Surprises in the local density of states of the interacting resonant level model

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We present results of the impurity local density of states of the interacting resonant level model at zero temperature. We concentrate on low-energy properties and predominantly use the numerical renormalisation group technique. As interaction is increased, we find that the resonance peak at zero energy disappears, while two new peaks at finite energy emerge. This is in the absence of any field breaking the resonance. We further show that the height of the spectral function does not scale in the same way as the width, and in fact defines a second distinct exponent. We back up our results with analytic strong-coupling calculations as well as an analytic diagrammatic renormalisation group calculation that rather surprisingly gets the second exponent exactly, even for strong interactions.

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Introduction - Since the times of Kondo\textsuperscript{1} and Anderson\textsuperscript{2}, physicists have been fascinated by the possible effects of embedding a correlated quantum impurity in a metallic host \textsuperscript{3–6}. Recently, a lot of work in this area has also concentrated around the Interacting Resonant Level model (IRLM) \textsuperscript{7–22}; first introduced in 1978\textsuperscript{7} as formally equivalent to the anisotropic Kondo model, it gained a lot of interest in its own right since various exact solutions out of equilibrium were proposed for it \textsuperscript{13–15}. Despite a lot of progress being made on non-equilibrium transport in the IRLM\textsuperscript{8–22}, there remains open questions about equilibrium properties.

Many studies \textsuperscript{7–22,26} have shown that certain ground state properties such as the local susceptibility depend on a single energy scale, the equivalent of the Kondo temperature. This energy scale has a power law dependence on the hybridisation between the impurity and the leads; in a recent work\textsuperscript{27} we showed that this power can be calculated exactly, even for strong interactions. We also showed that the shape of this susceptibility as a function of a local field only varies slightly as a function of interaction, through a formula originally given in \textsuperscript{28,29}, with the profile shape being Lorentzian.

In this work, we study the local density of states (LDoS) of the IRLM in the ground state, which unlike the susceptibility, also depends on excitations. Without interactions, these two properties are identical, and in some previous work on the IRLM they are used interchangeably. We show that in the presence of interactions, while the susceptibility is always scaled by the Kondo temperature, the local density of states depends on an additional (emergent) energy scale with a different exponent. In addition, strong interaction values split the central resonance peak of the LDoS, thus changing the Lorentzian profile.

Model - The interacting resonant level model consists of a one-dimensional non-interacting lead of spinless fermions coupled to a single level via a weak hybridisation $t'$ and an interaction $U$, as illustrated in Fig. 1. The Hamiltonian for the single lead IRLM is written in second quantised notation as:

\[
\mathcal{H} = -\sum_{n=0}^{N-1} t_n (c_{n+1}^\dagger c_n + h.c) + \varepsilon_0 d^\dagger d + t' (c_0^\dagger d + h.c) + U (d^\dagger d - 1/2) \left(c_0^\dagger c_0 - 1/2\right). \tag{1}
\]

The $c$ and $d$ operators are of fermionic nature: $d$ is the resonant level annihilation operator, and $c_n$ are (spinless) fermion annihilation operators at a site $n$ on the lead. The impurity level is resonant if its energy $\varepsilon_0$ is equal to the Fermi level on the lead, in this case both will be zero.

For convenience we use a tight binding model for the lead; in the ideal case the lead is uniform $t_n \equiv t$ and semi-infinite $N \to \infty$. Numerics are performed using the Numerical Renormalisation Group (NRG)\textsuperscript{30} which has finite $N$ and introduces a logarithmic discretization of the lead band by taking hopping amplitudes $t_n$ depend on $\Lambda$ as $t_n \sim \Lambda^{-n/2}$ where $\Lambda$ is the discretisation parameter; the uniform lead limit corresponds to $\Lambda \to 1$. The main property of the lead relevant for this work is the density of states at the Fermi level $\nu \sim t^{-1}$, which corresponds to a bandwidth of $2t$ in the uniform lead. Throughout

\begin{figure}[h]
\centering
\includegraphics[width=0.8\textwidth]{fig1}
\caption{NRG approach for the IRLM. Adding a new site to the existing chain of $N$ sites + impurity enlarges the Hilbert space at lower energy scales, from which only the lowest $S_K$ energy states are kept after truncation.}
\end{figure}
this work, we will focus on the repulsive regime $U \geq 0$ of the interaction.

**Local density of states** – The main object of study in this work is the local density of states, defined by:

$$A(\omega) = \text{Im} \left[ \frac{i}{\pi} \int_0^\infty dt e^{i\omega t} \langle d(t)d(0) + d^\dagger(0)d(t) \rangle \right]$$  \hspace{1cm} (2)

This quantity is a measure of excitations in the ground state of the system, and may be directly measured in scanning tunneling microscopy experiments. In the non-interacting system ($U = 0$), this is given by a Lorentzian with $T_0 = \pi \nu(t')^2$ representing the resonance width. To study the change in the resonance shape as interaction is increased we use the NRG, referring the reader to [6] for details on the method.

In Fig. 2 we plot $A(\omega)$ for different values of $U$ over a large energy range. The main thing to notice is that the spectral weight shifts from the central resonant peak towards high energies. These side peaks appearing at roughly $\omega = \pm U/2$ are equivalent physics to the Hubbard bands in the Anderson impurity model; similar physics has also been previously seen in a two-lead version of the model. In this work, we study the evolution of the low energy resonant peak for $\omega \nu \ll 1$, always keeping in mind that for large interactions, most spectral weight is not in the low-energy sector.

**Resonant peak** – For low energy properties, the bare interaction strength $U$ is not a particularly useful parameter, and it is better to use a dimensionless quantity $g$ defined as:

$$g = \frac{2\delta}{\pi} = \frac{2}{\pi} \arctan \left( \frac{U\pi \nu}{2} \right) \hspace{1cm} g \in [0, 1] \leftrightarrow U \geq 0. \hspace{1cm} (3)$$

In this expression, $\delta$ represents the scattering phase shift of fermions at the Fermi level when reaching the lead boundary, which is given by the above expression for a tight-binding lead. For leads with a different band structure or field theories with a different regularisation, the relationship between $g$ and $U$ would change, however the low-energy physics for a given phase shift is universal.

If scaled correctly, the low-energy shape of the spectral function is independent of the $t'$ parameter. The resonance width $T_K$ (equivalent to the Kondo temperature and known from previous works) defines a natural dimensionless variable $\omega/T_K$. We define another energy scale as $T_A = 1/A(\omega = 0)$, meaning that the scaled spectral function is always 1 at zero energy. If we look at data plotted in Fig. 3, we see that curves for different values of $t'$ collapse onto universal curves dependent only on the interaction strength $g$.

We defer analysis on the scaling behavior for the next section; for now we concentrate on the most obvious feature of this plot which is that the (low-energy) central peak splits in two as interaction strength is increased. We stress that this splitting is nothing to do with the Hubbard bands in Fig. 2 which occur at much larger energy – this is an intrinsic splitting of the low-energy resonant peak. We also emphasise that unlike previous work on the splitting of the resonance peak in the Kondo model, this occurs without an external field splitting the energies of the resonant level, or coupling to any other degree of freedom. Another aspect that makes this evolution particularly surprising is that it is not seen in the susceptibility $\chi = -(\partial^2 d^\dagger d/\partial \varepsilon_0)$ which remains approximately in Lorenzian shape for all values of interaction.

The physics of this splitting is relatively straightforward to see in the strong interaction $g \to 1$ ($U \to \infty$) limit, where the resonant level and the final site of the lattice must contain exactly one electron between them at low-energy to avoid paying the high interaction cost $U$. The effective model consists on a two-level system weakly coupled to the rest of the lead; however this two-level system is not resonant as the energies are split by the hybridisation $t'$ (which is equivalent to $T_K$ in the strong interacting limit). This accounts for the splitting in the strong coupling limit.

To investigate the splitting numerically, we have plotted the scaled spectral function $A(\omega/T_K,g) T_A(g)$ in Fig. 5 as a density plot, with $T_A(g) \equiv \max(A(\omega, g))$. We superimpose on top of the density plot the locations of local minima and maxima as a function of $\omega$ for a given interaction strength. This shows a somewhat surprising feature – the central peak doesn’t in fact split. Rather, side peaks appear at $\omega \sim \pm T_K$ at some critical interaction strength $g_{c1} \approx 0.454$, with the central peak turning into a local minimum at a slightly higher interaction $g_{c2} \approx 0.463$. This evolution of the shape near
the critical interaction strengths is shown in more detail in Fig. 3, where it is seen that a shoulder develops a little bit before the side-peaks appear.\cite{53}

This supports a scenario of a general shape of the spectral function consisting of one peak centered on \( \omega = 0 \) with another two centered at \( \omega \sim \pm T_K \). As interaction is increased, the relative weight of the central peak (corresponding to the weak-coupling resonant dot) decreases, while that of the side peak (corresponding to the strong-coupling off-resonant effective dot) increase. In this sense, the transitions should be thought of more as a crossover, with there being no particular significance to \( g_{c1} \) or \( g_{c2} \). On the other hand, exactly at \( g_{c2} \) when the curvature at \( \omega = 0 \) changes, the low-energy behavior of the spectral function is not \( \omega^2 \), which could be considered a defining property of a non-Fermi liquid \cite{37,38}.

Such a potential non-Fermi liquid is only at a single point in parameter space, making it different from, for example, the non-Fermi liquid behavior of the two-channel Kondo model\cite{39,43}. However, over this range of intermediate interactions, the coefficient of the \( \omega^2 \) term in the spectral function is much smaller than would be expected by the width of the resonance (i.e. the scale \( T_K \)). It is an open question how this region with relatively incoherent electronic excitations would manifest itself in observable properties.

Energy scales – In previous works on thermodynamic quantities, it has been observed that \( T_K \) is the only low energy scale in the system, with a collapse of data for different values of \( t' \) so long as energies are scaled by \( T_K \)\cite{21,44}. Numerical studies have even shown the single energy scale scaling for non-equilibrium steady state transport\cite{12,17,21,22}, sub-leading corrections to full-counting statistics\cite{45,46}, quenches\cite{16,47,48} and out-of-equilibrium entanglement entropy growth\cite{49}.

We will show however for the spectral function, one needs to define two distinct energy scales which depend on the hybridisation \( t' \) in different ways. To be precise, these are defined as

\[
T_K^{-1} = \chi(\epsilon_0 = 0), \quad T_A^{-1} = A(\omega = 0). \tag{4}
\]

The scale \( T_K \) is given by a power law in the hybridisation \( T_K \sim (t')^\alpha \), where \( \alpha = 2 \) for the non-interacting case, while previous work\cite{27} has given an exact expression \( \alpha = 2/(1 + 2g - g^2) \) when interactions are present. We use the known expression for \( T_K \) from previous work\cite{54}, which collapses multiple data sets for different hybridisations \( t' \) onto single curves.

If one tries to scale the vertical axis with the same \( T_K \) however, one does not get collapse. Defining \( T_A \) as in Eq. (4), we can extract this scale from NRG simulations\cite{54} for multiple values of \( t' \) and fit \( T_A = C(t')^\gamma \) for each value of interaction. The results are shown in Fig. 4 where empirically, we can fit

\[
\gamma = \alpha(1 - g^2) = \frac{2(1 - g^2)}{1 + 2g - g^2}, \tag{5}
\]
a relationship we will analytically derive shortly. In the inset, we show that even for small interactions, we...
At energy scales of the bandwidth, $\hbar \gamma$, while $\hbar$ is lowered, interactions these parameters will flow as energy to the renormalisation group paradigm, in the presence of interactions this limit of the exponent by using non-perturbative techniques such as bosonization is an open question; however, it seems likely that in this case, the equivalence to the sine-Gordon model that works so well for the exact mapping between the IRLM and the anisotropic Kondo model [7], we believe that an interesting question in which situations this limit of the exponent by using non-perturbative techniques such as bosonization is an open question; however, it seems likely that in this case, the equivalence to the sine-Gordon model that works so well for the Kondo model might arise naturally, allowing for experimental realisation of the physics described here.

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**Final remarks and outlook** – We have studied the impurity spectral function of the interacting resonant level model over the full range of interactions from weak to strong. Our two main results are:

1. As interaction is increased, the spectral function begins to deviate significantly from a Lorentzian shape, eventually splitting into two separate peaks at $\omega \sim T_K$ for interactions $U \nu \sim 1$.

2. The height of the spectral function $A(\omega)$ defines a new energy scale $T_A$ which scales with the hybridisation $t'$ with a different exponent than $T_K$. The expression for the exponent which is obtained from perturbative RG appears to work for all interaction strengths.

It is an open question whether such features of the spectral function would also manifest in any other observable quantities either in equilibrium or out. Finally, due to the exact mapping between the IRLM and the anisotropic Kondo model [7], we believe that such features should emerge in the case of strong $S_z$ interaction with perturbative $S_{xy}$ exchange. It is an interesting question in which situations this limit of the Kondo model might arise naturally, allowing for experimental realisation of the physics described here.

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**FIG. 4:** The scaling exponent $\gamma$ associated to the energy scale $T_A$, Eq. (3) for different NRG parameter sets. The $\alpha$ exponent curve is included for comparison. Inset: NRG data for the weak coupling sector, showing the deviation of data points from the $\alpha$ curve at $(O(g^2))$ in the interaction.
