Comment on “Scaling feature of magnetic field induced Kondo-peak splittings”[1]

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In a recent work[1] Zhang and coworkers (PRB 82, 075111 (2010)) studied the Zeeman splitting of the Kondo resonance for the single impurity Anderson model (SIAM) in a finite magnetic field $B$. They employed the numerical renormalization group (NRG) method to obtain spectral functions and discussed the position of the Kondo resonance in the spin-resolved spectral function at large magnetic fields. Additionally, they report a discrepancy between the position of the Kondo resonance in the total spectral function and the position in the spin resolved spectral function at large magnetic fields.

We show in the following, that both these conclusions cannot be drawn from the data presented in the publication, since they originate from the specific choice of NRG parameters.

We can indeed reproduce the published data[1] for the SIAM at $T = 0$ with $U = -2eV = 1$ and $\Gamma = 0.16$, which are depicted as set #1 in Fig. 1. However, we reproduce the crossover in the splitting from Kondo-like behavior to a non-universal splitting larger than the Zeeman energy, but this crossover occurs at much larger fields of the order of the charge scale.

In a recent work[1] Zhang and coworkers studied the Zeeman splitting of the Kondo resonance for the single impurity Anderson model (SIAM) in a finite magnetic field $B$. They employed the numerical renormalization group (NRG) to obtain spectral functions and discussed the position of the Kondo resonance in the spin-resolved and total spectral function, $\rho_\uparrow(\omega)$ and $\rho(\omega) = \sum_\sigma \rho_\sigma(\omega)$, respectively. Two important points made in the work are:

(i) With increasing magnetic field $B$ the position $\delta_\uparrow$ of the Kondo resonance in the total spectral function $\rho(\omega)$ does not approach its position $\Delta_\uparrow$ in the spin resolved spectral function, but instead $\Delta_\uparrow > \delta_\uparrow$.

(ii) The positions $\delta_\uparrow$ and $\Delta_\uparrow$ exceed the Zeeman energy, i.e. $\delta_\uparrow, \Delta_\uparrow > B$ for $B/T_K \gtrsim 5 − 10$, where $T_K$ is the low energy Kondo scale of the model ($g = 2, \mu_B = k_B = \hbar = 1$).

We show in the following, that both these conclusions cannot be drawn from the data presented in the publication, since they originate from the specific choice of NRG parameters.

We can indeed reproduce the published data[1] for the SIAM at $T = 0$ with $U = -2eV = 1$ and $\Gamma = 0.16$, which are depicted as set #1 in Fig. 1. For this set the discretization parameter is $\Lambda = 2.5$, only a small number of states $N_s = 150$ are retained in each NRG iteration, a large broadening of $\alpha = 0.8$ is used, $N_z = 20$ different discretizations are averaged ($z$-averaging), and an additional shift $\gamma = \alpha/4$ is employed in the broadening procedure.

In the following, however, we demonstrate the strong sensitivity of peak maxima on the NRG parameters. While set #2 differs from set #1 only by setting $\gamma = 0$, for set #3, a discretization parameter $\Lambda = 2$ is used, $N_s = 1800$ states are kept, $\alpha = 0.075$, and $N_z = 12$ different conduction band discretizations are averaged. All data are calculated within the complete Fock-space algorithm[2] also employed by Zhang et al. [1] which coincides with full density-matrix approach[2] at $T = 0$.

The spin-resolved spectral function $\rho_\uparrow(\omega)$ in a finite magnetic field $B = 0.003273 \approx 2.2T_K$ is shown in (a), where $\Delta_\uparrow$ is the low energy Kondo scale of the model. In this case we argue that both these findings are a result of the specific choice of NRG parameter values. However, we reproduce the crossover in the splitting from Kondo-like behavior to a non-universal splitting larger than the Zeeman energy, but this crossover occurs at much larger fields of the order of the charge scale.

**FIG. 1:** (Color online) (a) Spectral function of the SIAM in a finite magnetic field for three different NRG parameters (see main text). The inset displays a close-up of the region around the Fermi energy and the arrows indicate the position of the latter is much narrower for set #3 and, most important for the present discussion, the positions of the maximum differ (indicated by the arrows in the inset). The inset shows for set #3 the position of the magnetic field. $\Delta_\uparrow/B = 1$ corresponds to the Zeeman field. The inset shows for set #3 the position normalized with the magnetic field. $\Delta_\uparrow/B = 1$ corresponds to the Zeeman field. The inset shows for set #3 the position of the magnetic field. $\Delta_\uparrow/B = 1$ corresponds to the Zeeman field.
and spin-resolved spectral functions are compared. For set #3, $\delta_\uparrow$ and $\Delta_\uparrow$ very quickly approach each other and are indistinguishable for $B \gtrsim 0.004 \approx 3T_K$ (see upper scale in the plots). In contrast, the curves for set #1 do not approach each other as observed in Ref. 1. Panel (c) displays the maximum of the Kondo resonance $\Delta_\uparrow$ in $\rho_\uparrow(\omega)$ as function of the applied magnetic field $B$. The curve of set #3 increases almost linearly for all fields. It is slightly below the Zeeman splitting and exceeds it only for very large fields $B \gtrsim 0.2 = 1.25\Gamma \approx 150T_K$ (see inset). In contrast, the curves for sets #1 and #2 increase much faster and exceed the Zeeman-splitting already for fields $B \gtrsim 0.02 \approx 15T_K$.

The discretization of the conduction band[4] within NRG represents a severe approximation and recovering the correct continuum limit (e.g. $\Lambda \rightarrow 1^+$ and $N_s \rightarrow \infty$) is conceptually far from trivial. The broadening procedures adopted in the standard approaches[4, 5] offer no concise method, how to choose specific values for the parameters involved. But as these parameters are artificial and remain $\Lambda$ dependent, the physical phenomenon of interest must not depend on the actual value of these parameters. In Fig. 1 we demonstrate that the results of Zhang et al.[1] are non-universal since they are strongly dependent on the broadening parameters. Even changing only the artificial shift from $\gamma = \alpha/4$ (as in set #1) to $\gamma = 0$ (as in set #2) considerably changes the peak positions. In contrast, changing the same parameter for set #3 (within reasonable bounds, e.g. $0 \leq \gamma < \alpha$) does not change the spectral functions. This also holds for the other parameters, where the artificial broadening $\alpha$ is most critical. Increasing $\alpha$ reduces the critical field, where the $\Delta_\uparrow$ exceeds the Zeeman splitting. Generally, the accurate extraction of Zeeman-split peak positions from NRG spectral functions is a very delicate task as these always occur at finite energies, where the discretization errors are in principle not negligible.

We therefore argue that the two results of Zhang et al.[1] stated above are inconclusive and have been obtained by a particular choice of NRG parameters. Since there does not exist a “correct” choice for these parameters, physical conclusions must only be drawn from NRG spectra which are robust to changes of NRG parameters or error bars should be given. Neither requirement appears to be fulfilled by Ref. [1] as demonstrated above.

However, we reproduce the crossover in the Zeeman splitting from Kondo-like behavior, $\Delta_\uparrow/B < 1$, to a non-universal splitting with $\Delta_\uparrow/B > 1$ [see inset in Fig 1(c)]. But this crossover occurs at fields of the order of the charge scale, $B \sim \Gamma$, that is for fields two orders of magnitude larger than reported in Ref. [1].

ACKNOWLEDGMENTS

We thank Hui Zhang for helpful discussions and for sharing the details of his calculations with us. We acknowledge financial support from the Deutsche Forschungsgemeinschaft under AN 275/6-2.

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We show in the following, that both these conclusions cannot be drawn from the data presented in the publication, since they originate in an improper choice of NRG parameters.

We can indeed reproduce the published data [1] for the SIAM at $T = 0$ with $U = -2\epsilon = 1$ and $\Gamma = 0.16$, which are depicted as set #1 in Fig. 1. For this set the discretization parameter is $\Lambda = 2.5$, only a small number of states $N_s = 150$ are retained in each NRG iteration, a large broadening of $\alpha = 0.8$ is used, $N_z = 20$ different discretizations are averaged ($z$-averaging), and an additional shift $\delta = \alpha/4$ is employed in the broadening procedure. In the following, however, we demonstrate the strong sensitivity of peak maxima on the NRG parameters.

While set #2 differs from set #1 only by setting $\gamma = 0$, for set #3, a discretization parameter $\Lambda = 2$ is used, $N_s = 1800$ states are kept, $\alpha = 0.075$, and $N_z = 12$ different conduction band discretizations are averaged. All data are calculated within the complete Fock-space algorithm [2] also employed by Zhang et al. [1] which coincides with full density-matrix approach [2] at $T = 0$.

The spin-resolved spectral function $\rho_\uparrow(\omega)$ in a finite magnetic field $B = 0.003272 \approx 2.2T_K$ is shown in Fig. 1(a) for these three different parameter sets. While the results share the same qualitative features, they still differ considerably. The differences do not only affect high energy features like the Hubbard satellites, but also the low energy Kondo resonance (see inset). The width of the latter is much narrower for set #3 and, most importantly for the present discussion, the positions of the maximum differ (indicated by the arrows in the inset).

In panel (b) the positions of the Kondo maxima in total and spin-resolved spectral functions are compared. For set #3, $\delta_\uparrow$ and $\Delta_\uparrow$ very quickly approach each other and are indistinguishable for $B \gtrsim 0.004 \approx 3T_K$ (see upper scale in the plots). In contrast, the curves for set #1 do not approach each other as observed in Ref. [1]. Panel (c) displays the maximum of the Kondo resonance $\Delta_\uparrow$ in $\rho_\uparrow(\omega)$ as function of the applied magnetic field $B$. The curve of set #3 increases almost linearly for all fields. It is slightly below the Zeeman splitting and exceeds it only for very large fields $B \gtrsim 0.2 = 1.25T_K \approx 150T_K$ (see inset). In contrast, the curves for sets #1 and #2 increase much faster and exceed the Zeeman-splitting already for fields $B \gtrsim 0.02 \approx 15T_K$.

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