Josephson Effect Between Triplet Superconductors: A Self-Test for the Order Parameter Symmetry of Bechgaard Salts

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(March 22, 2002)

We show that the Josephson effect between triplet superconductors is sensitive to the relative orientation of the \( \mathbf{d} \)-vectors across the junction. In addition, we point out that the temperature and angular dependence of the Josephson effect can help distinguish between different order parameter symmetries. We discuss coherent and incoherent tunneling processes, and the role of surface bound states within the framework of non-local lattice Bogoliubov-deGennes equations.

Recent upper critical field and NMR experiments in \((\text{TMSTTF})_2\text{X}\) [1–3], where \( \text{X} = \text{ClO}_4, \text{PF}_6 \) have indicated that they may be unconventional triplet superconductors, while low temperature thermal conductivity experiments [4] suggest that the superconducting state is gapped. These experiments were inspired by early suggestions of triplet superconductivity in Bechgaard salts [5–8], and served as inspirations for the intense theoretical efforts [9–14] that followed. Lebed, Machida, and Ozaki (LMO) [11] proposed a “p-wave” triplet order parameter for \((\text{TMSTSF})_2\text{PF}_6\), where the \( \mathbf{d} \)-vector had a strong component along the \( \mathbf{a} \) direction, thus producing a strongly anisotropic spin susceptibility with \( \chi_a \ll \chi_N \) and \( \chi' \approx \chi_N \). A fully gapped singlet “d-wave” order parameter for \((\text{TMSTSF})_2\text{ClO}_4\) was proposed by Shimahara [12], while gapless triplet “f-wave” superconductivity for \((\text{TMSTF})_2\text{PF}_6\) was proposed by Kuroki, Arita, and Aoki (KAA) [13]. Duncan, Vaccarella and Sá de Melo (DVS) [14] performed a detailed group theoretical analysis and suggested that a weak spin-orbit fully gapped triplet “\( p_{xz} \)-wave” order parameter, where \( \chi_a \approx \chi_N \) and \( \chi' \approx \chi_N [10,15] \), would be a good candidate for superconductivity in Bechgaard salts.

Here we propose a test for the order parameter symmetry of Bechgaard salts which is based on the Josephson effect between two TS exists in the simplest case where the tunneling matrix element is spin-conserving (with or without time-reversal invariance), and that it depends on the relative orientation of the \( \mathbf{d} \)-vectors of the TS. In addition, we show that the temperature and angular dependence of the Josephson effect can also help distinguish between different triplet states. We include coherent and incoherent tunneling processes and the effects of surface bound states (within the framework of non-local lattice Bogoliubov-deGennes equations).

In anticipation of the existence of surface bound states in particular geometries of unconventional superconductors [18,19], we prefer to use a real space representation of the left \((L)\) and right \((R)\) superconductors Hamiltonian

\[
H_j = \sum_{r_j,r_j'} \mathcal{H}(r_j,r_j') \langle c_{j,\alpha_j}^\dagger (r_j) c_{j,\alpha_j} (r_j') \rangle + \sum_{r_j,r_j'} \left[ \Delta_j,\beta_j (r_j,r_j') c_{j,\alpha_j}^\dagger (r_j) c_{j,\beta_j} (r_j') + \text{H.C.} \right],
\]

where indices \( \alpha_j \) and \( \beta_j \) (with \( j = L,R \)) are spin labels, \( r_j, r_j' \) are position labels. Repeated Greek indices indicate summation. The first term of \( H_j \) contains \( \mathcal{H}(r_j,r_j') = [t_j(r_j,r_j') - \mu \delta_{r_j,r_j'}] \), where \( t_j(r_j,r_j') \) are transfer integrals confined to nearest neighbors and \( \mu \) is their chemical potential. The second term of \( H_j \) contains the order parameter matrix \( \Delta_j,\beta_j (r_j,r_j') = \langle c_{j,\alpha_j}^\dagger (r_j) c_{j,\beta_j} (r_j') \rangle \), where \( V_{j,\alpha_j,\beta_j,\gamma_j}(r_j,r_j') \) is the two-body pairing interaction. The tunneling Hamiltonian connecting \( L \) and \( R \) superconductors is

\[
H_T = \sum_{\mathbf{r}_L, \mathbf{r}_R} \left[ T_{\alpha_L \alpha_R}(\mathbf{r}_L,\mathbf{r}_R) c_{L,\alpha_L}^\dagger (\mathbf{r}_L) c_{R,\alpha_R} (\mathbf{r}_R) + \text{H.C.} \right],
\]

where the matrix element for tunneling is \( T_{\alpha_L \alpha_R}(\mathbf{r}_L,\mathbf{r}_R) = T_s(\mathbf{r}_L,\mathbf{r}_R) \delta_{\alpha_L,\alpha_R} + T_v(\mathbf{r}_L,\mathbf{r}_R) \cdot \sigma_{\alpha_L,\alpha_R} \), with the first term \( T_s \) corresponding to spin-conserving tunnelling, and the second term \( T_v \) corresponding to spin-dependent tunnelling. The pair current through the junction is (to second order in the tunneling matrix element)

\[
J_s(V,T) = \frac{2e}{\hbar} \text{Im} \left[ \exp(i \omega_f t) \sum_{\mathbf{r}_L, \mathbf{r}_R} T_{\alpha_L \alpha_R}(\mathbf{r}_L,\mathbf{r}_R) T_{\alpha_L,\beta_R}(\mathbf{r}_L,\mathbf{r}_R') P_{\alpha_R \beta_R}(\mathbf{r}_L,\mathbf{r}_R,\mathbf{r}_L',\mathbf{r}_R', i \omega_n) \right],
\]

where \( i \omega_n \) corresponds to Matsubara frequencies continued to \((-eV/\hbar + i \delta)\), and \( \omega_f = 2eV/\hbar \) with \( V \) being the voltage applied across the junction. The tensor \( P_{\alpha_R \beta_R}^{\alpha_L \beta_L} \) can be written in terms of the anomalous Green’s matrices as
\[ F_{\alpha\beta R}^{\delta \lambda L}(r_L, r_R, r'_L, r'_R, i\omega_n) = T \sum_{\delta^\prime} F_{\alpha\beta R}^{\delta \lambda L}(r_L, r'_L, i\omega_n) F_{R\delta^\prime R}^{\delta^\prime \lambda R}(r_R, r'_R, i\omega_n - i\nu_m) \text{, where } F_{j,\alpha\beta}(r_j, r'_j, i\nu_m) = T\int dt \exp(i\nu_m t) F_{j,\alpha\beta}(r_j, r'_j, \tau, \text{ with } F_{j,\alpha\beta}(r_j, r'_j, \tau)) = (Tc_{j,\alpha}(r_j, \tau)c_{j,\beta}(r'_j, 0)) \].

The general form of the order parameter matrix \( \Delta_{j,\alpha\beta}(r_j, r'_j) = i\Delta_{\alpha\beta}(r_j, r'_j) [\sigma_2]_{\alpha\beta} + i\delta_{j}^{\dagger}(r_j, r'_j) [\sigma_2]_{\alpha\beta} \), where the first term corresponds to the singlet (pseudo-singlet) state and the second to the triplet (pseudo-triplet) state in the case of weak spin-orbit coupling (in the case of strong spin-orbit coupling). The order parameter matrix \( \Delta_{j,\alpha\beta}(r_j, r'_j) \) satisfies the Pauli exclusion principle, since the function \( \Delta_{\alpha\beta}(r_j, r'_j) \) represents singlet pairing is symmetric under the exchange \( r_j \leftrightarrow r'_j \), and the vector \( \delta_{j}^{\dagger}(r_j, r'_j) \) which represent triplet pairing is antisymmetric under the exchange \( r_j \leftrightarrow r'_j \).

The reduced Hamiltonians on both sides of the junction can be separated diagonally via the lattice Bogoliubov-de Gennes transformation \( c_{j,\alpha}(r_j) = \sum N_j \left[ u_{N_j,\alpha}(r_j) \gamma_{N_j} + v_{N_j,\alpha}^{\dagger}(r_j) \gamma_{N_j}^{\dagger} \right] \), where \( u_{N_j,\alpha} \) and \( v_{N_j,\alpha} \) are two component spinors for each value of \( \alpha \) and satisfy the corresponding non-local Bogoliubov-deGennes (BdG) equation

\[ E_{N_j} u_{N_j,\alpha}(r_j) = \sum_{r_j'} \mathcal{H}(r_j, r'_j) u_{N_j,\alpha}(r'_j) + \sum_{r_j'} \Delta_{j,\alpha\beta}(r_j, r'_j) v_{N_j,\beta}(r'_j) \]

\[ -E_{N_j} v_{N_j,\alpha}(r_j) = \sum_{r_j'} \mathcal{H}^{\ast}(r_j, r'_j) u_{N_j,\alpha}(r'_j) + \sum_{r_j'} \Delta_{j,\alpha\beta}^{\ast}(r_j, r'_j) u_{N_j,\beta}(r'_j). \]

This set of equations must be solved self-consistently together with the order parameter equation

\[ \Delta_{j,\alpha\beta}(r_j, r'_j) = \frac{1}{4} V_{j,\alpha\beta\gamma\delta}(r_j, r'_j) \sum_{N_j} (1 - 2f_{N_j}) \left[ v_{N_j,\gamma}(r_j) u_{N_j,\delta}(r'_j) - v_{N_j,\delta}(r_j) u_{N_j,\gamma}(r'_j) \right] , \]

where the two-body potential is written under the assumption of weak spin-orbit coupling as \( V_{j,\alpha\beta\gamma\delta}(r_j, r'_j) = 2f_{1j}(r_j, r'_j) \delta_{\alpha\beta}\delta_{\gamma\delta} + 2f_{2j}(r_j, r'_j) \delta_{\alpha\gamma}\delta_{\beta\delta} \). From now on we will assume that the superconductors on either side of the junction are in (a) a triplet unitary state (time reversal invariant state in the bulk); (b) characterized by weak spin-orbit coupling; (c) the tunnel matrix element \( T_{\alpha\beta\gamma\delta}(r_j, r'_j) \) is spin conserving, i.e., the tunnel barrier preserves spin, and thus it is not magnetically active; and (d) the \( \delta_{j} \)-vector is weakly locked to the \( c_j \) axis by the weak spin-orbit coupling, a choice that is consistent with Knight shift experiments of Lee et al. [3]. All these assumptions seem to be applicable to the Bichgalds. We model these quasi-one-dimensional salts via the bulk dispersion \( \delta_{j}(k_j) = -|t_{x,j}| \cos(k_{x,j}a_j) - |t_{y,j}| \cos(k_{y,j}b_j) - |t_{z,j}| \cos(k_{z,j}c_j) \), where \( t_{x,j} \gg |t_{y,j}| \gg |t_{z,j}| \), corresponding to an orthorhombic crystal (D2h group) with lattice constants \( a, b \) and \( c \) along the \( a, b \) and \( c \) axis respectively. In the \( D_{2h} \) point group all representations are one dimensional and non-degenerate [14], which means that the \( \delta_{j} \)-vector in momentum space for unitary triplet states in the weak spin-orbit coupling limit is characterized by one of the four states: (1) \( 3A_{1u}(a) \), with \( \delta_{j}(k_j) = \hat{n}_j \Delta_{fxyz,j}X_jY_jZ_j \) ("\( f_{x,y,z} \" state); (2) \( 3B_{1u}(a) \), with \( \delta_{j}(k_j) = \hat{n}_j \Delta_{p_{x},j}Z_j \) ("\( p_{x} \" state); (3) \( 3B_{2u}(a) \), with \( \delta_{j}(k_j) = \hat{n}_j \Delta_{p_{y},j}X_j \) ("\( p_{y} \" state); (4) \( 3B_{3u}(a) \), with \( \delta_{j}(k_j) = \hat{n}_j \Delta_{p_{z},j}Y_j \) ("\( p_{z} \" state). Since, the Fermi surface touches the Brillouin zone boundaries the functions \( X_j, Y_j, \) and \( Z_j \) need to be periodic and can be chosen to be \( X_j = \sin(k_{z,j}a_j), \) \( Y_j = \sin(k_{y,j}b_j), \) and \( Z_j = \sin(k_{x,j}c_j) \). The unit vector \( \hat{n}_j \) defines the direction of \( \delta_{j}(k_j) \). Next, we discuss the Josephson effect in two situations, first neglecting, and second including surface bound state effects.

The Josephson effect neglecting surface bound states: In this approximation only the contribution from scattering states with well defined momentum is included. Under this assumption the BdG amplitudes become \( u_{N_j,\alpha}(r_j) = \exp(i\mathbf{k}_j \cdot \mathbf{r}_j) \tilde{u}_{N_j,\alpha}/\sqrt{V} ; v_{N_j,\alpha}(r_j) = \exp(i\mathbf{k}_j \cdot \mathbf{r}_j) \tilde{u}_{N_j,\alpha}/\sqrt{V} \), where quantum indices \( N_j \) are represented by momentum \( k_j \) and discrete index \( n_j = 1, 2 \). In this case, the expression for \( J_s(V, T) \) defined in Eq. (3) becomes

\[ J_s(V, T) = \frac{2e}{h} \left[ \sin(\phi) \sum_{k_L, k_R} \Re \{ W(k_L, k_R, i\omega_n) \} + \cos(\phi) \sum_{k_L, k_R} \Im \{ W(k_L, k_R, i\omega_n) \} \right] , \]

after summations over spin indices \( \alpha, \beta, \) indices \( n_j \), Matsubara frequencies \( i\nu_m \), and the U(1) gauge transformation \( \delta_{j} \rightarrow \delta_{j} \exp(i\phi) \) are performed. Note that this dot product \( \delta_{j}(k_L) \cdot \delta_{R}(k_R) \) appears in \( J_s(V, T) \), and thus \( J_s(V, T) \) is very sensitive to the relative orientation between \( \delta_{j}(k_L) \) and \( \delta_{R}(k_R) \) [20]. For instance, if \( \delta_{j}(k_L) \perp \delta_{R}(k_R) \) then \( J_s(V, T) \) vanishes identically for any \( V \) and \( T \). Furthermore \( J_s(V, T) \) (for fixed \( V \) and \( T \)) changes sign depending if the vectors \( \delta_{j}(k_L) \) and \( \delta_{R}(k_R) \) are aligned or anti-aligned. It is this sensitivity to the relative orientation of the \( \delta \)-vectors across
the junction that makes the Josephson effect between TS a crucial test for triplet superconductivity itself. The function $P(k_L, k_R, \omega_n) = T \sum_{i\nu_m} \left[ (\hbar \nu_m)^2 + E_{k_L}^2 \right]^{-1} \left[ (\hbar \omega_n - \hbar \nu_m)^2 + E_{k_R}^2 \right]^{-1}$ is a sum over Matsubara energies $\hbar \nu_m = (2m + 1)\pi k_B T$. The excitation energies are $E_{k_L} = \sqrt{E_{k_L}^2 + |d_j(k)|^2}$. Notice that $J_s(V, T)$ also vanishes identically if $W(k_L, k_R, \omega_n \rightarrow -eV/h + i\delta)$ is odd under inversion for $k_L \rightarrow -k_L$ or $k_R \rightarrow -k_R$. Since $d_j(k)$ is odd, $E_{k_L}$ is even under inversion $k_L \rightarrow -k_L$, and $P(k_L, k_R, \omega_n \rightarrow -eV/h + i\delta)$ is even under $k_L \rightarrow -k_L$ or $k_R \rightarrow -k_R$, a non-vanishing $J_s(V, T)$ requires $Q(k_L, k_R)$ to have contributions which are odd in both $k_L$ and $k_R$. Therefore, $J_s(V, T)$ depends crucially on the magnitude and symmetry properties of $Q(k_L, k_R)$ defined above, which contains the tunneling matrix element $T_s(k_L, k_R)$. Since all the $D_{2h}$ point group representations are one dimensional and non-degenerate [14], $T_s$ can be expanded as $T_s(k_L, k_R) = \sum_{k, L, R} T_{L, R, k_L}^T(k_L, k_R) \bar{\psi}_L^\dagger \psi_R^{\dagger}(k_L) \bar{\psi}_R \psi_L(k_R)$, in the case of weak spin-orbit coupling. Here $\psi_L^T(k)$ are the basis functions of of the $D_{2h}$ (orthorhombic) point group [14]. In the particular case of time reversal symmetry $T_s(-k_L, -k_R) = T_s^T(k_L, k_R)$ and $Q(k_L, k_R) = |T_s(k_L, k_R)|^2 \geq 0$.

For the weak spin-orbit “$p_x$”, “$p_y$”, “$p_z$” and “$f_{xyz}$” states, where the direction of the $d$-vectors is independent of momentum, a simple expression for $J_s(T)$ at zero bias can be obtained

$J_s^{(\lambda)}(T) = \bar{J}^{(\lambda)}(T) \times (\hat{n}_L \cdot \hat{n}_R) \times \sin(\phi)$, \hspace{2cm} (8)

where $\bar{J}^{(\lambda)}(T) = (2e/h) \Delta_L(T) \Delta_R(T) S^{(\lambda)}_{LR}(T)$, $\hat{\phi} = \phi_R - \phi_L$, and the label $\lambda$ identifies incoherent ($\lambda = inc$) or coherent ($\lambda = coh$) processes. Here, 

\[ S^{(\lambda)}_{LR}(T) = \sum_{k_L, k_R} Q^{(\lambda)}(k_L, k_R) \bar{\psi}_L \psi_{R,L}^{\dagger}(k_L) \bar{\psi}_R \psi_{L,R}^{\dagger}(k_R) P(k_L, k_R), \]

where $P(k_L, k_R) = 4T \sum_{m=0}^{\infty} (h^2 \nu_m^2 + E_{k_L}^2)^{-1} (h^2 \nu_m^2 + E_{k_R}^2)^{-1}$, and $\bar{\psi}_R \psi_{L,R}^{\dagger}(k_L) = X_L, Y_L, Z_L$ or $XY_L, XZ_L, YZ_L$. Notice that $\hat{n}_L \cdot \hat{n}_R = \cos(\theta_{LR})$, where $\cos(\theta_{LR})$ is the angle between the two $d$-vectors, and describes a polarization angle just like the Malus’s law of electric polarization. $J_s(T)$ depends crucially on the tunneling matrix elements $Q(k_L, k_R)$. For purely incoherent processes the only terms that contribute to $J_s^{(inc)}(T)$ come from $Q^{(inc)} = 2T_s^{1L,1R} T_s^{T_L, T_R} - 2T_s^{1L,1R} T_s^{T_L, T_R}$, where $\bar{\Gamma}_J$ are appropriate odd representations of the $d_j$-vectors. For the “$p_x$” symmetry $\psi_{L,R}^{\dagger}(k_L) = X_L$, and $\psi_{L,R}^{\dagger}(k_R) = X_R$, thus (a) $Q^{(inc)}_{p_x}(k_L, k_R) = \bar{Q}_{p_x} X_L X_R$ produces a non-vanishing $J_s(T)$, while (b) $Q^{(inc)}_{p_y}(k_L, k_R) = \bar{Q}_{p_y} 1_L 1_R$ produces a trivially vanishing $J_s(T)$. Similarly for the “$p_y$” symmetry $\bar{\psi}_{L,R}^{\dagger}(k_L) = Y_L$, and $\bar{\psi}_{L,R}^{\dagger}(k_R) = Y_R$, 

FIG. 1. Plot of $J_s(T)/J_s(0)$ versus $T/T_c$. Inset shows $J_s(0, \alpha_{LR})/J_s(0, 0)$ versus $\alpha_{LR}$ at $T = 0$. Several $a$ axis tunneling processes are illustrated for “$p_x$” and “$p_y$” symmetries. Incoherent processes: “$p_x$” with (a) $Q^{(inc)} \propto X_L X_R$ (solid line) and (b) $Q^{(inc)} \propto 1_L 1_R$ (trivially zero); “$p_y$” with (c) $Q^{(inc)} \propto Y_L Y_R$ (dashed line) and (d) $Q^{(inc)} \propto 1_L 1_R$ (trivially zero). Coherent processes: “$p_x$” with (a) $Q^{(coh)} \propto X_L X_R$ (dotted line) and (b) $Q^{(coh)} \propto 1_L 1_R$ (trivially zero); “$p_y$” with (c) $Q^{(coh)} \propto Y_L Y_R$ (dot-dashed line) and (d) $Q^{(coh)} \propto 1_L 1_R$ (double-dotted line). The $L$ and $R$ superconductors are assumed to be identical quarter-filled systems, with $T_s = 1.5 K$, and parameters $t_x = 5800 K$, $t_y = 1226 K$, $t_z = 48 K$.
thus (c) $Q^{(inc)}(J_L, k_R) = \tilde{Q}_{p_\parallel 1L1R}$ produces a non-vanishing $J_s(T)$, while (d) $Q^{(inc)}(k_L, k_R) = \tilde{Q}_{p_\parallel 1L1R}$ produces a trivially vanishing $J_s(T)$. For comparison purposes, we analyse next four coherent tunneling processes allowed by group theory corresponding to matrix elements (a) $Q^{(coh)}_{p_\parallel 1L1R}$, for the “$p_x$” symmetry; (b) $Q^{(coh)}_{p_\parallel 1L1R}$, for the “$p_y$” symmetry; and (c) $Q^{(coh)}_{p_\parallel 1L1R}$, for the “$p_y$” symmetry, where the momentum parallel to the junction is conserved. In Fig. 1 we show both the temperature and angular dependence of $J_s(\lambda)$ for the case of $a$ axis tunneling, assuming that $d_j \parallel c_j$ ($j = L, R$), $J_s(\lambda)(T)/J_s(\lambda)(0)$ is shown for $\alpha_L = 0$, where all L and R axes coincide. In the inset, we show $J_s(\lambda)(0, \alpha_L)/J_s(\lambda)(0, 0)$ for $T = 0$. For coherent processes $k_{\parallel LL} = k_{\parallel RR}$ and the parallel momenta are related by $k_{\parallel y} = \cos(\alpha_L)k_{\parallel y} - \sin(\alpha_L)k_{\parallel z}$, and $k_{\parallel z} = \sin(\alpha_L)k_{\parallel y} + \cos(\alpha_L)k_{\parallel z}$, where $\alpha_L$ is the angle between $k_{\parallel L}$ and $k_{\parallel R}$. For $a$ axis tunneling $\theta_{LR} = \alpha_L$. Notice in the inset of Fig. 1 that the Josephson current does not change sign for the “$p_y$” with $Q^{(coh)} \propto 1L1R$ (double-dotted line). This is a direct manifestation of the polarization effect of the $d$ vector. It is important to emphasize that both the temperature and the angular dependencies of $J_s(T, \alpha_L)$ can help distinguish different symmetries, and different (coherent or incoherent) tunneling processes (see Fig. 1), as seen experimentally for $c$ axis tunneling of cuprate superconductors[21]. The approach used for $a$ axis tunneling is good only in the cases of “$p_y$” or “$p_x$” symmetry but not for “$p_x$” or “$p_{xyz}$”, since the $d$ vector changes sign upon reflection at the interface, and leads to low energy surface bound states to be discussed next.

The Josephson effect including surface bound states: To obtain $J_s(T)$ for the “$p_x$” symmetry in the case of $a$ axis tunneling it is crucial to solve Eqs. (4), (5) and (6) self-consistently. We solve the non-local lattice BdG equations and compare our results with standard local quasi-classical continuum approximations [22-24]. First, we take advantage of the translational invariance along the direction parallel to the interface and write the BdG amplitudes as $\tilde{u}_{N_j,0,j}(r_j) = \exp(i\mathbf{k}_{\parallel} \cdot r_j) \tilde{u}_{k_j,\parallel N_j,0}(r_\perp)/\sqrt{V}$; $v_{N_j,0,j}(r_j) = \exp(i\mathbf{k}_{\parallel} \cdot r_j) \tilde{v}_{k_j,\parallel N_j,0}(r_\perp)/\sqrt{V}$, where quantum indices $N_j$ are represented by momentum $k_j$ and discrete index $n_j = 1, 2, 3$. After a Fourier transform in the parallel coordinates the lattice BdG equations (4) and (5) become one-dimensional in the perpendicular coordinates $r_\perp, r_\perp'$. We choose hard boundary conditions, where the BdG amplitudes vanish when $r_\perp = r_\perp' = 0$ (at the center of the insulating barrier). Second, only the triple channel component $V^{(t)}(r_j, r_j')$ of the general weak spin-orbit coupling interaction $V_j,0,j,\gamma_j,\gamma_j(\gamma_j, r_j, r_j')$ is considered. The triple component is $V^{(t)}(r_j, r_j') = I_{1,j}(r_j, r_j') + I_{2,j}(r_j, r_j')$, and it is assumed that $V^{(t)}(r_j, r_j')$ has an on-site ($r_j' = r_j$) repulsion $U_j$ and nearest neighbor attractions ($r_j' = r_j + a_n$) $V_j, x, V_j, y$, and $V_j, z$ only. In addition, we assume that the direction of the $d(r, r')$ is independent of position and points along the $c$ axis. Furthermore, we choose the spin quantization axis to be along the direction of $d(r, r')$. Under these conditions the order parameter matrix $\Delta_{j,0,j,\gamma_j}(r_j, r_j')$ for the “$p_y$” symmetry vanishes identically when $r_j' = r_j$, and has only off-diagonal matrix elements $\Delta_{j,0,j,\gamma_j}(r_j, r_j') = V_j, x \langle c_{j,\gamma_j}(r_j') c_{j,\gamma_j'}(r_j) \rangle + \langle c_{j,\gamma_j'}(r_j') c_{j,\gamma_j}(r_j) \rangle / 2$ and $\Delta_{j,0,j,\gamma_j}(r_j, r_j') = \Delta_{j,0,j,\gamma_j}(r_j, r_j')$ when $r_j' = r_j + a_n$. $J_s(T)$ is calculated numerically using Eq. (3) with $T_{aL,0}(r_L, r_R) = T_{s}(r_L, r_R) \delta_{aL,0}$. For definiteness and simplicity we also assumed that $T_{s}(r_L, r_R) = T \delta_{r_L, r_R}$ for $r_{LL} = -d/2$ and $r_{RR} = +d/2$; $T_{s}(r_L, r_R) = 0$ otherwise. Here, $d$ is the separation between the last layer of the L and the first layer of the R superconductor, and corresponds to the thickness of the insulating layer. This simple choice guarantees that the parallel momentum $k_{\parallel}$ is conserved across the junction, and thus correspond to a coherent process. Since the tunneling matrix elements connect mostly states that have appreciably large BdG amplitudes near the junction, we use a mixed representation of Eq. (3) expressed in terms of the parallel momenta $k_{\parallel} = k_{\parallel R} = k_{\parallel L}$ and the perpendicular coordinates $r_{\perp L}$ and $r_{\perp R}$ to calculate numerically $J_s(T)$. In Fig. 2 we compare our results for $J_s(T)$ using the non-local lattice BdG equations and the local quasiclassical approaches [22-24].
FIG. 2. Plots of $J_s(T)/J_{\text{ref}}(0)$ versus $T/T_c$ for for coherent “$p_x$” (“$p_z$”) a (c) axis tunneling, where $J_{\text{ref}}(0)$ is the Landau critical current for a singlet s-wave superconductor with the same $T_c$. Quasiclassical results are indicated by dashed (dotted) lines for “$p_x$” (“$p_z$”), while the non-local BdG results are represented by solid (double-dotted) lines for “$p_x$” (“$p_z$”), for the parameters of Fig 1.

The local quasiclassical approximation is only strictly valid when $k_F \xi \rightarrow \infty$, but it leads to zero energy bound states in the case where the quasiclassical order parameter $\Delta(k, \mathbf{r})$ changes sign upon $\mathbf{r} \rightarrow -\mathbf{r}$ [22–24] (as in the case of the a axis tunneling for the “$p_x$” symmetry). However, in the non-local lattice BdG equations (4) and (5) there are only finite energy bound states. The non-existence of zero energy bound states in the non-local lattice BdG equations can be understood as follows. Because the order parameter is non-local, it can be described in terms of the center of mass $\mathbf{R} = [\mathbf{r} + \mathbf{r}]/2$ and relative $\mathbf{r}_{\text{rel}} = [\mathbf{r}' - \mathbf{r}]$ coordinates. Near the surface these two coordinates are entangled and thus lift the zero energy bound states degeneracy found in the local theory. This produces, perturbatively, finite energy bound states of the order $|\Delta_0|/\gamma$ where $\gamma = \xi/a$, with $\xi$ and $a$ being the coherence and unit cell lengths, respectively. The finiteness of the energy of the bound states cuts off the low temperature $1/T$ divergence of $J_s(T)$ calculated in the quasiclassical approach at small transparencies [22–24]. For a axis tunneling and the “$p_x$” symmetry this amounts to a small correction to the quasiclassical results, as $\gamma = \xi/a_x \approx 106$ for the Bechgaard salts and $\Delta_{0,p_x} = 3.73$ K, leading to the lowest bound state energy to be approximately $T_{p_x}^* = 35.2$ mK. Which means that for $T < T_{p_x}^*$ the quasiclassical results are not reliable (see Fig. 2). The quasiclassical results fail in a more dramatic way, when we consider c axis tunneling for the “$p_z$” symmetry. In this case $\xi_z = 21.5$ Å, $a_z = 13.5$ Å, $\gamma_z = \xi_z/a_z \approx 1.59$ and $\Delta_{0,p_z} = 3.21$ K, resulting in $T_{p_z}^* = 2.02$ K, which is larger than the critical temperature $T_c = 1.5$ K used here. Thus, perturbative corrections to quasiclassical zero energy bound states are enormous, and the quasiclassical approximation can not be used except for $T \approx T_c$ (see Fig. 2).

In summary, we have discussed the Josephson current $J_s$ in TS/I/TS junctions, and indicated that the triplet nature of the order parameter for Bechgaard salts could be tested in such an experiment. We emphasized that the temperature and angular dependence of $J_s$ can help distinguish between different triplet order parameter symmetries, and we discussed the role of surface bound states within the non-local lattice BdG equations. We would like to thank NSF (Grant No. DMR-980311) for financial support.

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