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Realizing a Kondo-correlated state with ultracold atoms

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We propose a novel realization of Kondo physics with ultracold atomic gases. It is based on a Fermi sea of two different hyperfine states of one atom species forming bound states with a different species, which is spatially confined in a trapping potential. We show that different situations displaying Kondo physics can be realized when Feshbach resonances between the species are tuned by a magnetic field and the trapping frequency is varied. We illustrate that a mixture of 40K and 23Na atoms can be used to generate a Kondo correlated state and that momentum resolved radio frequency spectroscopy can provide unambiguous signatures of the formation of Kondo resonances at the Fermi energy. We discuss how tools of atomic physics can be used to investigate open questions for Kondo physics, such as the extension of the Kondo screening cloud.

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Introduction - Significant advances in quantum optics, such as in cooling, trapping and manipulating ultracold atoms, have lead to the realization of a plethora of exciting many-body phases in a controlled manner. An important drive for this field is that many of these phases and their description in terms of model Hamiltonians are of great interest in condensed matter physics, such that a fruitful interplay of these fields has developed. It has, for instance, been possible to realize supersolid phases both in fermionic and bosonic systems and the transition to a Mott insulating regime.

An intriguing many-body effect in condensed matter physics is the Kondo effect. It occurs when itinerant fermions interact with magnetic impurities, such as, for instance, a small concentration of Fe in Au. The orbital occupation of the impurity must be such that there is an unscreened spin present, i.e., in the simplest case a localized state occupied by a single electron. The essence of the Kondo effect is then that at low temperature this electron spin forms a many-body bound state with the itinerant electrons and becomes magnetically screened. Crucial for this magnetic screening are second order processes which lead to frequent spin flips. This Kondo correlated state leads to a distinctive feature in the resistivity (Kondo minimum) and was also observed as enhanced transport in quantum dots.

In spite of decades of intense research, there remain unresolved questions. For instance, a Kondo screening cloud with a certain spatial extent and characteristic oscillations was predicted, however, its experimental observation has remained elusive. On increasing the impurity concentration from very few to a full lattice, the Kondo clouds overlap and the localized spins interact with each other via the so-called Ruderman-Kittel-Kasuya-Yoshida (RKKY) coupling, mediated by the itinerant fermions. This generates a competing effect to the Kondo screening and leads to a transition to a magnetically ordered state of the spins. The Kondo lattice problem is of paramount importance for the understanding of heavy fermion systems and quantum criticality, however, it is very hard to analyze it theoretically beyond the mean field level. Here, we propose an experimental setup based on ultracold atoms to realize single impurity and lattice Kondo situations. The Kondo scale is shown to be accessible by current experimental techniques.

In the field of ultracold atoms, a lot of progress has recently been made for manipulating mixtures of different species that offer the unique possibility to selectively trap one species and to handle heteronuclear Feshbach resonances producing molecular bound states. These developments are important ingredients for our proposal. The main idea is to allow atoms of a Fermi sea to form bound states with a different, spatially confined atom, the impurity [see Fig. 1(a)]. We consider two species of ultracold atoms with mass $m_a, m_b$. Species $a$ is fermionic and is prepared in two different hyperfine states labeled by a spin index $\sigma$. Species $b$, which can be a fermion or boson, is subject to a strong harmonic confining potential. The bound states for the hyperfine states cor-
To tune the bare scattering lengths $a_{0,\sigma}$ by a magnetic field $B$, we assume that there is a Feshbach resonance, 

$$a_{0,\sigma}(B) = a_{bg} \left(1 - \frac{\Delta B_{0,\sigma}}{B - B_{0,\sigma}}\right),$$  

(4)

where $a_{bg}$ is the background scattering length, $\Delta B_{0,\sigma}$ the width and $B_{0,\sigma}$ the position of the resonance.

We describe the low energy physics of the system by an Anderson impurity model (AIM) [26] of the form,

$$H = \sum_{k,\sigma} \varepsilon_{k} c_{k,\sigma}^{\dagger} c_{k,\sigma} + \sum_{\sigma} \varepsilon_{b,\sigma} c_{b,\sigma}^{\dagger} c_{b,\sigma} + U n_{b,\uparrow} n_{b,\downarrow}$$

$$+ \sum_{k,\sigma} V_{k,\sigma} c_{k,\sigma}^{\dagger} c_{b,\sigma} + \text{h.c.} \ .$$  

(5)

Here, $c_{k,\sigma}^{\dagger}$ creates an itinerant fermion with momentum $k$ and spin projection $\sigma$, and $c_{b,\sigma}$ a bound state with energy $\varepsilon_{b,\sigma}$. The states are mixed by the hybridization $V_{k,\sigma}$. Three-particle bound states are assumed to be highly unstable due to rapid decay into deep two-body bound states [27,28]. Under such conditions it has been shown [24] that the system corresponds to $U \to \infty$, where the occupation of those states is suppressed. Particle loss is inhibited in such situations [24]. The effect of the shallow trapping potential on the atoms with mass $m_a$ is neglected, and hence the dispersion is $\varepsilon_{k} = \hbar^2 k^2/2m_r$ [59]. We focus on the case of three spatial dimensions, where the corresponding density of states (DOS) per spin is $\rho_{0}(\varepsilon) = c_3 \sqrt{\varepsilon}$, with $c_3 = V_{0} k_{F}^3/(4\pi^2 \varepsilon_{F}^{3/2})$, and $\varepsilon_{F} = \hbar^2 \pi^2 n^{2/3}$. Here, $n = N_a/V_{0}$, where $V_{0}$ is the volume of the system and $N_a$ the number of particles of species $a$.

**Relation of AIM parameters to scattering parameters** - The scattering amplitude is related to the $T$-matrix by

$$f_{\sigma}(k, k) = -V_{0} \frac{m_{\sigma}}{2\pi\hbar^2} T_{k,k}^{\sigma}.$$  

(6)

We can express the right hand side in terms of scattering properties of the AIM, $T_{k,k}^{\Lambda}(\omega = \xi_k)$, and from this determine the model parameters in Eq. 5. The $T$-matrix of the AIM is given by [11],

$$T_{k,k}^{\Lambda}(\omega) = V_{k,\sigma}^{*} G_{b,\sigma}(\omega) V_{k',\sigma},$$  

(7)

where $G_{b,\sigma}(\omega)$ is the retarded bound state Green’s function, $\eta \to 0$,

$$G_{b,\sigma}(\omega) = \omega + i\eta - \varepsilon_{b,\sigma} - K_{\sigma}(\omega) - \Sigma_{\sigma}(\omega).$$  

(8)

Generally, impurity properties only depend on the integrated hybridization term $K_{\sigma}(\omega) = \sum_{k} \frac{|V_{k,\sigma}|^2}{\omega + i\eta + \xi_k}$, where we defined $\xi_k = \varepsilon_k \pm \mu$.

A full solution of the scattering problem in Eq. 6 yields $f_{\sigma}$ [24] such that the AIM parameters can be determined numerically via Eq. 7. Here we take a simplified form, $V_{k,\sigma} = V_{\sigma}$, which is real and constant for

$$a_{0,\sigma}(B) = a_{bg} \left(1 - \frac{\Delta B_{0,\sigma}}{B - B_{0,\sigma}}\right),$$  

(4)

$$H = \sum_{k,\sigma} \varepsilon_{k} c_{k,\sigma}^{\dagger} c_{k,\sigma} + \sum_{\sigma} \varepsilon_{b,\sigma} c_{b,\sigma}^{\dagger} c_{b,\sigma} + U n_{b,\uparrow} n_{b,\downarrow}$$

$$+ \sum_{k,\sigma} V_{k,\sigma} c_{k,\sigma}^{\dagger} c_{b,\sigma} + \text{h.c.} \ .$$  

(5)
\[ \varepsilon_k < \Lambda_{\sigma, \sigma} \] and zero otherwise. This allows us to derive explicit analytical expressions. For generic forms of free states and an s-wave bound state, one sees that the overlap integrals \( V_{k, \sigma} \) vanish when the wave length \( 1/k \) becomes much shorter than the typical extension of the bound state \( a_\sigma \). From this follows that a reasonable assumption is \( \Lambda_{\sigma, \sigma} = \frac{a^2}{2 \pi [k_\nu a_\sigma]} \), with \( \alpha \approx 1 \), used in the following. From Eq. (9), we find then for small \( k \) with Eq. (2) and Eq. (7) with \( \mu = 0 \),
\[ V^2 = \frac{8 \pi}{V_0 k_\nu} \frac{2}{\pi |k_\nu a_\sigma| - k_\nu r_{c, \sigma}}, \]

such that \( V^2 \sim 1/N_\alpha \) and
\[ \frac{\varepsilon_{b, \sigma}}{\varepsilon_\sigma} = \frac{V_0 k_\nu^3}{4 \pi} \left( \frac{2}{\pi |k_\nu a_\sigma|} - \frac{1}{k_\nu a_\sigma} \right) V^2 = 2 \frac{2}{\pi |k_\nu a_\sigma|} - \frac{2}{\pi |k_\nu a_\sigma|} \]

(10)

Useful quantities are the hybridization parameter, \( \Gamma_{\sigma} = \pi p_\theta (\varepsilon_\nu) V^2 \), which is independent of the volume of the system, and the important ratio
\[ -\frac{\varepsilon_{b, \sigma}}{\pi \Gamma_{\sigma}} = \frac{1}{\pi} \left( \frac{1}{k_\nu a_\sigma} - \frac{2}{\pi |k_\nu a_\sigma|} \right), \]

(11)

which only depends on \( k_\nu a_\sigma \). We can see how the AIM model parameters depend on \( a_\sigma \) and \( r_{c, \sigma} \), for instance, \( -\varepsilon_{b, \sigma} \) increases with \( 1/a_\sigma \) for \( a_\sigma > 0 \). As discussed, \( a_\sigma \) and \( r_{c, \sigma} \) depend on \( a_0, \sigma \) and thus on the magnetic field \( B \) and the trapping frequency \( \omega_\infty \), and this allows to tune the model parameters in Eq. (9). We see that in general both \( h = (\varepsilon_{b, \uparrow} - \varepsilon_{b, \downarrow})/2 \), which acts as a local magnetic field, and \( \Delta \Gamma = (\Gamma_{\uparrow} - \Gamma_{\downarrow})/2 \) can be non-zero. For studies of the AIM the latter is unusual, but it has been discussed in situations of quantum dots coupled to partly polarized leads. As discussed in the SM, this implies that in general due to second order processes in the hopping an effective local magnetic field \( \tilde{h}_{ef} \) is generated. There, also the mapping of the general AIM in Eq. (5) to an anisotropic Kondo model with spin-spin couplings \( J_\perp \neq J_z \) and the derivation of the Kondo scale \( T_K \) from scaling equations are explained.

**Tuning to the Kondo state** - We now discuss appropriate parameter regimes to observe the Kondo-correlated state in more detail. These are meant as guidelines and not strict boundaries. The first condition (I) is to have small fluctuations of the occupation of the bound state, which can be expected if \( -\varepsilon_{b, \sigma}/(\pi \Gamma_{\sigma}) > c_1 \). A naive estimate is \( c_1 \approx 1/2 \), however, smaller values, \( c_1 \approx 0.25 \), also work well as shown later. The second condition (II) is to have the Kondo scale in a regime where it can be observed experimentally, i.e., the experimental temperature \( T_{\text{exp}} \sim T_K \). We assume \( T_{\text{exp}} = \alpha T_{\varepsilon_\sigma} \), where \( \alpha T_{\varepsilon_\sigma} \approx 0.01 \) can be achieved. To achieve this the bound state must not lie too deep. More formally, \( T_K \) depends exponentially on the Kondo coupling \( J_z \) and the asymmetry \( x = J_\perp/J_z < 1 \). It follows that \( J_z \) must not be too small and the asymmetry should not be too large. These couplings depend on the AIM parameters \( \varepsilon_{b, \sigma}, \Gamma_{\sigma} \) (see SM) and we can obtain a condition of the form \( -1/2 \sum_{\sigma} \varepsilon_{b, \sigma}/(\pi \Gamma_{\sigma}) < c_2 \) with a numerical estimate \( c_2 \approx 0.6 \). Hence, together with (I) we define an interval for values of \( -\varepsilon_{b, \sigma}/(\pi \Gamma_{\sigma}) \), and with the help of Eq. (11) we can state it as a condition for \( k_\nu a_\sigma \),
\[ c_1 < k_\nu a_\sigma < c_u, \]

(12)

where \( c_1 = \frac{\pi - 2}{\pi \sigma c_1} \), \( c_u = \frac{\pi - 2}{\pi \sigma c_1} \) are lower/upper boundaries [see Fig. 1(b)]. \( \Delta \Gamma \neq 0 \), an effective magnetic field is generated, which suppresses Kondo correlations. It is possible to offset the effective field with a local magnetic field \( h \), and thus, we define a third condition (III), \( \Delta \Gamma = \alpha_h h \). For a symmetric DOS, \( \alpha_h \approx 0.2 \) was found numerically \([31]\), however, for a general DOS and different cut-offs this may vary (see SM).

To be able to tune to the Kondo-correlated state, it is necessary to have a system, where the Feshbach resonances for \( |\uparrow\rangle \) and \( |\downarrow\rangle \) with the impurity atom have some overlap. Using the form in Eq. (4) for \( a_0, \sigma \), \( \Delta B_{0, \uparrow} \) and \( \Delta B_{0, \downarrow} \) need to have the same sign and \( |B_{0, \sigma} + \Delta B_{0, \sigma}| > |B_{0, -\sigma}| \). Given the bare scattering lengths \( a_0, \sigma \) the effective scattering length including the hybridizing potential can be calculated. For simplicity we use the Born approximation in Eq. (5) in the following, which was shown to give reasonably accurate results \([24]\). Hence, the effective scattering lengths can be tuned close to the Feshbach resonance and it is possible that at the intersection, \( \sigma_1 = \sigma_1 \), Eq. (12) is satisfied. This is illustrated in Fig. 1(b). As \( a_0, \uparrow = a_0, \downarrow \), Eq. (3) implies \( r_{c, \uparrow} = r_{c, \downarrow} \), such that \( h = \Delta \Gamma = 0 \) and automatically conditions (I-III) are satisfied. Note that if \( a_1 = a_1 \), but \( k_\nu a_\sigma > c_u \), we can satisfy Eq. (12) by reducing the density \( n \) and thus \( k_\nu \).

**Experimental system and probe** - For the experimental realization of our proposal we focus on a system of 40K with \( |\downarrow\rangle \equiv |9/2, -7/2 \rangle \) and \( |\uparrow\rangle \equiv |9/2, -5/2 \rangle \) hyperfine states and 23Na in the hyperfine state \( |1, 1 \rangle \). In this system recently molecular states were successfully produced using interspecies Feshbach resonances \([24]\). For our purpose, the Feshbach resonances with \( B_{0, \uparrow} = 106.9 \text{G}, B_{0, \downarrow} = 108.6 \text{G}, \Delta B_{0, \uparrow} = -1.8 \text{G}, \) and \( \Delta B_{0, \downarrow} = -6.6 \text{G} \[19] \) are suitable. The background scattering length is \( a_{bg} = -900 \text{ab} \), where the Bohr radius is \( a_B = 0.53 \cdot 10^{-10} \text{m} \). In the following we use common values in ultracold gas experiments, \( n \approx 10^{13} \text{m}^{-3} \), \( k_0 = [3\pi^2 n]^{1/3} = 1.6 \cdot 10^{-4} \text{ab} \). A typical trapping frequency is \( \omega_\infty \approx 100 \text{kHz} \[11] \), such that for 23Na we have \( a_{bg, \sigma} = 3.12 \cdot 10^{-4} \text{ab} \). One has \( a_{0, \uparrow} = a_{0, \downarrow} = -1.82 a_{bg} \) for

\[ B_\sigma = \frac{B_{0, \uparrow} \Delta B_{0, \uparrow} - B_{0, \downarrow} \Delta B_{0, \downarrow}}{\Delta B_{0, \uparrow} - \Delta B_{0, \downarrow}} = 106.26 \text{G}. \]

(13)

With Eq. (4), this implies \( k_\nu a_\sigma = 0.55 \). Employing the numerical renormalization group (NRG) \([33, 34]\), we cal-
FIG. 2: (Color online) (a) Spectral function $\rho_{b,\sigma}(\omega)$ for different values of $\varepsilon_b/\pi T$ obtained for $k_F = 1.075, 0.45 k_F^0$. The corresponding values are $k_F a_0 = 0.55, 0.41, 0.25$ and the complete set of AIM parameters is given in Table I in the SM. The magnetic field $B$ has been tuned such that $a_1 = a_2$. (b) Momentum resolved spectral function $\rho_{k,\sigma}(\omega)$ as calculated from Eq. (13) for the case $\varepsilon_k/\pi T = -0.21$ with $n_{imp}$ as discussed below Eq. (14).

We have demonstrated how to realize a Kondo-correlated state for a mixture of ultracold atoms. The proposed setup, different from a previous proposal based on alkaline-earth atoms, is the decay of the equal time spin correlation function $\langle S_z(r) S_z(0) \rangle$, which is difficult to access in condensed matter systems. In contrast, in the proposed ultracold gas system this correlation function should become accessible by spectroscopic tools, such that $\xi_K$ could be determined and this fundamental question of Kondo physics could be settled. Since our setup allows to switch the impurity on and off by optically changing the hyperfine state of the $b$ species, it would also be curious to analyze the time scale on which the Kondo cloud builds up. The proposed setup has also great potential to shed light on a number of intriguing issues for the Kondo lattice including the observation of a fractionalized Fermi liquid (FL$^*$) phase and the occurrence of superconductivity close to a quantum phase transitions.
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S1 Hybridization function

The hybridization function was defined as,

$$K_\sigma(\omega) = \sum_k \frac{|V_{k,\sigma}|^2}{\omega + i\eta - \varepsilon_k + \mu}.$$  (15)

We write $K_\sigma(\omega) = \Lambda_\sigma(\omega) - i\Gamma_\sigma(\omega)$. If we assume that $V_{k,\sigma} = V_\sigma$ is constant and is cut off by $\Lambda_{v,\sigma}$, then the imaginary part becomes,

$$\Gamma_\sigma(\omega) = -\pi |V_{\omega,\sigma}|^2 \rho_0(\omega + \mu) \text{arctan}\left(\frac{\Lambda_{v,\sigma}}{-\omega - \mu}\right).$$  (16)

The real part can also be evaluated in terms of principle value integrals and we find for $\omega < -\mu$,

$$\Lambda_\sigma^<(\omega) = -2|V_\sigma|^2 c_3 \left[\sqrt{\Lambda_{v,\sigma} - \sqrt{-\omega - \mu}} \arctan\left(\frac{\Lambda_{v,\sigma}}{-\omega - \mu}\right)\right].$$  (17)

and for $\omega > -\mu$,

$$\Lambda_\sigma^>(\omega) = -2|V_\sigma|^2 c_3 \left[\sqrt{\Lambda_{v,\sigma} + \sqrt{\omega + \mu}} \log\left(\frac{\sqrt{\Lambda_{v,\sigma} + \sqrt{\omega + \mu}}}{\sqrt{\Lambda_{v,\sigma} - \sqrt{\omega + \mu}}}\right)\right].$$

The function is continuous at $\omega \to -\mu$ but not smooth. A schematic plot with $\mu = \varepsilon_F$ is shown in Fig. 3.

![Schematic plot of the hybridization function](image)

FIG. 3: (Color online) Schematic plot of the hybridization function $\Gamma(\omega)$ and $\Lambda(\omega)$ indicating the boundaries of the continuum states $-\varepsilon_F$ and upper cutoff $\Lambda_v$ and the energy of the bare bound state $\varepsilon_b$, generally below the continuum. At the sharp positive edge $\Lambda(\omega)$ has a logarithmic singularity. This can lead to bound states outside the continuum [49]. The sharp cut-off can be softened without changing any of the results qualitatively. For simplicity we have omitted the index $\sigma$.

S2 Kondo physics with additional resonances

In the main text it was discussed how the system of $^{40}\text{K}$ and $^{23}\text{Na}$ atom can be tuned into a Kondo-correlated state employing two Feshbach resonances. It is fortunate
in this situation that the effective scattering lengths intersect in a suitable regime as shown in Fig. 1(b). However, for other systems this will not generally be the case. For instance, two hyperfine states of $^6\text{Li}$ have a number of Feshbach resonances with $^{133}\text{Cs}$ between 800-900G with promising features [21], but the intersection does not directly lie in a suitable regime. Here we show that it can nevertheless be possible to tune the system into a Kondo-correlated state with the help of confinement induced additional resonances [23, 24].

To see how the confining potential can help to align the bound state energies in the right regime, we consider for each component $\sigma$ the two-particle scattering problem between species $a$ and $b$. Without the harmonic confinement ($\omega_{\text{ho}} = 0$) the scattering problem for each $\sigma$ is characterized by the bare s-wave scattering length $a_{0,\sigma}$. For $a_{0,\sigma} > 0$, the effective scattering length $a_{\sigma}$ is found to have many sharp resonances [24], which can be understood as follows. A molecular bound state, where only $b$ feels the confinement has the harmonic oscillator energy $E_n = (2n + \frac{3}{2})\sqrt{\frac{m_b}{M}}\hbar\omega_{\text{ho}}$, with $M = m_a + m_b$. This energy reduced by the binding energy $E_{b,\sigma}$ can become resonant with the ground state energy of oscillator and atom, $E_n + E_{b,\sigma} = \frac{3}{2}\hbar\omega_{\text{ho}}$, which leads to the resonance for the effective scattering length $a_{\sigma}$. From this we obtain the condition [24],

$$a_{0,\sigma}^\text{res}(n) = \frac{a_{\text{ho}}}{\sqrt{\frac{2m_b}{m_b}}\sqrt{(2n + \frac{3}{2})\sqrt{\frac{m_b}{M}} - \frac{3}{2}}}$$

(18)

where $n = 1, 2, \ldots$. Hence, in a situation where one scattering length is in suitable regime the second one can be tuned there by one of those additional resonances.

In Fig. 4(a) we show schematically the bare scattering lengths $a_{0,\sigma}$ close to Feshbach resonances. We have also indicated values of the magnetic field where the resonance condition, Eq. (18), is satisfied. Now let us assume that on tuning $B$ we have satisfied $c_1 < k_b a_1(B_K) < c_2$, but $k_b a_1(B_K) < c_1$ [see Fig. 4(b)]. Then one can change $\omega_{\text{ho}}$ by the laser power to bring a sharp resonance in the vicinity, i.e., change $a_{\text{ho}}$ such that $a_0(B_K) \approx a_0^\text{res}(n_K)$ for some $n_K$. Then some further fine tuning to $B_K - \delta B$ will satisfy the condition $a_1(B_K - \delta B) = a_1(B_K - \delta B)$, such that conditions (I) and (II) are satisfied [see Fig. 4(c)]. Since we have used the additional resonance we have $r_{e,\uparrow} \neq r_{e,\downarrow}$, and thus in general $h, \Delta \Gamma \neq 0$. There are two different cases to consider: (i) $|r_{e,\sigma}| \ll a_{\sigma}$, in this case, $\Delta \Gamma \approx 0$ and $h \approx 0$, such that conditions (I-III) are satisfied. Note that $r_{e,\sigma}$ can be reduced by decreasing $a_{\text{ho}}$ as seen in Eq. (3). (ii) $|r_{e,\sigma}| \sim a_{\sigma}$ or $|r_{e,\sigma}| > a_{\sigma}$, in this case we have to tune $B$ further to satisfy the condition (III), $\Delta \Gamma = a_b h$. We can focus on the fast variation of $a_{1}$ close to the resonance, and assume the other quantities in this regime as constant. Depending on the strength of the asymmetry $r_{e,\uparrow}/r_{e,\downarrow}$ a solution which still respects Eq. (12) can be found.

### S3 Properties of the AIM and mapping to the Kondo model

Here we discuss some properties of the AIM in Eq. (5). First, we show how an effective magnetic field emerges for the case $V_\uparrow \neq V_\downarrow$. This is seen directly from the scaling equations for the Anderson model [11, 50]. For a general DOS one finds,

$$\frac{dh}{d\Lambda} = \frac{1}{2\pi} \left[ \frac{\Gamma_\uparrow(\Lambda)}{\Lambda - \varepsilon_{b,\uparrow}} - \frac{\Gamma_\downarrow(\Lambda)}{\Lambda - \varepsilon_{b,\downarrow}} \right] + \frac{1}{2\pi} \left[ \frac{\Gamma_\downarrow(-\Lambda)}{\Lambda + \varepsilon_{b,\downarrow} + U} - \frac{\Gamma_\uparrow(-\Lambda)}{\Lambda + \varepsilon_{b,\uparrow} + U} \right].$$

We introduced $\Gamma_\sigma(\Lambda) = \Gamma_\sigma \rho_0(\Lambda + \mu)$. When considering the situation $U \to \infty$ the last two terms can be neglected. In the special case of a particle-hole symmetric model, $\varepsilon_b = -U/2$, $\varepsilon_b = (\varepsilon_{b,\uparrow} + \varepsilon_{b,\downarrow})/2$, with symmetric and constant DOS, $\rho_0 = 1/W$, and initially zero field $h = 0$, no effective field is generated. We can see this from

$$\frac{dh}{d\Lambda} = \frac{\Gamma_\uparrow - \Gamma_\downarrow}{2\pi} \left( \frac{2\varepsilon_b + U}{(\Lambda + \varepsilon_b + U)(\Lambda - \varepsilon_b)} \right),$$

(19)

where the right hand side vanishes in the particle hole symmetric case. In all other cases for $\Gamma_\uparrow \neq \Gamma_\downarrow$ an effective field $h_{\text{eff}}$ is generated as a second order effect in the
hybridization. From Eq. (19) we can see that the effective field is proportional to ΔΓ, such that the form ΔΓ = αh, to offset the field is appropriate. We see that for ΔΓ > 0, U + 2ε > 0, reducing Λ leads to a negative h, such that the form

This term vanishes for a symmetric model εb = −U/2, a symmetric DOS and Vγ = Vγ. However, in general it is finite and acts like a local magnetic field as discussed above for the AIM. Generally, there are also terms ~ c′b,σc′b,−σ, which change the impurity occupation by 2. In the regime of single occupancy they are neglected. We also take the Kondo couplings independent of k. We define J⊥ = J⊥,± = J⊥,± and Jz = (J⊥,± + J⊥,±)/2.

In general J⊥ ≠ Jz and hence we have to deal with an anisotropic Kondo model.

S4 Scaling of the anisotropic Kondo model and TK

We can define the Kondo scale TK where Jz diverges in the scaling equations [11, 52]. In the isotropic case for constant DOS, the result is

Here, Λ0 is a suitable high energy cutoff. The square root DOS of the three dimensional systems leads to minor modifications which can be included in a prefactor. In the anisotropic case the equations read,

Using Jz = Jz, Kondo scale TK is found to be

for x = J⊥/Jz < 1 and γ = atan(√(1 − x2)/x) for x > 1. The coefficient αK accounts for the varying DOS and possibly different upper and lower cutoffs.

Having established these relations, we can derive a condition for Jz, such that TK is of the order of the experimental temperature (see main text). It can be written in the form −1/2 ∑σεb,σ/(πΓσ) < c2. If one assume that the asymmetry is not very large, that is x > 1/2 in Eq. (27), one can find the estimate c2 ≈ 0.6.

S4 NRG calculations for bound state spectral functions

We have done NRG calculations for the AIM in Eq. (5) and computed the low temperature bound state spectral function ρh,σ(ω). The ω-dependence of Kσ(ω) is dealt with as in NRG applications for dynamical mean field
calculations [34]. The first set of parameter is for the situation, where $B = B_s$ in Eq. (13) and we vary $k_{\pi}/k_{\pi}^0$, where $k_{\pi}^0 = 1.6 \cdot 10^{-4}/a_B$. The parameters are calculated as follows: $a_{\pi}$ and $r_{e,\sigma}$ are calculated from Eq. (3), and the AIM model parameters $\varepsilon_{b,\sigma}/\varepsilon_F$, and $V_{\sigma}/\varepsilon_F$ are computed from Eq. (10) and Eq. (9). The ratio $\bar{\Gamma}$ is given in Eq. (11), the upper cutoff $\Lambda_{e,\sigma} = \frac{\pi(2k_{\pi}a_{\pi})^2}{2}$, and $\varepsilon_F = 1$ sets the energy scale in the calculations. We chose $U$ large enough that double occupancy is strongly suppressed. The numerical values for the parameters are given in Table I. The value for $V_{\sigma}$ corresponds to the choice $V_0 k_F^3 = 1000$.

$$
| \begin{array}{cccc}
 k_{\pi}/k_{\pi}^0 & k_{\pi}a_{\pi} & \varepsilon_{b,\sigma}/\varepsilon_F & V_{\sigma}/\varepsilon_F & -\varepsilon_{b,\sigma}/(\pi \Gamma)
 \end{array} |
| \begin{array}{cccc}
 1 & 0.55 & -1.64 & 0.177 & 0.21 \\
 0.75 & 0.41 & -2.92 & 0.204 & 0.28 \\
 0.45 & 0.25 & -8.11 & 0.264 & 0.47 \\
 \end{array} |
$$

TABLE I: Values for the AIM model parameters, when varying the density.

$$
| \begin{array}{cccc}
 B(G) & k_{\pi}a_{\pi} & \varepsilon_{b,\sigma}/\varepsilon_F & h/\varepsilon_F & V_{\sigma}/\varepsilon_F & V_{\pi}/\varepsilon_F & -\varepsilon_{b,\sigma}/(\pi \Gamma) & \Delta \Gamma/\varepsilon_F
 \end{array} |
| \begin{array}{cccccc}
 106.25 & 0.55 & 0.55 & -1.64 & 0.000 & 0.177 & 0.177 & 0.000 \\
 106.2 & 0.48 & 0.53 & -1.78 & 0.075 & 0.174 & 0.176 & -0.029 \\
 106.1 & 0.38 & 0.50 & -1.96 & 0.175 & 0.167 & 0.175 & -0.111 \\
 106.0 & 0.30 & 0.47 & -2.12 & 0.243 & 0.157 & 0.174 & -0.219 \\
 \end{array} |
$$

TABLE II: Values for the AIM model parameters, when varying the magnetic field $B$.

In Table III the parameters are shown for the situation where the field is reduced from $B = 106.25G$ and $k_{\pi} = k_{\pi}^0$ is held fixed. The corresponding spectral functions are shown in Fig. 6.

The spectral functions show typical behavior of the AIM in a magnetic field [32][53]. We see that $\rho_{\sigma,\uparrow}(\omega)$ gains spectral weight at $\omega < 0$ on decreasing the field $h$, and the Kondo peak is shifted to negative energies. In contrast, there is a reduction of spectral weight for $\omega < 0$ in $\rho_{\sigma,\downarrow}(\omega)$ when $h$ becomes larger. At the same time the Kondo peak is shifted to positive energies and broadened. Note that $\Delta \Gamma < 0$ can reduce the magnetic field effect.

FIG. 5: (Color online) Spin resolved spectral functions $\rho_{\sigma,\uparrow}(\omega)$ (a) and $\rho_{\sigma,\downarrow}(\omega)$ (b) for decreasing magnetic field $B = 106.25, 106.2, 106.1, 106G$, which yields a number of different values for the $k_{\pi}a_{\pi}$ and the field $h$ and the other model parameters (see Table I), where $\Delta \Gamma \neq 0$. The Kondo resonance is split and suppressed.

In Table III the parameters are shown for the situation where the field is reduced from $B = 106.25G$ and $k_{\pi} = k_{\pi}^0$ is held fixed. The corresponding spectral functions are shown in Fig. 6.

FIG. 6: (Color online) Spectral functions $\rho_{\sigma,\uparrow}(\omega)$ and $\rho_{\sigma,\downarrow}(\omega)$ close to a resonance for a number of different values of $k_{\pi}a_{\pi}$ and the complete set of AIM parameters is given in Table III.

For illustration we also discuss a case where the additional resonances are used to tune into the Kondo-correlated state (cf. Fig. 4). We analyze the K-Na system and use $B = 106.2G < B_s$, where from Eq. (3) $k_{\pi}a_{\pi} = 0.475$ and $k_{\pi}a_{\pi} = 0.53$. Then we tune $k_{\pi}a_{\pi}$ with the additional resonance as discussed in Fig. 3(b,c) to satisfy conditions (I-III). The model parameters are given in Table III. We have for $B_K = 106.2G$ and $a_B = 3.12 \cdot 10^9 a_B$, the closest resonance at $\eta_K \approx 6$. We could also employ the resonance at a different value $\eta_K$ by suitably adjusting $\omega_{\eta_K}$ and hence $a_B$. We have assumed that $k_{\pi}a_{\pi} = 0.53, k_{\pi}r_{\sigma,\uparrow} = 0.52, k_{\pi}r_{\sigma,\downarrow} = 0.47$ are
In the limit of low temperature this becomes,

$$I_k = k_B a_\uparrow \text{shift of the dispersion and the imaginary part gives an}
$$

respect to the $$k$$ is the intensity and $$B$$ for

The spectral function for

transition rate from a hyperfine state

initially unoccupied, is given by [48],

that

leads to decreasing

Now decreasing

This leads to the expectation

$$\rho_{\sigma}(\omega) = \frac{(\eta + n_{\text{imp}} V_\sigma^2 \rho_{\sigma,\uparrow}( \omega ))/\pi}{(\omega - \varepsilon_k - n_{\text{imp}} V_\sigma^2 G_{b,\sigma}^R(\omega))^2 + (\eta + n_{\text{imp}} V_\sigma^2 \rho_{\sigma,\downarrow}( \omega ))^2}. \tag{29}$$

We see that the real part $$G_{b,\sigma}^R(\omega)$$ can contribute to a shift of the dispersion and the imaginary part gives an additional broadening. All terms in Eq. (28) depend on $$k$$ via $$\varepsilon_k$$ so we can introduce a density of states (DOS) $$\rho_0(\varepsilon)$$ and write,

$$I_\sigma(\omega) = \frac{\Omega^2}{2\pi} \int d\varepsilon \rho_0(\varepsilon) \rho_{\epsilon,\sigma}(\varepsilon - \mu + \omega_{3,\sigma} - \omega) n_F(\varepsilon - \mu + \omega_{3,\sigma} - \omega). \tag{30}$$

In the limit of low temperature this becomes,

$$I_\sigma(\omega) = \frac{\Omega^2}{2\pi} \int_{-\infty}^{\omega_{3,\sigma} - \omega} d\varepsilon \rho_0(\varepsilon + \mu) \rho_{\epsilon + \mu,\sigma}(\varepsilon + \omega_{3,\sigma} - \omega). \tag{31}$$

In the case of non-interaction fermions, $$\rho_{\epsilon + \mu,\sigma}(\varepsilon + \omega_{3} - \omega) = \delta(\varepsilon + \omega_{3,\sigma} - \omega - \varepsilon) = \delta(\omega_{3,\sigma} - \omega)$$, so the RF spectrum reads,

$$I_0(\omega) = \frac{2 \Omega^2}{3} \frac{k_B^3}{2\pi} \delta(\omega_{3,\sigma} - \omega). \tag{32}$$

The rf spectrum can be understood as the sum of all the transitions from the modified band dispersion $$E_{k,\sigma}$$ with a certain width $$\Delta k$$ for $$|\sigma, k\rangle$$ to a non-interacting dispersion $$\varepsilon_k$$ shifted by $$\omega_{3,\sigma}$$ for $$(3, \sigma)$$. A shift in the dispersion gives a shift of the rf signal, flattening of the dispersion can give additional weight at higher or lower energies, and broadening leads to a broadened rf signal. The Kondo peak on its own leads to a band bending and broadening and hence a rf peak which is shifted and has high energy tails.

The rf signal corresponding to Fig. 2(a) in the main text for an impurity concentration $$n_{imp}/N_a \approx 0.03$$ is shown in Fig. 7.

When comparing $$I_\sigma(\omega)$$ to the unperturbed signal $$I_0(\omega)$$ we find a broadened peak slightly shifted from $$\omega = \omega_{3,\sigma}$$. This shape can be traced back to the effect of the coupling of the itinerant states to the bound state spectral function. In Eq. (28) this leads to a broadening of the spectral function and a small band bending close to $$\varepsilon_k = \varepsilon_F$$, where the Kondo resonance lies. The signal in $$I_\sigma(\omega)$$ narrows for decreasing Kondo scale due to the reduced modification of $$\rho_{k,\sigma}(\omega)$$. The signals in Fig. 7 are rather characteristic for the two peak structure in Fig. 2(a), such that the Kondo-correlated state and position of the Kondo resonance can be identified well with rf spectroscopy.

In Fig. 8 we show the rf spectra when varying $$B$$ corresponding to the results in Fig. 5.

The peak in $$I_\uparrow(\omega)$$ is shifted to lower energies. This can be understood looking at the effect of the moving of the Kondo peak to lower energies and its effect on $$\rho_{k,\uparrow}(\omega)$$. In contrast, we find that $$I_\downarrow(\omega)$$ reverts to the non-interacting result $$I_0(\omega)$$ as the B field makes the relevant features disappear in the spectral function $$\rho_{k,\downarrow}(\omega)$$ and thus $$\rho_{b,\downarrow}(\omega)$$. The careful analysis of the $$I_\sigma(\omega)$$ signals as function of magnetic field should be provide a good picture of the tuning into the Kondo-correlated state.

FIG. 7: (Color online) rf spectrum corresponding to the spectral function in Fig. 2(a) in the main text and the values in Table II. We also show $$I_\downarrow(\omega)$$, (broadened delta-function) for comparison.

FIG. 8: rf spectrum when varying B corresponding to the results in Fig. 5.
FIG. 8: (Color online) rf spectra $I_1(\omega)$ (a) and $I_2(\omega)$ (b) for decreasing magnetic field $B$ as in Fig. 5 and model parameters in Table III. We also show $I_0(\omega)$, (broadened delta-function) for comparison.

FIG. 9: (Color online) rf spectra $I_1(\omega)$ (a) and $I_2(\omega)$ (b) close to a resonance for a number of different values of $k_x a_1$ as in Fig. 6 and the complete set of AIM parameters is given in Table III. We also show $I_0(\omega)$, (broadened delta-function) for comparison.

The rf signal corresponding to Fig. 6 (a)(b) is shown in Fig. 8 (a)(b). When comparing $I_2(\omega)$ to $I_0(\omega)$ we find a broadened peak slightly shifted from $\omega = \omega_{3,\sigma}$. Again we can understand the shape from the form of the spectral function and its effect on the itinerant states in Eq. (29). The signal in $I_1(\omega)$ broadens and shifts to smaller $\omega$ on decreasing $k_x a_1$, and the opposite happens for $I_2(\omega)$.

[40] C. Latta, F. Haupt, M. Hanl, A. Weichselbaum, M. Claassen, W. Wuester, P. Fallahi, S. Faelt, L. Glaz-


[56] This is justified by the local density approximation, which is usually a good description for trapped systems.

[57] The energy resolution required is set by the peak width in Fig. 2(b). For $n_{imp}/N_a \sim 0.1$ the width at $k = k_F$ is $\Delta/\varepsilon_F \sim 0.09$. 

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