From mixed valence to the Kondo lattice regime

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Abstract

Many heavy fermion materials are known to cross over from the Kondo lattice regime to the mixed valence regime or vice versa as a function of pressure or doping. We study this crossover theoretically by employing the periodic Anderson model within the framework of the dynamical mean field theory. Changes occurring in the dynamics and transport across this crossover are highlighted. As the valence is decreased (increased) relative to the Kondo lattice regime, the Kondo resonance broadens significantly, while the lower (upper) Hubbard band moves closer to the Fermi level. The resistivity develops a two peak structure in the mixed valence regime: a low temperature coherence peak and a high temperature 'Hubbard band' peak. These two peaks merge, yielding a broad shallow maximum upon decreasing the valence further. The optical conductivity likewise exhibits an unusual absorption feature (shoulder) in the deep mid-infrared region, which grows in intensity with decreasing valence. The involvement of the Hubbard bands in dc transport and of the effective f-level in the optical conductivity are shown to be responsible for the anomalous transport properties. A two-band hybridization-gap model, which neglects incoherent effects due to many-body scattering, commonly employed to understand the optical response in these materials is shown to be inadequate, especially in the mixed valence regime. Comparison of theory with experiment carried out for (a) dc resistivities of CeRhIn$_5$, Ce$_2$Ni$_3$Si$_5$, CeFeGe$_3$ and YbIr$_2$Si$_2$, (b) pressure dependent resistivity of YbInAu$_2$ and CeCu$_6$, and (c) optical conductivity measurements in YbIr$_2$Si$_2$ yields excellent agreement.

(Some figures may appear in colour only in the online journal)

1. Introduction

Rare earth lanthanides and actinides [1, 2] exhibit a wide range of behaviour such as heavy fermions (HFs), mixed valence (MV), proximity of superconductivity and magnetism, quantum critical points, etc. Such behaviour arises through an interplay of a variety of factors such as hybridization between conduction bands and deep f-levels, orbital degeneracy, crystal field effects, long range spin interactions and most importantly local Coulomb repulsion [3–7].

In this work, we present a detailed and systematic theoretical investigation of a regime that borders on heavy fermions at one end and on the mixed valence regime at the other. Experimentally, such a crossover from HFs to MV or vice versa has been observed to happen through pressure or doping [8–11]. The effects of such a crossover have been investigated for several materials [12–21]. For example, the first known HF superconductor CeCu$_2$Si$_2$ [9] when doped with yttrium (a non-magnetic homologue of Ce) shows increasing MV character. The resistivity exhibits a two peak structure in the temperature range 2–300 K. Varying doping concentration results in gradual coalescing of the two peak structure into a single broad peak. For the HF compound YbCu$_4$Ag [10], the ambient pressure resistivity as a function of temperature shows a broad peak which is characteristic of MV compounds. By applying pressure, the broad peak sharpens and the peak position also shifts to lower values of $T$, thus indicating a crossover to the Kondo lattice (KL) regime. The $T^2$ coefficient of the low temperature Fermi liquid resistivity also increases sharply with pressure, implying a decrease in the coherence scale. CeBe$_{13}$ [11] also shows a
pressure-induced crossover from the KL regime to the MV regime, as seen in the changes in the coherence peak in the resistivity. The trend in this material is opposite to that seen in the previous example, YbCu$_4$Ag [10].

Most previous theoretical attempts to describe the effects of pressure on HF materials have employed the single-impurity Anderson model [22–24]. An illustrative and important work in this context is that of Chandran et al [22]. They use a phenomenological model comprising competition between elastic energy cost and valence fluctuation induced magnetic energy gain. The magnetic energy for an Anderson lattice model was computed by using the free energy of an impurity Anderson model and ignoring lattice coherence effects. The free energy itself was arrived at through a slave-boson mean field approximation [25] which is a static approximation and is thus unable to treat dynamical effects of valence fluctuations. Phenomenological expressions were used to model the volume dependence of the parameters, and the pressure was obtained by using $P(T, V) = -\partial F/\partial V$. The authors were able to describe continuous and discontinuous valence transitions in a single framework. However, since the impurity Anderson model was used, lattice coherence effects were ignored. Transport quantities were not calculated. Recent years have seen the use of lattice models to describe the concentrated Kondo systems. The minimalist model that accounts for a large part of HF and MV behaviour is the periodic Anderson model (PAM) which represents a lattice of localized f-orbitals with a Hubbard repulsion $U$ hybridizing locally with a wide non-interacting conduction band. The PAM has of course been explored extensively using a wide range of methods and techniques such as dynamical mean field theory (DMFT) [26, 27], extended DMFT [28], cluster expansions [29], finite size simulations [30], etc. Within the framework of DMFT [26, 27], the self-energy becomes purely local or momentum-independent, which simplifies the problem significantly while retaining the competition between itinerancy and localization in a non-trivial way. The momentum independence of the self-energy implies that we can view lattice problems as locally self-consistent impurity problems, hence the solution of the PAM, for instance, reduces to that of a single-impurity Anderson model with a self-consistent hybridization. The various impurity solvers that have been adapted to solve the effective impurity problem are numerical renormalization group [31], exact diagonalization [32], perturbation theory methods such as iterated perturbation theory [33], local moment approaches [35], and slave-particle approaches [36].

The KL regime within the PAM has been investigated heavily by us [35, 37, 38] and the other groups [31, 39, 40] within DMFT and cluster extensions ignoring the d-f repulsion effects. We have used the local moment approach (LMA) within the DMFT framework previously to understand the PAM in the KL limit [37]. The LMA is a non-perturbative diagrammatic theory based approach developed by Logan et al [41]. This approach has been benchmarked extensively against methods such as the Bethe ansatz [41] and the numerical renormalization group [42]. Excellent quantitative agreement has been found, thus providing justification for its use as an impurity solver within DMFT. Further advantages of using LMA are that real frequency quantities are obtained directly with reasonable computation expense at all temperature and interaction strengths. Our focus in the LMA + DMFT approach to the PAM was on universality and scaling in dynamics and transport. A single low energy scale was found to characterize the spectra and transport in the KL regime [35]. The MV regime was not our focus; nevertheless, our studies indicated the absence of universality and scaling, although adiabatic continuity to the non-interacting limit was seen. The dc and optical transport properties were compared to several Kondo insulators and HF metals and excellent quantitative agreement was found [38, 43]. A few MV materials such as YbAl$_3$ and the skutterudite compound CeO$_x$Sb$_{12}$ were also considered [44], and again good agreement between theory and experiment was found. In a recent work, valence transition in ytterbium and europium intermetallics was studied by Zlatic and Freericks [45] employing a multi-component Falicov–Kimball (FK) model within DMFT. The authors argue that a complete description would entail a solution of the periodic Anderson model combined with the FK model. However, since this is challenging, they choose to solve just the FK model, albeit a multi-component one. Transport quantities like dc and optical conductivity, thermopower and magnetoresistance etc were calculated and qualitatively compared to the experiment. Using an equation of motion decoupling approximation, Bernhard and Coqblin [46] have investigated the PAM and explored the variation of the f-valence with various parameters of the model. They use the results of this study to understand pressure dependent valence changes. Miyake and co-workers [47] have used a variety of methods including the slave-boson approximation, the density matrix renormalization group, etc, to investigate the one-dimensional extended PAM (EPAM), which includes the d–f repulsion effects represented by $U_{cf}$. The EPAM has been investigated within DMFT by Sugibayashi and Hirashima [48] using quantum Monte Carlo methods. Their focus has been to understand the interplay between $U_{cf}$, valence fluctuations and superconductivity. In a recent work Ylvisaker et al [49] combined local density approximation with DMFT to understand the valence fluctuation and the valence transition in Yb metal. For the impurity solver, they have used Hirsch–Fye quantum Monte Carlo and continuous time quantum Monte Carlo. They reproduce the experimentally observed valence transition, and conclude that Yb metal is a fluctuating valence material rather than an intermediate valence one. As mentioned before, and as illustrated through the above mentioned studies, there has been substantial work on the valence transition and its effect on the spectral quantities within the PAM; however, the effects on transport quantities due to valence fluctuations and the crossover regime between the KL and the MV regime have received scant attention.

In this work, we focus on such a KL–MV crossover using the LMA + DMFT approach to the PAM. We assume that the effects of pressure/doping would be to change the model parameters, and hence a scan of the parameter space within
the PAM framework should be able to provide insight into the crossover regime. We highlight the changes occurring in the dynamics and transport properties as a result of this crossover. We find several new results such as a two peak resistivity and anomalous absorption features in the optical conductivity in certain parameter regimes. We provide theoretical explanations for these anomalies, and show that such behaviour does indeed exist in real materials and may be explained quantitatively using the present approach. The paper is structured as follows. We present the model and formalism in section section 2. The results and discussions are in sections 3 and 4, respectively. A comprehensive range of experimental measurements is shown to be described by our theoretical results in section 5. We conclude in section 6.

2. Model and formalism

The PAM is one of the simplest models representing a paradigm for understanding the physics of HF compounds. In standard notation, the Hamiltonian for the PAM is given by

\[
\hat{H} = \epsilon_c \sum_\sigma c_\sigma^\dagger c_\sigma - t \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{h.c.)}) + V \sum_\sigma (f_{i\sigma}^\dagger f_{i\sigma} + \text{h.c.)}) + \sum_\sigma \left( \epsilon_f + \frac{U}{2} f_{i,\sigma}^\dagger f_{i,-\sigma} \right) f_{i,\sigma}^\dagger f_{i,\sigma}. \tag{1}
\]

The first two terms describe the c-orbital energy (\(\epsilon_c\)) and the kinetic energy of the conduction band arising from nearest neighbour hopping \(t\), which is scaled as \(t \propto \frac{\ell}{\sqrt{N}}\) (\(\ell^2\) is the unit of energy) in the large dimension limit where the coordination number \(Z_c \rightarrow \infty\). We choose the hypercubic lattice for our calculation, for which the non-interacting energies \(U\) and \(V\) are in sections 3 and 4, respectively. A comprehensive range of experimental measurements is shown to be described by our theoretical results in section 5. We conclude in section 6.

2.1. Local moment approach: theory and practice

As mentioned in section 1, within DMFT the lattice model is mapped onto an impurity model with a self-consistently determined hybridization. And the solution of the resulting impurity problem is the most challenging step in the solution of the lattice model. We choose the LMA within DMFT to solve the PAM. The LMA has been benchmarked extensively in case of the SIAM with other exact methods such as NRG and Bethe ansatz. While in case of the PAM, excellent agreement with experiments for a wide variety of materials ranging from Kondo insulators to HF metals and for a range of experiments such as dc and optical transport as well as magnetotransport justifies its use to understand the crossover from the KL regime to the empty orbital regime via the MV regime. The theoretical formalism and practical implementation are described in [35, 37, 43], and the reader is referred to these works for details.

2.2. Transport: linear response

Within DMFT, vertex corrections are absent, hence the single-particle Green’s functions are sufficient within Kubo formalism to obtain transport quantities such as dc resistivity and optical conductivity. The expressions derived previously [37] can be brought into a simpler form (derived in the appendix) given below:

\[
\sigma(\omega) = \frac{\sigma_0}{2\pi^2} \text{Re} \int_{-\infty}^{\infty} \text{d}\omega' \frac{n_F(\omega') - n_F(\omega + \omega')}{\omega} \times \left[ \frac{G^*(\omega') - G^*(\omega + \omega')}{\gamma(\omega + \omega') - \gamma(\omega')} - \frac{G^*(\omega') - G^*(\omega + \omega')}{\gamma(\omega) - \gamma(\omega')} \right] \tag{5}
\]
where \( \sigma_0 = 4\pi e^2t^2a^2n/h \) for lattice constant \( a \), electronic charge \( e \), and electron density \( n \) and \( \gamma(\omega) = \omega^2 - \epsilon_\text{c} - V^2 [\omega^2 - \epsilon_\text{f} - \Sigma(\omega)]^{-1} \). The dc conductivity is obtained by considering the \( \omega \to 0 \) limit (see appendix for more details) of the above equation as

\[
\sigma_{\text{DC}} = \frac{\sigma_0}{2\pi} \Re \int_{-\infty}^{\infty} \frac{d\omega}{\omega} \left( \frac{d\Gamma}{d\omega} \right) \times \left[ \frac{\pi D^f(\omega)}{\Im \gamma(\omega)} + 2(1 - \gamma(\omega)G^f(\omega)) \right]
\]

where \( D^f(\omega) = -\Im G^f(\omega)/\pi \) is the spectral function of the retarded Green’s function \( G^f(\omega) \) and \( n_f(\omega) = (e^{\beta\omega} + 1)^{-1} \) is the Fermi function.

3. Results

In this section, we show results for spectral functions, i.e. the DOS, at both zero and finite temperature, optical conductivity again for \( T \geq 0 \), and dc resistivity. We work with a reasonably large interaction strength \( (U \simeq 4.5t_a) \) and a hybridization strength of \( V^2 = 0.6t^2 \). The crossover from the KL regime to the MV regime is investigated by varying \( \epsilon_\text{c} \) and \( \epsilon_\text{f} \) such that the total occupancy \( n_{\text{tot}} = n_\text{c} + n_\text{f} \) is fixed, and \( n_\text{f} \) is decreased. This is done because pressure experiments would be expected to keep the total occupancy fixed. The practical details of implementation are given in \[35, 37\]. We begin with the low energy scale and the spectra.

3.1. Coherence scale

The low energy coherence scale has been identified in previous studies to be \( \omega_L = ZV^2/t_a \), where \( Z = (1 - \partial \Sigma/\partial \omega|_{\omega=0})^{-1} \) is the quasiparticle weight (inverse effective mass). This scale is exponentially small in the strong coupling KL regime \( (n_f \to 1) \). Spectral functions, optical conductivities and resistivity were shown to be universal functions of \( (T/\omega_L, \omega/\omega_L) \) in our previous studies \[35, 37, 43\]. Figure 1 shows the variation of the lattice coherence scale \( \omega_L \) with the f-orbital occupancy \( n_f \) for fixed \( n_{\text{tot}} = 1.25 \) (filled circles) and 1.1 (squares). A crossover from the KL regime \( (n_f \to 1) \) through the MV regime \( (0.3 \lesssim n_f \lesssim 0.8) \) to the empty orbital regime \( (n_f \ll 1) \) manifests in a rapid increase in \( \omega_L \). A lowering of the f-orbital occupation implies greater local charge fluctuations, implying an effective decrease of correlation effects. This in turn implies a decrease in effective mass or an increase in \( Z \) and hence an increase in \( \omega_L \) with decreasing \( n_f \).

3.2. Density of states: zero temperature

The DOS for the spectral functions are considered next. Changes in the low frequency Kondo resonance and in the high frequency Hubbard bands are identified.

We show the \( T = 0 \) spectral functions \( (D^f(\omega; T = 0) = -\Im G^f(\omega, T = 0)/\pi \nu = f, c) \) as a function of the absolute frequency \( \omega/t_a \) in the left panel of figure 2. In the f-DOS (solid line), a usual three peak structure with high energy Hubbard bands and a narrow Kondo resonance at the Fermi level is seen for higher \( n_f (\gtrsim 0.7) \). For lower \( n_f \), a new spectral feature (marked by an arrow) appears above the Fermi level, the weight of which grows with decreasing \( n_f \). The lower Hubbard band (LHB) moves closer to the Fermi level, while the upper Hubbard band (UHB) shifts to higher energies with decreasing \( n_f \). The middle panel in figure 2 shows the Kondo resonance in greater detail as a function of the scaled frequency \( \omega/\omega_L \). Close to the KL regime, a pseudogap is seen straddling the resonance, which gets progressively filled up and for the lower values of \( n_f \), there is no trace of a pseudogap. Such a transfer of spectral weight is very non-trivial and is a very significant feature since it manifests clearly in a second peak in optical conductivity, as will be discussed in sections 3.4 and 4.2.

The conduction band DOS, \( D^c(\omega; T = 0) \), shown in the left panel (red dashed lines) of figure 2, has an overall Gaussian envelope, with spectral weight carved out at the effective f-level, \( \epsilon_f^* \) (seen clearly in the right panel of figure 2 and further discussed in section 4.1) in the form of a pseudogap and small Hubbard bands flanking the envelope. In contrast to the f-DOS (left panel of figure 2), the Hubbard bands here possess a very small fraction of the total spectral weight. The LHB is distinct from the envelope at higher \( n_f (\gtrsim 0.6) \), and merges into the envelope at lower \( n_f (\lesssim 0.5) \). The pseudogap fills up with decreasing \( n_f \) and for the lowest \( n_f \) values shown there is indeed no trace of a pseudogap (see inset). The position of the Kondo resonance, the Hubbard bands and a few other aspects are discussed in greater detail in section 4.1.

3.3. Density of states: temperature dependence

In figure 3, we show the evolution of the f-DOS as a function of temperature for \( n_f = 0.8 \) and 0.3 in the left and right panels, respectively. The insets in the panels show the low frequency, low temperature \( ((\omega/\omega_L, T/\omega_L) \sim \mathcal{O}(1)) \) part more clearly.

The left inset shows that the pseudogap proximal to the Fermi level fills up, while a thermal broadening of the Kondo resonance is clearly visible in the f-DOS. At any given
Figure 2. Left panel: the zero temperature spectral functions, $D^\nu(\omega; T=0)$, $\nu = c$ (dashed), $f$ (solid) are shown as a function of ‘absolute’ frequency $\omega/t_s$ for various $f$-occupancies ($n_f$, indicated in the boxes and in the legends) and a fixed $n_{tot}=1$.25. The middle and the right panels show the same spectra as the left panel, but as a function of the scaled frequency $\omega/\omega_L$ highlighting the changes in the Kondo resonance and the pseudogap.

Figure 3. The $f$-electron spectral function at temperatures $\tilde{T}=T/\omega_L=0, 2, 5, 10, 20$ (indicated in legends) and for all scales in the main panel. The insets show the low frequency part as a function of scaled frequency for lower temperatures. The left panel is for $n_f=0.80$ and the right panel is for $n_f=0.30$ (with fixed $n_{tot}=1.25$).

temperature $T$, it is expected that changes in the spectral function will occur in the frequency range $\omega \lesssim T$. And indeed, this is seen in the KL regime as discussed below and in [37]. The main left panel shows spectra for three different temperatures, which are hard to distinguish. This implies that there has hardly been any spectral weight transfer on a scale of $t_s$, even at the highest temperature shown ($\tilde{T}=10$, equivalent to $\sim 0.18 t_s$).

The physics in the MV regime is, naturally, different. The coherence scale is not exponentially small (see figure 1). In this regime, spectral weight transfer occurs in an energy interval that is far greater than the thermal energy scale. This may be seen in the right panel of figure 3, where at a temperature of $5\omega_L(\sim 0.77 t_s)$, the UHB which is at $\sim 6t_s$ and hence about 15 times the temperature, is strongly affected. In fact, the integrated spectral weight in the UHB is found to decrease with $T$. Such differences in terms of spectral weight transfer between the KL and MV regime have been noted previously [37]. The new spectral feature above the Fermi level (marked by an arrow in the left panel of figure 2) that emerges distinctly in the MV regime gains spectral weight and grows with increasing $T$. The reason for the growth of this feature is not completely clear; however, since the total spectral weight is conserved, the melting of Kondo resonance and the loss of spectral weight in the UHB with increasing $T$ must be compensated by gain in spectral weight elsewhere, and this could be one of the reasons for the growth of this feature with increasing $T$. Angle-resolved photoemission experiments should be able to easily identify such a feature. The conduction band DOS exhibits similar temperature dependence as the $f$-DOS and is hence not shown.

3.4. $T=0$ optical conductivity

As mentioned before, the zero temperature Green’s functions are sufficient within DMFT to compute the $T=0$ optical conductivity, $\sigma(\omega; T=0)$ (equation (5)) [26, 27]. In figure 4, we show $\sigma(\omega; T=0)$ as a function of frequency ($\omega/t_s$) for various values of $n_f$ and a fixed $n_{tot}=1.1$. For $n_f \rightarrow 1$, a familiar structure of a single mid-infrared peak (MIR) arising due to interband transitions [51], marked with a thin dashed
Figure 4. The zero temperature optical conductivity $\sigma(\omega; T=0)$ as a function of frequency ($\omega/t_*$) for various $n_f$, and fixed $n_{\text{tot}} = 1.1$ (left panel) and 1.25 (right panel). The MIR peak is marked with a thin dashed arrow, while the DMIR feature is marked with a thick solid arrow.

Figure 5. The dc resistivity for various $n_f$ values (mentioned next to the curve) as a function of temperature $T/t_*$ for a fixed $n_{\text{tot}} = 1.25$. The theoretically computed $\rho(T)$ all have zero residual values, but for visual clarity they have been appropriately vertically offset. For example in the left panel we add a temperature-independent $\rho_0$ that is zero for $n_f = 0.65$ and increases by unity for every higher $n_f$ ($\rho_0 = 1, 2, 3, \ldots$ for $n_f = 0.7, 0.75, 0.8, \ldots$).

arrow in figure 4, is obtained. As we decrease $n_f$, the MIR peak shifts to higher frequencies. A Drude peak is obtained at the lower frequencies for all $n_f$, but it cannot be shown here since it is a Dirac delta function for $T = 0$.

The lower $n_f$ values hold a surprise. A deep mid-infrared (DMIR) absorption feature or a shoulder, marked with a thick solid arrow in figure 4, emerges for lower $n_f$ values. This is distinct from the above mentioned MIR peak. Such a two peak structure has been reported earlier for the classic MV compound CePd$_3$ [52] and recently for YbIr$_2$Si$_2$ [12]. For the former compound, spin–orbit splitting was argued to be responsible for the two peaks, but the latter has not been understood quantitatively. Recently it has been pointed out through band structure studies that the DMIR feature could be due to transitions to the effective f-level [53]. Here we confirm that this feature could indeed arise from absorption into the effective f-level at $\epsilon_f^* = \epsilon_f + \Sigma(0)$, at which frequency a pseudogap appears in the spectral functions (figure 2). Thus the scenario proposed here could be relevant for both CePd$_3$ and YbIr$_2$Si$_2$. A detailed discussion of the effective f-level, the pseudogap and transfer of spectral weight into the pseudogap region is given in section 4.2.

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Here we must add that a two peak structure is indeed obtained for higher $n_{\text{tot}}$, such as $n_{\text{tot}} = 1.25$ shown in the right panel of figure 4, and hence is a generic feature in the crossover regime. Furthermore, with decreasing $n_f$, the DMIR feature merges into the MIR peak, without being able to develop into a full distinct peak for lower $n_f$, and hence gets harder to distinguish for higher $n_{\text{tot}}$.

We now move on to finite temperature transport.

3.5. dc resistivity as a function of temperature

In figure 5, we show the dc resistivity as a function of temperature $T/t_*$. The left panel shows the resistivity for 0.65 $\leq n_f \leq$ 0.95, while the right panel is for 0.30 $\leq n_f \leq$ 0.60. The theoretically computed $\rho(T)$ all have zero residual values, but for visual clarity they have been appropriately vertically offset (mentioned in the caption). There is a clear
shift of the coherence peak (low temperature peak) to higher temperatures since its position correlates with the low energy scale [37], and $\omega_{\ell}$ itself increases sharply with decreasing $n_{t}$. For $n_{t} \lesssim 0.8$, a second maximum begins to form at higher temperature. This second peak becomes easily distinguishable in the MV regime and merges into the coherence peak to yield a broad maximum close to the empty orbital regime (see right panel, $n_{t} \lesssim 0.45$). Here we have shown that the crossover from the KL regime to the MV regime involves the coalescing of the coherence peak and a high temperature peak into a single broad peak. This high temperature peak is not present in the KL regime or the empty orbital regime, and appears in the MV regime only due to the proximity of the Hubbard band to the Fermi level (discussed in detail in section 4.3). Although we have displayed data in figure 5 for $n_{\text{tot}} = 1.25$, the two peak structure is a generic feature of the MV regime for other $n_{\text{tot}}$ as well. However, the degree to which the two peaks can be distinguished and identified varies in different parameter regimes.

Pressure/doping dependent resistivity measurements in CeCu$_2$Si$_2$ [8, 9, 20] show similar behaviour. For low pressure, a two peak resistivity is observed. As a function of increasing pressure, the two peaks merge and a single broad peak is seen. In section 5, the effect of pressure was ascribed to a crossover from KL to intermediate valence; however, the second peak was argued to arise from higher lying crystal field multiplets. Here, although we do concur with the crossover phenomenon, we present an alternative scenario for a two peak resistivity structure. The scenario is that with increasing pressure, the valence decreases, bringing the Hubbard band into the proximity of the Fermi level, thus leading to a second peak arising due to the Hubbard band state contribution. We emphasize here that a two peak structure is obtained in our theory despite the model Hamiltonian (equation (1)) not containing crystal field effects.

We now move on to finite temperature optical transport.

3.6. $T > 0$ optical transport

We now show the temperature dependence of the optical conductivity in figure 6 for two different f-occupancies, 0.75 and 0.4 (other parameters are mentioned in the figure caption) in the left and right panels, respectively. The $\sigma(\omega; T)$ for the higher $n_{t}$ case has a usual prominent MIR peak, with a slight shoulder at lower frequencies. The inset shows the low temperature evolution of $\sigma(\omega)$, while the main panel shows $T \leq 10\omega_{L}$. With increasing temperature, a transfer of spectral weight over all energy scales is seen. The lower $n_{t}$ (0.4) optical conductivity shown in the right panel of figure 6 is qualitatively different from that of the left panel. The shoulder like structure seen in the KL regime (left panel) develops into a full peak in the MV regime, while the MIR peak diminishes in intensity and gets broader. The analysis at $T = 0$ shows (see section 4) that the lower frequency peak occurs at the effective f-level $\epsilon_{f}^*$. The inset shows that the DMIR peak or the shoulder only appears below a temperature $T = 0.08\omega_{L}$, even though it is positioned at a frequency $\omega$ equal to the coherence scale $\omega_{L}$ (since here $\epsilon_{f}^* + \Sigma(0) \approx 1$). This precise behaviour is seen in recent optical conductivity measurements in YbIr$_2$Si$_2$ [12] (see section 5).

4. Discussion

4.1. Spectral features: Kondo resonance and Hubbard bands

In this subsection, we discuss the positions and weights of the various features seen in the spectra in section 3.2. At high energies, the prominent spectral features are the Hubbard bands. In figure 2, it is seen that the Hubbard bands shift to the right with decreasing $n_{t}$. This is expected from the atomic limit, since in that limit the Hubbard bands occur at $\epsilon_{f}^*$ and $\epsilon_{f}^* + U$, and $\epsilon_{f}$ moves closer to the Fermi level when $n_{t}$ decreases. However, we find from our calculations, that in the displayed spectra, the Hubbard bands are not at the positions predicted by the atomic limit, as must be expected, due to a combination of shifts in the levels arising through hybridization and self-energy effects. We see that even for $n_{t} \sim 0.8$, the LHB and the UHB are not symmetrically placed about the Fermi level as would have been the case in the strong coupling KL regime. In fact, the LHB is at $\omega \lesssim -t_{s}$, while the UHB is at $\omega \gtrsim U$. The LHB is predicted very well by
the unrestricted Hartree–Fock (UHF) solution (not discussed here) which considers the static part of the self-energy and hybridization effects. For predicting the UHB, we can neglect hybridization effects; however, we need to retain the static part and most importantly the real part of the self-energy. The latter may be approximated by an expression obtained through high frequency moment expansion [54], and thus the UHB turns out to be at \( \sim (\varepsilon_f + \sqrt{\varepsilon_f^2 + U^2})/2 \), where \( \varepsilon_f = \varepsilon_f + U(\bar{n} + \bar{\mu})/2 \). \( U^2 = U^2\bar{n}(2 - \bar{n}) \) and \( \bar{n}, \bar{\mu} \) have been defined in section 4.2 of [35] as the fictitious occupation number and the moment obtained from the spin dependent host/medium propagators that are used to construct the LMA self-energies.

At the other extreme, i.e. close to the Fermi level, a low frequency form of the Green’s functions using a Fermi liquid self-energy \( \Sigma(\omega) = \Sigma(0) + \omega(\frac{1}{2} - 1) + O(\omega^2) \) may be derived that enables us to understand most of the features of the Kondo resonance. The resulting spectral functions in the neighbourhood of the Fermi level are given by

\[
D^f(\omega) \sim \rho_0 \left( \frac{\omega - \varepsilon_c}{\omega - Z\varepsilon_f} \right)^2
\]

\[
V^2D^f(\omega) \sim \frac{Z^2}{\omega - Z\varepsilon_f} D^f(\omega)
\]

(7)

where \( \varepsilon_f = Z\bar{\varepsilon}_f = Z(\varepsilon_f + \Sigma(0)) \) is the effective f-level. These equations show that the low energy (\( \omega \lesssim \omega_b \)) spectral features are precisely those of a non-interacting (\( U = 0 \)) PAM with renormalized parameters \( V^2 \rightarrow ZV^2 \), \( \varepsilon_f \rightarrow Z\varepsilon_f \) and \( (\varepsilon_c \rightarrow \varepsilon_{c0}) \) [35]. Thus, this is the renormalized non-interacting limit (RNIL). A scaling collapse of the numerically obtained spectra with the analytical expressions above would be a demonstration of adiabatic continuity of the interacting system to the non-interacting limit. Indeed, we do see such a collapse (not shown), implying adiabatic continuity, although the range of frequencies over which such a collapse occurs decreases from \( \omega \lesssim \omega_b \) in the KL regime, to \( \omega \ll \omega_b \) in the empty orbital regime.

As \( \omega \rightarrow \varepsilon_f \) in equations (7), the RNIL spectral functions also vanish, thus the pseudogap seen in the spectra is positioned at the effective f-level, \( \varepsilon_f = Z(\varepsilon_f + \Sigma(0)) \). Transfer of spectral weight into the pseudogap happens with decreasing \( n_f \) as seen in figure 2, which implies that the frequency interval in the neighbourhood of \( \varepsilon_f \) is gaining spectral weight. This spectral weight transfer is completely missed by theories that are equivalent to the RNIL. This includes approaches such as slave-boson theories or two-band models of HF systems, which ignore the imaginary part of self-energy. The variation of \( \varepsilon_f \) with \( n_f \) may be easily predicted using the Luttinger theorem which states [35]

\[
\frac{1}{2}(n_f + n_c) = \int_{-\infty}^{-\varepsilon_c + V^2/\bar{\varepsilon}_f} \rho_0(\epsilon) \, d\epsilon + \theta(-\bar{\varepsilon}_f).
\]

(8)

For fixed \( n_{tot} = n_f + n_c \), the upper limit of integration on the right-hand side of equation (8) is also crossed. Crossing over from the KL to MV regime would require decreasing \( n_f \) and increasing \( n_c \), which in turn would require decreasing \( \varepsilon_c \). Thus to keep \(-\varepsilon_c + V^2/\bar{\varepsilon}_f \) fixed, the \( \bar{\varepsilon}_f = \varepsilon_f + \Sigma(0) \) must increase, and hence the effective f-level, \( \varepsilon_f = Z\bar{\varepsilon}_f \), also increases as \( n_f \) decreases. This is indeed seen in figure 2 because the position of the pseudogap does indeed shift to higher frequencies as \( n_f \) is decreased.

### 4.2. Inadequacy of the renormalized non-interacting limit

In [37], it was shown that the two-band model or the RNIL predicts a square root singularity at the minimum direct gap (\( \sim 2\sqrt{ZV} \)), and hence the MIR peak is generally attributed to the direct gap. A simple Fermi liquid analysis \( \Sigma(\omega) \approx \text{Re}\Sigma(0) + \omega(1 - 1/Z) \) of the poles of the \( k \) dependent conduction electron Green’s function

\[
G_k(\omega; \epsilon_k) = \left[ \frac{\omega - \epsilon_c - \epsilon_k - \frac{V^2}{\omega - \epsilon_f - \Sigma(\omega)}}{\omega - \epsilon_f - \Sigma(\omega)} \right]
\]

(9)

yields a two-band model

\[
\omega_{\pm}(\epsilon_k) = \frac{(\epsilon_c + \epsilon_k - \epsilon_f^\pm) \pm \sqrt{(\epsilon_c + \epsilon_k - \epsilon_f^\pm)^2 + 4ZV^2}}{2}
\]

(10)

The minimum direct gap is given by \( \min(\omega_{+}(\epsilon_k) - \omega_{-}(\epsilon_k)) \). The square root singularity at the direct gap appears in the two-band model because the imaginary part of the self-energy is neglected, and the resulting spectral functions are Dirac delta functions. Including incoherent effects due to electron–electron scattering results in broadening of the MIR peak and cutting off the square root singularity.

At the lowest \( n_f \) values, a clear two peak structure is visible in the optical conductivity displayed in the figure 4 (especially for \( n_f = 0.45 \) in the left panel). The low frequency peak is in fact at the effective f-level, as argued below, while the high frequency peak is the usual MIR peak. Naively, finding an absorption peak at \( \epsilon_f^\pm \) is counter-intuitive, because the RNIL (equations (7)) shows that a pseudogap exists at \( \epsilon_f^\pm \), implying that there is no DOS at that energy. So how can absorption into a gap happen? The answer is of course that the RNIL, which is equivalent to a slave-boson mean field theory, which in turn is equivalent to a two-band model [51], are not totally correct in their predictions. These approaches neglect the imaginary part of the self-energy (scattering rate).

So even though the RNIL predicts a gap, there is in fact no gap at \( \epsilon_f^\pm \) when self-energy effects are included (see the pseudogap feature in the DOS in figure 2 and the discussion in section 4.1). And in fact, it may be shown rigorously, without recourse to LMA that absorption to \( \epsilon_f^\pm \) will happen provided the imaginary part of the self-energy is non-zero at that energy. To see this, consider the roots of the real part of the denominator of the conduction electron Green’s function, \( G^c(\omega, \epsilon_k) \) (equation (9)), given by

\[
\text{Re}[\omega - \epsilon_c - \epsilon_k - \frac{V^2}{(\omega - \epsilon_f - \Sigma(\omega)^{-1})}] = \omega - \epsilon_c - \frac{V^2}{\omega - \epsilon_f - \text{Re}\Sigma(\omega)^2} = \epsilon_k.
\]

(11)

If the imaginary part of the self-energy is completely neglected and a first order Taylor expansion is carried out for the real part of the self-energy, we get back equation (10).
However, retaining the imaginary part, however small it might be, results in an equation that is at least cubic in order. And for $\varepsilon_k = \varepsilon_c = Z(\varepsilon_f + \Sigma(0))$, one of the roots is just $\varepsilon^*_n = Z(\varepsilon_f + \Sigma(0))$.

We support the arguments above with LMA results below. The dispersion $\omega(\varepsilon_k)$ is computed for $n_f = 0.95$ ($n_c = 0.58$, $n_f = 0.7$ for $n_c = 0.63$, and $n_f = 0.4$ for $n_c = 0.71$ with $\varepsilon_c = 0.5$, $U = 4.7t_c$ through equation (11) and shown in the top, middle and bottom panels respectively in figure 7. The two bands obtained at the RNIL (equation (10)) are also superimposed in red. It is clear from the figure that the agreement of the two-band model with the full dispersion gets progressively worse as $n_f$ decreases. For $n_f = 0.4$, the middle band is clearly visible in the full dispersion, while being completely absent in the two-band picture. This third band, as argued above, is centred at $\omega = \varepsilon^*_f$. It is the excitations from the ‘band’ below the Fermi level to $\varepsilon^*_f$, that appears as an additional ‘anomalous’ absorption peak in the DMIR (as a shoulder). This anomalous peak is seen to become prominent in the MV regime and is very small or invisible in the KL regime. We refer the reader to figure 4, where an extra absorption feature is easily discernible for lower $n_f$ values, while for higher $n_f$ values just a weak shoulder is observed. As we will see later, such a two peak optical conductivity has indeed been observed in recent experiments (section 5).

**4.3. Two peak resistivity: why?**

We have shown previously that the coherence peak (low temperature peak) in the resistivity, which would be a minimum in the conductivity [37], occurs at a temperature comparable to $\omega_c$, the low temperature scale. A second peak (high temperature peak) has indeed been observed in experiments and has been attributed to crystal field split levels (for example in [8]). Notwithstanding the foregoing possibility, we find an alternative and far simpler explanation for the existence of the second peak even within the single band PAM. The second peak occurs at a temperature that is roughly half of the LHB energy scale. It might at first seem surprising to note that the Hubbard band is contributing to transport. The Hubbard bands are usually at an energy scale of $U/2$ in the strong coupling KL regime, which being of the order of a few eV remain untouched until room temperature. Nevertheless, for MV systems, even if the $U$ is large, either the LHB or the UHB moves close enough to the Fermi level so as to be affected at room temperature scales.

To show the contribution of the Hubbard band states to the conductivity, we consider expression (6) again. On the right-hand side, the integration is carried out over all frequencies. However, if we introduce an upper and a lower cutoff in the integration limits, we can isolate the contribution of individual spectral features within those limits. In figure 8, we show the calculated dc resistivity for $n_f = 0.6$, $n_c = 0.65$ (same as that in figure 5), with three different cutoffs: (i) the solid line being no cutoff (full resistivity), (ii) the dashed line having limits such that the LHB is excluded but the new ‘non-Hubbard band’ feature above the Fermi level (marked with an arrow in figure 2) is included, and (iii) the dotted line having limits such that both the LHB and the new feature is excluded. It is seen that excluding the spectral weight of the Hubbard band and the new feature enhances the resistivity systematically. This shows that the Hubbard band contribution to the dc conductivity is substantial in MV compounds. The two peak behaviour of resistivity is not specific to the parameter regime for which the dc resistivity has been displayed ($U/V^2 \sim 8$, $n_{tot} = 1.25$). In other parameter regimes, such as $n_{tot} = 1.1$, our calculations demonstrate (not shown here) that the dc resistivity crosses over from a single sharp coherence peak to a broad peak

![Figure 7](image-url)

**Figure 7.** The dispersion $\omega(\varepsilon_k)$ computed from equation (11) (black) and from the RNIL (equation (10)) (red) for $\varepsilon_c = 0.5$, $U = 4.7t_c$ and $n_f = 0.95$, $n_c = 0.58$ (top panel), $n_f = 0.7$, $n_c = 0.63$ (middle panel) and $n_f = 0.4$, $n_c = 0.71$ (bottom panel).

![Figure 8](image-url)

**Figure 8.** The second peak in the dc resistivity seen most clearly in the right panel of figure 5 for $n_f = 0.6$ disappears progressively by excluding the LHB and other spectral features. The solid line is for $n_f = 0.6$, $n_c = 0.66$ and is the full resistivity. The dashed and the dotted lines are obtained by excluding the LHB below the Fermi level and with decreasing cutoff above the Fermi level (see text for discussion).
lineshape with decreasing valence, going via a two peak structure but with very faint or hard to distinguish features.

5. Comparison to experiments

5.1. dc resistivity: ambient pressure

In figure 9, we have superposed theoretically computed dc resistivity (solid lines) with the experiments (circles) for CeRhIn₅ [55], Ce₂NiSi₅ [56], CeFeGe₃ [57] and YbIr₂Si₂ [12]. To find the appropriate theoretical parameters for each material, we had to adopt a trial and error approach. However, a surprising similarity in the dc resistivity of CeRhIn₅ and Ce₂NiSi₅ reduced our effort substantially. We found that we could take the experimentally measured dc resistivity for the two materials and scale them onto each other simply by rescaling the x- and y-axes. CeRhIn₅ has anisotropic resistivity, nevertheless the $\rho_x$ and $\rho_y$ may also be scaled onto each other, thus showing that qualitatively, they are also similar. We find that these two materials have $f$-occupancy $n_f \sim 0.7$, with the rest of the parameters being $n_g \sim 0.55, U/V^2 \sim 8, \epsilon_c = 0.5$. For CeFeGe₃, we found that the mixed valence resistivities do not fit the data well. Rather, the best fit was found using parameters ($n_f \sim 1, n_c \sim 0.77, U/V^2 \sim 5, \epsilon_c = 0.3$) that signify an intermediate correlation with $f$-occupancy being nearly unity. The optical transport data for YbIr₂Si₂ (see below) show a two peak structure very similar to that seen in figure 4 for $n_f = 0.4$ and $n_{\text{mag}} = 1.1$. Thus we take the same resistivity and superimpose that onto the experimentally measured one, and we see very good agreement.

5.2. dc resistivity: pressure dependence

Hydrostatic pressure dependence measurements of the dc resistivity of YbInAu₂ and its non-magnetic homologue LuInAu₂ have been carried out by Fuse et al [58]. The experimental magnetic resistivity along with the residual resistivity ($\rho_{\text{mag}} + \rho_0$) is shown in the inset of figure 10. The main panel shows a comparison of theory (solid lines, $n_{\text{tot}} = 1.1, U/V^2 \sim 8$) with experiment (symbols). The agreement is seen to be excellent. The $T_{\text{max}}$ is seen to decrease with pressure, and the material appears to be progressing towards a Yb$^{3+}$ state with increasing pressure, as conjectured in the experimental paper. Nevertheless, the valence remains in the MV regime ($\leq 0.4$), even with pressures up to 20 kbar. We now move on to CeCu₆, which has attracted a lot of attention in the past decade as a material that can be tuned to a quantum critical point with Au doping. Pressure dependent resistivity measurements on CeCu₆ were carried out in 1985 by Thompson and Fisk [59]. They found that with increasing pressure, the material crosses over from a KL like to an MV like regime. In the left panel of figure 11, we show the experimental graph, while in the right panel the theory (same data as for figure 5) is shown. The experiment shows that with increasing pressure, the temperature dependence follows the $P = 0$ curve to some temperature and then deviates. In the inset of the left panel, the experimental data for $0 \leq P \leq 17.4$ kbar are shown to collapse when plotted as $R/R_{\text{max}}$ versus $T/T_{\text{max}}$ for $T \leq 4T_{\text{max}}$. The theoretical curves in the right panel correspond very closely to those seen in the experiment. The agreement between theory and experiment shows that indeed, with increasing pressure, the occupancy does change from $n_f \rightarrow 1$ to $n_f \sim 0.75$, thus implying that the valence of Ce changes from $\sim 3+ \rightarrow 2.75+$. The theoretical curves decrease more rapidly (than the experimental one) with increasing temperature beyond the coherence peak, and the reason for this is that the phonon contribution is not subtracted in the experiment. The inset in the theoretical panel has five different valencies plotted together, namely, $n_f = 0.90, 0.85, 0.80, 0.78$ and $0.75$. Except for $n_f = 0.75$, the rest of the data are seen to collapse onto a single curve, as seen in the experiment. The $n_f = 0.75$ curve does collapse up to a certain temperature and then deviates from the universal curve.

5.3. Optical transport: YbIr₂Si₂

The recently discovered HF system YbIr₂Si₂ [60] has a crystal structure similar to the well studied YbRh₂Si₂. The
latter exhibits a field-tuned quantum critical point, while the former has a pressure-tuned first order phase transition to a ferromagnetic phase. The experimentally measured optical conductivity [12] is shown in the top panel of figure 12. A clear two peak structure is evident, and a large scale spectral weight transfer occurs as temperature is increased from 0.4 to 300 K. An important characteristic of the temperature dependence of $\sigma(\omega; T)$ is that, as temperature is increased, the lower frequency peak (shoulder) merges into the continuum at $T \sim 60$ K, at which temperature the higher frequency peak remains untouched.

We note that the theoretically computed optical conductivity shown in figure 6 does appear to resemble the experimentally measured $\sigma(\omega; T)$. In the experiment, the shoulder peak appears only for $T \lesssim 30$ K, which, according to theory, should be roughly 0.08 times the peak frequency for the chosen parameters (see the discussion for figure 6). Thus, theoretically, we can predict that the shoulder should appear at $\sim 30.0/0.08$ K $\simeq 32$ meV. The shoulder peak position as predicted by theory indeed agrees very well with the experimentally observed shoulder position ($\sim 30$ meV). The bottom panel of the same figure shows the optical conductivity computed for $U/t_0 = 5, V^2 = 0.6t_0^2$ and $\epsilon_c = 0.5t_0$, which yields $n_f = 0.4$ and $n_c = 0.7$, thus classifying YbIr$_2$Si$_2$ as an MV material. These parameters were chosen using the results shown in figure 4, and for consistency, we note that the dc resistivity in the experiment has a broad and shallow peak (see bottom right panel of figure 9) which indicates that YbIr$_2$Si$_2$ belongs to the MV regime. The dc conductivity obtained through a low frequency limit in the theory is higher than the corresponding experimental values. This is natural, since the theory neglects electron–phonon scattering, which if included would reduce the theoretical conductivities. Apart from this disagreement, an excellent agreement between theory and experiment is seen in quantitative terms for both the lineshape and the temperature dependence. A phenomenological analysis [12] of the experimental optical conductivity using the Drude and extended Drude formalisms has been used to infer a non-Fermi liquid nature of the quasiparticles in this material. However, if the quantitative agreement between theory and experiment is any indication, this material is a perfect Fermi liquid. The self-energy has the correct Fermi liquid form for the parameters used to compute the optical conductivity in the bottom panel of figure 12. In our approach, the Luttinger theorem is used as a constraint, which also supports the inference of Fermi liquid behaviour. The low temperature resistivity also exhibits a clean $T^2$ behaviour, both in the experiment [13] and theory (shown to agree well in the inset of the bottom right panel in figure 9), which again supports a Fermi liquid ground state. Additionally, we conclude that this material is in the MV regime with an effective f-occupancy of $n_f \approx 0.4$, which would correspond to an effective valence $\text{Yb}^{2.4+}$. (Naturally, the $n_f$ given here must be interpreted as hole occupancy for Yb compounds.) This effective valence predicted by our theory disagrees with the inference from susceptibility measurements, which yields a Yb valence close to 3+. Further theoretical and experimental investigations are needed to resolve this. We can also infer that the effective f-level given by $\epsilon_f^* = Z(\epsilon_f + \Sigma(0))$ in YbIr$_2$Si$_2$...
is located at roughly 25–30 meV. The dc resistivity calculated from theory for the parameters mentioned in figure 12 does agree qualitatively with experiment in terms of a broad peak and the lineshape (see figure 9); however, the scale inferred from fitting to the experimental data does not agree with that obtained from optical conductivity. There appears to be an inconsistency in theory, in terms of an ambiguity in the parameters that can fit the experiment. The implication is, we believe, minor. It should be possible by a better scanning of the parameter space to find a ‘right’ set of parameters that can fit the optical and dc conductivity consistently with the same scale. We believe that finding this right set of parameters will surely make the theory more convincing, but probably not by a great measure, since almost all aspects of the experiment are quantitatively captured by the current set of parameters. The new set of parameters would probably change the numbers (e.g. for the $U$, $V$ values); nevertheless, the major conclusions such as that of YbIr$_2$Si$_2$ being a Fermi liquid and an MV system should remain unscathed.

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Appendix

The expression for dynamical conductivity (hypercubic lattice) in [37] is

$$\sigma(\omega; T) = \frac{\sigma_0}{\omega} \int_{-\infty}^{\infty} d\omega_1 \left[ n_F(\omega_1) - n_F(\omega_1 + \omega) \right] \times \int_{-\infty}^{\infty} d\epsilon \rho_0(\epsilon) D^*(\epsilon; \omega_1) D^*(\epsilon; \omega + \omega_1)$$

where $D^*(\epsilon; \omega) = -i\text{Im}G^*(\epsilon; \omega)/\pi$; $G^*(\epsilon; \omega) = (\gamma(\omega) - \epsilon)^{-1}$ and $\gamma(\omega)$ is defined below equation (4). The identity $\text{Im}z_1\text{Im}z_2 = \text{Re}(z_1^*z_2 - z_1z_2)/2$ for $z_1, z_2 \in \mathbb{C}$ may be used to get

$$D^*(\epsilon; \omega_1)D^*(\epsilon; \omega + \omega_1) = \frac{1}{2\pi^2} \times \text{Re} \left( \frac{G^*(\epsilon; \omega + \omega_1) - G^*(\epsilon; \omega_1)}{\gamma(\omega_1) - \gamma^*(\omega + \omega_1)} \right).$$

The Hilbert transform integral over $\epsilon$ in equation (12) may be carried out to give the expression equation (5). The $\omega \rightarrow 0$ second limit of the equation (5) yields the dc conductivity. The second term involves using L'Hopital’s rule which in turn requires the knowledge of $dG^*(\omega)/d\omega$, which we derive below. The c-Green’s function is given by a Hilbert transform over the Gaussian DOS. The result is expressed in terms of the complementary error function as [26]

$$G^*(\omega) = H[\gamma] = -is\sqrt{\pi} \exp(-\gamma^2)\text{erfc}(-is\gamma)$$

where $s = \text{sgn}(\text{Im}\gamma) = +1$ for the retarded functions considered here. The derivative of this with respect to $\gamma$ is straightforward and is given by

$$\frac{dG^*(\omega)}{d\gamma} = -2\gamma G^*(\omega) - is\sqrt{\pi} \exp(-\gamma^2)(-is) \times \frac{\text{derfc}(x)}{dx} \bigg|_{x=-is\gamma} = 2(1 - \gamma G^*(\omega)).$$

Using this yields equation (6).

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