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Effective Interactions and the Nature of Cooper Instability of Spin Polarons in the 2D Kondo Lattice

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It has been shown that two- and three-center interactions arise in the strong-coupling regime for the 2D Kondo lattice; these interactions both induce and suppress the Cooper instability. It is important that, in contrast to the *t*–*J** model, the three-center interactions promote the Cooper pairing and ensure the appearance of the superconducting phase with a high critical temperature T_c. The calculated concentration dependences of T_c agree well with the experimental data for the cuprate superconductors.

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1. It is known that the electron structure of the CuO_2 plane of high-temperature superconductors (HTSCs) can be adequately described in the Emery model [1, 2]. At a low doping level, the relation between the parameters of the model allows the passage to the effective Hamiltonian. In this Hamiltonian, the Cu ions are in the homeopolar states, they are characterized by the spin $S = 1/2$ and coupled through the mechanism of indirect exchange interaction. The hole current carriers of the oxygen subsystem interact with the localized spins of the Cu ions through the *s*–*d* exchange coupling. Therefore, the Kondo lattice is a good model for the low-energy spectrum of HTSC Fermi excitations.

For the normal phase, the peculiarities of the elementary excitations found for the Kondo lattice have been adequately studied. The key idea in this approach is the spin polaron concept [3]. According to this concept, an elementary excitation in the 2D antiferromagnet (AFM) can be represented as a particle (electron or hole) surrounded by a cloud of spin fluctuations. This complicated quasiparticle, which has the renormalized mass and moves against the background of the AFM order, is the spin polaron [4].

This description of the Fermi excitations in the HTSC is justified if the *s*–*d* exchange coupling constant is larger than the hopping integral, and the current carrier concentration is relatively low. In this case, the spin polaron concept ensures a comparatively simple reproduction of the features of the HTSC pseudogap behavior [5]. In view of this circumstance, the problem of the description of the superconducting phase under the conditions where the Cooper instability is developed not for the bare fermions but in the subsystem of the spin polarons is of current interest. The objective of this work is to consider the above problem.

2. To describe the superconducting phase in the ensemble of the spin polarons, we write the Hamiltonian of the Kondo lattice as

$$\begin{aligned}\hat{H} &= J\sum_f \mathbf{S}_f\mathbf{s}_f + U\sum_f \hat{n}_{f\uparrow}\hat{n}_{f\downarrow} + \hat{H}_{\text{int}},\\ \hat{H}_{\text{int}} &= \sum_{fm\alpha} t_{fm}c^{\dagger}_{f\alpha}c_{m\alpha} + \frac{1}{2}\sum_{fm} I_{fm}\mathbf{S}_f\mathbf{S}_m.\end{aligned} \tag{1}$$

Here, the first two terms of the Hamiltonian describe the *s*–*d* exchange coupling of the AFM type ($J > 0$) between the localized spins of the Cu ions and the spins of the holes, as well as the Hubbard repulsion of two holes with the Hubbard energy U in the same site; $\mathbf{S}_f$ is the vector operator of the localized spin; and $\mathbf{s}_f$ is the vector operator of the hole spin. In the atomic representation, these terms correspond to the Hamiltonian $\hat{H}_0$. The interaction operator includes the kinetic energy of the holes written in the Wannier representation, as well as the Heisenberg exchange interaction of the AFM type in the subsystem of the localized spins; $c^{\dagger}_{f\alpha}$ and $c_{f\alpha}$ are the creation and annihilation operators, respectively, for the hole on site f with the spin projection α.

The deduction of the effective interactions arising between the spin-polaron quasiparticles is based on the condition that the *s–d* exchange integral J and Hubbard energy U are the highest energy parameters of the system under study. In this case, it is natural to pass to the representation where the strong interactions become diagonal. To this end, we introduce a complete set of eight single-site states. Let $|\uparrow\rangle$ and $|\downarrow\rangle$ be the hole-free single-site states, where the localized spin projections are +1/2 and –1/2, respectively. Below in this section, the site index will be omitted. The states with a single hole on the site are classified according to the values of the total angular momentum and its projection. The vector

$$|S\rangle = \frac{1}{\sqrt{2}}(c^{\dagger}_{-1/2}|\uparrow\rangle - c^{\dagger}_{1/2}|\downarrow\rangle)$$

corresponds to the state of the spin singlet with zero total angular momentum. The triplet states with the total angular momentum projection ±1, 0 are described by the vectors

$$|\pm 1\rangle = c^{\dagger}_{\pm 1/2}|\uparrow,\downarrow\rangle, \quad |0\rangle = \frac{1}{\sqrt{2}}(c^{\dagger}_{-1/2}|\uparrow\rangle + c^{\dagger}_{1/2}|\downarrow\rangle).$$

Two states with the opposite projections of the localized momentum and two holes on the same site are described in terms of the vectors

$$|+\rangle = c^{\dagger}_{1/2}c^{\dagger}_{-1/2}|\uparrow\rangle, \quad |-\rangle = c^{\dagger}_{1/2}c^{\dagger}_{-1/2}|\downarrow\rangle.$$

We construct the Hubbard operators $X^{pq} = |p\rangle\langle q|$ [6, 7] on the introduced basis of the single-site states and implement the representation for the spin operators,

$$\begin{aligned} S^{\dagger} &= X^{\uparrow\downarrow} + \frac{1}{\sqrt{2}}(X^{S,-1} + X^{0,-1} + X^{10} - X^{1S}) + X^{+-}, \\ S^{z} &= \frac{1}{2}(X^{\uparrow\uparrow} - X^{\downarrow\downarrow} + X^{0S} + X^{S0} \\ &\quad + X^{11} - X^{-1,-1} + X^{++} - X^{--}), \end{aligned} \tag{2}$$

and Fermi operators,

$$\begin{aligned} c^{\dagger}_{\uparrow} &= X^{1\uparrow} + X^{-,-1} + \frac{1}{\sqrt{2}}(X^{0\downarrow} - X^{S\downarrow} + X^{+S} + X^{+0}), \\ c^{\dagger}_{\downarrow} &= X^{-1\downarrow} - X^{+1} + \frac{1}{\sqrt{2}}(X^{0\uparrow} + X^{S\uparrow} + X^{-S} - X^{-0}). \end{aligned} \tag{3}$$

The two-hole states and triplet states are separated from the singlet one by the energy values $U + 3J/4$ and J, respectively.

3. When U and J are large, we can pass to the effective Hamiltonian $\hat{H}_{\text{eff}}$, where the contributions from the upper single-site states are taken into account in the operator form of the perturbation theory. Introducing the projection operator onto three lower single-site states $P = \prod_f (X^{\uparrow\uparrow}_f + X^{\downarrow\downarrow}_f + X^{SS}_f)$ and, using the smallness conditions,

$$\frac{t_{fm}}{J} \ll 1, \quad \frac{t_{fm}}{U + 3J/4} \ll 1, \quad \frac{I_{fm}}{J} \ll 1,$$

the effective Hamiltonian

$$\begin{aligned} \hat{H}_{\text{eff}} &= PHP + PH_{\text{int}}(H_0 - E^{(0)}_0)^{-1} \\ &\quad \times (PH_{\text{int}}P - H_{\text{int}}P) + \ldots \end{aligned} \tag{4}$$

can be written (up to the terms of the second order in the mentioned parameters) as

$$\begin{aligned} \hat{H}_{\text{eff}} &= \sum_f (\varepsilon_{sp} - \mu) X^{SS}_f + \frac{1}{2}\sum_{fm\sigma} t_{fm} X^{S\sigma}_f X^{\sigma S}_m \\ &\quad + \frac{1}{2}\sum_{fm} I_{fm}\tilde{\mathbf{S}}_f\tilde{\mathbf{S}}_m + \frac{1}{2}\sum_{fm} V_{fm} X^{SS}_f X^{SS}_m + \hat{H}_{(3)}, \end{aligned} \tag{5}$$

where $\sigma = \uparrow, \downarrow$ and the first term describes the set of noninteracting spin polarons (the structure of these quasiparticles in the initial basis is discussed in the Conclusions) with the renormalized energy $\varepsilon_{sp} = -3J/4 + \Delta\varepsilon$. The renormalization

$$\Delta\varepsilon = -\frac{3}{4}\sum_m \left(\frac{t_{fm}t_{mf}}{J} + \frac{I_{fm}I_{mf}}{4J}\right) \tag{6}$$

is determined by the quantum processes of virtual transitions to the triplet states due to hops and the exchange interaction (see the representations for the spin and Fermi operators) and μ is the chemical potential of the system. The second term describes the kinetic energy of the spin-polaron quasiparticles with the renormalized hopping integral (spin-polaron narrowing of the band). The exchange interaction is represented by the third term of $\hat{H}_{\text{eff}}$, which involves the quasispin operators $\tilde{S}^{\dagger}_f = X^{\uparrow\downarrow}_f$ and $\tilde{S}^{z}_f = \frac{1}{2}(X^{\uparrow\uparrow}_f - X^{\downarrow\downarrow}_f)$ reduced with respect to the initial representation. As a result of the virtual quantum "throws" to the upper single-site states, interaction between the spin polarons arises; this interaction is represented by the fourth term in $\hat{H}_{\text{eff}}$. The intensity of this interaction is determined by the matrix element

$$V_{fm} = \frac{3}{2}\frac{t_{fm}t_{mf}}{J} - \frac{t_{fm}t_{mf}}{U + 3J/4} + \frac{9}{32}\frac{I_{fm}I_{mf}}{J}. \tag{7}$$

It is seen that the processes of virtual throws to the triplet states induce the repulsion of the spin polarons, while the virtual transitions to the states with two holes on the site lead to their attraction. At the specified relations between the parameters, the total result of the processes considered is the repulsion of the spin-polaron quasiparticles. This interaction affects the Cooper instability conditions, because it results in more strin-

gent conditions compared to the limiting case $U, J \longrightarrow \infty$. The last term in $\hat{H}_{\text{eff}}$ describes the three-center interactions,

$$\hat{H}_{(3)} = \sum_{\substack{fmg\sigma \\ f\neq g}} \left(\frac{t_{fm}t_{mg}}{4J}\right) X_f^{S\sigma} X_m^{\sigma\bar{\sigma}} X_g^{\bar{\sigma}S} - \sum_{\substack{fmg\sigma \\ f\neq g}} \left(\frac{t_{fm}t_{mg}}{2J}\right) X_f^{S\sigma}\left(X_m^{\bar{\sigma}\bar{\sigma}} + \frac{1}{2}X_m^{\sigma\sigma}\right) X_g^{\sigma S} - \sum_{\substack{fmg\sigma \\ f\neq g}} \left(\frac{t_{fm}t_{mg}}{4(U+3J/4)}\right) X_f^{S\sigma} X_m^{SS} X_g^{\sigma S} - \sum_{\substack{fmg\sigma \\ f\neq g}} \left(\frac{I_{fm}I_{mg}}{4J}\right) \tilde{\mathbf{S}}_f \tilde{\mathbf{S}}_g X_m^{SS}, \quad (8)$$

which are important for the HTSC implementation (see below). We note that the operator $X_f^{\sigma S}$ acts as the annihilation operator for the hole with the spin projection $-\sigma$, performing the transition of site f from the singlet state to the hole-free state. The operator $X_f^{S\sigma}$ corresponds to the creation of the hole with spin projection $-\sigma$, because its action reduces to the addition of the hole to site f, which is thus transferred from the state $|\sigma\rangle$ to the singlet $|S\rangle$.

4. To obtain the self-consistency equations in the superconducting phase, we used the method of the irreducible Green's functions [8]. Introducing the normal $\langle\langle X_f^{\downarrow S}|X_{f'}^{S\downarrow}\rangle\rangle_\omega$ and anomalous $\langle\langle X_f^{S\uparrow}|X_{f'}^{S\downarrow}\rangle\rangle_\omega$ Green's functions, the equations of motion were written for them. Further, we used the scheme of projecting these equations onto the introduced basis of the spin-polaron Green's functions. This procedure resulted in the Gor'kov equations

$$(\omega - \tilde{\varepsilon}_{\mathbf{k}})\langle\langle X_{\mathbf{k}\uparrow}|X_{\mathbf{k}\uparrow}^\dagger\rangle\rangle = \left(\frac{1+n}{2}\right) + \Delta_{\mathbf{k}}\langle\langle X_{-\mathbf{k}\downarrow}^\dagger|X_{\mathbf{k}\uparrow}^\dagger\rangle\rangle,$$
$$(\omega + \tilde{\varepsilon}_{\mathbf{k}})\langle\langle X_{-\mathbf{k}\downarrow}^\dagger|X_{\mathbf{k}\uparrow}^\dagger\rangle\rangle = \Delta_{\mathbf{k}}\langle\langle X_{\mathbf{k}\uparrow}|X_{\mathbf{k}\uparrow}^\dagger\rangle\rangle \quad (9)$$

for the Fourier images of the normal and anomalous Green's functions,

$$\langle\langle X_f^{\downarrow S}|X_{f'}^{S\downarrow}\rangle\rangle_\omega = \frac{1}{N}\sum_{\boldsymbol{\kappa}} e^{i\boldsymbol{\kappa}(\mathbf{R}_f - \mathbf{R}_{f'})}\langle\langle X_{\mathbf{k}\uparrow}|X_{\mathbf{k}\uparrow}^\dagger\rangle\rangle,$$
$$\langle\langle X_f^{S\uparrow}|X_{f'}^{S\downarrow}\rangle\rangle_\omega = \frac{1}{N}\sum_{\boldsymbol{\kappa}} e^{i\boldsymbol{\kappa}(\mathbf{R}_f - \mathbf{R}_{f'})}\langle\langle X_{-\mathbf{k}\downarrow}^\dagger|X_{\mathbf{k}\uparrow}^\dagger\rangle\rangle. \quad (10)$$

In the system of equations, $\tilde{\varepsilon}_{\mathbf{k}} = -3J/4 + V_0 n + [(1+n)/4]t_{\mathbf{k}}$ is the renormalized spectrum of the Fermi excitations determined by the polaron band; $t_{\mathbf{k}}$ is the Fourier image of the hopping integral; V_0 is the Fourier image of the matrix element of the spin polaron coupling for zero quasi-momentum; and n is the hole concentration per site. The superconducting gap appeared in the introduction of the anomalous Green's function is determined as

$$\Delta_{\mathbf{k}} = \frac{1}{N}\sum_{\mathbf{q}}\left(2t_{\mathbf{q}} + 2\tilde{V}_{\mathbf{k}-\mathbf{q}} - \frac{3}{2}I_{\mathbf{k}-\mathbf{q}}\right)\frac{\langle X_{-q\downarrow}X_{q\uparrow}\rangle}{1+n}. \quad (11)$$

The function $\tilde{V}_{\mathbf{k}-\mathbf{q}}$ in the kernel of this integral equation is associated with the repulsion of the spin polarons (the effective Hamiltonian term $\sim V_{fm}$) and with the three-center interactions. In this case, some contributions from $H_{(3)}$, which do not contribute to the superconducting gap with the $d_{x^2-y^2}$ symmetry, are omitted here to shorten the expression. In the Wannier representation, the matrix element $\tilde{V}_{fm}$ renormalized owing to $H_{(3)}$ has the form

$$\tilde{V}_{fm} = \frac{2-n}{2}\frac{t_{fm}t_{mf}}{J} - \frac{(1-n/4)t_{fm}t_{mf}}{U+3J/4} + \frac{5-4n}{32}\frac{I_{fm}I_{mf}}{J}. \quad (12)$$

Calculating the anomalous Green's function and using the spectral theorem, the self-consistency equation for the superconducting gap $\Delta_{\mathbf{k}} = \Delta\cdot(\cos k_x - \cos k_y)$ can be written as

$$\Delta_{\mathbf{k}} = \frac{1}{N}\sum_{\mathbf{q}}\left(\frac{3}{2}I_{\mathbf{k}+\mathbf{q}} - 2\tilde{V}_{\mathbf{k}+\mathbf{q}}\right)\left(\frac{\Delta_{\mathbf{q}}}{4E_{\mathbf{q}}}\right)\tanh\left(\frac{E_{\mathbf{q}}}{2T}\right). \quad (13)$$

Hence, the transition temperature to the superconducting phase with the $d_{x^2-y^2}$ symmetry of the order parameter is determined by the solution of the equation

$$1 = \frac{\tilde{G}}{N}\sum_{\mathbf{q}}\frac{3}{8}\frac{(\cos q_x - \cos q_y)^2}{(\tilde{\varepsilon}_{\mathbf{q}} - \mu)}\tanh\left(\frac{\tilde{\varepsilon}_{\mathbf{q}} - \mu}{2T_c}\right), \quad (14)$$

where the coupling constant can be represented as

$$\tilde{G} = I - \frac{2(2-n)t^2}{3J} + \frac{(4-n)t^2}{3(U+3J/4)} - \frac{(5-4n)I^2}{24J}. \quad (15)$$

Here, the contributions determined by the hopping integrals and the exchange parameters between the sites of the long-range coordination spheres are neglected. This simplification is possible because the mentioned parameters decrease rather rapidly with the internodal distance. For comparison, we note that the coupling

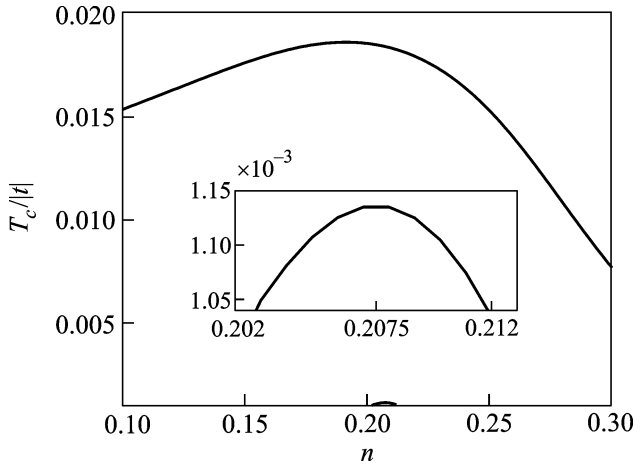

Fig. 1. Concentration dependence of the critical temperature calculated (upper curve) including and (lower curve) disregarding $H_{(3)}$ for $t = 1$ eV, $t' = 0.6|t|$, $t'' = 0.22|t|$, $J = 5|t|$, $U = 5|t|$, and $I = 0.33|t|$. The lower curve is shown enlarged in the inset.

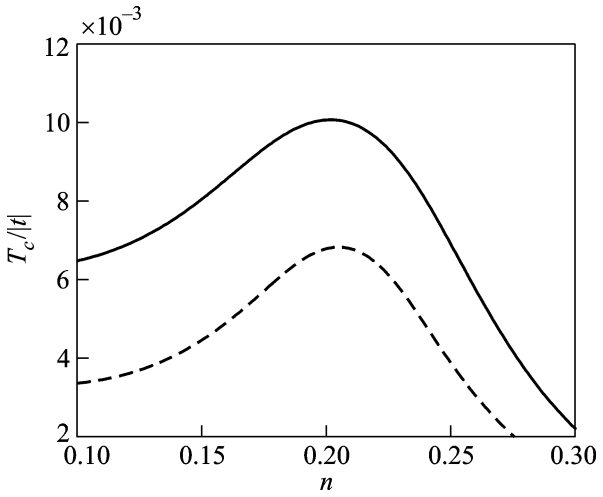

Fig. 2. Concentration dependence of the critical temperature calculated for $t = 1$ eV, $t' = 0.6|t|$, $t'' = 0.22|t|$, $J = 5|t|$, $I = 0.3|t|$ at $U =$ (solid curve) $7|t|$ and (dashed curve) $10|t|$.

constant in the absence of three-center interactions would be given by the expression

$$G = I - \frac{2t^2}{J} + \frac{4t^2}{3(U + 3J/4)} - \frac{3I^2}{8J}. \qquad (16)$$

The effective coupling constant $\tilde{G}$ is formed due to several factors. The first term I corresponds to the spin polaron attraction and provides the positive contribution to the total mechanism of the Cooper pairing. The physics of this attraction is simple and is associated with the fact that the spin of the site occupied by the polaron is zero. Therefore, if two polarons are at a distance longer than the interatomic distance, then the exchange energy loss is ~8I. If the spin polarons are in the nearest sites, then this loss is ~7I. Thus, the characteristic attraction energy is I, which is represented by the coupling constant. We note that the relative energy increase in the 2D case exceeds the corresponding increase for the 3D case.

The second contribution to the constant $\tilde{G}$ is caused by the two- and three-center interactions of the spin polarons. The resulting interaction consists of three terms. The first and third terms result from the processes of the virtual transitions to the triplet spin-polaron states due both to the hole hops and to the exchange interaction. These contributions form the repulsion of the spin polarons. The second term in the expression for $\tilde{V}_{fm}$ results from the processes of throw into the single-site states with two holes (this explains the presence of U in the denominator). It is seen that these processes lead to the mutual attraction of the polarons. Therefore, the three-center interactions partially compensate for a decrease in the coupling constant caused by the spin polaron repulsion and thereby (see below) considerably affect the conditions of the superconducting phase implementation.

We note that the importance of the three-center interactions for the t–J* model was mentioned earlier in [9]. However, in the case of the t–J* model, the three-center interactions reduced the coupling constant (and, thus, heavily reduced the critical temperature), while the three-center interactions in the spin polaron system have an opposite effect, considerably increasing the critical temperature. This statement is illustrated in Fig. 1. In the calculation of the critical temperature as a function of the concentration, the parameters were chosen so that the superconducting phase region could exist in the absence of the three-center interactions. It is seen that, when the three-site interactions are taken into account, the critical temperatures T_c become sufficiently high in the given range of the parameters and in the optimal doping region (~170 K). If the three-center interactions are neglected, then the maximum critical temperature is about 13 K.

If the parameters are chosen so that the critical temperatures typical of the cuprate semiconductors could be reached in the optimal doping region, then the superconducting phase appears to be suppressed if the three-center interactions are disregarded. Figure 2 shows the calculated $T_c(n)$ dependences with allowance for the three-center interactions for two values of the Hubbard parameter U. Clearly, an increase in U reduces the critical temperature because the efficiency of the virtual throws to the states with two holes is suppressed under this variation of U, and the total coupling constant decreases. It follows from the concentration dependences of the critical temperature that the concept of Cooper instability considered in the system of spin polarons can be an actual alternative in the HTSC interpretation in cuprate oxides.

5. To conclude, we consider the structure of the spin polaron quasiparticles. First of all, we note that all calculations after the passage to the effective Hamiltonian are performed in the new basis. This means that, to construct the function of a certain state in the initial representation, it is necessary to perform the corresponding transformations (this corresponds to conventional procedures under unitary rotations). Hence, to determine the form of the wavefunction of the spin polaron in the initial basis, it is necessary to perform the corresponding transformations. Let the state with a single polaron in the new basis be described by the function $|1_{sp}\rangle = X_m^{S\sigma}|0\rangle$. Here, $|0\rangle$ corresponds to the polaron-free state. In the initial basis, this state is described with the accepted accuracy by the wavefunction

$$\begin{aligned}|\Psi\rangle &= X_m^{S\sigma}|0\rangle + \frac{1}{H_0 - E_0^{(0)}}(PH_{\text{int}}P - H_{\text{int}}P)X_m^{S\sigma}|0\rangle \\ &= X_m^{S\sigma}|0\rangle + \sum_{f\sigma_1}\frac{t_{fm}}{J}\left(\frac{1}{\sqrt{2}}X_f^{\eta(\bar{\sigma}_1),\bar{\sigma}_1} + \frac{1}{2}X_f^{0\sigma_1}\right)X_m^{\sigma_1\sigma}|0\rangle \\ &\quad - \sum_f \frac{I_{fm}}{2J}\left(\frac{1}{\sqrt{2}}\tilde{S}_f^+ X_m^{-1\sigma}\right. \\ &\quad \left. - \frac{1}{\sqrt{2}}\tilde{S}_f^- X_m^{1\sigma} + \tilde{S}_f^z X_m^{0\sigma}\right)|0\rangle,\end{aligned} \tag{17}$$

where $\eta(\sigma) = \pm 1$ at $\sigma = \uparrow, \downarrow$, respectively. It is seen that the spin polaron state in the initial basis is a coherent mixture of the bar state and the states where the hole is in the m triplet-state sites adjacent to the initial site (the terms t_{fm}), as well as the states for which site m is transferred to the triplet states (the terms I_{fm}), while the neighboring sites are in the hole-free states correlated with the value of the triplet momentum projection and a certain projection of the spin. The Cooper instability mechanism leading to HTSC is considered in this work as applied to those complicated quasiparticles.

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