Poor Man’s Understanding of Kinks Originating from Strong Electronic Correlations

K. Held, R. Peters, and A. Toschi

1 Institute of Solid State Physics, Vienna University of Technology, A-1040 Vienna, Austria
2 Department of Physics, Kyoto University, Kyoto 606-8502, Japan

(Dated: May 22, 2014)

By means of dynamical mean field theory calculations, it was recently discovered that kinks generically arise in strongly correlated systems, even in the absence of external bosonic degrees of freedoms such as phonons. However, the physical mechanism behind these kinks remained unclear. On the basis of the perturbative and numerical renormalization group theory, we herewith identify these kinks as the effective Kondo energy scale of the interacting lattice system which is shown to be smaller than the width of the central peak.

PACS numbers: 71.27.+a, 71.10.Fd

Kinks in the energy vs. momentum dispersion-relation indicate deviations from a quasiparticle renormalization of the non-interacting system. Hence, these kinks provide valuable information of many-body effects. The textbook example is the coupling of the electronic system to external, bosonic degrees of freedom such as e.g. phonons. In this situation, a kink naturally develops at the bosonic eigenenergy. The low-energy kinks in high-temperature superconductors at 40-70 meV are hence taken as evidence for an electron-phonon or a spin-fluctuation pairing mechanism. Besides these low-energy kinks, kinks at higher energies have been reported, not only in cuprates but also in various transition metals and transition metal oxides. These kinks are at 50-800 meV, often beyond the relevant bosonic energy scales associated with phonons or non-local spin fluctuations.

On the theoretical side, kinks at similarly high energies have been found by serendipity in local density approximation plus dynamical mean field theory (LDA+DMFT) calculations of SrVO$_3$. In these calculations the aforementioned bosonic degrees of freedom are clearly absent, and the physical origin is to be found in the strongly correlated electronic system itself. It was shown mathematically that a three peak spectrum with a lower and upper Hubbard band and a well pronounced central peak in-between generically results in a kink in the energy-momentum dispersion of the one-particle excitations. While it was clear, given the structure of the DMFT equations, that the central peak of width $\Gamma$ was associated with Kondo physics, the physical origin of the emergence of a second (kink) energy scale $\omega^* < \Gamma$ remained mysterious. This kink also reflects in other quantities, most notably the specific heat. It has been observed as well in other materials and models such as LaNiO$_3$, $f$-electron systems, and the two-band Hubbard model. At the kink energy there is a maximum in the local spin susceptibility, which was considered to represent “emergent collective spin-fluctuations”. For two bands of different width a single maximum in the spin susceptibility along with a single kink energy scale has been found, which put the generalizability of into question. Most of all, a physical understanding was hitherto missing: Why is there a second energy scale besides the width of the central peak?

In this paper, we identify the physical origin to be the crossover to the strong coupling fix point. That is, the kink corresponds to the effective Kondo energy scale which, for the Hubbard model, is different from the width of the central peak in the spectral function. Our conclusions are based on a very simple, albeit analytical approach, Anderson’s poor man scaling as well as numerically precise numerical renormalization group (NRG) calculations. In the following, we will first provide for a qualitative overview by means of Fig. 1. Next we present the perturbative renormalization group calculation. Thereafter, we discuss its relevance for Hubbard-type models and transition metal oxides; and finally the NRG results corroborating the analytical calculation.

Overview. The usual Kondo system consists of an interacting impurity site which is coupled to a non-
interacting conduction band by a hybridization amplitude $V$. Usually, the conduction electron bandwidth is the largest energy scale of the system, see Fig. 1 (left hand side). At the Kondo energy scale a central quasiparticle peak develops. At the same energy scale the imaginary part of the susceptibility $\text{Im}\chi(\omega)$ exhibits a peak [33], which can be understood as an effective scattering of quasiparticles and quasi-holes at each other. One can also consider this as a bosonic mode emerging from local spin fluctuations similar to those reported in [28]. However, this is the relevant situation for strongly correlated lattices, e.g., for describing an iron impurity in gold. Moreover, in this case, there is no kink in the real part of the self energy, separating two different linear behaviors.

The situation is very different if we instead consider a Kondo system with a very narrow conduction electron band, which is strongly coupled to the impurity site, see Fig. 1 (right hand side). Let us stress that this is not the usual situation considered for the Anderson impurity model, e.g., for describing an iron impurity in gold. However, this is the relevant situation for strongly correlated lattice models, describing e.g. transition metal oxides. For such a model or material an electron leaving a site with hopping amplitude $\sim D$ enters a strongly correlated lattice. Also on other lattice sites, there are hence correlation effects which lead to a renormalized, very narrow bandwidth for the central peak of the spectrum around the Fermi level. The electron considered is moving within this very narrow band. At a later time the electron might return to the original site and, possibly, interact (by local interaction $U$) with a second electron on the depicted site.

This description of locally interacting electrons, which can propagate via the (self-energy renormalized) other sites is at the heart of DMFT [17]; DMFT even maps the correlated lattice problem onto an Anderson impurity whose local propagator includes the described self-energy contributions from all other sites. This Anderson impurity model is calculated self-consistently and for strong electronic correlations has a non-interacting density of states (DOS) as depicted in Fig. 1 (right hand side) [17, 29]. This DMFT description neglects non-local correlations such as the mentioned non-local spin fluctuations [4, 5]. At least in three dimensions, one can however expect DMFT to yield reliable results at sufficiently high temperatures or energies, such as the few hundred meV of high energy kinks.

As we will show below, there are two energy scales in the narrow, correlated band situation: one associated with the width of the central peak and one associated with the Kondo energy scale which is again connected to a maximum in $\text{Im}\chi(\omega)$, as well as to a stronger quasiparticle renormalization. This explains the observations of [28] and [22, 23], respectively. In contrast, for the usual impurity situation considered (Fig. 1 left hand side) the first energy scale, i.e., the bandwidth of the central peak is missing, since the conduction electron bandwidth is essentially infinite. Here, only the Kondo energy scale remains.

**Poor man’s scaling.** In Anderson’s perturbative renormalization group approach, the conduction electrons are eliminated step-by-step by reducing the bandwidth of the conduction electrons from $[-D, D]$ to $(-\delta D, (D - \delta D))$ in the Kondo model [30, 31]. This renormalizes the interaction $J = 4V^2/U$ between impurity spin and conduction spin by

$$dJ(D)/d\ln D = -2\rho(D)J^2(D). \quad (1)$$

Here, $\rho(D)$ is the DOS of the conduction electrons at the energy $D$ and $-\delta D$ around which the conduction electrons are integrated out by second order perturbation theory.

Usually, $\rho(D)$ is taken constant which results in a Kondo temperature $T_K = D_0 e^{-1/(\rho_0 J(D_0))}/\Gamma$ [30, 31]. In our case, a constant density of states is, however, certainly not appropriate. Hence, we now employ Anderson’s poor man scaling for the situation depicted in Fig. 1 (right hand side) instead of the constant one (left hand side). A reasonable description for the conduction electron DOS arising from strong correlations is a Lorentzian $\rho(D) = \rho_0 \pi/(D^2 + \Gamma^2)$ of width $\Gamma$, the width of the central spectral peak. In this case the integration of Eq. (1) from the initial band edge $D_0$ to $D$ yields

$$\frac{1}{J(D)} - \frac{1}{J(D_0)} = \rho_0 \ln \left( \frac{D^2}{D^2 + \Gamma^2} \right)^{D_0} . \quad (2)$$

Collecting all terms with cutoff $D$ and $D_0$ on the left and right hand side, respectively, yields,

$$\frac{D^2}{D^2 + \Gamma^2} e^{-1/(\rho_0 J(D_0))} = \frac{D_0^2}{D_0^2 + \Gamma^2} e^{-1/(\rho_0 J(D_0))}, \quad (3)$$

$$D_0 \to \infty \quad e^{-1/(\rho_0 J(D_0))} = \text{const.} \quad (4)$$

Here, we have set the initial cut-off $D_0$ to infinity in the second line, and identified the combination of $D$ and $J(D)$ on the left hand side to be invariant under the renormalization group flow. This can be compared to the usual poor man’s scaling result [30, 31] for a constant DOS, i.e., $\rho(D) = \rho_0$:

$$D e^{-1/(\rho_0 J(D_0))} = D_0 e^{-1/(\rho_0 J(D_0))} = \text{const.} \equiv T_K. \quad (5)$$

If the energy (cutoff) $D$ approaches the Kondo temperature in Eq. (5), the coupling $J(D)$ diverges. This marks the crossover to the strong coupling fix point in the renormalization group flow.

For the narrow conduction band case Eq. (3) on the other hand, this divergence of $J$ and hence the strong coupling fix point is approached for

$$D = D^* = \sqrt{\eta/(1 - \eta)} \Gamma \quad \text{with } \eta = e^{-1/(\rho_0 J(D_0))}. \quad (6)$$

That is besides the conduction electron (half) bandwidth $\Gamma$, there is a second energy scale $\omega^*$ in the problem, at which the Kondo effect marks the crossover to the
strong coupling fix point. This crossover is accompanied by strong local spin fluctuations, connected to the above mentioned maximum in \( \Im \chi \), and the stronger quasi-particle renormalization of the strong coupling fix point.

Relevance for DMFT and kinks in transition metal oxides. The two energy scales \( \Gamma \) and \( \omega^* \) are relevant for strongly correlated electron systems with a central peak. For the one-band Hubbard model with semicircular DOS (Bethe lattice) and half bandwidth \( D \), the DMFT self-consistent Anderson impurity model has the following non-interacting Green function \([12]\):

\[
G_0^{-1}(\omega) = \omega + \mu - (D/2)^2 G(\omega). \tag{7}
\]

For a general DOS, there are corrections to Eq. (7), which however still remains the leading term in a momentum expansion of the DOS.

At the same time, this non-interacting Green function \( G_0 \) is connected to the hybridization \( V \) and the non-interacting conduction-electron Green function \( G_0 \) of the Anderson impurity model through

\[
G_0^{-1}(\omega) = \omega + \mu - V^2 G_0(\omega). \tag{8}
\]

As already depicted in Fig. 1 (right hand side), this local non-interacting Green function \( G_0 \) stems from hopping processes, with electrons leaving the impurity site with amplitude \( D \) (\( V \)), moving through a narrow conduction band with DOS \( \rho(\omega) = -\frac{1}{2\pi} \Im G_0(\omega) = -\frac{1}{2\pi} \Im G(\omega) \) if we take \( V = D/2 \), note that only the combination \( \rho(\omega)V^2 \) is relevant in Eq. (8).

We can disregard the Hubbard side bands of DMFT in \( \Im G(\omega) \) or \( \rho(\omega) \) since virtual excitations at large energies are suppressed in the renormalization group flow (only yield a negligible renormalization of \( J \)). Therefore, we can concentrate on the central peak whose spectral function \( A(\omega) = -\frac{1}{2\pi} \Im G(\omega) \) can be approximated by a Lorentzian of width \( \Gamma \) and height \( \rho(0) = 2/(\pi D) \). The latter is pinned to its non-interacting value \([12]\).

For half-filling and a narrow enough central peak, we are in the Kondo regime so that we can map the Anderson impurity model directly onto a Kondo model with \( J = 4V^2/U \). In other cases, this is also possible but only after first renormalizing the parameters of the Anderson impurity model itself \([31]\). For this \( J \) and a typical value of \( U = 2D \) for a three peak spectrum, we obtain \( \omega^* = 0.21\Gamma \) from Eq. (6); for a larger value of \( U = 2.8D \) we obtain \( \omega^* = 0.11\Gamma \). Hence, the Kondo and kink energy scale \( \omega^* \) is directly related to the (half)width of the central peak \( \Gamma \); and both of them get smaller and smaller when we approach the Mott-Hubbard transition. Note, also \( Z_{FL}D \) is directly related to \( \Gamma \) (or \( Z_{CP}D \)), see \([23, 37]\).

What do we have in the energy region \( \omega^*, \Gamma \) if the Kondo effect only sets in at \( \omega^* \)? Here, in the DMFT the parameters are such that \( J \) and \( \rho(\omega) \) are large even without a renormalization of \( J \) as soon as \( \omega \lesssim \Gamma \). Hence, even without the Kondo effect, there is already spectral weight in the central peak for \( \omega \in [\omega^*, \Gamma] \). At \( \omega^* \), the Kondo effect then strongly renormalizes \( J \), which translates into a much stronger renormalization of the quasiparticles and a kink in the self energy.

Indeed, in DMFT we have necessarily \( \Gamma > \omega^* \). Otherwise, i.e., for \( \omega^* = \Gamma \), the renormalization group flow from an infinitesimally small energy interval around \( \omega^* = \Gamma \) would strongly renormalize \( J \) to the strong coupling fix point, which is mathematically not possible. The bandwidth of the central peak hence defines the second energy scale \( \Gamma > \omega^* \). While the Kondo energy is \( \omega^* \), the Kondo effect indirectly generates also the energy scale \( \Gamma \) through the DMFT self-consistency, which physically describes that there is similar Kondo physics on the neighboring sites. There is a strongly enhanced coupling even above the Kondo scale \( \omega^* \) but not beyond \( \Gamma \).

Numerical renormalization group. It is well known \([31]\) that terms in 3rd order perturbation theory and beyond may modify the Kondo temperature. Hence, we have also employed the numerical renormalization group (NRG) \([34, 36]\) with cutoff parameter \( \Lambda = 2 \). Fig. 2 shows the DMFT(NRG) self energy, spectral function and spin susceptibility for the Hubbard model at \( U = 2D \) with Bethe DOS. Clearly, there is a kink at \( \omega^* \) in the real part of the self energy. The slopes of the self energy before and after the kink define two different renormalization factors \( Z_{FL(CP)} = \left[ 1 - \frac{\partial \Re \Sigma(\omega)}{\partial \omega}|_{\omega^*} \right]^{-1} \) with \( Z_{FL} < Z_{CP} \). The overall halfwidth of the central peak is \( \Gamma = Z_{CP}D \) so that we can read of the kink energy in Fig. 2 as \( \omega^* \approx 0.21\Gamma \), in agreement with the poor man’s scaling prediction. The same holds for \( U = 2.8D \), where NRG yields \( \omega^* = 0.004D \) and \( \Gamma = 0.036D \), i.e., \( \omega^* \sim 0.11\Gamma \) in unexpectedly good agreement with poor man’s scaling.
to the strong coupling fix point. That the kink energy \( \omega^* \) scale which is smaller than the (half)width \( \Gamma \) of the central peak of a strongly correlated electron system. At \( \omega^* \), we find the crossover to the strong coupling fix point which enhances the coupling strength and with this the quasiparticle renormalization. Hence, there is a kink in the self energy. Let us emphasize that this is a radically new insight; the present-day DMFT understanding is that the Kondo effect sets in already at \( \Gamma \). The crossover to the strong coupling fix point naturally leads to a maximum in the local spin susceptibility at \( \omega^* \) as was reported in [27, 28]. The same maximal spin susceptibility is also found at the Kondo energy scale of the usual Anderson impurity model with a wide conduction electron bandwidth [32]. However, in the latter case, there is no kink since the Kondo energy scale is the only low energy scale. In a two orbital model, there will be typically a joint SU(4) Kondo effect of all orbitals, which explains the single kink energy found in [27].

This explanation allows for distinguishing this kink from other kinks of different origin by searching in experiment for the typical Kondo physics [31] (keeping in mind the additional physics emerging between \( \omega^* \) and \( \Gamma \)). If one observes a kink in the energy-momentum relation of angular resolved photoemission spectroscopy (ARPES), the origin as a Kondo kink will be demonstrated by a simultaneous observation of a maximum in the frequency or temperature dependence of the susceptibility, the temperature dependence of the nuclear magnetic resonance (NMR) \( T_1 \) relaxation time, a change of the \( T^2 \) behavior in the resistivity, and a kink in the electronic specific heat.

**Acknowledgements.** This work has been supported by the European Research Council under the European Union’s Seventh Framework Programme (FP/2007-2013)/ERC through grant agreement n. 306447 (KH), the Japan Society for the Promotion of Science (JSPS) through the FIRST Program (RP), and the Austrian Science Fund (FWF) via Research Unit FOR 1346 (AT, FWF project ID I597).

---

1. See, e.g., N. W. Ashcroft and N. D. Mermin, Solid State Physics. Holt, Rine hart and Winston, USA, (1976).
2. A. Lanzara, P. V. Bogdanov, X. J. Zhou, S. A. Kellar, D. L. Feng, E. D. Lu, T. Yoshida, H. Eisaki, A. Fujimori, K. Kishio, J.-I. Shimoyama, T. Noda, S. Uchida, Z. Hussain, and Z.-X. Shen, Nature 412, 510 (2001).
3. Z.-X. Shen, A. Lanzara, S. Ishihara, and N. Nagaosa, Philos. Mag. B 82, 1349 (2002).
4. H. He, Y. Sidis, P. Bourges, G. D. Gu, A. Ivanov, N. Koshizuka, B. Liang, C. T. Lin, L. P. Regnault, E. Schoenherr, and B. Keimer, Phys. Rev. Lett. 86, 1610 (2001).
5. J. Hwang, T. Timusk, and G. D. Gu, Nature 427, 714 (2004).
6. J. Graf, G.-H. Gweon, K. McElroy, S. Y. Zhou, C. Jozwiak, E. Rotenberg, A. Bill, T. Sasagawa, H. Eisaki,
