









## Universal scaling of tunable Yu-Shiba-Rusinov states across the quantum phase transition

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Quantum magnetic impurities give rise to a wealth of phenomena attracting tremendous research interest in recent years. On a normal metal, magnetic impurities generate the correlation-driven Kondo effect. On a superconductor, bound states emerge inside the superconducting gap called the Yu-Shiba-Rusinov (YSR) states. Theoretically, quantum impurity problems have been successfully tackled by numerical renormalization group (NRG) theory, where the Kondo and YSR physics are shown to be unified and the normalized YSR energy scales universally with the Kondo temperature divided by the superconducting gap. However, experimentally the Kondo temperature is usually extracted from phenomenological approaches, which gives rise to significant uncertainties and cannot account for magnetic fields properly. Using scanning tunneling microscopy at 10 mK, we apply a magnetic field to several YSR impurities on a vanadium tip to reveal the Kondo effect and employ the microscopic single impurity Anderson model with NRG to fit the Kondo spectra in magnetic fields accurately and extract the corresponding Kondo temperature unambiguously. Some YSR states move across the quantum phase transition (QPT) due to the changes in atomic forces during tip approach, yielding a continuous universal scaling with quantitative precision for quantum spin- $\frac{1}{2}$  impurities.

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Quantum impurity problems deal with impurities featuring a small number of intrinsic quantum degrees of freedom connected to a continuous bath. The complexity lies in the quantum nature of such impurities resulting in correlations and many-body effects as well as the concomitant breakdown of a perturbative or mean field treatment<sup>1</sup>. Magnetic impurities attract particular attention as it is not a priori clear whether a fully quantum theory is necessary or a semiclassical treatment on the spin degrees of freedom suffices to describe the system. In some instances, the spin can be treated classically, as in the case of the in-gap Yu-Shiba-Rusinov (YSR) states generated from magnetic impurities on superconducting surfaces<sup>2–5</sup>. There, correlation effects play a subordinate role and, therefore, the YSR states can be treated well within the mean-field approximation<sup>6–15</sup>. However, in other cases the spin needs to be treated fully quantum mechanically and correlation effects are indispensable to describe the observations, such as the Kondo effect, which emerges when magnetic impurities are placed on normal conducting surfaces<sup>16–21</sup>.

The only difference between YSR and Kondo physics is a superconducting instead of a normal conducting bath. Thus, both phenomena can be theoretically described in a unified framework within the single impurity Anderson model (SIAM). A solution of such a model including full correlations can be achieved by means of numerical renormalization group (NRG) theory<sup>22–24</sup>. The hallmark of this theory is a universal scaling relation between the normalized YSR energy  $\varepsilon_{\text{YSR}}/\Delta$  and  $k_{\text{B}}T_{\text{K}}/\Delta$ , where  $\varepsilon_{\text{YSR}}$  is the YSR energy,  $T_{\text{K}}$  is the Kondo temperature,  $k_{\text{B}}$  is the Boltzmann constant and  $\Delta$  is the superconducting order parameter. The quantum phase transition (QPT) associated with YSR-physics is predicted to occur at  $k_{\text{B}}T_{\text{K}}/\Delta = 0.24$ <sup>1,25–27</sup>.

Despite these convincing theoretical predictions for the universal scaling, there are different aspects of uncertainty in existing experimental results, especially in atomic junctions where fitting the tunneling spectra is essential for extracting the Kondo temperature<sup>28–32</sup>. One reason is that the commonly reported Kondo systems are not purely spin- $\frac{1}{2}$ , which complicates the analysis. Another reason is that the experimental procedures followed for the extraction of the Kondo temperature are usually phenomenological, either done by simply taking the half width half maximum of the Kondo peak or by fitting with rather phenomenological functions like Fano or Frota functions<sup>21,33</sup>, while a much better solution is to employ NRG directly<sup>31,34,35</sup>. Furthermore, the finite experimental temperature results in a thermal broadening obscuring the spectral peak. These obstacles as well as the existence of various definitions of the Kondo temperature result in an ambiguity of the obtained Kondo temperature, up to a factor of four<sup>29</sup>.

Here, we follow a more rigorous procedure and extract the Kondo temperature unambiguously by employing the full NRG theory on the microscopic SIAM to directly fit the Kondo spectra on spin- $\frac{1}{2}$  YSR impurities on the vanadium tip<sup>11,15,36</sup> in magnetic fields at low temperatures (10 mK). We compare the Kondo temperature with the YSR energy at zero field and demonstrates the universal scaling. Since both phenomena are treated within one microscopic framework, the ambiguity of the Kondo temperature is eliminated. Using this approach, we analyze various YSR impurities on the vanadium tip, especially those moving across the QPT with varying tip-sample distance, which has been observed in a number of YSR states before<sup>37–42</sup>, and reveal a continuous and quantitative universal scaling behavior.

## Results

**Quantum phase transition and the Kondo effect.** The magnetic impurity is introduced onto the apex of the vanadium scanning

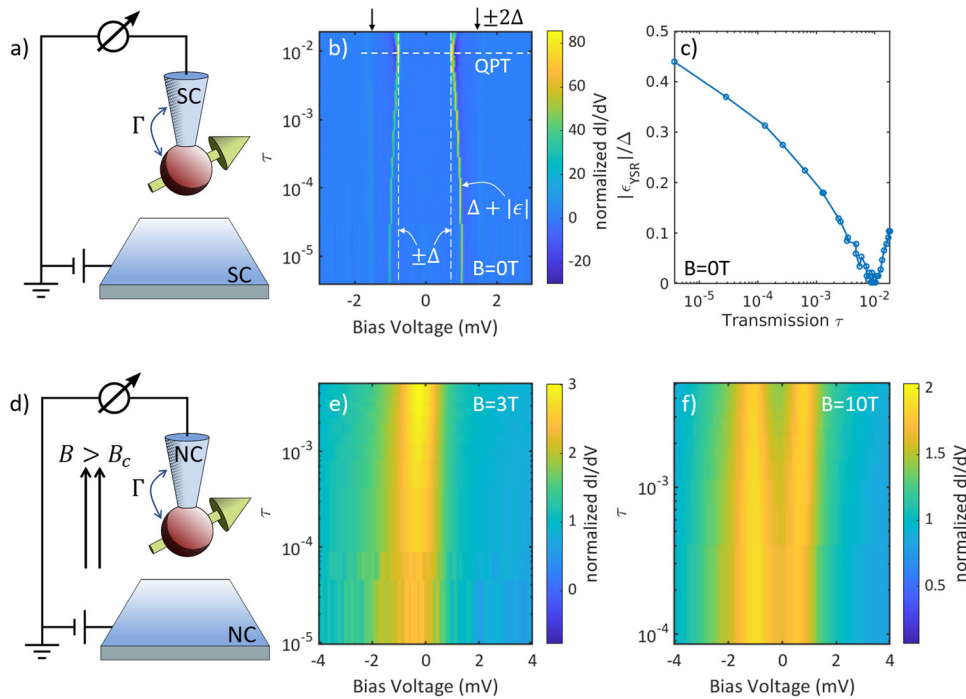
tunneling microscope tip producing a YSR state on the tip apex using the method described in refs. <sup>11</sup> and <sup>15</sup> (see Supplementary Note 1, schematics see Fig. 1a). The sample is also vanadium, having the same order parameter  $\Delta = 750 \mu\text{eV}$  as the tip. At zero magnetic field and a base temperature of 10 mK, the junction is well superconducting. The tunneling between the tip YSR state with the energy  $\varepsilon_{\text{YSR}}$  and the coherence peak of the sample at  $\Delta$  yields the most prominent spectral feature shown in Fig. 1b at bias voltages of  $eV = \pm(\Delta + |\varepsilon_{\text{YSR}}|)$  (YSR-BCS peaks with BCS meaning Bardeen-Cooper-Schrieffer superconductors). The tunneling between the coherence peaks (BCS-BCS peaks) at bias voltages of  $eV = \pm 2\Delta$  is largely suppressed compared to the YSR-BCS tunneling due to the presence of YSR states. Notice that from the YSR-BCS peak positions it is not possible to extract the sign of the YSR energy  $\varepsilon_{\text{YSR}}$ . We, therefore, use its absolute value in Figs. 1, 2. Conventionally,  $\varepsilon_{\text{YSR}}$  acquires a negative sign after the QPT (in the screened spin regime) to indicate the fact that the ground state and the excited state interchange at the QPT. After we obtain more information with respect to the two domains of the QPT from Kondo spectra, we add the proper signs to  $\varepsilon_{\text{YSR}}$  (Figs. 3, 4).

In this example, the YSR state moves across the QPT when approaching the tip to the sample and increasing the normal state transmission  $\tau = G_{\text{N}}/G_0$ , where  $G_{\text{N}}$  is the normal state conductance measured well above the superconducting gap and  $G_0 = 2e^2/h$  is the quantum of conductance ( $e$  is electron charge and  $h$  is Planck constant). The clear indication of this QPT is the zero crossing of  $\varepsilon_{\text{YSR}}$  signaled by the point where the YSR-BCS peaks touch  $eV = \pm \Delta$  (dashed vertical line in Fig. 1b). We further find  $|\varepsilon_{\text{YSR}}|$  by subtracting  $\Delta$  from the YSR-BCS peak position and plot the normalized YSR energy  $|\varepsilon_{\text{YSR}}|/\Delta$  in Fig. 1c, which clearly shows the zero crossing.

Then we apply magnetic fields from 1.5 T to 10 T perpendicular to the sample surface, which exceed the critical field and quench superconductivity in both the tip and the sample making them both normal conducting (Fig. 1d). At a magnetic field of 3 T, a Kondo peak is observed around zero bias voltage (Fig. 1e), whose width decreases with increasing transmission, indicating a decreasing Kondo temperature. Increasing the magnetic field to 10 T, the Kondo peak splits into two peaks due to the Zeeman effect (Fig. 1f).

## The single impurity Anderson model and the universal scaling.

For a quantitative modeling, we use the SIAM with the Hamiltonian  $H_{\text{SIAM}} = H_{\text{s}} + H_{\text{i}} + H_{\text{c}}$ , where  $H_{\text{s}} = \sum_{k\sigma} \xi_k c_{k\sigma}^\dagger c_{k\sigma}$  represents the band dispersion of the normal conducting substrate with  $c$  and  $c^\dagger$  being the annihilation and creation operators for electrons with momentum  $k$  and spin  $\sigma$ ,  $H_{\text{i}} = \varepsilon_{\text{d}}(n_{\uparrow} + n_{\downarrow}) + Un_{\uparrow}n_{\downarrow}$  denotes the Anderson impurity with impurity level  $\varepsilon_{\text{d}}$ , on-site Coulomb term  $U$  and the electron occupation number operator  $n$ , and  $H_{\text{c}} = \sum_{k\sigma} V_k(c_{k\sigma}^\dagger d_{\sigma} + \text{H.c.})$  represents the coupling between the impurity and the substrate with  $d$  being the annihilation operator on the impurity site<sup>43,44</sup>. Assuming a constant density of states  $\rho$  and constant hybridization strength  $V_k$  near the Fermi level, we further define the parameter  $\Gamma = \pi\rho|V_{k_{\text{F}}}|^2$  quantifying the impurity-substrate coupling. Therefore, the behavior of the SIAM is essentially defined by the three parameters  $U$ ,  $\varepsilon_{\text{d}}$  and  $\Gamma$  (Fig. 2a). Note that all parameters are energies in units of the half bandwidth  $D$  of the bulk conduction electrons. Among these three parameters,  $\Gamma$  is of special experimental interest, because the movement of the YSR state shown in Fig. 1b originates from a changing impurity-substrate coupling  $\Gamma$  due to the changing atomic forces acting in the junction between tip and sample<sup>15,41</sup>. Therefore, we will use  $\Gamma$  as the variable to fit



**Fig. 1** **A Yu-Shiba-Rusinov (YSR) impurity moving through the quantum phase transition (QPT).** **a** The schematics of the experiment at zero field, where the junction is superconducting. During tip approach, the atomic force exerted on the magnetic impurity changes resulting in a varying coupling  $\Gamma$  and therefore a moving YSR energy. **b** YSR spectra across the QPT during tip approach. Here, since both tip and sample are superconducting, the spectral peaks involving the YSR states are at  $\pm(\Delta + |\epsilon_{\text{YSR}}|)$ , where  $\Delta$  is the superconducting order parameter and  $\epsilon_{\text{YSR}}$  is the energy of the tip YSR state. Therefore, the QPT happens when such spectral peaks touch  $\pm\Delta$ . **c** The extracted YSR energy normalized by  $\Delta$  as a function of the transmission  $\tau$ . **d** The schematics of the experiment in a magnetic field higher than the critical magnetic field  $B_c$ , where superconductivity in both the tip and the sample are quenched. **e** Emerging Kondo peaks at 3 T. **f** The Kondo peaks further split at high magnetic field ( $B = 10$  T here). Note: the data presented in **(b, c)** are reproduced from ref. <sup>15</sup>.

the Kondo spectra in the following. For convenience, we also define the asymmetry parameter  $\delta = \epsilon_d + U/2$  to be used instead of  $\epsilon_d$  as it is easier to distinguish different scenarios. If  $\delta = 0$ , the impurity levels are symmetric around the Fermi energy resulting in electron-hole symmetry, yielding a symmetric spectral function. If  $\delta \neq 0$ , the spectral function will be asymmetric due to electron-hole asymmetry.

Through a Schrieffer-Wolff transformation<sup>27,45</sup>, an expression of the Kondo temperature in terms of the SIAM parameters can be derived as

$$k_B T_K = D_{\text{eff}} \sqrt{\rho J} \exp\left(-\frac{1}{\rho J}\right), \text{ with } \rho J = \frac{8\Gamma}{\pi U} \frac{1}{1 - 4(\delta/U)^2}. \quad (1)$$

The effective band width  $D_{\text{eff}}$  depends on  $U$ : If  $U \ll 1$ ,  $D_{\text{eff}} = 0.182U\sqrt{1 - 4(\delta/U)^2}$ <sup>25,44</sup>. If  $U \gg 1$ ,  $D_{\text{eff}}$  is a constant on the order of 1, whose exact value is fixed comparing with the situation  $U \ll 1$ . In the NRG implementation used in this paper  $D_{\text{eff}} = 0.5$  for  $U \gg 1$  (see Supplementary Note 2).

Further, to reflect the Kondo effect in a finite magnetic field (Fig. 1d–f), a Zeeman term needs to be added in the Hamiltonian

$$H_{\text{SIAM,B}} = H_{\text{SIAM}} + g\mu_B B S_z, \quad (2)$$

where  $g$  is the gyromagnetic ratio,  $\mu_B$  is the Bohr magneton,  $S_z$  is the spin component along the magnetic field  $B$ .

On the other hand, to account for superconductivity and YSR states (Fig. 1a–c), the Hamiltonian is modified to

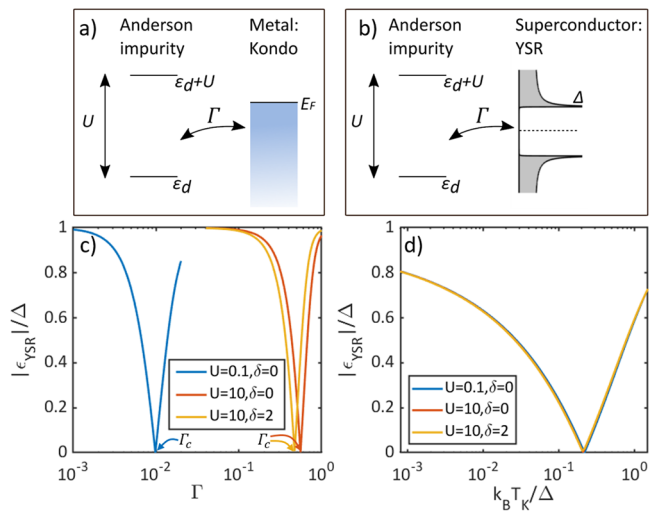
$$H_{\text{SIAM,SC}} = H_{\text{SIAM}} - \sum_k \left( \Delta c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger + \Delta^* c_{-k\downarrow} c_{k\uparrow} \right), \quad (3)$$

with  $\Delta$  being the superconducting order parameter (Fig. 2b).

Using the “NRG Ljubljana” package for NRG simulations<sup>46</sup>, we calculated the normalized YSR energy  $|\epsilon_{\text{YSR}}|/\Delta$  as a function of  $\Gamma$  for different  $U$  and  $\delta$  (Fig. 2c). With increasing  $\Gamma$ , the YSR energy always moves from the gap edge towards zero energy, across the QPT, and then from zero energy towards the gap edge again. The critical impurity-substrate coupling  $\Gamma_c$  at the QPT depends on both  $U$  and  $\delta$ .

We convert  $\Gamma$  to  $k_B T_K$  using Eq. (1) and plot  $k_B T_K/\Delta$  as the horizontal axis in Fig. 2d. All curves from Fig. 2c overlap now, demonstrating the universal scaling between the YSR energy and the Kondo temperature independent of the details of the SIAM parameters  $\delta$  and  $U$ . This is because the low energy physics including the YSR and Kondo phenomena is dominated by the Kondo temperature, which is much smaller than the energy scale of  $U$ ,  $\epsilon_d$  and  $\Gamma$  (see Supplementary Note 3). Therefore, according to Eq. (1) there are some redundant degrees of freedom in the SIAM in the context of the Kondo effect and YSR states. The parameter  $\delta$  is responsible for the asymmetry of the spectrum and remains thus relevant for fitting, but  $U$  can be chosen freely. In the following, we use  $U = 10$ , which is much larger than one, so that the impurity Hubbard satellite peaks, which are generally not observed in our experimental spectra, do not interfere with the fitting.

**Fitting the Kondo spectra directly using NRG theory.** The Kondo spectra from Fig. 1e, f are replotted as cascaded curves in Fig. 3a for  $B = 3$  T and (b) for  $B = 10$  T. We can directly fit the Kondo spectra in the magnetic field using NRG theory (black dashed lines in Fig. 3a, b). For the fit, we fix  $U = 10$ , and also fix a  $\delta$  that represents the asymmetry of the spectra for a certain



**Fig. 2** Single impurity Anderson model (SIAM). **a** The schematics of the SIAM for a normal metal giving rise to the Kondo effect. The parameters are the impurity level  $\epsilon_d$ , the on-site Coulomb  $U$  and the impurity-substrate coupling  $\Gamma$ . For convenience, in this paper we use the asymmetry parameter  $\delta = \epsilon_d + \frac{U}{2}$  instead of  $\epsilon_d$ . **b** The schematics of the SIAM including superconductivity giving rise to the YSR states. Here, there is one more parameter in the model which is the superconducting order parameter  $\Delta$ . **c** The normalized YSR energy  $|\epsilon_{\text{YSR}}|/\Delta$  as a function of  $\Gamma$  calculated from the numerical renormalization group (NRG) theory. The critical  $\Gamma$  at the QPT ( $\Gamma_c$ ) depends on both  $U$  and  $\delta$ . **d** The normalized YSR energy as a function of  $k_B T_K/\Delta$  is a universal curve independent of  $U$  and  $\delta$ , indicating that the low energy physics is controlled by the Kondo temperature making not all parameters in the SIAM relevant.

impurity. For the impurity shown in Figs. 1 and 3, we choose  $\delta = -2$ .

The asymmetry of a Kondo peak is typically ascribed to a Fano line shape originating from the interference between different tunneling paths<sup>47–51</sup>. However, independent from these scattering and transport phenomena, an electron-hole asymmetry will also result in an asymmetric Kondo peak. The same electron-hole asymmetry will render the YSR peaks asymmetric, so a correlation between the asymmetry of a Kondo peak and the asymmetry of the corresponding YSR states is expected. In our experiment, the tunneling channel to the continuum is largely suppressed as evidenced by the faint BCS-BCS tunneling peaks in Fig. 1b. Consequently, we conclude that the transport is dominantly through a single YSR channel, and thus Fano-like interference is minimal, which is also supported by the clearly peaked Kondo features in Fig. 3a, b. A more detailed discussion of the alternative scenario considering Fano process is in the Supplementary Note 4, where we show that actually very similar Kondo temperatures are obtained for both scenarios<sup>52</sup>. For the following part here, however, we assume that the asymmetry of the Kondo peaks originates from the intrinsic asymmetry of the SIAM with parameter  $\delta$ . With  $U = 10$  and  $\delta = -2$  being fixed as outlined above, the only fitting parameter is  $\Gamma$ . The resulting fits agree well with the experimental spectra with quantitative precision, for both 3 T (Fig. 3a), and 10 T (Fig. 3b) magnetic fields. The general trend that the peak width reduces when increasing the normal state transmission  $\tau$ , the peak asymmetry, as well as the details of the Zeeman splitting at 10 T are precisely reproduced.

We plot the fitted values for the impurity-substrate coupling  $\Gamma$  as a function of transmission  $\tau$  in Fig. 3c. All fits for  $B = 1.5$  T, 3 T and 10 T are quite similar indicating consistency. The values also

reflect the observation in the raw data (Figs. 1e, 3a) that the impurity-substrate coupling  $\Gamma$  and concomitantly the Kondo temperature  $T_K$  as well as the peak width decrease with increasing transmission.

Combining Figs. 1c and 3c, we obtain the YSR energy  $\epsilon_{\text{YSR}}/\Delta$  as a function of the impurity-substrate coupling  $\Gamma$ , which is displayed in Fig. 3d. The expected dependence of  $\epsilon_{\text{YSR}}/\Delta$  vs.  $\Gamma$  predicted from the NRG model is shown as the purple dashed line. The experimental data generally follows the trend of the theoretical expectations and the critical impurity-substrate coupling  $\Gamma_c$  at the QPT agrees approximately. The relative deviation in  $\Gamma$  is quite small (<5%), which could be due to slightly different atomic forces acting on the impurity when the substrate is superconducting or normal conducting, which will be discussed in more detail below.

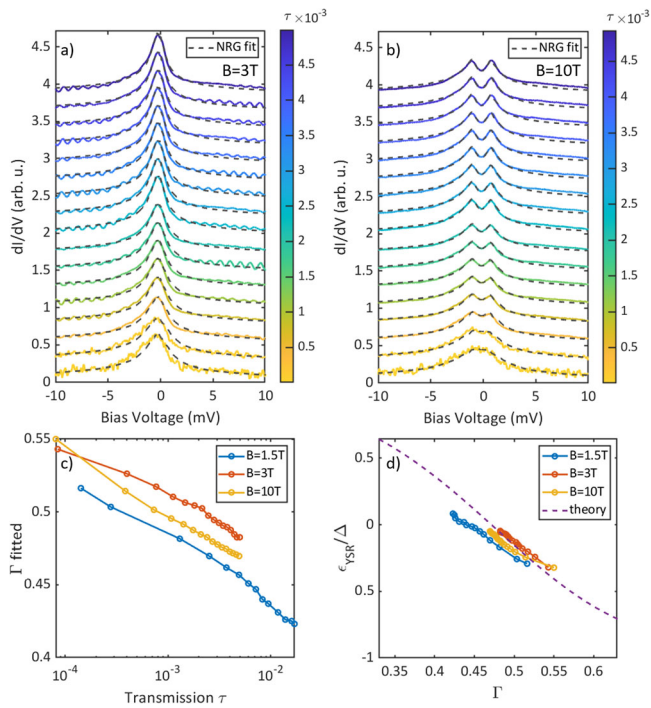
**Universal scaling in various YSR impurities.** Converting the fitted impurity-substrate coupling  $\Gamma$  to a Kondo temperature  $T_K$  through Eq. (1), we plot  $T_K$  as a function of the transmission  $\tau$  in Fig. 4(a) as well as the normalized YSR energy  $\epsilon_{\text{YSR}}/\Delta$  as a function of  $k_B T_K/\Delta$  in Fig. 4b. The different markers (six in total: +, ○, △, ×, ★, □) label the different YSR impurities, where the YSR states represented by the three markers +, ○, and △ move across the QPT while the other three ×, ★, and □ do not move significantly when approaching the tip to the sample. The impurity shown in Figs. 1 and 3 is presented with the marker +, which is the same impurity as in ref. 15. The different magnetic fields, in which the impurities have been measured, are color coded as shown in the figure colorbar.

Depending on the interactions in the junction, the impurity-substrate coupling  $\Gamma$  and concomitantly the Kondo temperature  $T_K$  decreases (+, ○) or increases (△) when approaching the tip to the sample<sup>41</sup>, indicating that the YSR state moves across the QPT from the screened spin regime to the free-spin regime or the other way around, respectively. Usually, the atomic forces at low conductance are attractive which pulls the impurity away during tip approach<sup>37,53</sup>, resulting in a decrease of the impurity-substrate coupling  $\Gamma$  and the Kondo temperature  $T_K$ . However, since  $\Gamma$  also depends on the local density of states  $\rho$ , small structural changes due to the atomic forces can lead to a change in  $\rho$ , such that in some cases they result in a net increase of  $\Gamma$  during tip approach<sup>39,41,54</sup>. In other cases the magnetic impurity is more rigidly bound to the tip, such that impurity is not susceptible to the atomic forces in the junction and the YSR energy does not depend on the junction transmission within the range of our measurements (×, ★, □).

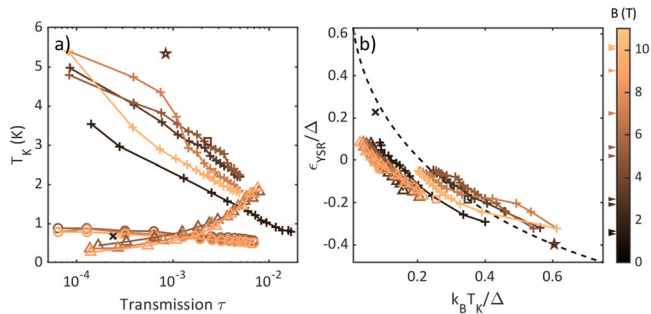
Despite the varying behavior of the impurities during tip approach, the scaling between the YSR energy and the Kondo temperature is generally universal (Fig. 4b). The theoretical curve predicted by the NRG theory is plotted as a dashed line. All experimental data generally reproduces the trend of the universal scaling.

## Discussion

There are multiple indications that the impurity induced YSR states in vanadium are spin- $\frac{1}{2}$  systems ranging from single quasiparticle level tunneling and its spin selection<sup>11,14</sup>, to the observation of a 0- $\pi$ -transition<sup>15</sup>. This is further corroborated by the observation of only one pair of YSR peaks on both sides of the QPT (see Fig. 1b, in contrast with high spin systems<sup>55</sup>) and the remarkable quantitative agreement when fitting the Kondo spectra with the spin- $\frac{1}{2}$  SIAM model using NRG theory (see Fig. 3a, b). This makes our system a model platform to study the relation between the Kondo effect and YSR states.



**Fig. 3** Fitting the Kondo spectra of a Yu-Shiba-Rusinov (YSR) impurity moving through the quantum phase transition using the microscopic numerical renormalization group (NRG) theory. **a** The Kondo spectra (colored solid lines) and their fits (black dashed lines) at  $B = 3$  T. **b** The Kondo spectra (colored solid lines) and their fits (black dashed lines) at external magnetic field  $B = 10$  T. **c** The fitted impurity substrate coupling  $\Gamma$  as a function of  $\tau$  shows a decreasing coupling during tip approach, indicating that the impurity is pulled away due to attractive forces in the junction. **d** Normalized YSR energy as a function of  $\Gamma$  extracted from Kondo peaks at  $B = 1.5$  T (blue curve), 3 T (red curve) and 10 T (yellow curve). The purple dashed line is the theoretical expectation from the NRG theory with the same asymmetry parameter  $\delta = -2$  as in the fits. Notice that the deviation in terms of  $\Gamma$  is quite small (below 5%).



**Fig. 4** The universal scaling of various Yu-Shiba-Rusinov (YSR) impurities on vanadium tip. **a** The extracted Kondo temperature  $T_K$  as a function of the normal state transmission  $\tau$ . Different markers denote different impurities. The plus sign (+) denotes the impurity shown in Figs. 1 and 3. Different colors represent different magnetic fields  $B$ , and the used magnetic fields are marked with arrows of corresponding colors on the left side of the colorbar.  $T_K$  of the same impurity extracted from data in different magnetic fields are comparable, showing consistency throughout each dataset. **b** The universal scaling of the normalized YSR energy as a function of  $k_B T_K/\Delta$ , where  $k_B$  is the Boltzmann constant and  $\Delta$  is the superconducting order parameter. All datasets show similar tendency agreeing with the theoretical universal scaling (black dashed line).

Similar scaling has been observed before for different kinds of impurities (not necessarily spin- $\frac{1}{2}$ )<sup>28–32,56</sup>. In most cases, the experimentally derived definition of the Kondo temperature leaves some ambiguity in the comparison with the universal scaling. Using the full microscopic NRG model we not only minimized the ambiguity but also accounted for the effect of the applied magnetic field in fitting the data. In addition, since our experimental temperature of 10 mK is much smaller than the Kondo temperature, the intrinsic temperature broadening of the Kondo peak is negligible<sup>20,57</sup>. Furthermore, the Fermi-Dirac broadening of the probing electrode can also be neglected due to our high energy resolution at mK temperatures. Consequently, we do not need any deconvolution to extract the real Kondo signal from the experimentally broadened peaks, further achieving quantitative accuracy.

Still, the remaining deviations from the universal scaling as displayed in Fig. 4b raise intriguing questions as to their origin. One possibility, as proposed in previous studies, is the validity of the universal scaling with respect to the parameter space of the SIAM<sup>26</sup>. For atoms on substrates in our case, both the impurity-substrate coupling  $\Gamma$  and the half band width  $D$  are always much larger than  $\Delta$ , such that the universal scaling is valid and precise independent of  $U$ <sup>26,27</sup>. Therefore, this reasoning can be ruled out as outlined in Supplementary Note 3. However, a realistic structured electronic band and non-constant density of states can modify the Kondo physics in a non-trivial way<sup>58–60</sup> and thus go beyond the simple assumption of the universal scaling. It is therefore intriguing to investigate the validity or breakdown of the universal scaling in weakly coupled systems like certain molecules and in systems with non-trivial band structure.

We further find that the fit for different magnetic fields differs slightly even for the same impurity. This indicates that the magnetic field may change the force exerted on the impurity and in turn the impurity-substrate coupling. Also, the quenching of the superconductivity could change the atomic forces modifying the impurity-substrate coupling. This is reasonable because the relative deviation in terms of the impurity-substrate coupling is only a few percent (see Fig. 3d), while the resulting response in the Kondo temperature is much larger due to the exponential dependence (Eq. (1)). Other mechanisms including residual interactions with nearby spins could also influence the universal scaling behavior.

## Conclusion

In summary, we have analyzed the scaling between the YSR energy and the Kondo temperature fits of Kondo spectra using microscopic model on the magnetic impurities at the apex of a vanadium tip. The impurities show spin- $\frac{1}{2}$  characteristics and some of them move across the quantum phase transition during tip approach allowing for a continuous control and investigation of the scaling behavior. Directly using NRG theory in the fitting of the Kondo spectra reduces the ambiguity in extracting the Kondo temperature compared to experimentally derived definitions of the Kondo temperature. Additionally, our experimental temperature in the mK regime minimizes the experimental broadening. With this, our results corroborate the universal scaling of the NRG theory at the atomic scale with quantitative precision. The observed deviations point to a degree of freedom not captured by the current theory like modified impurity-substrate coupling in a magnetic field, which calls for further investigations. A future direction would be to apply such analysis to other spin- $\frac{1}{2}$  systems as well as higher spin systems or coupled YSR dimers<sup>61</sup>.

## Methods

The sample used in the experiments was a vanadium (100) single crystal with >99.99% purity, which was prepared in ultrahigh vacuum (UHV) by multiple cycles of argon ion sputtering at around 1 keV acceleration energy in about  $10^{-6}$  mbar argon pressure followed by annealing at around 700 °C. The tip was cut from a polycrystalline vanadium wire of 99.8% purity and subsequently prepared in UHV by Argon sputtering. To obtain a tip exhibiting clean bulk gap as well as good imaging capabilities, several rounds of field emission as well as standard tip shaping techniques were conducted on V(100) surface. We repeatedly dipped the tip onto the sample surface to introduce YSR states with desired properties onto the apex of the tip<sup>11</sup>. We measured the tunneling between tip YSR states and clean sample superconductor in the absence of external magnetic field. Then we quenched superconductivity in both tip and sample to reveal the Kondo effect. Theoretical simulation of both YSR and Kondo spectra was conducted under the framework of the NRG theory with the implementation from the “NRG Ljubljana” package<sup>46</sup>.

## Data availability

The data that support the findings of this study are available from the corresponding author upon reasonable request.

## Code availability

The code that supports the findings of this study are available from the corresponding author upon reasonable request.

Received: 10 January 2023; Accepted: 1 August 2023;

Published online: 17 August 2023

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## Acknowledgements

We gratefully acknowledge stimulating discussions with Alfredo Levy Yeyati, Rok Žitko, Markus Ternes, and Robert Drost. This work was funded in part by the ERC Consolidator Grant AbsoluteSpin (Grant No. 681164) and by the Center for Integrated Quantum Science and Technology (IQ<sup>ST</sup>). J.A. acknowledges funding from the BMBF within the sub-project QCOMP (Cluster4Future QSENSE). C.P. acknowledges funding from the IQ<sup>ST</sup> and the Zeiss Foundation. J.C.C. acknowledges funding from the Spanish Ministry of Science and Innovation (grant no. PID2020-114880GB-I00) and the DFG and SFB 1432 for sponsoring his stay at the University of Konstanz as a Mercator Fellow.

## Author contributions

H.H. and S.K. performed the experiments with support from C.R.A. and K.K.. H.H., C.P., B.K., J.C.C. and J.A. provided theory support. H.H. and C.R.A. modeled and analysed the

data with support from all authors. All authors discussed the results. H.H. wrote the manuscript with input from all authors.

## Funding

Open Access funding enabled and organized by Projekt DEAL.

## Competing interests

The authors declare no competing interests.

## Additional information

**Supplementary information** The online version contains supplementary material available at <https://doi.org/10.1038/s42005-023-01332-8>.

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**Peer review information** *Communications Physics* thanks Rok Žitko and the other, anonymous, reviewers for their contribution to the peer review of this work.

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