omega_{-}+h}. \quad (2.8)$$

Here $\omega_{\pm}=i\omega\pm\xi(p)$, $\omega=\pi T(2n+1)$, $T_{q}=2t\cos(q/2)e^{iq/2}$ and $T_{q+k}=2t\cos[(q+k)/2]e^{i(q+k)/2}$.

The self-consistency equation for the order parameter is

$$|\triangle|=\frac{\Lambda T\rho(0)}{2\pi}\sum_{\omega}\int_{0}^{\infty}\int_{0}^{2\pi}d\xi dqF^{+}_{11}, \quad (2.9)$$

where $\rho(0)=m_{\parallel}/2\pi$ is the electron density of states at the Fermi level in the normal state.

III. SUPERCURRENT

The Josephson supercurrent in S/F superlattices is carried by Andreev bound states, similarly as in the S/N case. In the S layer the supercurrent is carried by Cooper pairs, but in the N layer it flows via quasiparticles, which recondensate in the next S layer; bound states represent this process.[11] Postponing the investigation of the bound states in the quasiparticle spectra to the next section, in this section we calculate the supercurrent flowing across the layers. In this case, the vector potential $A_{\perp}$ enters the Hamiltonian through the substitution $t\to te^{\pm iedA_{\perp}/c}$, where d is interlayer distance and the part of Hamiltonian depending on $A_{\perp}$ is

$$H_{A}=\frac{1}{d}\sum_{\vec{p},n,i,\sigma}t[a^{+}_{n,i,\sigma}(\vec{p})a_{n,-i,\sigma}(\vec{p})e^{iedA_{\perp}/c}+a^{+}_{n+1,-i,\sigma}(\vec{p})a_{n,i,\sigma}(\vec{p})e^{iedA_{\perp}/c}+\text{H.c.}]. \quad (3.1)$$

For the supercurrent

$$j_{\perp}=c\frac{\delta H_{A}}{\delta A_{\perp}}, \quad (3.2)$$

we get (for one spin orientation)

$$j_{\perp}=2iet\rho(0)T\sum_{\omega}\int\int d\xi\frac{dq}{2\pi}(G_{-1,1}-G_{1,-1}), \quad (3.3)$$

where $G_{i,j}$ are previously calculated Green's functions [Eqs. (2.4)–(2.8)] in the state with the current, i.e., with $\triangle=|\triangle|\exp(ikn)$.

For small values of the transfer integral t, we obtain an analytical result, performing in G_{ij} expansion over t/T_{c},

$$j_{\perp}=\left\{4e|\triangle|^{2}t^{4}\rho(0)T\sum_{\omega}\int d\xi\frac{\omega^{2}+\xi^{2}-h^{2}}{(\omega^{2}+\xi^{2}+|\triangle|^{2})^{2}[\omega^{2}+(\xi-h)^{2}][\omega^{2}+(\xi+h)^{2}]}\right\}\sin k. \quad (3.4)$$

As in the Josephson case, the supercurrent is proportional to $\sin k$, k being the phase change from one S layer to the neighboring one,

$$j_\perp = j_c \sin k, \tag{3.5}$$

where j_c is the critical current.

The order parameter $|\triangle|$ is small near T_c, and j_c reduces to

$$j_c = 2e|\triangle|^2 t^4 \pi\rho(0) T_c \sum_\omega \frac{12\omega^4 - 7\omega^2 h^2 - h^4}{|\omega|^3(\omega^2+h^2)(4\omega^2+h^2)^2}. \tag{3.6}$$

For $h=0$, j_c is positive; for h large, $h \gg T_c$, j_c becomes negative. The change of sign of j_c, which corresponds to the transition from $k=0$ to $k=\pi$ in the ground state,[2,5] occurs at $h=3.77\,T_{c0}$, in accordance with the $(T-h)$ diagram of Andreev *et al.*[5] (Note that the mean-field critical temperature T_{c0} at $t=0$ is equal to T_c up to second-order terms in t/T_c, see Ref. 5). At low temperatures, $T\to 0$, we calculate j_c by substituting in Eq. (3.4) the summation over ω_n by integration over ω

$$j_c = 4e|\triangle|^2 t^4 \rho(0) \int \frac{d\omega}{2\pi} d\xi \times \frac{\omega^2+\xi^2-h^2}{(\omega^2+\xi^2+|\triangle|^2)^2[(\omega^2+\xi^2+h^2)^2-4h^2\xi^2]}. \tag{3.7}$$

Here for $|\triangle|$ we take $\triangle_0$, its value in the absence of coupling, $t=0$. Performing the integration over ξ and ω, we get at $T=0$

$$j_c = 2e\triangle_0^2(0) t^4 \rho(0) \left\{ \frac{2}{(\triangle_0^2(0)-h^2)^2} \ln\left[\frac{\triangle_0(0)}{2h} + \frac{h}{2\triangle_0(0)}\right] - \frac{1}{\triangle_0^2(0)(\triangle_0^2(0)+h^2)} \right\}. \tag{3.8}$$

It can be seen that j_c goes to zero at $h/\triangle_0(0) \simeq 1/2$, which just corresponds to $h_{\rm crit}=0.87\,T_{c0}$ at $T=0$, again in accordance with Ref. 5.

At low temperatures, critical current increases logarithmically for small h,

$$j_c \approx 4e\triangle_0^2(0)\left(\frac{t}{\triangle_0(0)}\right)^4 \rho(0) \ln\frac{\triangle_0(0)}{h}, \quad h \ll \triangle_0(0). \tag{3.9}$$

Notice that the above result holds for $h \gg t$, since this is the condition for the expansion of Green's function over t.

From the above results for S/F superlattices it is easy to obtain the critical current in S/N superlattices taking the limit $h\to 0$. Near T_c, from Eq. (3.6) we find for the S/N case

$$j_c = 2e|\triangle|^2 t^4 \pi\rho(0) T_c \sum_\omega \frac{3}{4}\frac{1}{|\omega|^5} = e\triangle_0^2 \left(\frac{t}{T_c}\right)^4 \pi\rho(0) 3\zeta(5)\left(1-\frac{1}{32}\right). \tag{3.10}$$

At low T, for h small a cutoff in Eq. (3.9) is needed at $h \sim t$, giving for S/N multilayers

$$j_c = 2e\triangle_0^2(0)\left(\frac{t}{\triangle_0(0)}\right)^4 \rho(0)\ln\frac{\triangle_0(0)}{t}. \tag{3.11}$$

Comparing Eqs. (3.10) and (3.11) one can see that at low temperatures there is an anomalous (logarithmic) rise of j_c. This is related to the fact that at $T \ll t^2/T_c$ the density of superconducting electron of N layer increases.[15] This leads to different regimes in $j_c(T)$ dependences at $T<t^2/T_c$ and $T>t^2/T_c$. For the S/F multilayer the corresponding change of regimes should occur at $T\sim h^2/T_c$ for small h.

To investigate the case of arbitrary (not small) transfer integral t, we performed numerical calculations of the perpendicular supercurrent as a function of phase k for given values of h, t, and of the temperature T.

The total current (for both spin orientations) is calculated from Eq. (3.3) and the corresponding equation where $h\to -h$, using $\Delta(T)$ calculated from Eq. (2.9). Putting in Eq. (2.9) first $|\triangle|\to 0$ for $T\to T_c$, and then $|\triangle|\to|\triangle(T)|$, we eliminate Λ and get the equation

$$0 = T_c \sum_\omega \iint d\xi dq \left(\frac{QS+PR}{S^2+R^2}\right)\Bigg|_{|\triangle|=0} - T\sum_\omega \iint d\xi dq \left(\frac{QS+PR}{S^2+R^2}\right)\Bigg|_{|\triangle|=|\triangle(T)|}, \tag{3.12}$$

where $Q=\omega^2-h^2+\xi^2$, $P=-2\omega h$,

$$S = -|\triangle|^2(-\omega^2+\xi^2+\xi h) + (\omega^2-\xi^2-\xi h+|T_q|^2) \times(\omega^2-\xi^2+\xi h+|T_{k+q}|^2) - (2\omega\xi+\omega h)(-2\omega\xi+\omega h) \tag{3.13}$$

and

$$R = -2\omega h|\triangle|^2 + (2\omega\xi+\omega h)(-\omega^2+\xi^2-\xi h-|T_{k+q}|^2) + (-2\omega\xi+\omega h)(-\omega^2+\xi^2+\xi h-|T_q|^2). \tag{3.14}$$

The dependence of $j_\perp(k)$ for $t/T_c=1$, and for several values of the exchange field at temperatures $T/T_c=0.01$, and $T/T_c=0.8$ is presented in Fig. 1. One finds the (nearly) sinusoidal behavior of $j_\perp(k)$ in each case. This is at first glance surprising, since its differs from what is known from S/N superlattices with finite layer thickness. The atomic-scale models of superlattices, where the movement of quasiparticles perpendicular to the layers is characterized by the transfer energy t, differ from the usual models of weak links, which represent strongly coupled systems. In the latter case, electrons can travel through the link almost freely, so that higher-order processes, in which several Cooper pairs are involved, become important and $j_\perp(k)$ may deviate significantly from the simple sinusoidal function.[11] In our case, we obtain slight deviations from the sinusoidal behavior of $j_\perp(k)$ for $h/T_c \ll 1$ and $t/T_c \geq 3$, i.e., when the coupling between the layers is strong.

The supercurrent is positive for small h/T_c, where $k=0$ state is stable $[j_\perp(k=0)=0,\ j'_\perp(k=0)>0]$ and decreases with the rise of h to become negative at large h/T_c, where

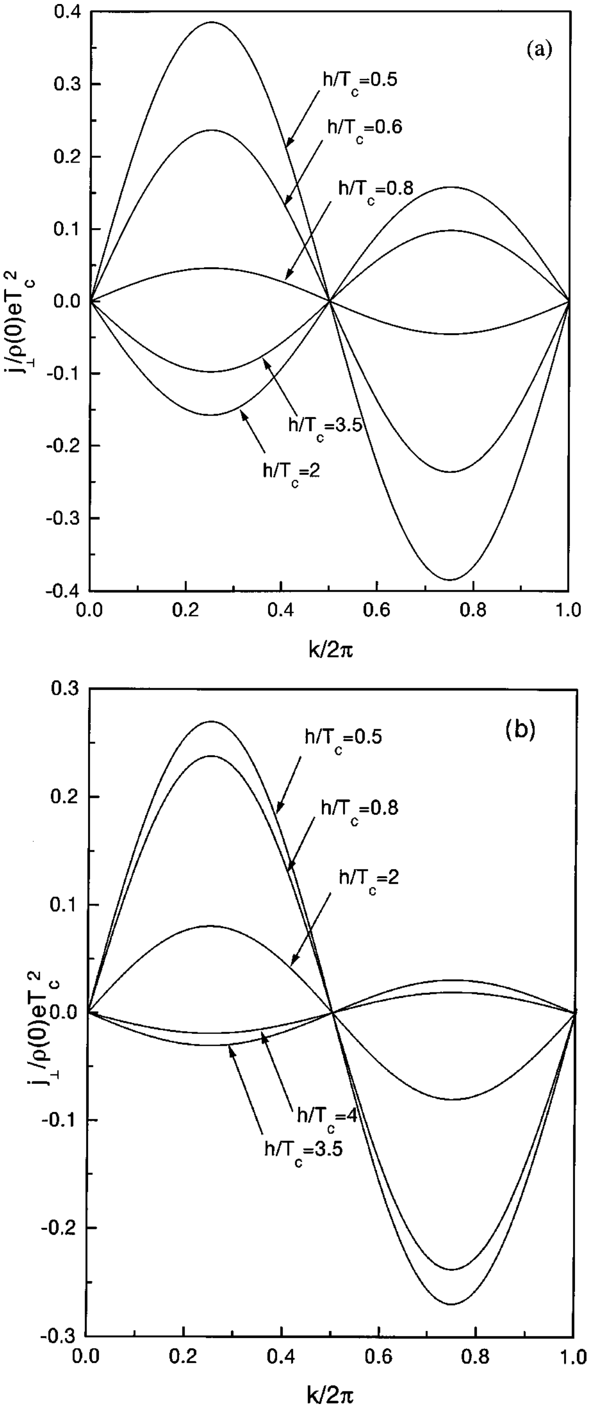

FIG. 1. Perpendicular current $j_{\perp}$ as a function of the phase k for $t/T_c=1$, $T/T_c=0.01$ (a), $T/T_c=0.8$ (b) for several values of h/T_c.

$k=\pi$ state is stable $[j_{\perp}(k=\pi)=0,\ j_{\perp}'(k=\pi)>0]$. The stability criterion used here, as in Ref. 5, is the minimum of the free energy (per unit area) $\mathcal{F}$: $\mathcal{F}'(k)=0$ and $\mathcal{F}''>0$, or, due to the Josephson relation $j_{\perp}(k)\propto\partial\mathcal{F}/\partial k$, $j_{\perp}(k)=0$, $j_{\perp}'(k)>0$. The corresponding dependence of the maximum supercurrent $|j_c(h)|$ is presented in Fig. 2 for $T/T_c=0.01$ and $T/T_c=0.8$. The transition from the $k=0$ to the $k=\pi$ state, where $j_c=0$, is clearly seen. The critical values $h_{\mathrm{crit}}(T=0.01)=0.88T_c$ and $h_{\mathrm{crit}}(T=0.8)=3.03T_c$ are practically the same as found in Ref. 5, for small t/T_c. At low T, a rise of $|j_c|$ at small h is found, similar to that predicted for $t/T_c\ll 1$.

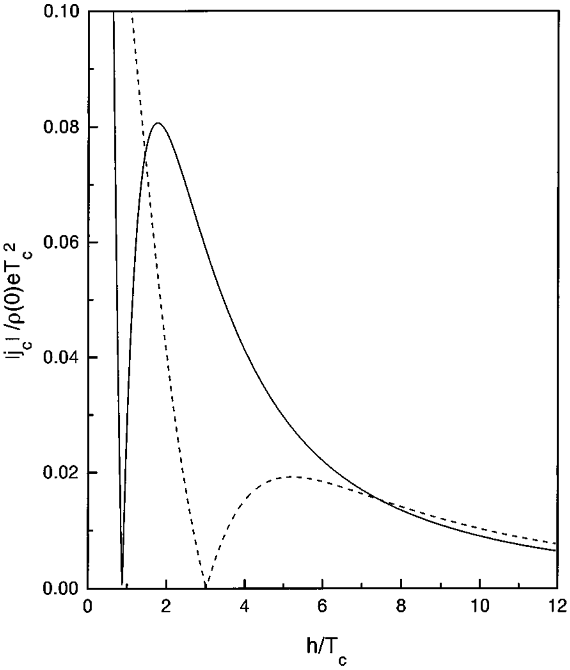

FIG. 2. Critical current j_c as a function of exchange field h/T_c for $t/T_c=1$, $T/T_c=0.01$ (solid line), and $T/T_c=0.8$ (dashed line).

The nonmonotonic variation of $j_c(h)$ is due to the appearance of the $k=\pi$ state, which in S/F superlattices has the same physical origin as the formation of the nonuniform superconducting state in bulk superconductors under Zeeman field (paramagnetic effect). Such a nonuniform state was predicted by Larkin and Ovchinnikov[16] and Fulde and Ferrell[17] a long time ago, but it is very difficult to meet the conditions for its appearance. In contrast, S/F superlattices provide a good opportunity to study one special kind of nonuniform superconducting state — the π state.

IV. DENSITY OF STATES

In S/F superlattices as in the S/N case[15,18] we expect that the quasiparticle spectra are drastically changed due to the coupling between layers, the bound states appearing as the result of Andreev reflections of electrons. However, it is a special case of this reflection since the exchange field is present in normal layers, opposite for the two electrons forming a Cooper pair. In this section we study the shape of the spectra as a function of the exchange field h, the transfer integral t, and the phase increment k. We calculate first the quasiparticles density of states for spin-up orientation, $\rho_i(E)=\rho_{i,\uparrow}(E)$ at $T=0$ on S and F layers, $i=\pm 1$.

In superconductor–normal-metal (S/N) superlattices[15,18] the quasiparticles excitations spectrum at $T=0$ is gapless in both layers and on N layer density of states increases as $\sqrt{E}$ from $E=0$. In S/F superlattices, as it was shown analytically in Ref. 5, for h small the density of states on F layer at $E=0$ is finite and the spectrum in both layers is gapless.

To investigate the general case [and in particular the case of large $h>h_{\mathrm{crit}}(0)$, where the transition from $k=0$ to $k=\pi$ occurs] we performed numerical calculations of $\rho_i(E)$. At zero temperature the density of states of energy E in layer i is given by[14]

$$\rho_i(E) = -\frac{\rho(0)}{\pi}\int_0^\infty d\xi \int_0^{2\pi}\frac{dq}{2\pi}\mathrm{Im}(G_{ii}(\omega,\xi,q)|_{i\omega\to E+i\delta}). \tag{4.1}$$

Using Eqs. (2.4)–(2.8) one obtains

$$\rho_i(E) = \frac{\rho(0)}{2\pi}\sum_n \int_0^{2\pi}\left(\frac{B_i \mathrm{sgn} C}{|D'|}\right)\bigg|_{\xi=\xi_n} dq. \tag{4.2}$$

Here ξ_n are the real solutions of a quartic equation in ξ, which corresponds to the poles of the retarded Green's function in Eq. (4.1),

$$D = \xi^4 + \xi^2(|\triangle(0)|^2 - 2E^2 - |T_q|^2 - |T_{k+q}|^2 - 2Eh - h^2) + \xi(2E+h)(|T_q|^2 - |T_{k+q}|^2) - |\Delta(0)|^2(E+h)^2 + (E^2 + Eh - |T_{k+q}|^2)(E^2 + Eh - |T_q|^2). \tag{4.3}$$

For the S layer,

$$B_1 = (E - \xi + h)(E^2 + \xi^2 + 2E\xi + hE + \xi h - |T_q|^2), \tag{4.4}$$

and for the F layer,

$$B_{-1} = (E + \xi + h)[E^2 - \xi^2 - |\triangle(0)|^2] - |T_q|^2(E - \xi), \tag{4.5}$$

where as C and D' are the same for the both layers,

$$C = -|\triangle(0)|^2(2E + 2h) + 4E^3 + 6hE^2 - 2\xi^2 h + 2h^2 E - 4\xi^2 E - |T_q|^2(2E - 2\xi + h) - |T_{k+q}|^2(2E + 2\xi + h), \tag{4.6}$$

$$D' = 4\xi^3 + 2\xi[|\triangle(0)|^2 - 2E^2 - 2Eh - h^2 - |T_q|^2 - |T_{k+q}|^2] + (2E+h)(|T_q|^2 - |T_{k+q}|^2). \tag{4.7}$$

Note that for given h, k and t, $D(E;\xi)$ in Eq. (4.3) is obtained by analytical continuation of $D(\omega;\xi)$ in Eq. (2.4). Since $D(\omega;\xi)$ appears in the denominator of the normal Green's functions $G_{i,-i}$, $i = \pm 1$, in Eq. (3.3), similarly as in the S/N case, it determines both the Josephson current, and the energy spectrum of the quasiparticles.[11] The bound states, seen as peaks or singularities in $\rho_i(E)$ after the integration over q, Eq. (4.2), occur at the energies E_b where (for some q) $D'(E;\xi=\xi_n)=0$, ξ_n being the solutions of $D(E;\xi_n)=0$. Simple explicit equations for E_b as functions of h and t can be obtained for $k=0$, see the Appendix.

To calculate from Eqs. (4.2)–(4.7) the densities of states $\rho_i(E)$, $i=\pm 1$, at $T=0$ we use numerical solutions of Eq. (3.12) for $|\triangle(0)|/T_c$ for given h,k as a function of t. An example of the dependence of $|\Delta(0)|/T_c$ on t for two different values of exchange field $h/T_c = 0.35$ and 1.5 is presented in Fig. 3. Similarly as in the S/N case, although both T_c and $|\Delta(0)|$ decrease due to the proximity effect when t rises, their ratio increases with t.

Results for the densities of states on S and F layers are presented in Figs. 4 and 5 for two fixed values of the exchange field ($h/T_c = 0.35$ and 1.5) and for two different values of the transfer integral ($t/T_c = 0.35$ and 1), for spin- up orientation. For each value of h we take the ground-

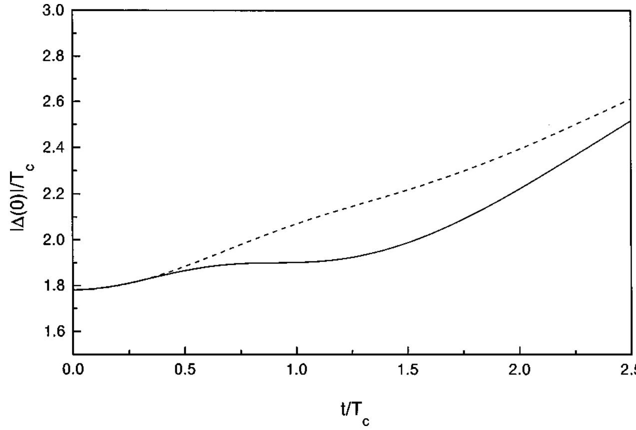

FIG. 3. The superconducting order parameter $|\Delta(0)|/T_c$ as a function of t/T_c for $h/T_c = 0.35$ (solid line) and $h/T_c = 1.5$ (dashed line).

state phase difference k according to the results of Sec. III, $k=0$ for $h/T_c = 0.35$ where h is below the critical value of the exchange field corresponding to the transition from $k=0$ to $k=\pi$ at $T=0$, $h < h_{\mathrm{crit}}(0) \approx 0.87T_c$, and $k=\pi$ for $h = 1.5T_c > h_{\mathrm{crit}}(0)$.

For $h/T_c = 0.35$ ($k=0$) different spectra are obtained for smaller ($t/T_c = 0.35$) and higher ($t/T_c = 1$) value of transfer integral. In the first case, Fig. 4(a), the density of states in S layer has two singularities at $|E| \cong |\Delta(0)|$ [corresponding to E_{b1} and E_{b4}, Eqs. (A2), (A3) in the Appendix], with some smaller structures in between. It is not changed very much with respect to the usual BCS shape,[19] but the singularities occur at the new value of $|\Delta(0)|$, obtained for the superlattice. On the F layer, the change of the spectrum (with respect to the normal ferromagnetic metal where the density of states is constant) is drastic: two large peaks appear inside the interval $|E| \leqslant |\Delta(0)|$ (corresponding to E_{b2} and E_{b3}) with two smaller peaks at the ends, $|E| \cong |\Delta(0)|$. In the second case, Fig. 4(b), the resemblance with the BCS case in S is lost, the density of states exhibits two resonant states (singularities) inside the interval $|E| < |\Delta(0)|$, jumps at $|E| \cong |\Delta(0)|$, and two singularities outside this interval. On F layer, there are two small peaks outside the interval $|E| \leqslant |\Delta(0)|$, and two singularities occur inside, at the same positions as for the S layer. These structures correspond to the (decreasing) energies E_{b1}, E_{b5}, E_{b6}, and E_{b4}. For larger t/T_c, the only "memory" of the BCS behavior in S is the jump at $|E| = |\Delta(0)|$.

We note also that for a fixed value of h/T_c (and k) a bound state may appear at the Fermi level ($E=0$), if t/T_c has an appropriate value (see the Appendix). An example of such a zero-energy bound state obtained for $h/T_c = 0.35$ is presented in Fig. 4(c).

For higher values of the exchange field, e.g., $h/T_c = 1.5$ ($k=\pi$), similar conclusions hold, i.e., new singularities appear when t/T_c is increased, see Fig. 5(a) ($t/T_c = 0.35$) and Fig. 5(b) ($t/T_c = 1.$). At fixed t/T_c, a characteristic consequence of the increase of exchange field is a shift of the positions of peaks on F, and the change of the spectrum shape on S, compare Figs. 4(a) and 5(a), and Figs. 4(b) and 5(b).

In the limit of high exchange field, $h/T_c \gg 1$, (and t/T_c

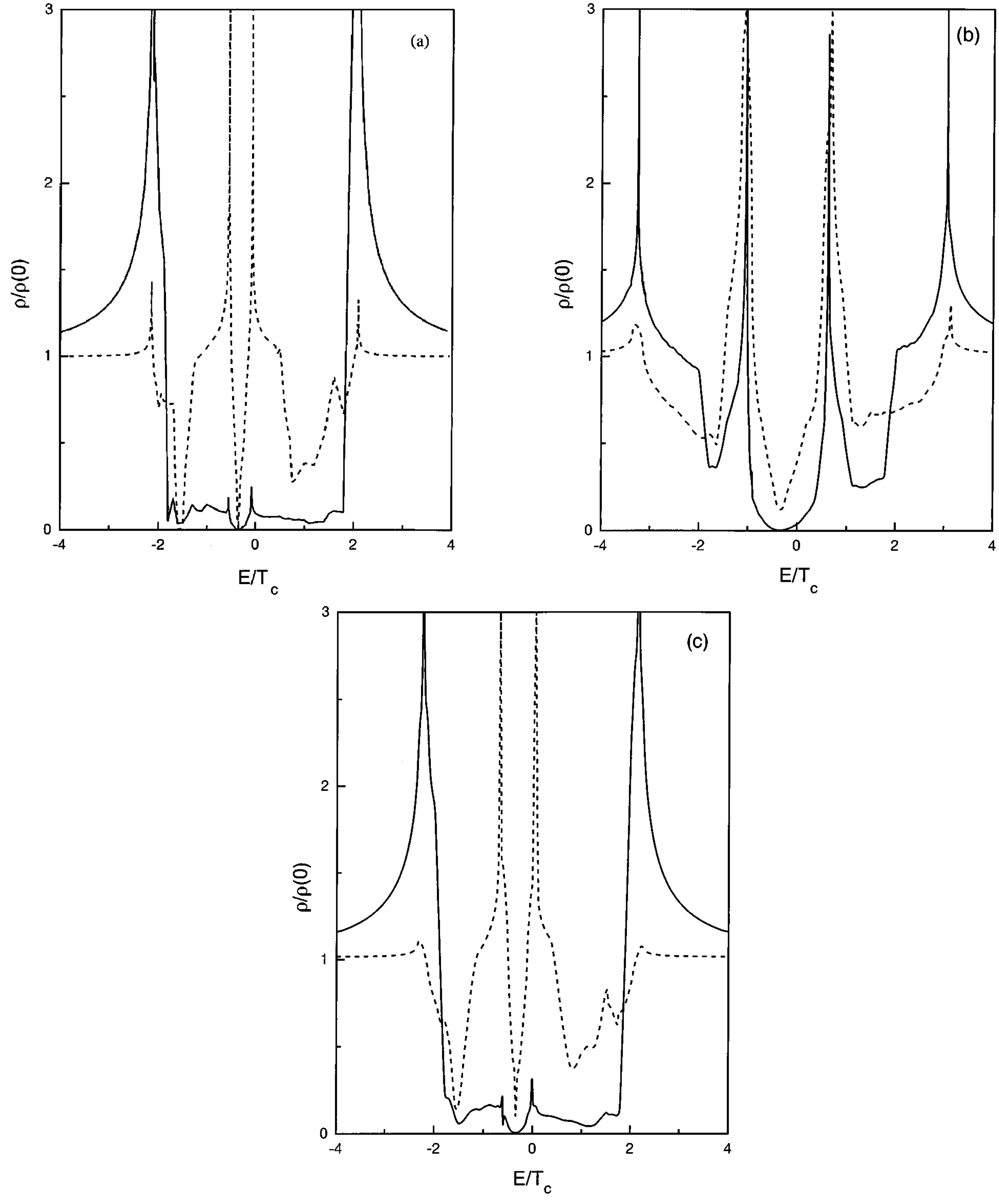

FIG. 4. Density of states $\rho_\uparrow(E,h)=\rho(E,h)$ at $T=0$ for $h/T_c=0.35$ and $t/T_c=0.35$ (a), $t/T_c=1$ (b), and $t/T_c=0.4$ (c). In the latter case, zero-energy peaks corresponding to the condition in the Appendix are shown. Full lines indicate S layers, dashed lines indicate F layers.

<1), or of small transfer integral $t/T_c \ll 1$, the decoupling of S layers leads on S to the BCS spectrum, with the gap, whereas on F the density of states becomes constant. In the opposite case of large coupling, $t/T_c \geqslant 3$ (and $h/T_c \ll 1$) the system behaves as a single BCS superconductor with the same shape of the density of states S and on F layers. In all above cases, there is no true gap in the excitation spectrum, $\rho_i(E)$ can be very small, but is always finite.

The effect of changing the phase increment, at fixed h and t, from its ground state value is illustrated for S layers in Fig. 6 on the example $h/T_c=0.35$ and $t/T_c=1$. The spectra for $k=0$ and $k=\pi$ (where $j_\perp=0$) and for $k=\pi/2$ (where $j_\perp=j_c$) are presented.

For the other spin orientation (spin down) we do not plot the density of states, because the spectra $\rho_{i\uparrow}(E,h)$ and $\rho_{i\downarrow}(E,h)=\rho_{i\uparrow}(E,-h)$ are (almost) symmetrical with respect to $E=0$ axes. However, since there is a spin splitting in the spectra it is evident that the Andreev reflection at the S/F

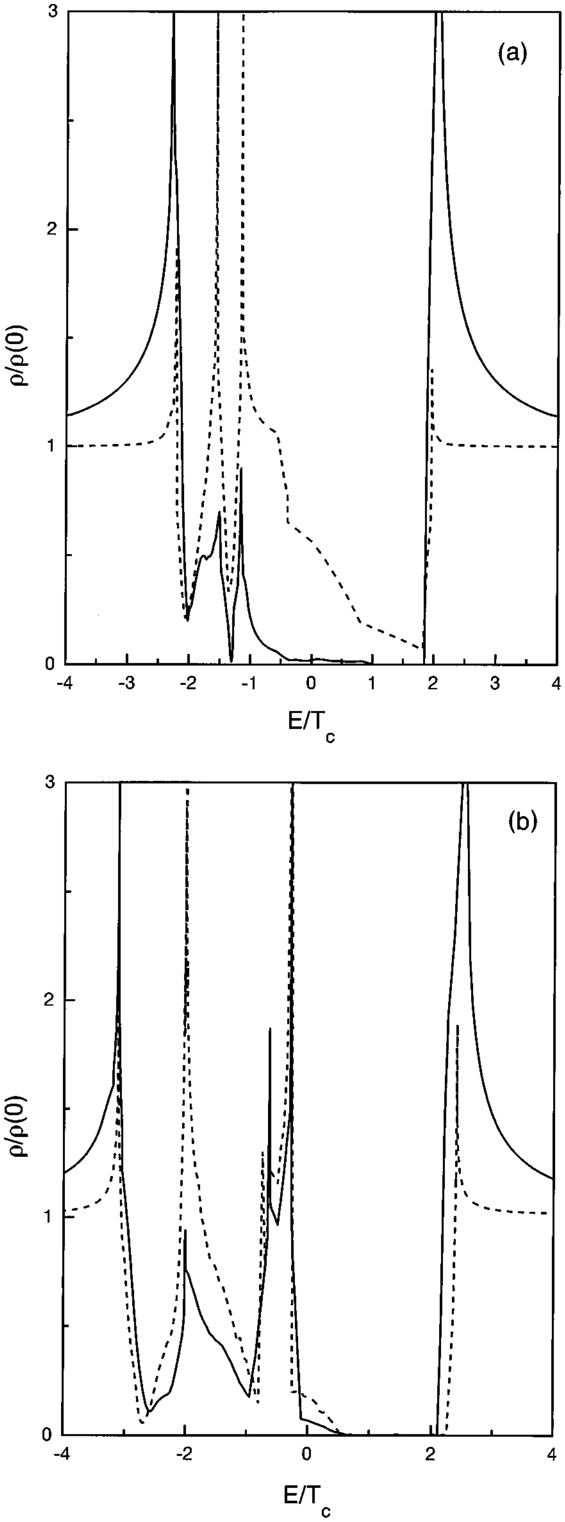

FIG. 5. Density of states $\rho_{\uparrow}(E,h)=\rho(E,h)$ at $T=0$ for $h/T_c=1.5$ and $t/T_c=0.35$ (a) and $t/T_c=1$. (b). Full lines indicate S layers, dashed lines indicate F layers.

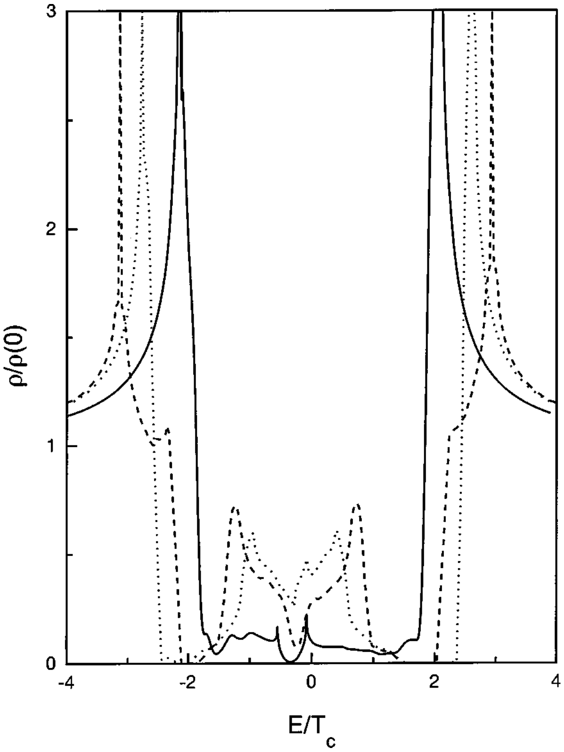

FIG. 6. Density of states $\rho_{\uparrow}(E,h)=\rho(E,h)$ on S layers at $T=0$ for $h/T_c=0.35$ and $t/T_c=1$. The preferred value of the phase increment in the ground state, $k=0$ (solid line), and nonpreferred values, $k=\pi/2$ (dashed line) and $k=\pi$ (dotted line).

interface is strongly affected by the presence of the exchange field in F, so that the number of peaks in the total density of states $\rho=\rho_{\downarrow}+\rho_{\uparrow}$ is increased.

V. SUMMARY AND CONCLUSION

In conclusion, we have studied a microscopic mechanism of formation of π junctions in atomic-scale S/F superlattices. It is related to the presence of the exchange field in F layers, S layers having the s-wave order parameter symmetry.

The main result of our calculation of the perpendicular supercurrent is that the critical current has a nonmonotonic dependence on h, and becomes zero at $h=h_{\mathrm{crit}}(T)$, corresponding to the transition from $k=0$ to $k=\pi$ in the ground state. Even for $t/T_c=1$, where the perturbation approach is not valid, we obtain numerically a $(T-h)$ diagram quite similar to that of Ref. 5. If a nonmonotonic $j_c(h)$ would be observed experimentally, this would be a clear signature of the appearance of the $k=\pi$ ground state in the S/F superlattice.

We have found the relationship between the Josephson supercurrent and the quasiparticles bound states, appearing as peaks or singularities in the density of states: both the supercurrent and the quasiparticle energy spectrum are determined by the poles of the normal Green's functions of the superlattice.

Using the obtained criterion for the transition from $k=0$ to $k=\pi$ at $T=0$, we calculated the densities of states on S and F layers in the ground state for different values of h and t. The spectra are gapless, as in the S/N case.[15,18] However, whereas in the latter case the gapless character of the spectrum is due to the presence of electron eigenstates localized on N layers only so that the electrons do not feel the pairing potential and have no gap in the superconducting phase,[15] in the present case the gapless character is due, in addition, to the exchange field breaking the time-reversal symmetry.[20]

Taking the nonpreferred values of the phase increment k, the spectra do not change very much, whereas they are strongly influenced by the values of the exchange field and of the transfer integral. For example, the appearance of singularities inside the ''gap'' on the S layer is an indication of relatively large t, whereas the decoupled case corresponds to sufficiently large h, or very small t. The appearance of a peak at the Fermi level, which is in S/N junctions formed when S has the d-wave symmetry,[21] in the present case is related to the presence of the exchange field h in F layers, with s-wave pairing in S layers. Another consequence of $h \neq 0$ is the removal of degeneracy in the spectra for two spin orientations. Due to the spin splitting, the number of peaks (singularities) in the total (spin up and spin down) quasiparticle density of states is increased.

The quasiparticle spectra can be probed by tunneling spectroscopy, which is the common method of measuring the superconducting quasiparticle density of states.[19] However, the determination of the ''gap'' $|\Delta(0)|$ may be complicated by appearance of bound states at higher energies, similarly as in the S/N case.[18] For experimental testing, the desirable S/F interfaces should be atomically flat with well lattice matched layers, as, e.g., in high-T_c cuprate superconductor/colossal magnetoresistance ferromagnet superlattices.[13] Also, our results (at least for t small) could describe superconductor/antiferromagnet (S/AF) superlattices, such as the layered compound $Sm_{1.85}Ce_{0.15}CuO_4$, which consists of ferromagnetic sheets within the a-b planes, with Sm spin direction along the c axes and spins in alternate layers aligned antiparallel.[22]

APPENDIX

In this Appendix we calculate explicitly the bound-state energies E_b for $k=0$ (and spin-up orientation), from Eqs. (4.3) and (4.7). In this case Eq. (4.3) becomes

$$D(E,\xi)=\xi^4+b\xi^2+c=0, \tag{A1}$$

where

$$b=|\Delta|^2-2E^2-2Eh-h^2-2|T_q|^2,$$

$$c=(E^2+Eh-|T_q|^2)^2-|\Delta|^2(E+h)^2.$$

and $\Delta=\Delta(0)$ everywhere. Eq. (4.7) can be written in the form

$$D'(E,\xi_n)=2\xi_n(2\xi_n^2+b)=0.$$

Thus, we have two types of solutions:

(a) $\xi_n=0$, $c=0$, which gives

$$E_{b1/2}=\frac{1}{2}[(|\Delta|-h)\pm\sqrt{(|\Delta|+h)^2+4|T_q|^2}], \tag{A2}$$

and

$$E_{b3/4}=\frac{1}{2}[-(|\Delta|+h)\pm\sqrt{(|\Delta|-h)^2+4|T_q|^2}], \tag{A3}$$

(b) $2\xi_n^2+b=0$, $b^2=4c$, which gives

$$E_{b5/6}=\frac{-h(|\Delta|^2+h^2+4|T_q|^2)\pm2\sqrt{|\Delta|^2|T_q|^2(h^2-|\Delta|^2+4|T_q|^2)}}{2(h^2+4|T_q|^2)}, \tag{A4}$$

Real solutions given in Eq. (A4) are obtained for $h^2+4|T_q|^2\geqslant|\Delta|^2$, i.e., for sufficiently large h and/or t. Here for $q=0$ $|T_q|^2=4t^2$. For $h=0$ and $q=0$ the solutions for E_b coincide with those obtained in Ref. 18, for the S/N case. Note that the bound states at $E=0$ may be obtained by choosing h and t according to the conditions (a) $c=0$, $t=\sqrt{|\Delta|h}/2$, and (b) $b^2=4c$, $h^2=-(|\Delta|^2+8t^2)+4t\sqrt{2|\Delta|^2+4t^2}$, which requires $t\geqslant|\Delta|/4$.

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