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Employing confinement induced resonances to realize Kondo physics with ultracold atoms

J Bauer and E Demler

Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA

C Salomon

Laboratoire Kastler Brossel, CNRS, UPMC, Ecole Normale Superieure, 24 rue Lhomond, 75231 Paris, France

E-mail: jbauer@physics.harvard.edu

Abstract. We recently proposed a novel realization of Kondo physics with ultracold atomic gases and illustrated that a mixture of ^{40}K and ^{23}Na atoms has suitable properties for the generation of a Kondo-correlated state with experimentally accessible scales. This system fortuitously satisfies rather special conditions. Here we discuss an alternative realization based on confinement induced resonances which could also be applicable for other mixtures. We first explain the general principle of how to engineer the Kondo correlated state like this. Then we present results for local spectral functions from numerical renormalization group (NRG) calculations for the appropriate effective Anderson impurity model and also predict the experimentally measurable radio frequency response.

1. Introduction

In spite of decades of intense research Kondo physics [1] attracts a lot interest in condensed matter physics. One reason is that there remain unresolved questions. For instance, a Kondo screening cloud with a certain spatial extent and characteristic oscillations was predicted [1, 2, 3, 4], however, its experimental observation has remained elusive. For a periodic lattice of Kondo impurities 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 can lead 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 [5, 6], however, it is very difficult to analyze it theoretically beyond the mean field level. We have recently proposed an experimental setup [7] based on ultracold atoms to realize single impurity and lattice Kondo situations. We hope that such an experimental realization of Kondo physics will shed light on some of these open issues. In particular, for certain hyperfine states of a system of ^{40}K and ^{23}Na atoms the effective scattering lengths have suitable properties when tuned close to Feshbach resonances such that Kondo physics is directly possible. However, many other systems will not meet these conditions. Here we show that additional resonances of the confining potential [8, 9] for the "impurity atom" can be employed to tune the system into the Kondo-correlated state.

2. Idea and formal setup

We consider a situation with 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 σ. Species b, which can be a fermion or boson, is subject to a strong harmonic confining potential. The bound states for the hyperfine states correspond to the unscreened spin in the Kondo problem. In order for the Kondo effect to occur the bound states need to obey certain conditions [7] which will be explained below.

For a quantitative discussion we first introduce the atomic scattering problem and parameters. Consider for each component σ the two-particle scattering between species a and b described by a Hamiltonian of the form,

$$H_{\rm scat} = \frac{p_b^2}{2m_b} + \frac{1}{2}m_b\omega_{\rm ho}^2 r_b^2 + \frac{p_a^2}{2m_a} + V(\boldsymbol{r}_a - \boldsymbol{r}_b), \tag{1}$$

where $\boldsymbol{p}_\alpha$, $\boldsymbol{r}_\alpha$ are momenta and positions of the particles, $V(\boldsymbol{r})$ is the interspecies potential and $\omega_{\rm ho}$ a scale for the harmonic confinement. A corresponding length scale is the harmonic oscillator length $a_{\rm ho} = \sqrt{\hbar/m_b\omega_{\rm ho}}$. The low energy form of the effective s-wave scattering amplitude $f_\sigma(k)$ in terms of a_σ and the effective radius $r_{e,\sigma}$ is $f_\sigma(k)^{-1} = -\frac{1}{a_\sigma} + r_{e,\sigma}\frac{k^2}{2} - ik$. Without the harmonic confinement ($\omega_{\rm ho} = 0$) the scattering problem for each σ is characterized by the bare s-wave scattering length $a_{0,\sigma}$. In presence of the harmonic trap the effective parameters a_σ and $r_{e,\sigma}$ can be calculated depending on the bare scattering length $a_{0,\sigma}$ [9, 10]. One finds,

$$a_\sigma = \frac{m_a}{m_r}a_{0,\sigma}, \quad r_{e,\sigma} = -\frac{m_r}{m_a}\frac{a_{\rm ho}^2}{a_{0,\sigma}}. \tag{2}$$

To tune the bare scattering lengths $a_{0,\sigma}$ by a magnetic field B, we assume that there is a Feshbach resonance,

$$a_{0,\sigma}(B) = a_{\rm bg}\Big(1 - \frac{\Delta B_{0,\sigma}}{B - B_{0,\sigma}}\Big), \tag{3}$$

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

To make the connection to Kondo physics explicit, we describe the low energy physics of the system by an Anderson impurity model (AIM) [11] of the form,

$$H = \sum_{\boldsymbol{k},\sigma}\varepsilon_{\boldsymbol{k}}c^\dagger_{\boldsymbol{k},\sigma}c_{\boldsymbol{k},\sigma} + \sum_\sigma \varepsilon_{b,\sigma}c^\dagger_{b,\sigma}c_{b,\sigma} + Un_{b,\uparrow}n_{b,\downarrow} + \sum_{\boldsymbol{k},\sigma}V_{\boldsymbol{k},\sigma}c^\dagger_{\boldsymbol{k},\sigma}c_{b,\sigma} + \text{h.c.}\,. \tag{4}$$

Here, $c^\dagger_{\boldsymbol{k},\sigma}$ creates an itinerant fermion with momentum $\boldsymbol{k}$ and spin projection σ, and $c^\dagger_{b,\sigma}$ a bound state with energy $\varepsilon_{b,\sigma}$. The states are mixed by the hybridization $V_{\boldsymbol{k},\sigma}$. 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 $c_3 = V_0k_{\rm F}^3/(4\pi^2\varepsilon_{\rm F}^{3/2})$, and $\varepsilon_{\rm F} = \frac{\hbar^2}{2m_r}\left(3\pi^2 n\right)^{2/3}$. 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. We have shown [7] that the parameters in Eq. (4) are related to the scattering quantities by

$$\frac{V_\sigma^2}{\varepsilon_{\rm F}^2} = \frac{\frac{8\pi}{V_0k_{\rm F}^3}}{\frac{2}{\pi}|k_{\rm F}a_\sigma| - k_{\rm F}r_{e,\sigma}}, \qquad \frac{\varepsilon_{b,\sigma}}{\varepsilon_{\rm F}} = 2\frac{\frac{2}{\pi|k_{\rm F}a_\sigma|} - \frac{1}{k_{\rm F}a_\sigma}}{\frac{2}{\pi}|k_{\rm F}a_\sigma| - k_{\rm F}r_{e,\sigma}}. \tag{5}$$

We introduce the hybridization parameter, $\Gamma_\sigma = \pi\rho_0(\varepsilon_{\rm F})V_\sigma^2$ and the ratio

$$\frac{-\varepsilon_{b,\sigma}}{\pi\Gamma_\sigma} = \frac{1}{\pi}\left(\frac{1}{k_{\rm F}a_\sigma} - \frac{2}{\pi|k_{\rm F}a_\sigma|}\right), \tag{6}$$

which only depends on $k_{\rm F}a_\sigma$. We can see how the AIM model parameters depend on a_σ and $r_{e,\sigma}$, for instance, $-\varepsilon_{b\sigma}$ increases with $1/a_\sigma$ for $a_\sigma > 0$. As discussed, a_σ and $r_{e,\sigma}$ depend on $a_{0,\sigma}$ and thus on the magnetic field B and the trapping frequency $\omega_{\rm ho}$, and this allows to tune the model parameters in Eq. (4).

Appropriate parameter regimes to observe the Kondo-correlated state have been discussed in detail in Ref. [7]. The first condition (I) is to have small fluctuations of the occupation of the bound state, which can be expected if $-\varepsilon_{b,\sigma}/(\pi\Gamma_\sigma) > c_1$. The second condition (II) is to have the Kondo scale in a regime where it can be observed experimentally, i.e., the experimental temperature $T_{\rm exp} \sim T_{\rm K}$. These can be stated as a condition for $k_{\rm F}a_\sigma$,

$$c_l < k_{\rm F}a_\sigma < c_u, \tag{7}$$

where c_l, c_u are lower/upper boundaries. For $\Delta\Gamma = (\Gamma_\uparrow - \Gamma_\downarrow)/2 \neq 0$, 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), $\Delta\Gamma = \alpha_h h$.

3. Kondo physics with additional resonances

In Ref. [7] it was discussed how the system of ^{40}K with $|\downarrow\rangle \equiv |9/2, -7/2\rangle$ and $|\uparrow\rangle \equiv |9/2, -5/2\rangle$ hyperfine states and ^{23}Na in the hyperfine state $|1, 1\rangle$ can be tuned into a Kondo-correlated state employing two close-by Feshbach resonances. It is fortunate in this situation that the effective scattering lengths intersect in a suitable regime. However, for other systems this will not generally be the case. For instance, two hyperfine states of ^{6}Li have a number of Feshbach resonances with ^{133}Cs between 800-900G with promising features [12], 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 [8, 9].

To see how the confining potential can help to align the bound state energies in the right regime, we consider for each component σ the two-particle scattering problem between species a and b. Without the harmonic confinement ($\omega_{\rm ho} = 0$) the scattering problem for each σ is characterized by the bare s-wave scattering length $a_{0,\sigma}$. For $a_{0,\sigma} > 0$, the effective scattering length a_σ is found to have many sharp resonances [9], which can be understood as follows. A molecular bound state, where only b feels the confinement has the harmonic oscillator energy $E_n = (2n + \frac{3}{2})\sqrt{\frac{m_b}{M}}\hbar\omega_{\rm ho}$, 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, $E_n + E_{b,\sigma} = 3/2\hbar\omega_{\rm ho}$, which leads to the resonance for the effective scattering length a_σ. From this we obtain the condition [9],

$$a_{0,\sigma}^{\rm res}(n) = \frac{a_{\rm ho}}{\sqrt{\frac{2m_r}{m_b}}\sqrt{(2n+\frac{3}{2})\sqrt{\frac{m_b}{M}} - \frac{3}{2}}} \tag{8}$$

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. 1 (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. (8), is satisfied.

Now let us assume that on tuning B we have satisfied $c_l < k_{\rm F}a_\downarrow(B_{\rm K}) < c_u$, but $k_{\rm F}a_\uparrow(B_{\rm K}) < c_l$ [see Fig. 1 (b)]. Then one can change $\omega_{\rm ho}$ by the laser power to bring a sharp resonance in the vicinity, i.e., change $a_{\rm ho}$ such that $a_0(B_{\rm K}) \simeq a_0^{res}(n_{\rm K})$ for some $n_{\rm K}$. Then some further fine tuning to $B_{\rm K} - \delta B$ will satisfy the condition $a_\downarrow(B_{\rm K} - \delta B) = a_\uparrow(B_{\rm K} - \delta B)$, such that conditions (I) and (II) are satisfied [see Fig. 1 (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 be considered: (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

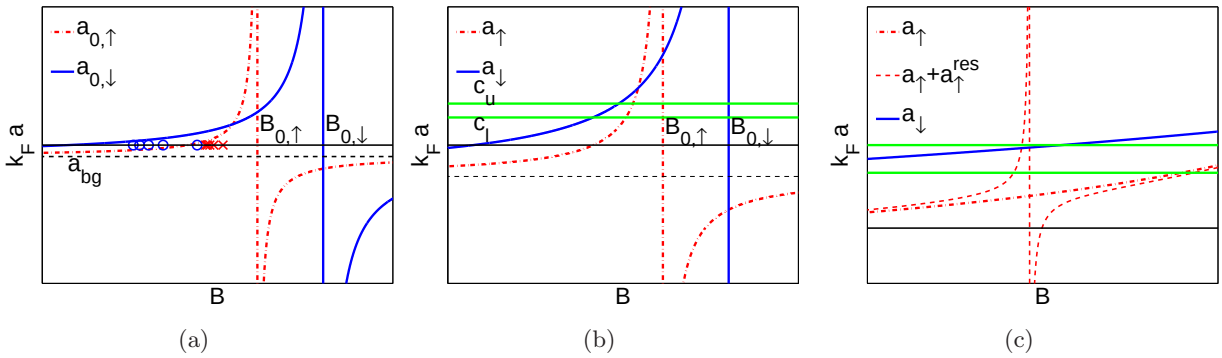


Figure 1. (Color online) (a) Schematic plot of the bare scattering length $a_{0,\sigma}$ for two interspecies Feshbach resonances, with $B_{0,\uparrow} < B_{0,\downarrow}$, and $|\Delta B_{0,\uparrow}| < |\Delta B_{0,\downarrow}|$, $\Delta B_{0,\sigma} < 0$, $a_{\rm bg} < 0$. The circles (crosses) indicate the first 5 magnetic fields where the resonance condition in Eq. (8) is satisfied for $a_{0,\downarrow}$ ($a_{0,\uparrow}$). (b) Schematic plot of the effective scattering length a_σ for a situation where the condition $a_\uparrow = a_\downarrow$ is not satisfied within the Kondo boundaries (c_l, c_u). (c) Close-up of (b), where a resonance has been tuned to $B = B_{\rm K}$.

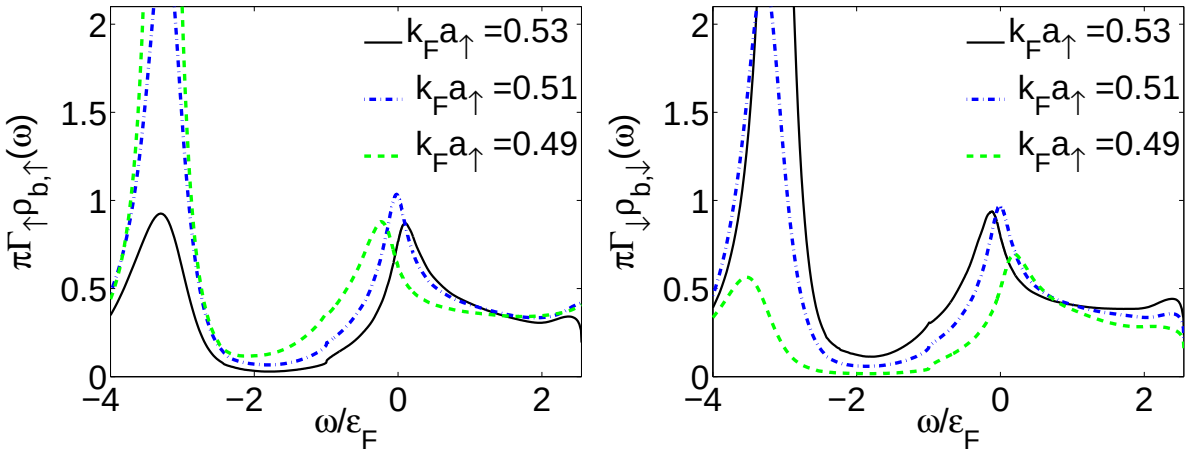
$r_{e,\sigma}$ can be reduced by decreasing $a_{\rm ho}$ as seen in Eq. (2). (ii) $|r_{e,\sigma}| \sim a_\sigma$ or $|r_{e,\sigma}| > a_\sigma$, in this case we have to tune B further to satisfy the condition (III), $\Delta\Gamma = \alpha_h h$. We can focus on the fast variation of $a_\uparrow$ close 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. (7) can be found.

4. NRG calculations for bound state spectral functions

To make the above discussion more quantitative, we have done numerical renormalization group (NRG) calculations for the AIM in Eq. (4) and computed the low temperature bound state spectral function $\rho_{b,\sigma}(\omega)$. We analyze the above mentioned K-Na system and use $B = 106.2\text{G} < B_s$, where $B_s = 106.26\text{G}$ [7]. We have from Eq. (2) $k_{\rm F} a_\uparrow = 0.475$ and $k_{\rm F} a_\downarrow = 0.53$. Then we tune $k_{\rm F} a_\uparrow$ with the additional resonance as discussed in Fig. 1(b,c) to satisfy conditions (I-III). We have for $B_{\rm K} = 106.2\text{G}$ and $a_{\rm ho} = 3.12 \cdot 10^3 a_{\rm B}$, the closest resonance at $n_{\rm K} \approx 6$. We could also employ the resonance at a different value $n_{\rm K}$ by suitably adjusting $\omega_{\rm ho}$ and hence $a_{\rm ho}$. We have assumed that $k_{\rm F} a_\downarrow = 0.53$, $k_{\rm F} r_{e,\uparrow} = -0.52$, $k_{\rm F} r_{e,\downarrow} = -0.47$ are held constant and only $k_{\rm F} a_\uparrow$ varies close to the resonance. Similar tuning is possible for other values of B and $a_{\rm ho}$. Generically, for $a_{0,\uparrow} < a_{0,\downarrow}$ one has $|r_{e,\uparrow}| > |r_{e,\downarrow}|$, which leads to $\Delta\Gamma < 0$ and $h > 0$. This leads to the expectation value $n_\uparrow - n_\downarrow < 0$. Now decreasing $a_\uparrow$ close to the resonance from $a_\uparrow \simeq a_\downarrow$ leads to decreasing h, increasing $\Delta\Gamma$, and $\Lambda_{v,\uparrow} > \Lambda_{v,\downarrow}$. This will lead eventually to a situation, where the field effect is canceled such that $n_\uparrow - n_\downarrow \simeq 0$. Since in this situation still $V_\uparrow \neq V_\downarrow$, in general anisotropic Kondo physics is realized. The parameters of the AIM are calculated as in Ref. [7]. $\varepsilon_{\rm F} = 1$ sets the energy scale in the calculations. We chose U large enough that double occupancy is strongly suppressed. The results for the spectral functions are shown in Fig. 2.
We identify a clear Kondo peak close to $\omega = 0$. The other features are typical for the Kondo effect in a magnetic field [13, 14, 15] with a slightly shifted resonance and shifted spectral weight. For $k_{\rm F} a_\uparrow \simeq 0.51 < k_{\rm F} a_\downarrow$ the field effect is roughly canceled and $\rho_{b,\uparrow}(\omega) \sim \rho_{b,\downarrow}(\omega)$.

5. RF spectroscopy and experimental signature

The spectral functions discussed above are clear signatures for the Kondo effect, however, they are currently not directly measurable in experiment. In contrast, a well-established experimental technique for ultracold atomic gases is radio frequency (rf) spectroscopy. The retarded Green's



(a) (b)

Figure 2. (Color online) Spectral functions $\rho_{b,\uparrow}(\omega)$ and (b) $\rho_{b,\downarrow}(\omega)$ close to a confinement induced resonance for a number of different values of $k_{\rm F}a_\uparrow$.

function of itinerant states in presence of $n_{\rm imp}$ impurities is given by [1],

$$G_{\boldsymbol{k},\sigma}(\omega)^{-1} = \omega + i\eta - \xi_{\boldsymbol{k}} - n_{\rm imp}V_\sigma^2 G_{b,\sigma}(\omega), \tag{9}$$

and $\rho_{\boldsymbol{k},\sigma}(\omega) = -\frac{1}{\pi}{\rm Im}G_{\boldsymbol{k},\sigma}(\omega)$, $\eta \to 0$, is the momentum resolved spectral function. $n_{\rm imp}/N_a \approx 0.03$ is chosen in subsequent calculations. In ultracold gas experiments, $\rho_{\boldsymbol{k},\sigma}(\omega)$ can be measured directly by momentum resolved photo-emission spectroscopy [16, 17, 18]. Here we discuss the integrated rf response. The transition rate from a hyperfine state $|\sigma, \boldsymbol{k}\rangle$ to a different one $|3, \boldsymbol{k}\rangle$, which does not interact with others and is initially unoccupied, is given by [19],

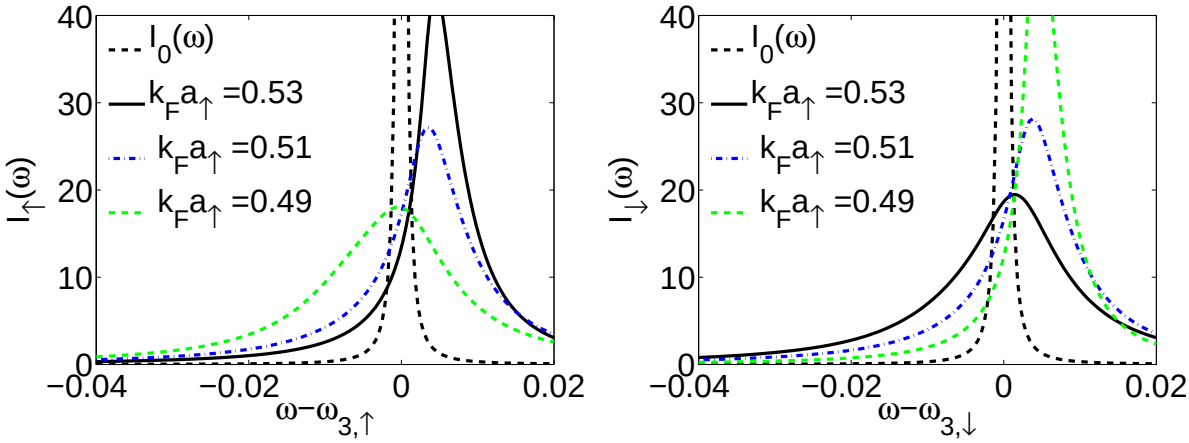
$$I_\sigma(\omega) = \frac{\Omega^2}{(2\pi)^4}\int {\rm d}^3k \int {\rm d}\omega'\ \rho_{\boldsymbol{k},\sigma}(\omega')\rho_{3,\boldsymbol{k}}(\omega+\omega')n_{\rm F}(\omega'). \tag{10}$$

Ω is the intensity and ω the rf frequency. We assume that $|3, \boldsymbol{k}\rangle$ is a free state shifted in energy by $\omega_{3,\sigma}$ with respect to the $|\sigma, \boldsymbol{k}\rangle$ states, $\rho_{3,\boldsymbol{k}}(\omega) = \delta(\omega - (\xi_{\boldsymbol{k}} + \omega_{3,\sigma}))$. In the case of non-interacting fermions, the RF spectrum $I_0(\omega)$ is proportional to a delta-function. The rf signal corresponding to Fig. 2(a)(b) is shown in Fig. 3(a)(b).

When comparing $I_\sigma(\omega)$ to $I_0(\omega)$ 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. This leads to a broadening of the spectral function $\rho_{\boldsymbol{k},\sigma}(\omega)$ and a small dispersion bending close to $\varepsilon_{\boldsymbol{k}} = \varepsilon_{\rm F}$, where the Kondo resonance lies. The signal in $I_\uparrow(\omega)$ broadens and shifts to smaller ω on decreasing $k_{\rm F}a_\uparrow$, and the opposite happens for $I_\downarrow(\omega)$. The signals in Fig. 3 are rather characteristic for the two peak structure in Fig. 2, such that the Kondo-correlated state and position of the Kondo resonance can be identified well with rf spectroscopy.

6. Conclusions

We have demonstrated how to realize a Kondo physics for a mixture of ultracold atoms employing confinement induced resonances. The proposed setup can be realized with experimental techniques currently available and the Kondo scale is accessible. In general, this allows one to analyze field dependent and anisotropic Kondo physics. There are numerous possible extension of our work including the study of non-equilibrium Kondo physics, Kondo lattice systems and signatures of quantum criticality.



(a) (b)

Figure 3. (Color online) rf spectra $I_\uparrow(\omega)$ (a) and $I_\downarrow(\omega)$ (b) close to a resonance for a number of different values of $k_F a_\uparrow$ as in Fig. 2. We also show $I_0(\omega)$, (broadened delta-function) for comparison.

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