# Author comments upon resubmission:

We thank the referees for their work and for their recommendation to publish in SciPost Physics. In particular, the reviews motivated us to check the interesting conjecture raised by referee 1 regarding the connection between the Kondo temperature and relaxation timescale. Please see our response below.

**Referee 1**

> The authors gave a elaborate answer and addressed the questions raised by both referees.
>
> To make the long story below short: Overall it is an very good paper, employing a difficult technique to a tough problem. The authors did their best to answer all questions to the best of their abilities. I can recommend the paper for publication in the revised version. However, personally I would reconsidering their definition of the Kondo temperature by carefully gauging it against other useful definitions that are developed for various numerical and experimental approaches.

We are thankful for this comment. Please see more about the definition of the Kondo scale and its relationship with the relaxation time below.

> In more detail:
>
> The authors gave a reasonable answer concerning their definition of the Kondo temperature. Apparently, they used the definition from the Bethe-ansatz also requering $U$ to be large! A different estimate is found in chapter 3 in Hewsons book. Here one has to bear in mind that additional corrections to these large $U$ formulas come into play since $U/\pi\Gamma$ is not very large for the parameters in the manuscript. The Kondo temperature is a crossover scale and can always be defined with some arbitrariness.

It is true that the Kondo temperature is a crossover scale and its various definitions agree only up to a constant even in the scaling regime. Our estimate for the Kondo temperature is indeed based on the Bethe-ansatz in the large $U$ limit (with some corrections for intermediate $U$), but is consistent with the appearance of the Abrikosov–Suhl resonance in the spectral function. As this is an essential and potentially confusing point, we have added this information to the revised version of the manuscript.

> I am a bit confuse by the statement in the reply: $\Delta = 2\Gamma$ as stated in the replay or $2 \times \Gamma/2 = \Gamma$ as written below Eq (58) of the manuscript?

We apologize for this not being entirely clear, but there is no typographic error. First off, we want to emphasize that the quantity $\Delta$ from the reply letter does not appear in the manuscript itself. It appears only in the reply letter, where we have copied the equation directly from Hewsons's book and subsequently identified the parameters in this formula with the ones used in our manuscript. The factor of 2 in the expression $\Delta = 2\Gamma$ stems from different conventions for the definition of coupling strength. This differs slightly depending on the field and the previous work that one wants to be consistent with. It has nothing to do with the factor of 2 arising from the fact that we consider a setup comprising two leads, which sets the sum (over leads) of the maximum coupling strength to $2 \times \Gamma/2 = \Gamma$. We hope that this explanation clarified the meaning of the formulas provided in the manuscript and the reply letter.

> Importantly, all parameters are stated clearly so that the reader can make up her/his own mind.

We agree that this is crucial.

> The spectrum shown in Fig R1 of the reply suggests that indeed the strongly correlated regime is addressed but the AS resonance is still very small (peak hight well below the Hubbard site peaks) and well below the zero temperature limit predicted by the Friedel sum rule. This is very encouraging since the NCA is operated in local moment regime in the vicinity or above $T_K$ as I suspected. One can also read off that the NCA underestimates the width of the Kondo resonance as expected for a second order approach in the hybridization strength: higher order processes contribute to the resonance as well.

Once again, we are in perfect agreement with the referee.

> Just a personal remark: It might be useful for the authors to consult PRL 81, 5226 (1998) for an operative experimental definition of $T_K$ exploiting the universality of the zero-bias conductance. It was gauged using the results of Costi and Hewson from 1994 and

works remarkable well. Employing Goldhaber-Gordon's approach immediately reveals that the choice of T must be above $T_K$.

We thank the referee for this comment. The 1998 Goldhaber-Gordon paper (now reference 99 in the revised manuscript) operationally defined $T_K$ as the temperature where the zero-bias conductance is $G_0/2$; here, that would give $T_K \simeq \Gamma$, consistent with our result. The expression used there, for $\epsilon_0 = -U/2$, can be written as $T_K = \frac{\sqrt{\Gamma' U}}{2} e^{-\frac{\pi U}{4\Gamma'}}$. If we had $\Gamma' = \Gamma$, this would indeed give a much lower Kondo temperature. However, the result from Hewson is very similar to this, except for a correction term that is only important at small values of $U$. It can be written as $T_K = \sqrt{\frac{\Delta U}{2}} e^{-\frac{\pi U}{8\Delta} + \frac{\pi \Delta}{2U}}$. Clearly this is consistent with Goldhaber-Gordon at large $U$ if and only if $\Gamma' = 2\Delta$. In turn, therefore, $\Gamma' = 2\Delta = 4\Gamma$ and the Kondo temperature using the formula in the Goldhaber-Gordon paper is $\sim 0.58\Gamma$: reasonable, but less accurate than the number we used, because it does not include the small-$U$ correction term. This shows that we are farther from the strong coupling regime than might be thought without carefully examining the choice of units, just as the very high Kondo temperature suggests. Once again, this choice of parameters is dictated by the desire to avoid pushing against the limits of the NCA's accuracy.

Why do I emphazise the importance of a proper identification of $T_K$? That becomes clearer when looking into the real-time dynamics which is the main focus of this paper. The other referee asked "What sets the time scale for the relaxation to the equilibrium? The Kondo temperature is set to 0.8 Gamma, nearly Gamma." and the authors answer "At equilibrium and in the scaling limit, we typically expect all time and energy scales to be universally determined by $T_K$".

This is only correct when focusing only on the dynamics govern by the low energy excitations of the system which excludes the charge dynamics. Also the spectral function does not only contain a Kondo resonance but also high energy features whose broadening is governed by $\Gamma$. Typically NEQ dynamics of local charges are governed by $\Gamma$, even below for $T \ll T_K$, while the spin dynamics is governed by $T_K$. The reason is obvious: local charge fluctuations are suppressed in the scaling limit. Clearly

> the charge susceptibility is governed by $1/\Gamma$ while the spin susceptible approaches $1/T_K$in the scaling limit.

We thank the referee for this comment. Indeed our statement was too broadly phrased and what the referee says is true, and even seen clearly in some of our own former papers.

> The authors continue in their reply " However, unlike the low-energy features, the transient peak in the energy-resolved singlet weight when starting from an empty dot clearly decays much more slowly (Fig. 3(a))"
>
> I also noticed this slow dynamics when reading the first version of the paper and that was the reason why I instigated a discussion on $T_K$. I suspected that the spin dynamics reported by the authors indeed governed by $T_K$. However, the authors' estimate for $T_K$ is simply to high such that this point was not recognised by the authors. The authors write in their reply "one can extract a timescale of $\sim 25\Gamma$", I guess they mean $\tau \approx 25/\Gamma$ which would be comparable with my estimate of $T_K$ in my first report, suggesting that $\tau \approx 1/T_K$
>
> Question: which other low energy scale should drive the long time dynamics? I suspect that there is non!

We appreciate this very insightful comment, which pushed us to reexamine some of our assumptions. The Kondo temperature is only defined up to an observable-dependent constant. To answer whether it controls the long relaxation timescale we observed, one must therefore consider scaling behavior. With this in mind, we investigated the relationship between the low-temperature decay time $\tau$ and $T_K$ (as obtained from the Bethe ansatz formula) for several values of $U$ between $4\Gamma$ and $10\Gamma$. Our preliminary results reveal that, at least within the NCA, $1/\tau$ is essentially *linear* in $T_K$ over this parameter range. So, even though the $T_K$ relevant to transport and given by the formulas above is rather large, this validates the referee's suspicion! The timescale is controlled by the Kondo temperature, but the relevant Kondo scale varies by a constant factor. We have included this information in the revised version of the manuscript and thank the reviewer for this comment. However, we chose not to include the plot or investigate the prefactor in too much detail until a more reliable method is available. Finally, we apologize for the mix-up in the units of $\tau$. Indeed, we meant $\tau \approx 25/\Gamma$.

**Referee 2**

> The authors have put much effort into answering the questions of the referees. I accept the authors' explanation that this manuscript goes beyond existing nonequilibrium studies of the Kondo effect and that the singlet-weights might be a useful tool for future theoretical and experimental studies. Thus, the manuscript fulfills the criteria of SciPost Physics. I recommend this manuscript for publication in SciPost Physics.

We thank the referee for this comment and for recommending publication in SciPost Physics.

# List of changes:

- at the top of page 14:
  We replaced the sentence

  > At equilibrium, these parameters suggest a Kondo temperature $T_K \approx 0.8\Gamma$ [3].

  by the more detailed statement:

  > We use the Kondo temperature as a measure for the emergence of correlation effects. The Kondo temperature is a crossover scale and its definition carries a degree of arbitrariness. A commonly used large $U$ estimate based on the Bethe ansatz suggests a Kondo temperature $T_K \approx 0.8\Gamma$ at equilibrium [3]. We found that this is consistent with the temperature at which the Abrikosov–Suhl resonance appears in the spectral function (data not shown) and in the differential conductance. This is also consistent with the operational definition used in Ref. [99].

- at the top of page 16:
  We have added the following statement to the revised manuscript:

Preliminary investigations of the scaling behavior of this timescale with $U$ reveal a linear relationship between the relaxation time and $1/T_K$. The relaxation dynamics is therefore fully determined by the Kondo temperature, albeit with a prefactor that remains to be understood. Further analysis will await numerically exact results.