Microscopic theory of the dc Josephson effect in clean superconductor/insulator and superconductor/semiconductor multilayers

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We have constructed a fully microscopic self-consistent theory of the dc Josephson effect in clean periodic superconducting multilayers with realistic finite-size repulsive barriers, at arbitrary temperatures. We have derived an explicit analytical expression for the critical Josephson current j_c as a function of the superconductor-layer thickness a. In the limit $a \ll \xi_0$, we have found fundamental differences with the Ambegaokar-Baratoff relation: a strong reduction of j_c and an unusual temperature dependence. In this limit, we also predict an exponential decrease of the critical temperature and the gap parameter due to the depairing effect of the Josephson current. [S0163-1829(97)04037-X]

In the last years considerable effort was concentrated on the fabrication of high-quality superconducting periodic multilayers with Josephson coupling through insulating[1] and semiconducting[2] barriers. These devices are believed to be of great importance for future microelectronics.[3] On the other hand, experimental and theoretical studies of artificial Josephson coupled multilayers may contribute to the understanding of some of the intriguing features of high-T_c superconductors exhibiting the intrinsic Josephson effect.[4]

It is well known[5] that the principal physical characteristic of any weakly coupled superconducting system is the critical Josephson current j_c. Unfortunately, the problem of the microscopic calculation of j_c in weakly coupled *periodic multilayers* has not so far received proper attention. However, the very first theoretical results reveal dramatic differences with respect to single-junction behavior. Thus two of the authors (S.V.K. and S.V.N.) have recently proposed a self-consistent microscopic theory of current-carrying states in Josephson- and proximity-effect-coupled multilayers near the bulk critical temperature T_{c0}.[6] Regarding j_c, they found drastic deviations from a single-junction case: unusual temperature dependence for superconductor/normal metal (S/N) multilayers, and a strong reduction of j_c for S/I multilayers in the limit $a \ll \xi_0$ (a for the S-layer thickness, ξ_0 for the BCS coherence length). The latter result, explained in terms of the nonlocality of j_c, suggests that at lower temperatures ($T \ll T_{c0}$) qualitative deviations from the Ambegaokar-Baratoff relation[7] for a single SIS junction should be expected. Our aim here is to clarify this situation in detail.

In this paper, we derive an explicit analytical expression for j_c as a function of a for *arbitrary* temperatures in the framework of a microscopic model with a periodic repulsive *finite-size* barrier, typical of superconductor/semiconductor (S/Sem) multilayers. In the limit $a \ll \xi_0$, we investigate the effect of the suppression of the critical temperature and the gap parameter by the supercurrent. Mathematically, we circumvent a very difficult problem of finding the full Green's function and use a powerful analytical method that is applicable even to barriers with an internal structure. Physically relevant elements of the Green's function are calculated on the basis of a perturbation procedure.

We begin by considering an infinite periodic in the x-direction superconducting (s-wave) system in the clean limit and in the absence of external magnetic fields. Complete structural homogeneity in the yz plane is implied, though the transverse dimensions of the system are taken to be small compared to the London penetration depth in order to discard the influence of self-induced fields. The S layers and the barriers occupy the regions $S_n = [-a + d/2 + nc, -d/2 + nc]$ and $B_n = [-d/2 + nc, d/2 + nc]$, respectively ($c = a + d$ is the period, and n is an integer). This system is described by the Gor'kov equations (Fourier transformed in y, z)

$$\left\{ i\omega + \left[E_F t^2 + \frac{1}{2m}\frac{d^2}{dx^2} - U(x) \right]\tau_3 + \frac{1}{2}(\tau_1 + i\tau_2)\Delta(x) + \frac{1}{2}(\tau_1 - i\tau_2)\Delta^*(x) \right\} \begin{bmatrix} G_\omega(x,x';t) \\ F_\omega(x,x';t) \end{bmatrix} = \begin{bmatrix} \delta(x-x') \\ 0 \end{bmatrix}, \quad (1)$$

$$\Delta^*(x) = |g(x)| \pi N(0) v_0 T \sum_\omega \int_0^1 dt\, t \langle F_\omega(x,x;t) \rangle, \quad (2)$$

$$g(x) = -|g| \sum_n \delta_{S_n}(x), \quad U(x) = U_0 \sum_n \delta_{B_n}(x), \quad U_0 > 0,$$

$$\delta_\Omega(x) = \{1 \quad \text{for } x \in \Omega, \quad 0 \quad \text{for } x \notin \Omega\}.$$

Here $\hbar = 1$, τ_i ($i = 1,2,3$) are the Pauli matrices in the Gor'kov-Nambu space, $\omega = \pi T(2n+1)$ (n is an integer), E_F is the Fermi energy, $N(0) = m p_0 / 2\pi^2$ is the one-spin density of states at the Fermi level ($p_0 = m v_0$ being the Fermi momentum), g is the electron-electron coupling constant, U_0 is the barrier potential, $t \equiv \cos\theta$ is the cosine of the angle of incidence at the interface. In the self-consistency equation, $\langle \cdots \rangle$ denotes spatial averaging over atomic-scale oscillations. (We confine ourselves to the limit $p_0^{-1} \ll a$.) Because of the periodicity, the pair potential obeys the relation $\Delta(x+nc) = \Delta(x)\exp(in\phi)$. The functions G_ω, F_ω and their first derivatives G'_ω, F'_ω are subject to the usual continuity conditions at the interfaces $x = \pm d/2 + nc$.

As in the case of a single junction,[8] the supercurrent density can be written as

$$\begin{aligned} j &\equiv j(x \in B_0) \\ &= \frac{2iemE_F}{\pi} T \sum_\omega \int_0^1 dtt \int_{-\infty}^{-d/2} dx_1 \int_{d/2}^{+\infty} dx_2 [\Delta(x_1)\Delta^*(x_2) \\ &\quad \times \langle G^n_\omega(x_1,x_2;t) G_{-\omega}(x_2,x_1;t)\rangle - \Delta(x_2)\Delta^*(x_1) \\ &\quad \times \langle G^n_\omega(x_2,x_1;t) G_{-\omega}(x_1,x_2;t)\rangle], \end{aligned} \tag{3}$$

where G^n_ω is the Green's function of the system in the normal state. An obvious advantage of this representation is the proportionality of the integrand to the product of the Green's functions with $x_1 \in S_m$, $x_2 \in S_n$, where $m \neq n$, identically equal to zero in the absence of weak coupling: To calculate j_c in first order in the tunneling probability D, we must take Δ in zero order and substitute the expressions for G^n_ω, G_ω in first order in $\sqrt{D}$ (see below).

As we are not concerned with the Green's functions with coordinates inside the barriers, in what follows we shall consider only $G_\omega(x \in S_n, x' \in S_m; t)$, $F_\omega(x \in S_n, x' \in S_m; t)$. To derive the boundary conditions for these functions, we first solve Eq. (1) for $G_\omega(x \in B_n, x' \in S_m; t)$ and $F_\omega(x \in B_n, x' \in S_m; t)$. Making use of the full set of the boundary conditions, we arrive at the required relations

$$\begin{bmatrix} G_\omega \\ F_\omega \end{bmatrix}(nc+d/2,x') = \cosh(\lambda_B^{\mp} d)\begin{bmatrix} G_\omega \\ F_\omega \end{bmatrix}(nc-d/2,x') + \frac{\sinh(\lambda_B^{\mp} d)}{\lambda_B^{\mp}}\begin{bmatrix} G'_\omega \\ F'_\omega \end{bmatrix}(nc-d/2,x'), \tag{4}$$

$$\begin{bmatrix} G'_\omega \\ F'_\omega \end{bmatrix}(nc+d/2,x') = \cosh(\lambda_B^{\mp} d)\begin{bmatrix} G'_\omega \\ F'_\omega \end{bmatrix}(nc-d/2,x') + \lambda_B^{\mp}\sinh(\lambda_B^{\mp} d)\begin{bmatrix} G_\omega \\ F_\omega \end{bmatrix}(nc-d/2,x'), \tag{5}$$

where $\lambda_B^{\mp} = \sqrt{U_0 - E_F t^2 \mp i\omega}$. Equations (4) and (5) form a closed system of exact boundary conditions for the functions $G_\omega(x \in S_n, x' \in S_m; t)$ and $F_\omega(x \in S_n, x' \in S_m; t)$. In the limit $d \to +0$, $U_0 \to +\infty$, $dU_0 \equiv V = \text{const}$, they reduce to the boundary conditions for a periodic δ-function potential.

Assuming $\lambda_B^{\mp} \approx \lambda_B \equiv \sqrt{U_0 - E_F t^2}$, we proceed to the limit of a low-transparency barrier $\lambda_B d \gg 1$. We can now solve Eqs. (1) and (2) with the boundary conditions (4) and (5) by means of perturbation theory, with $\exp(-\lambda_B d) \propto \sqrt{D}$ being the expansion parameter. As expected, in zero order, $\Delta^{(0)}(x) = \Delta_0 \Sigma_n \exp(in\phi)\delta_{S_n}(x)$ (Δ_0 is the gap in the bulk, and ϕ is a phase shift at the interfaces), and only $G^{(0)}_\omega(x \in S_n, x' \in S_n; t)$ and $F^{(0)}_\omega(x \in S_n, x' \in S_n; t)$ are nonzero. The functions $G_\omega(x \in S_n, x' \in S_m; t)$ and $F_\omega(x \in S_n, x' \in S_m; t)$ with $|n-m| > 1$ are of order >1 in $\sqrt{D}$ and should be neglected. The first-order approximation to $G_\omega(x \in S_1, x' \in S_0; t)$, entering Eq. (1), is given by

$$\begin{aligned} G^{(1)}_\omega(x \in S_1, x' \in S_0; t) = -\frac{m\lambda_B e^{-\lambda_B d}}{\Omega^2} \Bigg\{ &\frac{(\Omega+\omega)^2 + \Delta_0^2 e^{i\phi}}{\lambda_+^2 + \lambda_B^2} \frac{\sin[\lambda_+(a+d/2-x+\alpha_+)]\sin[\lambda_+(a+d/2+x'+\alpha_+)]}{\sin^2[\lambda_+(a+\beta_+)]} \\ &+ \frac{\Delta_0^2(1-e^{i\phi})}{\lambda_+^2+\lambda_B^2}\sqrt{\frac{\lambda_+^2+\lambda_B^2}{\lambda_-^2+\lambda_B^2}} \frac{\sin[\lambda_+(a+d/2-x+\alpha_+)]\sin[\lambda_-(a+d/2+x'+\alpha_-)]}{\sin[\lambda_+(a+\beta_+)]\sin[\lambda_-(a+\beta_-)]} \\ &+ \frac{\Delta_0^2(1-e^{i\phi})}{\lambda_-^2+\lambda_B^2}\sqrt{\frac{\lambda_-^2+\lambda_B^2}{\lambda_+^2+\lambda_B^2}} \frac{\sin[\lambda_-(a+d/2-x+\alpha_-)]\sin[\lambda_+(a+d/2+x'+\alpha_+)]}{\sin[\lambda_+(a+\beta_+)]\sin[\lambda_-(a+\beta_-)]} \\ &+ \frac{(\Omega-\omega)^2 + \Delta_0^2 e^{i\phi}}{\lambda_-^2 + \lambda_B^2} \frac{\sin[\lambda_-(a+d/2-x+\alpha_-)]\sin[\lambda_-(a+d/2+x'+\alpha_-)]}{\sin^2[\lambda_-(a+\beta_-)]} \Bigg\}, \end{aligned} \tag{6}$$

where $\Omega = \sqrt{\omega^2 + \Delta_0^2}$, $\lambda_\pm = \pm\sqrt{E_F t^2 \pm i\Omega}$, $\alpha_\pm = \lambda_\pm^{-1}\arcsin[\lambda_\pm(\lambda_\pm^2+\lambda_B^2)^{-1/2}]$, and $\beta_\pm = \lambda_\pm^{-1}\arcsin[2\lambda_\pm\lambda_B(\lambda_\pm^2+\lambda_B^2)^{-1/2}]$. The function $G^{(1)}_\omega(x \in S_0, x' \in S_1; t)$, also entering Eq. (1), is obtained from Eq. (6) via the substitution $x \leftrightarrow x'$, $\phi \to -\phi$. The normal-state function $G^{n(1)}_\omega(x \in S_1, x' \in S_0; t)$ is a limiting case of Eq. (6) for $\Delta_0 = 0$. Note that the spatial dependence of Eq. (6) clearly indicates that in first order in D only two adjacent S layers contribute to the supercurrent (3).

Now one can benefit from the quasiclassical approximation $\lambda_\pm \approx \pm p_0|t| + i\Omega/v_0|t|$ $[|t| \gg (T_{c0}/E_F)^{1/2}]$. Inserting $\Delta^{(0)}$ and the quasiclassical expressions for $G^{n(1)}_\omega$, $G^{(1)}_\omega$ into Eq. (3), carrying out small-scale averaging, and performing spatial integration finally yields

$$j = \frac{\pi}{2} ev_0 N(0)\Delta_0^2 T \int_0^1 dttD(t) \sum_\omega \frac{\tanh^2[(2a\sqrt{\omega^2+\Delta_0^2})/v_0 t]}{\omega^2+\Delta_0^2} \sin\phi, \tag{7}$$

$$D(t)=\frac{16E_F t^2(U_0-E_F t^2)}{U_0^2}\exp[-2d\sqrt{2m(U_0-E_F t^2)}].$$

Equation (7) is the desired analytical expression for the dc Josephson current in clean S/I and S/Sem multilayers, valid for any $p_0^{-1}\ll a\leqslant\infty$ and arbitrary temperatures. We observe that Eq. (7) does not depend on concrete features of our model and should also hold for semiconducting barriers with internal structures of the type considered by Aslamazov and Fistul in the case of a single SSemS junction.[8] For temperatures close to T_{c0}, Eq. (7) reduces to the expression first derived in Ref. 6 for S/I multilayers. Equation (7) is independent of the period c. This is a direct consequence of the already-mentioned adjacent-layer coupling in first order in D. The period may enter higher-order corrections, when the effect of subgap current-carrying Bloch states[9] comes into play.

As expected, in the limit $a\gg\xi_0$, Eq. (7) goes over into the Ambegaokar-Baratoff relation

$$j=\frac{\pi e v_0 N(0)}{2}\int_0^1 dt t D(t)\Delta_0(T)\tanh\frac{\Delta_0(T)}{2T}\sin\phi. \quad (8)$$

To consider the opposite limit $p_0^{-1}\ll a\ll\xi_0$, one must transform the sum over ω with the aid of contour integration in the complex ω plane (because of the divergence at small a). After some simple algebra, one arrives at the fundamental result

$$j=\frac{7\zeta(3)}{\pi^3}\frac{e v_0 N(0)\Delta_0^2(T)}{T_{c0}}\frac{a}{\xi_0}\int_0^1 dt D(t)\sin\phi, \quad (9)$$

where $\zeta(m)$ is the Riemann zeta function and $\xi_0\equiv v_0/2\pi T_{c0}$. Equation (9) was first derived in Ref. 6 for S/I superlattices near T_{c0}, but now we have established its legitimacy for superstructures with *arbitrary* repulsive barriers in the *whole* temperature region $0\leqslant T<T_{c0}$. Three remarkable features are to be noted with regard to Eq. (9): (i) a strong reduction of j_c due to the emergence of the additional small factor a/ξ_0 (ii) the temperature dependence determined solely by the factor $\Delta_0^2(T)$ in the whole temperature range, and (iii) the occurrence of $\int_0^1 dt D(t)$ instead of $\int_0^1 dt t D(t)$ in the Ambegaokar-Baratoff regime. These results are a manifestation of the nonlocality of the supercurrent in its extreme: While the product of two Green's functions in the integrand Eq. (3) decays at distances on the order of ξ_0, the actual range of spatial integration is restricted by two adjacent S layers only. Thus, for instance, at $T=0$ we can rewrite Eq. (9) as

$$j=\frac{14\zeta(3)}{\pi^2}e v_0 N(0)\Delta_0(0)\int_0^1 dt t D(t)P(t)\sin\phi,$$

where $P(t)=a/v_0 t\Delta_0^{-1}(0)$ is the quasiclassical probability of finding an unscattered electron with the x component of the velocity $v_0 t$ within one S layer during the characteristic time $\Delta_0^{-1}(0)$. Finally, one must bear in mind that Eq. (9) has been derived in the clean mesoscopic regime. Considerable changes may occur in the dirty limit $l\ll\xi_0$ (l is the electron mean free path), when the fall off length of the integrand in Eq. (3) is of the order of $\sqrt{\xi_0 l}$. Actually, this limiting situation asks for further investigation.

Now we want to study the effect of the supercurrent on the critical temperature and the gap parameter, and establish a criterion of validity of our perturbation-theory approach in the limit $p_0^{-1}\ll a\ll\xi_0$. As is always the case in inhomogenous superconductors, the critical temperature T_c is given by the largest eigenvalue of the linearized self-consistency equation (2). Explicitly, for clean S/I multilayers with thin ($d\ll\min\{a,\xi_0\}$) repulsive barriers, such an equation was derived in Ref. 6. Expanded to first order in $D\ll 1$, it reads

$$\begin{aligned}\Delta(x\in S_0)=\frac{\pi N(0)|g|}{v_0}\Bigg[&\int_{-a+0}^{-0}dx'\Delta(x')T\sum_\omega\int_0^1\frac{dt}{t}\Bigg\{\exp\left[-\frac{2|\omega|}{v_0 t}|x-x'|\right][1-D(t)]\\&\times\frac{\exp[-2|\omega|a/v_0 t]\cosh[(2|\omega|/v_0 t)(x-x')]+\cosh[(2|\omega|/v_0 t)(x+x'+a)]}{\sinh(2|\omega|a/v_0 t)}\Bigg\}\\&+\int_{+0}^{a-0}dx'\Delta(x')T\sum_\omega\int_0^1\frac{dt}{t}D(t)\Bigg\{\frac{\exp[(-2|\omega|/v_0 t)(x'-x-a)]}{2\cosh(2|\omega|a/v_0 t)}\\&+\frac{\exp[-2|\omega|a/v_0 t]\cosh[(2|\omega|/v_0 t)(x-x'+a)]+\cosh[(2|\omega|/v_0 t)(x+x')]}{\sinh(4|\omega|a/v_0 t)}\Bigg\}\\&+\int_{-2a+0}^{-a-0}dx'\Delta(x')T\sum_\omega\int_0^1\frac{dt}{t}D(t)\Bigg\{\frac{\exp[(-2|\omega|/v_0 t)(x-x'-a)]}{2\cosh(2|\omega|a/v_0 t)}\\&+\frac{\exp[-2|\omega|a/v_0 t]\cosh[(2|\omega|/v_0 t)(x-x'-a)]+\cosh[(2|\omega|/v_0 t)(x+x'-2a)]}{\sinh(4|\omega|a/v_0 t)}\Bigg\}\Bigg],\end{aligned} \quad (10)$$

with a cutoff at the Debye frequency, ω_D, in the sum over ω implied. The restriction on spatial integration by two adjacent S layers is again a result of the first-order approximation. For $a \gg \xi_0$, Eq. (10) goes over into the very familiar equation for a single SIS junction.[10] The analysis of Eq. (10) in the limit $p_0^{-1} \ll a \ll \xi_0$ shows that in the current-carrying state its largest eigenvalue corresponds to a complex Δ, constant in each S layer with a phase shift ϕ at the interfaces. (Physically, but for the phase jumps ϕ no spatial variations can occur in the small-scale-averaged Δ over distances less than ξ_0.) Thus, substituting $\Delta(x) = \text{const}\sum_{n=-1}^{1} \exp(in\phi)\delta_{S_n}(x)$ yields

$$T_c = T_{c0}\exp\left[-\frac{1}{N(0)|g|}\int_0^1 dtD(t)(1-\cos\phi)\right], \quad (11)$$

where $T_{c0} = 2\omega_D\,(\gamma/\pi)\exp[-1/N(0)|g|]$ (γ is Euler's constant). The occurrence of the depairing factor $\int_0^1 dtD(t)(1-\cos\phi)$ in the exponent of Eq. (11) is quite unusual for weak superconductivity and signifies a strong suppression of T_c by the Josephson current. In this case, the influence of the Josephson current can even be regarded as effective weakening of the electron-electron coupling constant:

$$|g| \rightarrow |g|\left[1 - \int_0^1 dtD(t)(1-\cos\phi)\right].$$

[Analogous renormalization of $|g|$ owing to pair breaking is known for proximity-effect S/N bilayers in the so-called Cooper limit.[11] The expression for T_c in these structures is in a one-to-one correspondence with our Eq. (11).] By virtue of the BCS Ref. 12 relation $|\Delta(0)| = (\pi/\gamma)T_c$, we expect for the gap at $T=0$ the dependence

$$|\Delta(0)| = \Delta_0(0)\exp\left[-\frac{1}{N(0)|g|}\int_0^1 dtD(t)(1-\cos\phi)\right]. \quad (12)$$

Thus the effect of the Josephson current on T_c and $|\Delta|$ is by no means small unless the condition

$$\int_0^1 dtD(t) \ll N(0)|g| \quad (13)$$

is fulfilled. At the same time, Eq. (13) gives the desired criterion of the validity of our perturbation-theory approach in the limit $p_0^{-1} \ll a \ll \xi_0$. To conclude the discussion of Eqs. (11)–(13), we remark that as far as no specific features of the thin-barrier case enter these relations, they should also hold for any periodic structures with realistic finite-size repulsive barriers (S/Sem multilayers).

Summarizing, we have constructed a fully microscopic self-consistent theory of the dc Josephson effect in clean S/I and S/Sem multilayers. Reformulating the problem in terms of the relevant Green's functions and applying perturbation theory at an early stage of calculations, we managed to derive an explicit analytical expression for the Josephson current as a function of the S-layer thickness $a(p_0^{-1} \ll a \leq \infty)$, valid at arbitrary temperatures [Eq. (7)]. In the limit $p_0^{-1} \ll a \ll \xi_0$, we found fundamental differences with single-junction behavior, inherent to nonlocal nature of the Josephson current: a strong reduction of j_c and unusual temperature dependence [Eq. (9)]. In the latter limit, we also obtained exponential decrease of T_c and $|\Delta(0)|$ due to depairing effect of the Josephson current [Eqs. (11) and (12)] and checked the self-consistency of our calculations [Eq. (13)].

Our results may have important conceptual implications in physics of superconducting multilayers with Josephson coupling. For example, they establish a quantitative limit on decreasing the S-layer thickness in vertically stacked Josephson-junction arrays intended for superconducting microelectronic circuits of high integration,[3] if one looks for large values of j_c. Concerning high-T_c superconductors with the intrinsic Josephson effect such as $Bi_2Sr_2CaCu_2O_8$, it is a common practice[4] to estimate $|\Delta(0)|$ and the temperature dependence of j_c on the basis of the Ambegaokar-Baratoff relation (8). In view of the extremely thin CuO_2 double layers ($a=3$ Å), believed to be superconducting, one may question the legitimacy of this approach. Moreover, one cannot altogether exclude a possibility of gap measurements from I-V characteristics being affected by the tunneling supercurrent [if the transport current perpendicular to weak links exceeds j_c, this effect must be even more pronounced than given by Eq. (12)]. Finally, the above-discussed effects, resulting from spatial nonlocality combined with periodicity, must qualitatively hold also for anisotropic (d-wave) pairing. However, in this case the enhancement of predicted suppression of j_c and T_c is to be expected because of pair breaking by the interfaces themselves.[13]

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