Universal Thermal Entanglement of Multichannel Kondo Effects

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Quantum entanglement between an impurity and its environment is expected to be central in quantum impurity problems. We develop a method to compute the entanglement in spin-1/2 impurity problems, based on the entanglement negativity and the boundary conformal field theory (BCFT). Using the method, we study the thermal decay of the entanglement in the multichannel Kondo effects. At zero temperature, the entanglement has the maximal value independent of the number of the screening channels. At low temperature, the entanglement exhibits a power-law thermal decay. The power-law exponent equals two times of the scaling dimension of the BCFT boundary operator describing the impurity spin, and it is attributed to the energy-dependent scaling behavior of the entanglement in energy eigenstates. These agree with numerical renormalization group results, unveiling quantum coherence inside the Kondo screening length.

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Introduction.—Quantum entanglement has been used to identify and characterize many-body states [1–4]. It provides fundamental understanding especially when states possess maximal entanglement such as Bell entanglement [5–7]. An interesting direction is to see how entanglement changes as a state deviates from a fixed point, e.g., thermally. Entanglement in pure excited states or thermal states has not been much studied [8–10].

For this direction, there are a wide class of states in quantum impurity problems [11], including impurities in metals [12,13], spin chains [14,15], Luttinger liquids [16], and quantum Hall effects [17,18]. Here bipartite entanglement [see Fig. 1(a)] between an impurity and its environment will be central. This entanglement was studied in the single-channel Kondo effect (1CK). In the 1CK ground state [19], it is Bell entanglement and induces impurity-spin screening. Its thermal suppression, computed with numerical renormalization group methods (NRG) [20,21], shows Fermi liquid behavior [22–24]. The entanglement is used [25] for quantifying spatial distribution of Kondo clouds [26–30]. It is valuable to study the entanglement in other impurities, including multichannel Kondo effects that show non-Fermi liquids [31], boundary phase transitions [32], and fractionalization. The entanglement will have essential information about how boundary degrees of freedom quantum-coherently couple with the bulk in boundary critical phenomena [33,34].

However no approach for analytically computing the entanglement has been developed. In a boundary conformal field theory (BCFT) [35–37], a standard theory for quantum impurities and multichannel Kondo effects, the entanglement was not considered, since the impurity degrees of freedom are replaced by a boundary condition of the environment and the entanglement is for the partition inside

the Kondo cloud length. By contrast, entanglement for another partition [Fig. 1(b)] far outside the Kondo length has been extensively computed [38–42], revealing the "fractional ground-state degeneracy" [43].

Another difficulty arises in studying the entanglement in thermal states. Entanglement entropy, a widely used entanglement measure, cannot distinguish the entanglement from classical correlations [44–46] in the mixed states, overestimating the entanglement. Entanglement negativity [47–49] is then a good choice, as it is applicable to mixed states. This entanglement measure has been numerically computed for Kondo systems [14,21,41].

In this work we develop an approach for analytically computing entanglement negativity $\mathcal{N}_{I|E}$ for the partition [Fig. 1(a)] between the impurity and its environment in a one-dimensional spin-1/2 impurity problem described by a BCFT. The impurity part, replaced by a boundary condition in the BCFT, is restored in low-energy eigenstates, by identifying the impurity spin with BCFT boundary operators and computing its matrix elements with respect to the eigenstates. Then the thermal density matrix is constructed, to obtain $\mathcal{N}_{I|E}$.

We then analyze thermal decay of the negativity in the k-channel Kondo effects (kCK). At zero temperature, the



FIG. 1. Bipartition (dotted lines) for entanglement in a Kondo system. (a) It separates the impurity (circle) and the screening channels (rod). (b) It is located at distance *l* from the impurity far outside the Kondo cloud length ξ_K .

entanglement between the impurity and screening channels is maximal, $\mathcal{N}_{I|E} = 1$, regardless of the number *k* of the channels, although frustration in the impurity screening occurs *k* dependently. This is in stark contrast with the *k*-dependent impurity entropy for the partition in Fig. 1(b). At low temperature $T \ll T_K$, the entanglement has algebraic thermal decay

$$\mathcal{N}_{I|E}(T) = 1 - a_k \left(\frac{T}{T_K}\right)^{2\Delta} \tag{1}$$

with the exponent identical to two times of the scaling dimension Δ of the BCFT operator describing the impurity spin. $\Delta = 1$ for k = 1, $\Delta = 2/(2 + k)$ for $k \ge 2$, T_K is the Kondo temperature, and a_k is a k-dependent positive constant. We confirm Eq. (1), using the NRG method developed in Ref. [21]. We also find the scaling behavior of $\mathcal{N}_{I|E}$ in thermal crossover between different fixed points in channel anisotropic Kondo effects.

Interestingly, the power-law exponent of the thermal decay is determined by that of the energy dependence of the entanglement in energy eigenstates. This is valid for general spin-1/2 impurities described by BCFTs.

Computation of negativity.—We develop a method of computing the negativity $\mathcal{N}_{I|E} = \|\rho^{T_I}\| - 1$ between the impurity and the other part in a one-dimensional critical system having a spin-1/2 impurity described by a BCFT at temperature *T*. ρ is the density matrix of the whole system, $\|\cdot\|$ is the trace norm, and T_I is the partial transpose on the impurity. The maximum possible value of $\mathcal{N}_{I|E}$ is 1 in the system [50].

We organize steps for computing $\mathcal{N}_{I|E}$. (i) At a fixed point, the impurity spin \vec{S}_{imp} is identified with BCFT boundary operators ψ_{α} with scaling dimension Δ_{α} ,

$$S_{\rm imp}^{\alpha=x,y,z} = c_{\alpha} + d_{\alpha}\psi_{\alpha} + \cdots, \qquad (2)$$

with constants c_{α} , d_{α} and operators \cdots of dimension > Δ_{α} . (ii) The energy $E(\sim E_i, E_j)$ dependence of matrix elements $\langle E_i | \vec{S}_{imp} | E_j \rangle$ of the identified operator is studied for lowenergy eigenstates $|E_i\rangle$ of the BCFT Hamiltonian, which includes the irrelevant terms describing thermal deviation from the fixed point. For the purpose, we consider a finite system size L and choose $L \sim v/E$, where v is a relevant velocity (we set the Planck constant $\hbar \equiv 1$ and Boltzmann constant $k_B \equiv 1$). Using conformal transformation [50], we find

$$\langle E_i | S^{\alpha}_{imp} | E_j \rangle = c_{\alpha} \delta_{ij} + d_{\alpha} O(L^{-\Delta_{\alpha}}),$$
 (3)

and their energy dependence is obtained by replacing v/L by *E*. The replacement has been justified [35,57–62] such that the states of energy *E* in an infinite-size system, e.g., obtained with the NRG, are well described by the

corresponding BCFT or bosonization of finite size $L \sim v/E$; the region outside *L* negligibly affects the states of energy *E* at positions near the impurity. It is because correlations exponentially decay with distance $x \gtrsim v/T$ at temperature *T*. The replacement allows us to avoid numerical calculations [63] of the matrix elements.

(iii) The energy eigenstates $|E_i\rangle$'s are represented [50] in the bipartite basis states of the impurity and the environment, utilizing Eq. (3). The impurity degrees of freedom are restored in the representation. Energy dependence in the representation of $|E_i\rangle$ is found as in Eq. (11) for the *k*CK.

Utilizing Schmidt decomposition [50], we find that each energy eigenstate $|E_i\rangle$ has the entanglement of

$$\mathcal{N}_{I|E}(|E_i\rangle) = \sqrt{1 - 4\langle E_i | \vec{S}_{\rm imp} | E_i \rangle^2} \tag{4}$$

between the impurity and the environment, showing that the entanglement directly relates to the expectation value of the impurity spin for each low-energy engenstate. This is a general relation applicable to any spin-1/2 impurities. Using Eq. (3) and expanding Eq. (4) up to possible leading contributions in the low-energy regime, we obtain

$$\mathcal{N}_{I|E}(|E_i\rangle) = \sqrt{1 - 4\sum_{\alpha=x,y,z} c_{\alpha}^2} + \sum_{\alpha} c_{\alpha} d_{\alpha} O(E_i^{\Delta_{\alpha}}) + \sum_{\alpha} d_{\alpha}^2 O(E_i^{2\Delta_{\alpha}}) + \cdots$$
(5)

The energy dependence of $\mathcal{N}_{I|E}(|E_i\rangle)$ follows $E_i^{\Delta_{\alpha}}$ or $E_i^{2\Delta_{\alpha}}$, depending on c_{α} 's.

(iv) The thermal density matrix is constructed, $\rho(T) = \sum_i w_i |E_i\rangle \langle E_i|$, with the eigenstates $|E_i\rangle$ of energy $E_i \sim T$, the Boltzmann weight $w_i = e^{-E_i/T}/Z$, and the partition function $Z = \sum_i e^{-E_i/T}$. This approximate density matrix was proved [57,60] to well describe thermodynamic properties associated with the impurity; the exact density matrix is governed mainly by the eigenstates $|E_i \sim T\rangle$, because w_i decays exponentially with $E_i \gtrsim T$ while the density of states increases with E_i . Then the negativity $\mathcal{N}_{I|E}(\rho) = \|\rho^{T_I}\| - 1$ is computed.

Combining these steps, we find [50] that the thermal behavior of the entanglement satisfies

$$\mathcal{N}_{I|E}[\rho(T)] = \sum_{i} w_i(E_i) \mathcal{N}_{I|E}(|E_i\rangle)|_{E_i \sim T} + f(T).$$
(6)

The first term of $\mathcal{N}_{I|E}(|E_i \sim T\rangle)$ is the leading contribution from the diagonal elements of ρ , while f(T) is the other contribution from the diagonal and off-diagonal elements. The first term is dominant at low temperature, since $w_i(E_i \sim T) \sim O(1), f(T) \sim T^{\kappa}$, and κ is larger than or equal to the minimum among $2\Delta_{\alpha}$'s. Therefore the powerlaw exponent of the thermal behavior of $\mathcal{N}_{I|E}(\rho)$ equals that of the energy dependence of $\mathcal{N}_{I|E}(|E_i\rangle)$. Namely, the temperature dependence of $\mathcal{N}_{I|E}(\rho)$ stems from the universal behavior of the pure energy eigenstates. This is a fixed-point property of general spin-1/2 impurities described by BCFTs. We below apply the findings to the *k*CK model.

Restoring the impurity state in BCFT.—In the kCK model, a spin-1/2 impurity \vec{S}_{imp} interacts with k channels of noninteracting electrons. Its Hamiltonian is

$$H_{kCK} = \sum_{i=1}^{k} [H_i + \lambda_i \vec{S}_{imp} \cdot \vec{S}_i]$$
(7)

with the *i*th-channel Hamiltonian H_i , the interaction strength $\lambda_i > 0$, and the *i*th-channel electron spin \vec{S}_i at the impurity position. We first consider isotropic couplings $\lambda_1 = \cdots = \lambda_k = \lambda$ at $T \ll T_K$. This regime is described by the BCFT Hamiltonian [35–37,64]

$$H_{\rm BCFT} = H_{\rm FP} + \bar{\lambda} H_{\rm LI}.$$
 (8)

 $H_{\rm FP}$ is the fixed-point Hamiltonian invariant under $U(1) \times SU(2)_k \times SU(k)_2$ Kac-Moody algebra, and $\bar{\lambda}H_{\rm LI}$ is the leading irrelevant term with coupling strength $\bar{\lambda} \propto (1/T_K)^{\Delta}$. Operators are labeled by quantum numbers (Q, j_s, j_f) with charge Q, spin j_s , flavor j_f , respectively, in the U(1), SU(2)_k, SU(k)_2 sectors.

As in Eq. (2), the impurity spin is identified [37,65] with a boundary operator $\vec{\psi}$ with scaling dimension Δ ,

$$S_{\rm imp}^{\alpha=x,y,z} \propto \frac{\psi^{\alpha}}{(T_K)^{\Delta}} + \cdots.$$
 (9)

In the 1CK, $\vec{\psi}$ is the local spin density operator \vec{J} with $\Delta = 1$ at the boundary. In the *k*CK with $k \ge 2$, $\vec{\psi}$ is the $(Q = 0, j_s = 1, j_f = 0)$ primary boundary operator $\vec{\phi}$ with $\Delta = 2/(2 + k)$. Using Eq. (3) and replacing 1/L by energy $E_i, E_j \sim E \ (\ll T_K)$, we find

$$\langle E_i | S_{\rm imp}^{\alpha=x,y,z} | E_j \rangle = O\left[\left(\frac{E}{T_K}\right)^{\Delta}\right],$$
 (10)

which agrees with NRG results [50].

Equation (10) implies that each eigenstate $|E_i\rangle$ with $E_i \ll T_K$ is composed of a maximally entangled state $(|\uparrow\rangle \otimes |\phi_{i\uparrow}\rangle + |\downarrow\rangle \otimes |\phi_{i\downarrow}\rangle)/\sqrt{2}$ and small deviation $|\delta E_i\rangle$,

$$|E_i\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |\phi_{i\uparrow}\rangle + |\downarrow\rangle \otimes |\phi_{i\downarrow}\rangle) + |\delta E_i\rangle.$$
(11)

 $|\mu = \uparrow, \downarrow\rangle$ is the impurity spin state and $|\phi_{i\mu}\rangle$'s are orthonormal states of the channels; the notation $|\phi_{i\mu}\rangle$ does not imply that the spin quantum number of $|\phi_{i\mu}\rangle$ is μ [66]. The

impurity state is restored in the energy eigenstates $|E_i\rangle$. Using Eq. (10) and a Gram-Schmidt process [50], we derive Eq. (11) and find the scaling of $\sqrt{\langle \delta E_i | \delta E_i \rangle} = O[(E/T_K)^{\Delta}]$ and $\langle \delta E_i | E_j \rangle = O[(E/T_K)^{\Delta}]$ in the restricted Hilbert space spanned by states of energy $E \sim E_i \sim E_j$.

Negativity at zero temperature.—Equation (11) shows that each pure ground state is in the form $(|\uparrow\rangle \otimes |\phi_{g\uparrow}\rangle +$ $|\downarrow\rangle \otimes |\phi_{g\downarrow}\rangle)/\sqrt{2}$, having maximal entanglement $\mathcal{N}_{I|E} = 1$ between the impurity and the channels. There can happen multiple N_0 degenerate ground states $|E_g = 0\rangle$'s in the *k*CK with $k \ge 2$, e.g., when the channels satisfy the antiperiodic condition [35]. Their thermal mixture $\rho(T = 0) =$ $\sum_{g=1}^{N_0} |E_g = 0\rangle \langle E_g = 0|/N_0$ has the maximal entanglement, $\mathcal{N}_{I|E} = 1$, because $|\phi_{g\mu}\rangle$'s are mutually orthonormal. This agrees with our NRG result in Fig. 2.

It is remarkable that the impurity is maximally entangled with the screening channels at zero temperature, independently of the channel number k. In the 1CK, the perfect impurity screening originates from the maximal entanglement. In the kCK with $k \ge 2$, $\mathcal{N}_{I|E} = 1$ still happens, although the impurity is overscreened with k-dependent frustration. This is in stark contrast with the impurity entropy [38] $\zeta_{imp} = \ln g$ for the partition far outside the Kondo length [Fig. 1(b)] which is k dependent; g = 1 for k = 1 and $g = 2 \cos[\pi/(2 + k)]$ for $k \ge 2$.



FIG. 2. Temperature dependence of the negativity $\mathcal{N}_{I|E}$ between the impurity and screening channels in the isotropic *k*CK effects. (a) NRG results [50], obtained by the method of Ref. [21]. At T = 0, $\mathcal{N}_{I|E} = 1$ independently of *k*. $\mathcal{N}_{I|E}$ rapidly decreases around T_K . (b),(c) NRG (dots) and BCFT (curves) results at $T \ll T_K$. $\mathcal{N}_{I|E}$ shows power-law scaling with T/T_K . The powerlaw exponents of the BCFT prediction in Eq. (1) agree with the NRG. (c) Log-log plot of $1 - \mathcal{N}_{I|E}(T)$.

 $\mathcal{N}_{I|E}$ and ζ_{imp} reveal different but complementary aspects of the Kondo effects. $\mathcal{N}_{I|E}$ measures how the impurity is coherently screened or quantum correlation between the impurity and its screening cloud, while ζ_{imp} counts the effective ground-state degeneracy induced by the impurity [43]. For example, $\mathcal{N}_{I|E} = 1$ shows that even at $k \to \infty$, the impurity is not free but maximally correlated with the channels. Hence $\zeta_{imp} \to \ln 2$ at $k \to \infty$ does not imply a residual free moment. This is expected from the behavior of the impurity magnetization [67,68].

And, at k = 2, $\zeta_{imp} = \ln \sqrt{2}$ implies fractionalization of the impurity into two Majorana fermions, a free Majorana γ_{i1} and another γ_{i2} coupled with the channels. Each ground state of the 2CK is a product state of a fermionic state by fusion of γ_{i1} and a free Majorana of the channel, and another fusion state of γ_{i2} and a Majorana of the channels [62]. In terms of the bipartite basis states for the partition in Fig. 1(a), the product state is written as the maximalentanglement form $(|\uparrow\rangle \otimes |\phi_{g\uparrow}\rangle + |\downarrow\rangle \otimes |\phi_{g\downarrow}\rangle)/\sqrt{2}$. Here the impurity states $|\uparrow\rangle$ and $|\downarrow\rangle$ are described by fusion of γ_{i1} and γ_{i2} . Hence, the fractionalization is reconciled with $\mathcal{N}_{I|E} = 1$. Similar maximal entanglement happens in a one-dimensional *p*-wave superconductor having free Majoranas [10].

Universal thermal decay of negativity.—Putting $c_{\alpha} = 0$ and $\Delta_{\alpha} = \Delta$ of the *k*CK [see Eq. (10)] into Eq. (5), we find that the entanglement becomes weaker in the eigenstates of higher energy, $\mathcal{N}_{I|E}(|E_i\rangle) = 1 - O[(E_i/T_K)^{2\Delta}]$. Then using Eq. (6), we obtain the algebraic thermal decay of the entanglement in Eq. (1). The decay is confirmed by the NRG in Fig. 2, and also by direct calculation [50] of $\mathcal{N}_{I|E} + 1 = ||\rho^{T_I}|| = 2 - O[(T/T_K)^{2\Delta}]$ that equals the sum of the square roots of the eigenvalues of $(\rho^{T_I})^2$.

The power-law exponent 2Δ of the thermal decay of $\mathcal{N}_{I|E}$ is a universal fixed-point behavior. Considering the energy dependence $\langle \delta E_i | E_j \rangle = O[(E/T_K)^{\Delta}]$ of the eigenstates in Eq. (11), it is nontrivial that the exponent of the entanglement decay is 2Δ rather than Δ ; the contributions of $O[(T/T_K)^{\Delta}]$ to $\mathcal{N}_{I|E}(\rho)$ exactly cancel each other. This relates with the fact that the entanglement is a nonlinear function of the density matrix. The exponent (Δ versus 2Δ) is determined by whether $c_{\alpha} = 0$ or not or equivalently by the ground-state expectation value of \vec{S}_{imp} ; see Eqs. (2)–(5). For example, we find [69] that the exponent of the algebraic thermal decay of $\mathcal{N}_{I|E}$ is Δ_z ($= \Delta_x$) in the Ising spin chain [33,34] with fixed boundary where $c_{x,z} \neq 0$ and $2\Delta_y > \Delta_{x,z}$.

Negativity between fixed points.—We study the temperature dependence of the negativity $\mathcal{N}_{I|E}(T)$ in the channel anisotropic Kondo model, where thermal crossover happens between different Kondo effects [31,32]. Figure 3 shows that the power-law exponent of $\mathcal{N}_{I|E}(T)$ accordingly changes, following Eq. (1).



FIG. 3. Temperature dependence of the negativity $\mathcal{N}_{I|E}$ in anisotropic (a) 2CK and (b) 3CK effects with the coupling strengths λ_1 and $\lambda_{i\geq 2} = \lambda$. The power-law exponent of $\mathcal{N}_{I|E}(T)$ changes, following crossover between different Kondo effects. The NRG results (points) agree with the BCFT prediction (lines). The isotropic case with $\lambda_1 = \lambda$ is shown for comparison. (a) When $\lambda_1 = 0.99\lambda$ or 1.01λ , the exponent changes from $2\Delta = 2$ (the 1CK behavior) to $2\Delta = 1$ (2CK) as *T* increases, passing the crossover temperature T^* . (b) When $\lambda_1 = 0.99\lambda$, the exponent changes from $2\Delta = 1$ (2CK) to $2\Delta = 4/5$ (3CK). When $\lambda_1 = 1.01\lambda$, the exponent changes from $2\Delta = 4/5$ (3CK).

We focus on the anisotropic 2CK model with the coupling strengths $\lambda_1 \neq \lambda_2$. Combining the finite-size bosonization method and our approach, we derive [50]

$$1 - \mathcal{N}_{I|E} \propto \begin{cases} \frac{T}{T_K} & (T^* \ll T \ll T_K), \\ \frac{\nu T^2}{T^*} & (T \ll T^*). \end{cases}$$
(12)

 $T^* \ [\propto \nu^2 (\lambda_2 - \lambda_1)^2 T_K]$ is the crossover temperature between the 1CK at lower temperature and the 2CK at higher temperature. ν is the local density of channel states at the impurity site. Interestingly, the scaling behavior $\nu T^2/T^*$ at $T \ll T^*$ is different from the known behavior of observables; at $T \ll T^*$, the decay of electron conductance in a setup follows $(T/T^*)^2$, while the magnetization follows $(T/T^*)^2 \sqrt{T^*T_K}$ [70]. This scaling behavior of $\mathcal{N}_{I|E}$ is attributed [50] to the scaling

$$\langle E_i | S_{\rm imp}^{\alpha} | E_j \rangle = \begin{cases} O\left(\sqrt{\frac{E}{T_K}}\right) & (T^* \ll E \ll T_K) \\ O\left(\frac{\sqrt{\nu}E}{\sqrt{T^*}}\right) & (E \ll T^*) \end{cases}$$
(13)

with $E \sim E_i \sim E_j$. This is confirmed by the NRG.

Conclusion.—We develop analytic computation of the entanglement $\mathcal{N}_{I|E}$ between the impurity and channels in the multichannel Kondo effects. $\mathcal{N}_{I|E}$ quantifies how the Kondo screening quantum coherently happens inside the screening length. Its thermal scaling is a universality of the fixed point and reflects non-Fermi liquids and fractionalization [71]. $\mathcal{N}_{I|E}$ and the impurity entropy show different but complementary aspects of the Kondo effects.

Our findings have implications. First, the direct relation in Eq. (4) between $\mathcal{N}_{I|E}$ and $\langle E_i | \vec{S}_{imp} | E_i \rangle$ for energy eigenstates means that the impurity spin screening originates from the entanglement $\mathcal{N}_{I|E}$ in general spin-1/2 impurities. It implies the possibility of accessing $\mathcal{N}_{I|E}$ by experimentally detecting impurity magnetization at sufficiently low temperature. For example, in a quantum dot [72,73] showing multichannel charge Kondo effects, the excess charge of the dot, corresponding to $\langle E_i | \vec{S}_{imp} | E_i \rangle$, is detectable. One can measure $\mathcal{N}_{I|E}$ with changing a gate voltage applied to the dot, which corresponds to a magnetic field applied to \vec{S}_{imp} .

Second, the entanglement $\mathcal{N}_{I|E}$ will be useful for quantifying the spatial distribution of multichannel Kondo clouds. The 1CK cloud was recently observed [30] with changing the location at which the screening channel is weakly perturbed. Similarly, we suggest [74] to observe *k*CK clouds by monitoring change of $\mathcal{N}_{I|E}$ or $\langle E_i | \vec{S}_{imp} | E_i \rangle$ with varying the perturbation position.

Third, the thermal scaling of $\mathcal{N}_{I|E}$ is a universal fixedpoint property. This scaling behavior can be different from that of states, since $\mathcal{N}_{I|E}$ is a nonlinear function of the states. Interestingly, the thermal scaling of $\mathcal{N}_{I|E}$ is estimated from the scaling of $\mathcal{N}_{I|E}$ of energy eigenstates. This suggests to study entanglement in pure excited states in other problems, which has been less studied [8–10] than ground states.

Finally, our approach is applicable to study coherent coupling between the boundary and bulk in spin chains or in other spin-1/2 impurities described by BCFT. The behavior of $\mathcal{N}_{I|E}$ will depend on different universality classes of boundary phenomena of different boundary conditions.

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