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A tunable two-impurity Kondo system in an atomic point contact

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Two magnetic atoms, one attached to the tip of a scanning tunnelling microscope and one adsorbed on a metal surface, each constituting a Kondo system, have been proposed as one of the simplest conceivable systems potentially exhibiting quantum critical behaviour. We have succeeded in implementing this concept experimentally for cobalt dimers clamped between a scanning tunnelling microscope tip and a gold surface. Control of the tip–sample distance with subpicometre resolution enables us to tune the interaction between the two cobalt atoms with unprecedented precision. Electronic transport measurements on this two-impurity Kondo system reveal a rich physical scenario, which is governed by a crossover from local Kondo screening to non-local singlet formation due to antiferromagnetic coupling as a function of separation of the cobalt atoms.

If a magnetic impurity is introduced into a non-magnetic metallic environment, its spin interacts with the conduction electrons of the host. Below a characteristic temperature T_K^0, this leads owing to the Kondo effect to a non-magnetic singlet ground state, where the spin of the magnetic impurity is completely screened[1]. As soon as two or more magnetic impurities are in proximity to each other, a competition between Kondo screening and magnetic interaction among the spins sets in and the ground state depends sensitively on their respective magnitude. Many of the peculiar properties of correlated electron materials are attributed to this competition between screening of local spins and magnetic interaction of neighbouring spins. Depending on which interaction dominates, the properties can vary, for example, between antiferromagnetic ordering and heavy-fermion behaviour, between being an insulator or a metal. Certain materials can be tuned continuously between the aforementioned phases through a quantum phase transition (QPT) as a function of an external control parameter, such as doping[2], pressure[3] or magnetic field[4]. The physics close to the quantum critical point is often described on the basis of models in which the formation of dimers governs the physics[5,6]. Thus the study of a model system consisting of a dimer, as presented here, with magnetically coupled spins can serve as a test ground for these theories.

The two-impurity Kondo problem

The physics of two Kondo impurities coupled by some interaction has been studied theoretically in great detail[7–13]. The relative strengths of an antiferromagnetic exchange interaction I and of the single-impurity Kondo temperature T_K^0 determines whether the ground state of the two-impurity system is governed by the formation of a singlet state between the two spins due to antiferromagnetic coupling or a Kondo singlet of each spin due to screening by the conduction electrons[10]. A schematic phase diagram of the two-impurity Kondo problem with antiferromagnetic coupling I is shown in Fig. 1a. If the transition between the two ground states is governed by quantum fluctuations it constitutes a QPT.

Despite intense theoretical research on the two-impurity Kondo problem, an experimental realization providing access to the full phase diagram and the transition between Kondo screening and antiferromagnetism has remained elusive. Studies of semiconductor structures containing two quantum dots with a tunable coupling have been able to reveal the splitting of the Kondo resonance in the limit of strong coupling[14,15]; however, they exposed difficulties in tuning the two quantum dots continuously through the full phase diagram: either the single-impurity regime was not accessible[15] or the splitting of the Kondo resonance, a measure for the exchange interaction, remained constant as a function of coupling in the strong-coupling regime[14], which is difficult to reconcile with theory[11,12]. Also, a realization with two magnetic atoms adsorbed on a metal surface has proven difficult. The limitation to a discrete set of interatomic separations imposed by the substrate lattice prevents a detailed investigation of the influence due to the exchange coupling in the interesting regime close to the quantum critical point[16–18]. Only recently the non-equilibrium transport properties of the two-impurity Kondo problem have been studied theoretically for a configuration where one magnetic atom is attached to the tip of a scanning tunnelling microscope (STM) and the other sits on a metal surface[19]. The coupling between the two atoms can be tuned continuously by varying the tip–sample separation, such that the system can be driven through the QPT (Fig. 1a). At the QPT, a further resonance is expected to appear in the differential conductance at zero bias whose width is only determined by the temperature of the experiment[13,19]. For the observability of the QPT the properties of the two Kondo impurities are not required to be identical, which facilitates an experimental realization. We have implemented this model system with two

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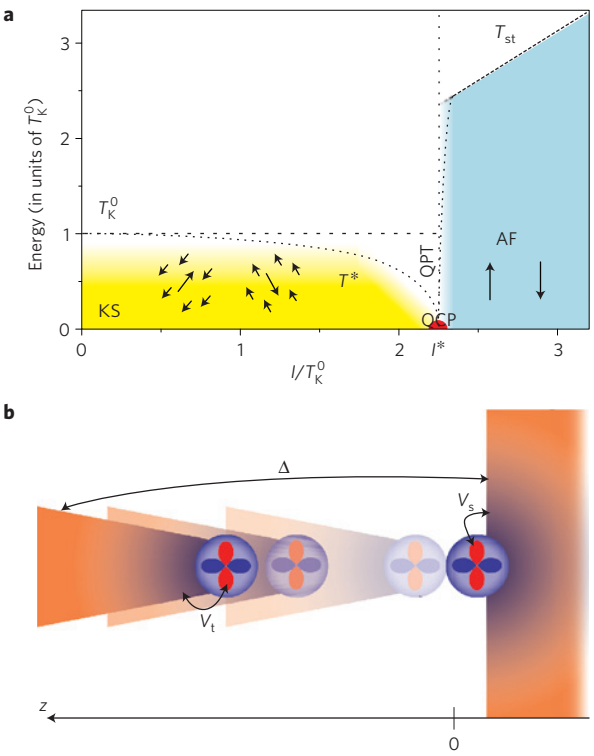

Figure 1 | Phase diagram and experimental realization of the two-impurity Kondo problem. a, Relevant energy scales and ground states as functions of coupling between the spins. KS—single-impurity Kondo screening dominates (with Kondo temperature T_K^0); the coupled system has a characteristic energy scale T^*. AF—owing to antiferromagnetic coupling, the two spins lock into a molecular singlet (the characteristic energy scale T_{st} is given by the single–triplet excitation). The vertical dotted line indicates the critical coupling I^* where the QPT occurs. The behaviour of T_{st} and T^* close to the QPT is unclear (indicated by dotted lines). **b**, Illustration of measurement set-up with one cobalt atom on the tip and one on the surface. The hybridization $V_{s,t}$ between the cobalt atoms and their respective electrodes leads to Kondo screening of the spins of the cobalt atoms. The coupling Δ between tip and sample results in an antiferromagnetic interaction I between the two spins. The strength of the interaction is varied by changing the tip–sample distance.

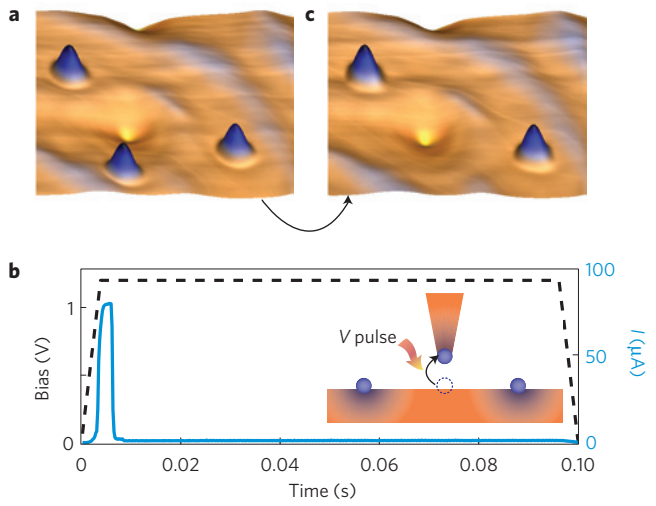

Figure 2 | Preparation of the tip Kondo system. a, STM image of three cobalt adatoms on Au(111) taken with a spectroscopically featureless tip; **b**, by applying a voltage pulse after approaching the tip towards a cobalt adatom, the atom is transferred to the tip—seen as a sudden change in the current trace; **c**, the atom has disappeared from the surface.

cobalt atoms as the Kondo impurities. The measurement set-up is depicted in Fig. 1b.

Tip Kondo system

Following sample preparation as described in the Methods section, in STM images measured at a sample temperature of 6.7 K we find single cobalt adatoms on the Au(111) surface (Fig. 2a), which can be identified by their characteristic Kondo resonance[20]. In tunnelling spectra, the Kondo resonance is detected as a Fano line shape (Supplementary Eq. S1) due to interference between electrons tunnelling into the conduction band of the substrate and into the Kondo state (Fig. 3b). Depending on the relative strengths of the two channels, the line shape of the Kondo resonance can be a dip, an asymmetric line shape or a peak[20]. The single-impurity Kondo resonance of a cobalt adatom on Au(111) has been determined previously to be around 75 K; there is some dependence on the adsorption site within the reconstruction of Au(111) (ref. 21). We have attached single cobalt atoms to the STM tip by positioning the tip on top of an adatom and applying a voltage pulse (Fig. 2b; ref. 22). After application of a successful pulse the cobalt atom disappears from the surface (see Fig. 2c) and the spectrum taken over a clean spot exhibits a resonance similar to the one found for cobalt atoms on the surface (see Fig. 3c). This suggests that the atom at the tip has an environment similar to that on the surface. Though the STM tip is made from a chemically etched tungsten wire, its apex is covered with gold owing to indentation of the tip into the sample, which we do for tip conditioning. As the precise environment of the adatom on the tip cannot be controlled well, there is some scattering in the appearance of the tip Kondo resonance for different tip preparations, which influences details of the spectra (see Supplementary Information S5 and Fig. S5 for statistics and typical spectra after pick-up). We found Kondo temperatures ranging between 100 and 230 K for tip-attached Kondo systems. When the tip with the cobalt atom is positioned on top of a cobalt atom on the surface, the tunnelling spectrum shows a superposition of the Kondo resonances of tip and sample, as is apparent from the larger amplitude of the resonance in the tunnelling spectrum (see Fig. 3d).

While approaching the two cobalt atoms towards each other, the junction makes a transition from the tunnelling to the point-contact regime (Fig. 4a). Reversible formation of point contacts between an STM tip and a single atom on a metal surface has been shown previously for both non-magnetic[23,24] and magnetic adatoms[25,26]. Recently, point-contact formation of a magnetic tip to a magnetic atom has also been shown[27]. Spectra acquired in the tunnelling regime for $z > 0$ Å (see Figs 3d, 4b) show a resonance similar to the one found for a single cobalt atom in the junction (compare Fig. 3b,c) but with a larger amplitude, as it is a superposition of the Kondo resonances of tip and sample. The shape and width of the feature change only little for rather large tip–sample distances $z > 2$ Å. Once the two atoms are moved within 2 Å of point contact the width of the resonance is reduced. Close to the transition to the point-contact regime, the resonance changes its shape from a dip to a peak of similar width (see Fig. 4b for $z \sim -30$ pm). On pushing the tip further in, the peak splits into two resonances at almost symmetric positions with respect to zero bias. The splitting increases with decreasing tip–sample distance (Fig. 4b). We note that all data shown in this work are obtained from reversible, non-destructive measurements, where STM images taken before and after formation of the point contact show no changes of the tip or the cobalt atom itself. The conductance traces during approach and withdrawal are apart from some vertical drift coincident with each other. Occasionally we observe lateral

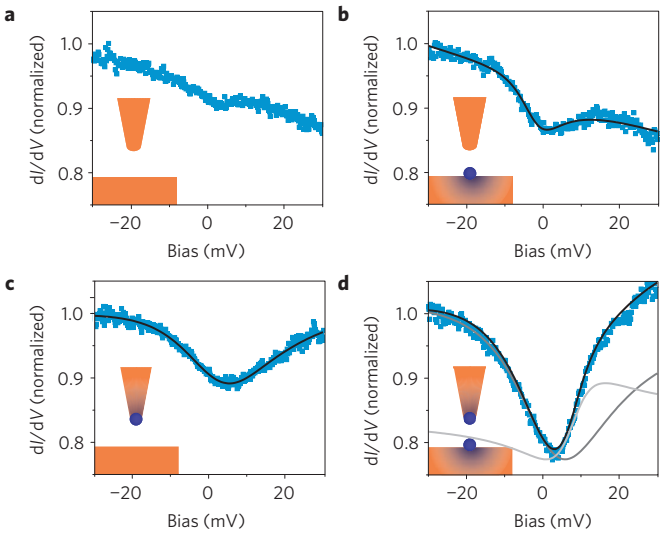

Figure 3 | Spectroscopy of the tip Kondo system. a, Spectrum recorded before picking up an atom on the clean surface. **b**, Spectra taken on cobalt adatoms show a Kondo resonance; the Kondo temperature T_K^0 is determined from the half-width Γ of the resonance[20] (here $\Gamma = 6.89 \pm 0.32$ mV, $T_K^0 = 80 \pm 4$ K). **c**, After picking up a cobalt atom, spectra taken on the clean surface show a resonance at the Fermi level, too. **d**, Spectra taken with a tip with a cobalt atom on top of a second cobalt atom on the surface show the two resonances superimposed, as seen from the amplitude. The solid black line is a fit of the sum of two Fano functions, fixing the parameters (ε_0, Γ, q) of the resonance of the tip atom (dark grey solid line) from a spectrum taken on the clean surface as in **c**, whereas the Fano function of the adatom (light grey solid line) on the surface has been fitted. The resulting width of the resonance of the adatom is $\Gamma = 7.73 \pm 0.24$ mV ($T_K = 90 \pm 3$ K).

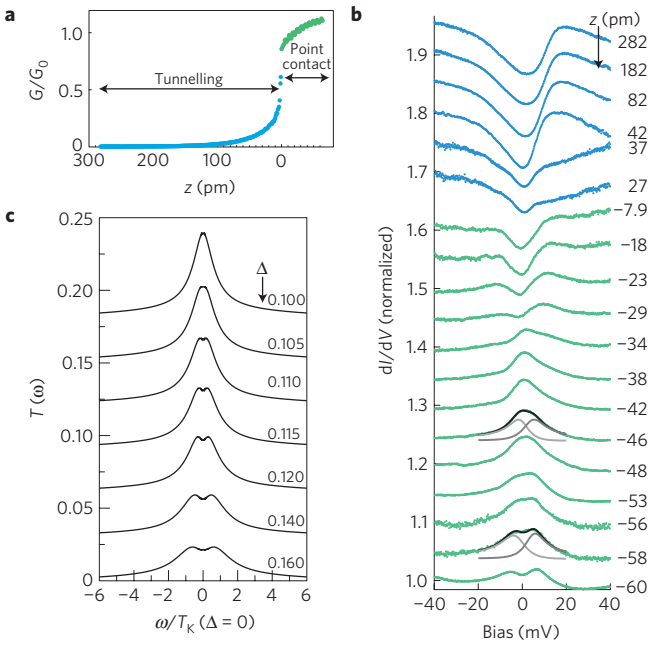

Figure 4 | Measurements on two-impurity Kondo system in tunnelling and transport. a, Approach curve acquired while moving the tip with a cobalt atom towards a cobalt atom on the surface. Conductance in units of the spin-degenerate conductance quantum $G_0 = 12.9$ kΩ as a function of tip–sample distance (relative to the transition from tunnelling (blue) to point contact (green)) at fixed bias voltage ($V_{bias} = 40$ mV). **b**, Spectra as a function of tip–sample distance (as indicated on the right) in the tunnelling and point-contact regimes. Spectra obtained with two different tips are shown. **c**, NRG calculation for the T-matrix, which is proportional to the LDOS, showing the transition from the Kondo resonance to a split peak on increasing the coupling Δ between the electrodes. Spectra in **b** and **c** are shifted vertically.

hops of the cobalt atom, which can however be directly detected in the conductance trace as well as from the STM images taken before and after the approach curve is acquired (for details see Supplementary Information S1).

With only one cobalt atom between tip and surface, we do not see a reduction of the width of the resonance (consistent with refs 25,26), a change in the line shape from dip to peak or a splitting (compare Supplementary Fig. S4). Thus these effects are related to the presence of two cobalt atoms in the tunnelling junction. This renders inelastic tunnelling due to vibrational excitations[28] unlikely as a possible source for the conductance curve. Effects due to contamination, for example with hydrogen[29], typically lead to characteristic spectra which are distinctly different from the conductance curves shown in Figs 3 and 4; Furthermore, in this case spectra should not depend on whether there are one or two cobalt atoms in the junction.

Comparison with theory

We can identify two regimes from the conductance traces: a weak-coupling regime, in which only one resonance is observed, and a strong-coupling regime, where we find a split resonance. To understand the evolution of the spectra we have carried out numerical renormalization group (NRG) calculations. NRG is a numerically exact and non-perturbative method to describe the physics of quantum impurities[30,31]. The NRG calculations have been carried out for two Kondo impurities each coupled to its own bath of conduction electrons. A coupling Δ between the two conduction-electron baths is accounted for (compare Fig. 1b). The magnetic coupling between the Kondo impurities results from the coupling Δ of the electrodes. In Fig. 4c, one diagonal element of the T-matrix is plotted, which is proportional to the local density of states (LDOS) at the two impurity sites. The parameters of the calculation are defined in Fig. 1b; different tip–sample distances are modelled by different couplings Δ between the two electrodes. We find qualitative agreement between our experiment and NRG calculations concerning the evolution from a single peak towards a split resonance.

The splitting of the resonance directly reflects the exchange interaction between the spins of the two cobalt atoms[11,12,17], which leads to a splitting of states with even and odd parity. We can extract its dependence on the vertical distance between the two electrodes by fitting a sum of two Fano line shapes to the experimental data[17]. The resulting splitting of the two resonances is plotted as a function of vertical tip position in Fig. 5a. It rises within 20 pm from 3 to 9 meV. For compact cobalt dimers on Au(111) and Cu(100), the Kondo resonance has been found to be completely suppressed[16,17], which has been attributed to a reduced coupling of the dimer magnetic moment to the conduction band[16] and strong magnetic interaction significantly larger than the Kondo energy[17]. We do not observe this suppression of the Kondo resonance. One possible reason for this apparently large difference in the interaction may be the relative spatial orientation of the d orbitals that contribute to the Kondo effect. In the case of a d_{xy} or d_{x2-y2} orbital (with x and y parallel to the surface), the direct interaction can be significantly smaller in the vertical direction than in the lateral direction. We note that for the data shown in Supplementary Fig. S6, which also shows a splitting but is obtained with a different tip, significantly larger magnetic exchange interactions compared with the data shown in Fig. 4c are reached. This is probably because the precise atomic configuration of the tip apex is not controlled—which will

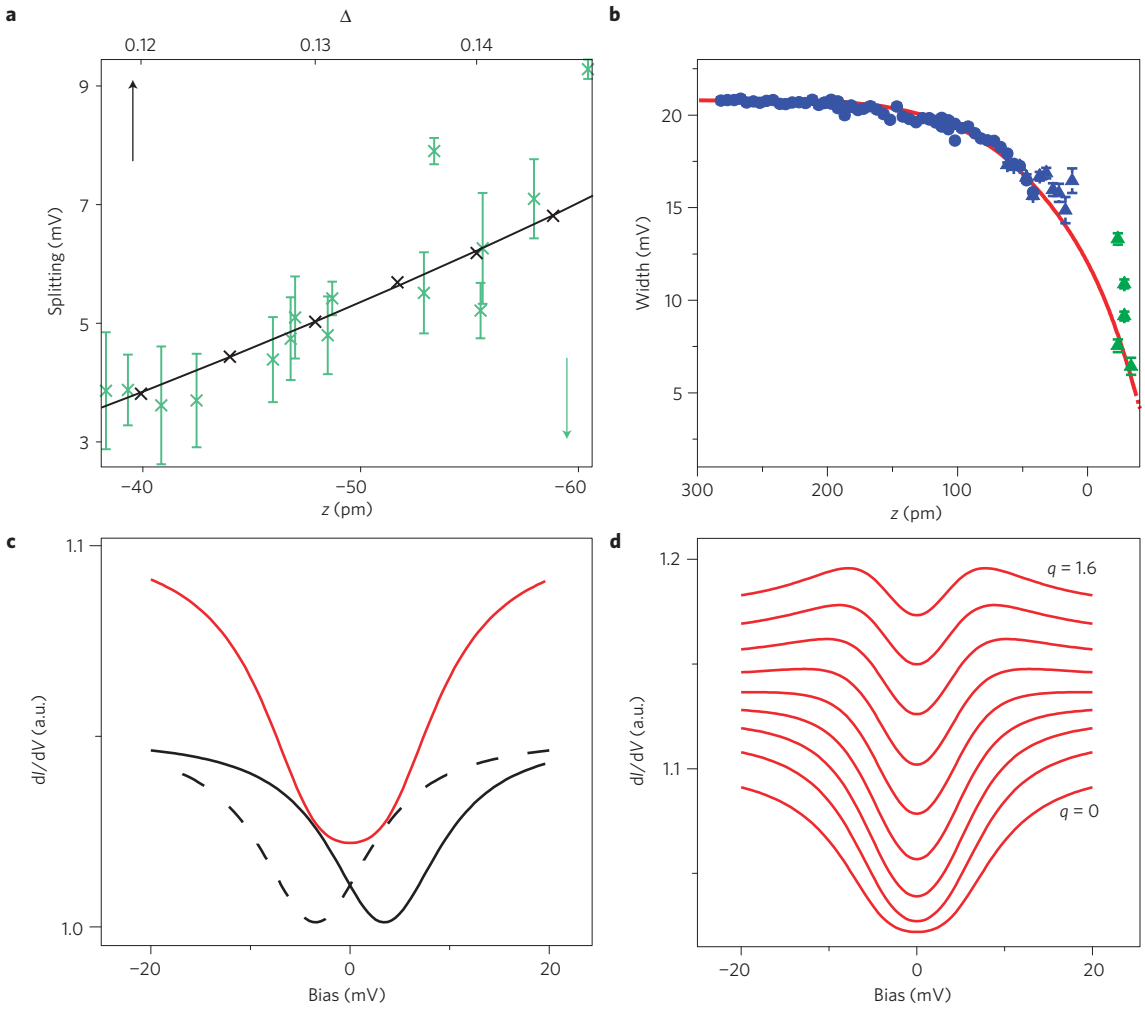

Figure 5 | Interaction effects between the cobalt atoms. a, Splitting of peaks seen in Fig. 4b as a function of tip–sample distance. Black crosses have been obtained from NRG calculations in Fig. 4c; for comparison with experimental data we assume $z \sim \log\Delta + z_0$. The solid line is a linear fit to the NRG calculations. **b**, Width of the resonance extracted from spectra as in Fig. 4b as a function of tip–sample distance; circles and triangles indicate separate sets of measurements following different sample preparations with different tips (colours as in Fig. 4a). The solid line shows the calculated width of the resonance, where the line-shape parameter q is assumed to depend on the tip–sample distance z as $q \sim \exp(-z/\kappa_d)$ (see also Supplementary Information S2C). Error bars in **a** and **b** represent the 68.1% confidence interval obtained from the least-squares fit. **c**, Superposition of the Kondo resonances of tip and sample (black lines) leads to tunnelling spectra (red line) as in Fig. 4b (for details see Supplementary Information S2B). **d**, Calculated tunnelling spectra as the line shapes of the single-impurity resonances change from dip to peak.

influence the strength of the coupling between the d orbitals of the two cobalt atoms.

To quantitatively analyse the behaviour of the resonance in the weak-coupling regime, we have fitted single Fano resonances to the spectra. The width of the resonance is reduced by up to ~70% (see Fig. 5b) when the two cobalt atoms are brought close to each other.

The NRG calculation does not show a significant change in the width of the resonance at weak coupling. However, as measurements with only one cobalt atom in the junction do not show a similar reduction of the width, it must be related to the presence of two cobalt atoms.

Modelling of the line shape

We can rationalize the reduction by the superposition of the Kondo resonances of tip and sample. In the spectra, only one resonance is observed because the resonances of the two cobalt atoms are both at the Fermi level (see Fig. 5c for an illustration). To assess the influence of their superposition on the overall spectrum, we have carried out a model calculation assuming that the tip and sample spectra can be described by Fano resonances (as with only one cobalt atom in the junction; see Fig. 3b,c; ref. 20). We assume that only the line shape of the individual resonances changes from a dip to a peak while approaching the two cobalt atoms towards each other, keeping the parameters of the Kondo resonances (that is width, amplitude and position) constant as found in the NRG calculation. With this model, we can recover the behaviour of the tunnelling spectra and of the overall width of the resonance. A change in the line shape of the Fano resonance with tip–sample distance has been predicted if there is substantial coupling of the tip to the Kondo state[32], because the vacuum tail of the conduction band and the Kondo state decay typically on different length scales. The observation of Fano resonances in the contact regime is consistent with earlier work with single cobalt atoms contacted by an STM tip[25,26] and theoretical predictions[33,34]; however, the interpretation in terms of different transport channels is less clear. The modelled spectra are shown in Fig. 5d and demonstrate that the overall shape of the measured spectra (Fig. 4b) is well reproduced. We have plotted the width extracted from fitting a single Fano resonance to the calculated spectra (for details see Supplementary Information S2B) on top of the width extracted

from the experimental data in Fig. 5b. The agreement is very good apart from deviations close to the transition to point contact. These could be due to mechanical relaxation effects of tip and sample, which are especially strong at the transition. The assumed increase of the single-impurity line-shape parameter q can be attributed to an increase in coupling between the d orbitals of the two cobalt atoms opening an extra direct channel contributing to the current[20,32]. This is supported by an increased conductance in point contact that we observe for junctions containing two cobalt atoms compared with junctions with only one cobalt atom or only gold atoms (see Supplementary Information S3 and Fig. S3). Though the interaction between the conduction band of one electrode and the d orbital of the cobalt atom on the opposite electrode might naively be expected to be stronger than direct interaction of the d orbitals, it seems to be negligible, as otherwise for a gold tip approaching towards a cobalt atom a change in the line shape should be observed. Alternatively, the reduction of the width could be explained by weak antiferromagnetic or ferromagnetic interaction, which can reduce the Kondo temperature[5,8,18]. We cannot resolve the single Kondo resonances but rather observe the superposition of the two in our spectra, thus we cannot rule out these possibilities. A ferromagnetic interaction, as has been predicted from calculations for a chromium tip above a cobalt atom on Cu(100) in the tunnelling regime for comparatively large tip–sample distances[35], would however imply that the exchange interaction oscillates through zero back to antiferromagnetic coupling for small tip–sample distances—for which we do not see evidence. Consistency with the NRG calculation as well as the increased conductance in point contact support our modelling of the reduction of the width as being due to the change in the line shape.

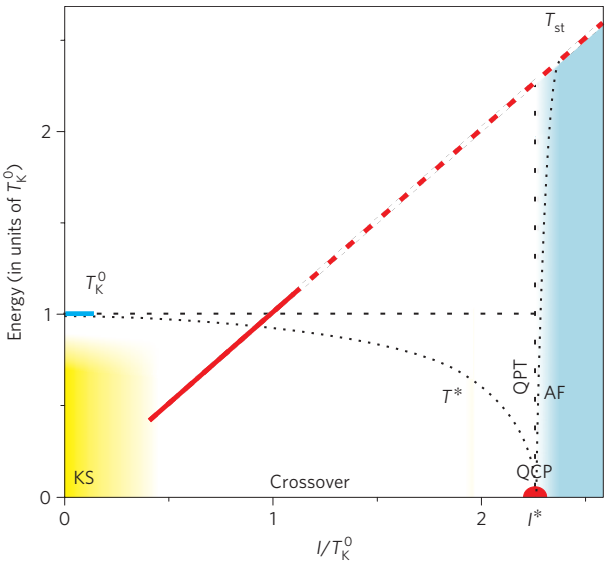

Figure 6 | Schematic phase diagram emerging from the experiment. The QPT at the critical coupling is suppressed owing to strong coupling between the conduction electrons at the tip and the sample; instead, the system exhibits a broad crossover region between the Kondo-screened and antiferromagnetically coupled regimes. Red and blue lines indicate the experimentally accessible lines of the diagram (the solid red line is extracted from data shown in Fig. 5b assuming that the exchange interaction is proportional to the splitting; the dashed red line indicates data shown in Supplementary Fig. S6c). The splitting is observed well below the critical coupling I^*. Symbols and abbreviations are as in Fig. 1a.

Conclusions

We can clearly identify two coupling regimes for the cobalt dimer. The resulting phase diagram is depicted in Fig. 6. Far out in the tunnelling regime, the two cobalt atoms behave as weakly interacting Kondo impurities, each with its own Kondo resonance. Approaching the two cobalt atoms towards each other, the interaction rises and the resonance splits owing to exchange interaction. Further reduction of the tip–sample distance increases the interaction and hence the separation of the two peaks.

Our data show a splitting of the Kondo resonance already for exchange interactions as small as 3 meV, significantly smaller than the characteristic energy scale of Kondo screening of about $k_B T_K^0 \sim 6.5$ meV and the predicted critical coupling beyond which a sudden splitting of the Kondo resonance is expected, $I^* \sim 2k_B T_K^0 \approx 13$ meV (refs 7,9–12; in the asymmetric case with differing Kondo temperatures T_K^{01}, T_K^{02} with $T_K^{02} < T_K^{01}$ the critical coupling I^* is $I^*/(k_B T_K^{01}) \approx 4/\pi(1+(T_K^{02}/T_K^{01}))$ (ref. 12), which in our case gives ~33 meV (using the parameters for tip 3 in Supplementary Table S1)). Both the appearance of the splitting at couplings smaller than the critical coupling and the shape of the resonances on approaching the antiferromagnetic regime are fully consistent with the NRG calculations shown in Fig. 4c. For much stronger exchange interactions, the spectra are expected to be governed by inelastic spin excitations[36] breaking the singlet rather than by a split Kondo resonance. Whereas the splitting extracted from the spectra in Fig. 4c is not sufficiently large to put the cobalt dimer in the antiferromagnetic regime, for the data shown in Supplementary Fig. S6c the splitting becomes more than 40 mV, which is larger than the critical coupling, indicating that the two cobalt atoms in contact are in the antiferromagnetic regime. Therefore, the coupling at which the quantum critical point (QCP) would occur is experimentally accessible.

Instead of showing a QPT, the cobalt dimer undergoes a crossover between the two regimes, Kondo screening and antiferromagnetism. By comparison with the NRG calculations, the crossover can be attributed to the strong coupling between the electrodes. For the system to reveal quantum critical behaviour, the coupling between the electrodes needs to be small compared with the single-impurity Kondo temperature[7,19]. One way to come closer to a system exhibiting critical behaviour is to use atoms as Kondo systems that exhibit a significantly lower Kondo temperature while still having substantial coupling to the electrodes (by which the magnetic coupling is mediated). This can be achieved for Kondo systems that have a Coulomb repulsion about a factor of two higher than cobalt atoms; possible candidates could be rare-earth atoms[37]. Another way would be to increase the direct coupling between the orbitals that form the Kondo state. Direct charge coupling also renders the QCP unstable[38], so it will only be observable for the right balance of direct hopping and exchange interaction[39].

The atomically precise engineering of a two-atom Kondo system provides a unique playground to probe electron correlations, complementing studies on semiconductor quantum dots. Our experiment provides a model system for studying the competition between electron correlation and local-moment antiferromagnetism, which eventually might enable study of quantum criticality on a two-impurity system. It also opens up new perspectives for atomic-scale magnetometry. The tip Kondo system can be used as a probe for magnetic interactions, yielding quantitative information about them. This offers the opportunity to study magnetic properties of atoms, magnetic molecules, clusters and islands with the high lateral resolution of STM.

Methods

Measurements have been made in a home-built low-temperature ultrahigh-vacuum STM which operates at temperatures down to a sample temperature of 6.7 K. The Au(111) single crystal has been prepared in ultrahigh vacuum by cycles of sputtering and annealing to 800 K. Cleanliness of the sample has been checked by STM after transferring the crystal into the cryostat. Cobalt atoms have been evaporated onto the gold surface *in situ* from a tungsten filament with a cobalt wire wound around it. Tunnelling and point-contact spectra have been acquired with

open feedback loop recording the dI/dV signal from a lock-in amplifier. For the experiments shown, we used lock-in modulations in the range of 1.43–2.15 mV_{RMS}. We have used a tungsten tip, cleaned by field emission and by bringing it in contact with the Au(111) surface before the experiments described in the main text. A tip is judged good if it exhibits a sufficiently flat tunnelling spectrum (apart from the onset of the surface state of Au(111) at −460 mV and a linear background) and images atoms on the surface as spherical protrusions.

To obtain the LDOS of the two-impurity problem, we have computed the local T-matrix containing many-body effects by Wilson's NRG technique[40,41]. The cornerstone of NRG is the logarithmic discretization of the conduction-electron band and mapping the system onto a semi-infinite chain with the impurity at the end. NRG has been successfully applied to the problem of two magnetic impurities, but only thermodynamic quantities were computed previously[42,43]. The main source of complication of the two-impurity model in our configuration is that the calculation is effectively a two-band calculation: the impurities couple to two semi-infinite chains. Consequently, the Hilbert space grows by a factor of 16 in each NRG step. This is still manageable with today's computer resources. Concerning the details of the present NRG calculation, we have chosen a discretization parameter $\Lambda = 2$, the number of iterations was $N = 50$ and we kept $M = 4{,}096$ states per iteration exploiting the charge and spin z-component U(1) symmetries.

In Fig. 4c, only one diagonal element of the T-matrix is plotted, as the two diagonal elements are (owing to symmetry) identical in the calculation. The diagonal elements are proportional to the LDOS at the impurity sites.

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References

1. Hewson, A. C. *The Kondo Problem to Heavy Fermions* (Cambridge Univ. Press, 1993).
2. Löhneysen, v. *et al.* Non-fermi-liquid behavior in a heavy-fermion alloy at a magnetic instability. *Phys. Rev. Lett.* **72,** 3262–3265 (1994).
3. Mathur, N. D. *et al.* Magnetically mediated superconductivity in heavy fermion compounds. *Nature* **394,** 39–43 (1998).
4. Grigera, S. A. *et al.* Magnetic field-tuned quantum criticality in the metallic ruthenate $Sr_3Ru_2O_7$. *Science* **294,** 329–332 (2001).
5. Klein, M. *et al.* Signature of quantum criticality in photoemission spectroscopy. *Phys. Rev. Lett.* **101,** 266404 (2008).
6. Sachdev, S. Quantum criticality: Competing ground states in low dimensions. *Science* **288,** 475–480 (2000).
7. Georges, A. & Meir, Y. Electronic correlations in transport through coupled quantum dots. *Phys. Rev. Lett.* **82,** 3508–3511 (1999).
8. Jayaprakash, C., Krishna-murthy, H. R. & Wilkins, J. W. Two-impurity Kondo problem. *Phys. Rev. Lett.* **47,** 737–740 (1981).
9. Jones, B. A. & Varma, C. M. Study of two magnetic impurities in a fermi gas. *Phys. Rev. Lett.* **58,** 843–846 (1987).
10. Jones, B. A., Varma, C. M. & Wilkins, J. W. Low-temperature properties of the two-impurity Kondo hamiltonian. *Phys. Rev. Lett.* **61,** 125–128 (1988).
11. López, R., Aguado, R. & Platero, G. Nonequilibrium transport through double quantum dots: Kondo effect versus antiferromagnetic coupling. *Phys. Rev. Lett.* **89,** 136802 (2002).
12. Simon, P., López, R. & Oreg, Y. Ruderman–Kittel–Kasuya–Yosida and magnetic-field interactions in coupled Kondo quantum dots. *Phys. Rev. Lett.* **94,** 086602 (2005).
13. De Leo, L. & Fabrizio, M. Spectral properties of a two-orbital Anderson impurity model across a non-Fermi-liquid fixed point. *Phys. Rev. B* **69,** 245114 (2004).
14. Craig, N. J. *et al.* Tunable nonlocal spin control in a coupled-quantum dot system. *Science* **304,** 565–567 (2004).
15. Jeong, H., Chang, A. M. & Melloch, M. R. Kondo effect in an artificial quantum dot molecule. *Science* **293,** 2221–2223 (2001).
16. Chen, W., Jamneala, T., Madhavan, V. & Crommie, M. F. Disappearance of the Kondo resonance for atomically fabricated cobalt dimers. *Phys. Rev. B* **60,** R8529–R8532 (1999).
17. Wahl, P. *et al.* Exchange interaction between single magnetic adatoms. *Phys. Rev. Lett.* **98,** 056601 (2007).
18. Néel, N. *et al.* Two-site Kondo effect in atomic chains, Preprint at http://arxiv.org/abs/1105.3301.
19. Sela, E. & Affleck, I. Nonequilibrium transport through double quantum dots: Exact results near a quantum critical point. *Phys. Rev. Lett* **102,** 047201 (2009).
20. Madhavan, V., Chen, W., Jamneala, T., Crommie, M. F. & Wingreen, N. S. Tunnelling into a single magnetic atom: Spectroscopic evidence of the Kondo resonance. *Science* **280,** 567–569 (1998).
21. Madhavan, V., Chen, W., Jamneala, T., Crommie, M. F. & Wingreen, N. S. Local spectroscopy of a Kondo impurity: Co on Au(111). *Phys. Rev. B* **64,** 165412 (2001).
22. Eigler, D. M., Lutz, C. P. & Rudge, W. E. An atomic switch realized with the scanning tunnelling microscope. *Nature* **352,** 600–603 (1991).
23. Limot, L., Kröger, J., Berndt, R., Garcia-Lekue, A. & Hofer, W. A. Atom transfer and single-adatom contacts. *Phys. Rev. Lett.* **94,** 126102 (2005).
24. Yazdani, A., Eigler, D. M. & Lang, N. D. Off-resonance conduction through atomic wires. *Nature* **272,** 1921–1924 (1996).
25. Néel, N. *et al.* Conductance and Kondo effect in a controlled single-atom contact. *Phys. Rev. Lett.* **98,** 016801 (2007).
26. Vitali, L. *et al.* Kondo effect in single atom contacts: The importance of the atomic geometry. *Phys. Rev. Lett.* **101,** 216802 (2008).
27. Néel, N., Kröger, J. & Berndt, R. Kondo effect of a Co atom on Cu(111) in contact with an iron tip. *Phys. Rev. B* **82,** 233401 (2010).
28. Stipe, B. C., Rezaei, M. A. & Ho, W. Single-molecule vibrational spectroscopy and microscopy. *Science* **280,** 1732–1735 (1998).
29. Gupta, J. A., Lutz, C. P., Heinrich, A. J. & Eigler, D. M. Strongly coverage-dependent excitations of adsorbed molecular hydrogen. *Phys. Rev. B* **71,** 115416 (2005).
30. Wilson, K. G. The renormalization group: Critical phenomena and the Kondo problem. *Rev. Mod. Phys.* **47,** 773–840 (1975).
31. Bulla, R., Costi, T. A. & Pruschke, T. Numerical renormalization group method for quantum impurity systems. *Rev. Mod. Phys.* **80,** 395–450 (2008).
32. Plihal, M. & Gadzuk, J. W. Nonequilibrium theory of scanning tunnelling spectroscopy via adsorbate resonances: Nonmagnetic and Kondo impurities. *Phys. Rev. B* **63,** 085404 (2001).
33. Lucignano, P., Mazzarello, R., Smogunov, A., Fabrizio, M. & Tosatti, E. Kondo conductance in an atomic nanocontact from first principles. *Nature Mater.* **8,** 563–567 (2009).
34. Jacob, D., Haule, K. & Kotliar, G. Kondo effect and conductance of nanocontacts with magnetic impurities. *Phys. Rev. Lett.* **103,** 016803 (2009).
35. Tao, K. *et al.* Switching a single spin on metal surfaces by a STM tip: *Ab initio* studies. *Phys. Rev. Lett.* **103,** 057202 (2009).
36. Heinrich, A. J., Gupta, J. A., Lutz, C. P. & Eigler, D. M. Single-atom spin-flip spectroscopy. *Science* **306,** 466–469 (2004).
37. van der Marel, D. & Sawatzky, G. A. Electron–electron interaction and localization in d and f transition metals. *Phys. Rev. B* **37,** 10674–10684 (1988).
38. Zaránd, G., Chung, C-H., Simon, P. & Vojta, M. Quantum criticality in a double-quantum-dot system. *Phys. Rev. Lett.* **97,** 166802 (2006).
39. Malecki, J., Sela, E. & Affleck, I. The prospect for observing the quantum critical point in double quantum dot systems. *Phys. Rev. B* **82,** 205327 (2010).
40. Wilson, K. G. The renormalization group: Critical phenomena and the Kondo problem. *Rev. Mod. Phys.* **47,** 773–840 (1975).
41. Bulla, R., Costi, T. A. & Pruschke, T. Numerical renormalization group method for quantum impurity systems. *Rev. Mod. Phys.* **80,** 395–450 (2008).
42. Jones, B. A. & Varma, C. M. Study of two magnetic impurities in a Fermi gas. *Phys. Rev. Lett.* **58,** 843–846 (1987).
43. Jones, B. A., Varma, C. M. & Wilkins, J. W. Low-temperature properties of the two-impurity Kondo Hamiltonian. *Phys. Rev. Lett.* **61,** 125–128 (1988).

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Author contributions

J.B. and Y-h.Z. carried out experiments, J.B. analysed the data, L.B. carried out the NRG calculations, P.S. and J.K. provided theoretical support, P.W. carried out the line-shape analysis and J.B., L.D. and P.W. wrote the manuscript. PW, L.D. and K.K. planned and supervised the project. All authors discussed the manuscript.

Additional information

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