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

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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.

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Kinks in the energy vs momentum dispersion-relation indicate deviations from a quasiparticle renormalization of the noninteracting system. Hence, these kinks provide valuable information of many-body effects. The textbook example [1] 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 [2–4] at 40–70 meV are hence taken as evidence for an electron-phonon [2,3] or a spin-fluctuation [4,5] pairing mechanism. Besides these low-energy kinks, kinks at higher energies have been reported, not only in cuprates [6–9] but also in various transition metals [10,11] and transition metal oxides [12–15]. These kinks are at 50–800 meV, often beyond the relevant bosonic energy scales associated with phonons or nonlocal 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 (DMFT) [16–21] calculations of $SrVO_3$ [22]. 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 [23] 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 (half)width Γ 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 noteworthy the specific heat [24]. It has been observed as well in other materials and models such as $LaNiO_3$ [25], f-electron systems [26], and the two-band Hubbard model [27]. At the kink energy there is a maximum in the local spin susceptibility [28], which was considered [28] to represent "emergent collective spin fluctuations." For two bands of a different width, a single maximum in the spin susceptibility along with a single kink energy scale has been found [27], which put the generalizability of [23] 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 Letter, 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 [29] 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

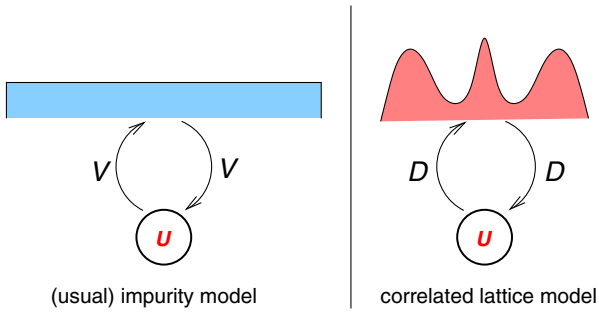

FIG. 1 (color online). Comparison of the usual Anderson impurity model of a strongly interacting site coupled via V to an uncorrelated featureless and wide conduction-electron band (left-hand side) and the Hubbard model situation (right-hand side). In the latter case, an electron leaving a correlated site moves within the strongly correlated and narrow band of the central peak. In this situation there is a kink at the effective Kondo energy scale which is smaller than the width of the narrow band.

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 noninteracting 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 $\mathrm{Im}\chi(\omega)$ exhibits a peak [30], which can be understood as an effective scattering of quasiparticles and quasiholes at each other. One can also consider this as a bosonic mode emerging from *local* spin fluctuations similar to those reported in [28]. However, 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 noninteracting density of states (DOS) as depicted in Fig. 1 (right-hand side) [17,31]. This DMFT description neglects *nonlocal* correlations such as the mentioned nonlocal 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 $\mathrm{Im}\chi(\omega)$, as well as to a stronger quasiparticle renormalization. This explains the observations of [22,23,28], 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, the conduction electrons are eliminated step-by-step by reducing the bandwidth of the conduction electrons from $[-\mathcal{D}, \mathcal{D}]$ to $[-(\mathcal{D}-d\mathcal{D}), (\mathcal{D}-d\mathcal{D})]$ in the Kondo model [29,32]. This renormalizes the interaction $J = 4V^2/U$ between the impurity spin and conduction spin by [29,33]

$$dJ(\mathcal{D})/d\ln\mathcal{D} = -2\rho(\mathcal{D})J^2(\mathcal{D}). \tag{1}$$

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

Usually, $\rho(\mathcal{D})$ is taken constant which results in a Kondo temperature $T_K = \mathcal{D}_0 e^{-1/[\rho_0 J(\mathcal{D}_0)]}$ [29,33]. 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 $\rho(\mathcal{D}) = \rho_0\Gamma^2/(\mathcal{D}^2+\Gamma^2)$ of width Γ, the width of the central spectral peak. In this case the integration of Eq. (1) from the initial band edge $\mathcal{D}_0$ to $\mathcal{D}$ yields

$$\frac{1}{J(\mathcal{D})} - \frac{1}{J(\mathcal{D}_0)} = \rho_0 \ln\left(\frac{\mathcal{D}^2}{\mathcal{D}^2+\Gamma^2}\right)\Bigg|_{\mathcal{D}_0}^{\mathcal{D}}. \tag{2}$$

Collecting all terms with cutoff $\mathcal{D}$ and $\mathcal{D}_0$ on the left- and right-hand sides, respectively, yields

$$\frac{\mathcal{D}^2}{\mathcal{D}^2+\Gamma^2} e^{-1/[J(\mathcal{D})\rho_0]} = \frac{\mathcal{D}_0^2}{\mathcal{D}_0^2+\Gamma^2} e^{-1/[J(\mathcal{D}_0)\rho_0]}, \tag{3}$$

$$\overset{\mathcal{D}_0\to\infty}{\longrightarrow} e^{-1/[J(\mathcal{D}_0)\rho_0]} = \text{const.} \tag{4}$$

Here, we have set the initial cutoff $\mathcal{D}_0$ to infinity in the second line, and identified the combination of $\mathcal{D}$ and $J(\mathcal{D})$ 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 [29,33] for a constant DOS, i.e., $\rho(\mathcal{D}) = \rho_0$:

$$\mathcal{D} e^{-1/[J(\mathcal{D})\rho_0]} = \mathcal{D}_0 e^{-1/[J(\mathcal{D}_0)\rho_0]} = \text{const} \equiv T_K. \tag{5}$$

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

For the narrow conduction band case Eq. (4) on the other hand, this divergence of J and hence the strong coupling fix point is approached for

$$\mathcal{D} = \omega^* = \sqrt{\eta/(1-\eta)}\Gamma \quad \text{with} \quad \eta = e^{-1/[J(\mathcal{D}_0)\rho_0]}. \quad (6)$$

That is besides the conduction-electron (half) bandwidth Γ, there is a second energy scale ω^* 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 $\mathrm{Im}\chi$ [30] and the stronger quasiparticle renormalization of the strong coupling fix point.

Relevance for DMFT and kinks in transition metal oxides.—The two energy scales Γ and ω^* 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 noninteracting Green function [17]:

$$\mathcal{G}_0^{-1}(\omega) = \omega + \mu - (D/2)^2 G(\omega). \quad (7)$$

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 noninteracting Green function $\mathcal{G}_0$ is connected to the hybridization V and the noninteracting conduction-electron Green function G_0 of the Anderson impurity model through

$$\mathcal{G}_0^{-1}(\omega) = \omega + \mu - V^2 G_0(\omega). \quad (8)$$

As already depicted in Fig. 1 (right-hand side), this local noninteracting Green function $\mathcal{G}_0$ stems from hopping processes, with electrons leaving the impurity site with amplitude D (V), moving through a narrow conduction band with DOS $\rho(\omega) = -(1/\pi)\mathrm{Im}G_0(\omega) = -(1/\pi)\mathrm{Im}G(\omega)$ [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 $\mathrm{Im}G(\omega)$ 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 $A(\omega) = -(1/\pi)\mathrm{Im}G(\omega)$ can be approximated by a Lorentzian of width Γ and height $\rho(0) = 2/(\pi D)$. The latter is pinned to its noninteracting value [17].

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 [33]. 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 ω^* is directly related to the (half)width of the central peak Γ, and both of them get smaller and smaller when we approach the Mott-Hubbard transition. Note also that $Z_{\mathrm{FL}}D$ is directly related to Γ (or $Z_{CP}D$); see [31,34].

What do we have in the energy region $[\omega^*, \Gamma]$ if the Kondo effect only sets in at ω^*? 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 ω^*, 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 ω^*, the Kondo effect indirectly generates also the energy scale Γ 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 ω^* but not beyond Γ.

Numerical renormalization group.—It is well known [33] that terms in third order perturbation theory and beyond may modify the Kondo temperature. Hence, we have also employed the NRG [35–37] with cutoff parameter $\Lambda = 2$. Figure 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 ω^* in the real part of the self-energy. The slopes of the self-energy before and after the kink define two different renormalization factors $Z_{\mathrm{FL}(CP)} = [1 - \partial\,\mathrm{Re}\,\Sigma(\omega)/\partial\omega|_{\omega<\omega^*(\omega>\omega^*)}]^{-1}$ with $Z_{\mathrm{FL}} < Z_{CP}$. The overall half width of the central peak is $\Gamma = Z_{CP}D$ so that we can read of the

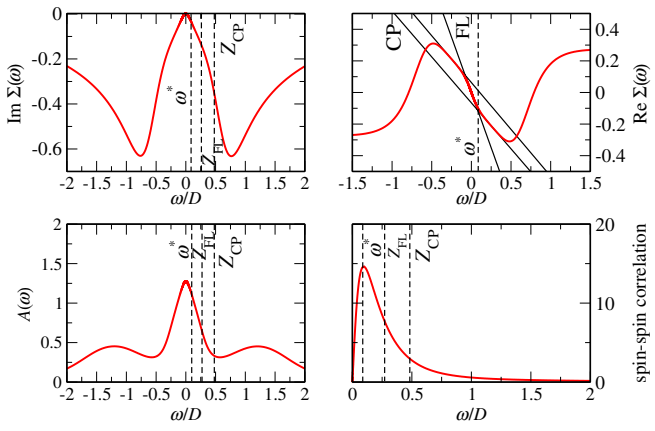

FIG. 2 (color online). DMFT(NRG) results for the Hubbard model at $U = 2D$. Upper panels: Imaginary (left) and real parts (right) of the self-energy. The latter shows a kink at ω^*; the linear slopes before and after ω^* (straight lines) define a Fermi liquid (Z_{FL}) and central peak renormalization factor (Z_{CP}), respectively, whose values are indicated in the other panels. Lower left panel: Spectral function $A(\omega)$. Lower right panel: Spin-spin correlation function with a maximum at ω^*.

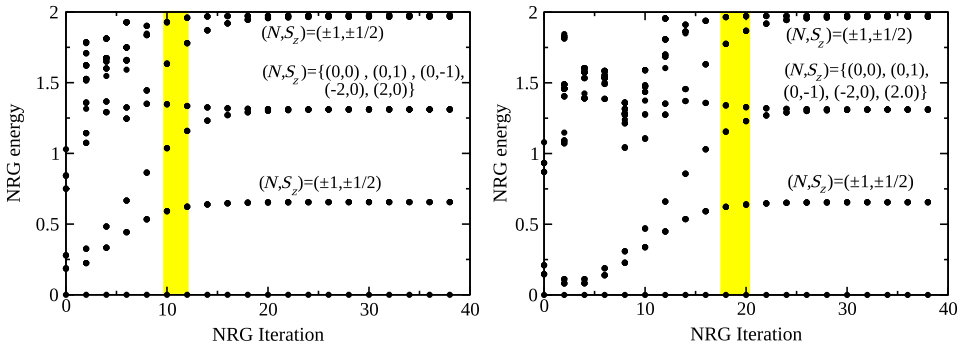

FIG. 3 (color online). DMFT(NRG) energy levels vs NRG iteration for the Hubbard model at $U = 2D$ (left panel) and $U = 2.8D$ (right panel). The quantum numbers in brackets indicate the difference in charge (N) and the spin-S_z component compared to the lowest energy level whose energy we fixed to zero. The kink energy ω^* corresponds to the NRG iterations highlighted in yellow or gray-shaded. The NRG energy levels indicate the crossover to the strong coupling fix point at ω^*.

kink energy in Fig. 2 as $\omega^* \sim 0.21\Gamma$, 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 the poor man's scaling. At the kink energy $\omega^* < \Gamma$, the spin susceptibility in the lower left panel of Fig. 2 has a maximum.

To further elucidate that ω^* indeed represents the crossover to the strong coupling fix point, we present in Fig. 3 the lowest NRG energy levels as a function of the NRG iteration. At iteration i, energies $\omega = 1/2(1 + 1/\Lambda)\Lambda^{-(i-2)/2}D$ become accessible within the NRG flow, and the iterations highlighted in Fig. 3 are those where the kink energy ω^* is reached. In this region, the NRG energy levels show a crossover to the strong coupling fix point. After this crossover, the energy levels remain constant, i.e., at the strong coupling fix point, for subsequent iterations.

At $U = 2.8D$ (right panel of Fig. 3), there is a considerable rearrangement of the energy levels around iterations 2–8. This might possibly correspond to a crossover from the free orbital to the local moment fix point of the Anderson impurity model. However, since this is restricted to a few iterations, there is no clear local moment plateau as in [36], where a larger ratio $U/(V^2\rho_0)$ has been employed. At larger iterations, which correspond to the kink energy ω^* at $U = 2.8D$, we see again the final crossover to the strong coupling fix point.

Conclusion.—Using poor man's scaling, we have shown that the kink energy ω^* is actually the Kondo energy scale which is smaller than the (half)width Γ of the central peak of a strongly correlated electron system. At ω^*, 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 Γ. The crossover to the strong coupling fix point naturally leads to a maximum in the local spin susceptibility at ω^* 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 [30]. 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 a different origin by searching in experiment for the typical Kondo physics [33] (keeping in mind the additional physics emerging between ω^* and Γ). If one observes a kink in the energy-momentum relation of angular resolved photoemission spectroscopy, 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 T_1 relaxation time, a change of the T^2 behavior in the resistivity, and a kink in the electronic specific heat.

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