Spectral properties of a narrow-band Anderson model

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We consider single-particle spectra of a symmetric narrow-band Anderson impurity model, where the host bandwidth $D$ is small compared to the hybridization strength $\Delta_0$. Simple 2nd order perturbation theory (2PT) in $U$ is found to produce a rich spectral structure, which leads to rather good agreement with extant Lanczos results and offers a transparent picture of the underlying physics. It also leads naturally to two distinct regimes of spectral behaviour, $\Delta_0 Z/D \gg 1$ and $\ll 1$ (with $Z$ the quasi-particle weight), whose existence and essential characteristics are discussed and shown to be independent of 2PT itself. The self-energy $\Sigma_i(\omega)$ is also examined beyond the confines of PT. It is argued that on frequency scales of order $\omega \sim \sqrt{\Delta_0 D}$, the self-energy in strong coupling is given precisely by the 2PT result, and we point out that the resultant poles in $\Sigma_i(\omega)$ connect continuously to that characteristic of the atomic limit. This in turn offers a natural rationale for the known inability of the skeleton expansion to capture such behaviour, and points to the intrinsic dangers of partial infinite-order summations that are based on PT in $U$.

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I. INTRODUCTION

Since its inception nearly forty years ago, the Anderson impurity model (AIM) has become one of the generic models of correlated electron physics, permitting at possibly the simplest level a detailed study of the competition between local interactions and electron itinerancy. The great majority of previous work, reviewed comprehensively in Ref. 3, has focused on an impurity coupled to a conduction band whose width ($D$) represents a large energy scale — large compared to the one-electron hybridization strength ($\Delta_0$) that characterizes the host/impurity coupling. The opposite extreme of a narrow-band AIM has however been invoked in relation to the Hubbard model in large dimensions, where the correlated lattice problem maps onto an effective impurity model coupled to a self-consistently determined bath. Here, in the vicinity of the Mott transition occurring in the particle-hole symmetric ($\frac{1}{2}$-filled) Hubbard model, an effective narrow-band AIM is generated self-consistently in the now widely accepted scenario for the transition that arose originally from the iterated perturbation theory (IPT) approach of Kotliar, Georges and coworkers.

Recently Hofstetter and Keheirein have undertaken a numerical study of the symmetric narrow-band AIM, freed from the additional complications of self-consistency and itself defined by $\Delta_0 \gg D$. Thermodynamic and spectral properties of the model were found thereby to exhibit a range of behaviour that is quite distinct from the conventional wide-band AIM. Single-particle spectra for example, determined via finite-size Lanczos calculations, show a much richer structure than their wide-band counterpart. At low frequencies in particular they exhibit an intricate competition between various physical effects and their associated energy scales, reflecting ultimately the importance in the narrow-band AIM of an energy scale $\omega_0 \sim \sqrt{\Delta_0 D}$ that while large compared to the host bandwidth $D$ is typically small compared to the on-site interaction $U$.

Spectral properties of the narrow-band AIM are discussed in the present paper, a complementary analytical study based in part upon 2nd order perturbation theory (2PT) in $U$. This is found to provide a qualitatively correct description on all energy scales, suggests a simple physical interpretation of the most prominent spectral features, and produces rather good agreement with the Lanczos results of Hofstetter and Keheirein. We also show, independent of the intrinsic limitations of 2PT, that spectral behaviour divides into two distinct regimes that are borne out by the calculations of Ref. 3. (a) weak-coupling for $\Delta_0 Z/D \gg 1$ (with $Z$ the quasi-particle weight), and (b) a strong coupling (Kondo) regime for $\Delta_0 Z/D \ll 1$.

For the weak to moderate interaction strengths reliably accessible by Lanczos calculations, Hofstetter and Keheirein have shown that pole contributions to the interaction self-energy $\Sigma_i(\omega)$, occurring on the scale $\omega_0 \sim \sqrt{\Delta_0 D}$, are an integral facet of the narrow-band AIM; but that they cannot be captured to any order in a skeleton expansion. Within 2PT, $\Sigma_i(\omega)$ is indeed found to be dominated entirely by poles on this order. However in strong coupling $U \gg \Delta_0$, 2PT will certainly be qualitatively deficient on the lowest energy scales $|\omega| \ll D$ characteristic of the Kondo resonance. We show nonetheless that in strong coupling the pole contributions to the self-energy are again given precisely by the result arising from 2PT. These poles are thus a ubiquitously dominant and essentially $U$-independent characteristic of the narrow-band AIM. They are moreover continuously connected to the atomic limit of the model, which sheds light on the inability of a skeleton expansion to recover them, and...
points to the intrinsic dangers of partial infinite-order summations based on PT in $U$.

The Hamiltonian for the AIM is given in standard notation by

$$
\hat{H} = \sum_{k\sigma} \varepsilon_k \hat{n}_{k\sigma} + \sum_{\sigma} \varepsilon_i \hat{n}_{i\sigma} + U \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_{k\sigma} (V_{ik} \hat{c}_{i\alpha}^+ \hat{c}_{k\sigma} + \text{h.c.})
$$

(1)

where the first term describes electrons (of spin $\sigma = \uparrow, \downarrow$) in a metallic host band of dispersion $\varepsilon_k$. The following two terms refer to the impurity, with $\varepsilon_i$ the impurity level and $U$ the on-site Coulomb interaction. The final term describes the one-electron hybridization between the impurity and the host. Throughout this article, as in Ref. 2, we study the particle-hole symmetric AIM where $\varepsilon_i = -U/2$. In this case, for all interaction strengths, the Fermi level remains fixed at its non-interacting value and the impurity charge $n_i = (\hat{n}_{i\uparrow} + \hat{n}_{i\downarrow}) = 1$; single-particle spectra are thus symmetric with respect to the Fermi level, $\omega = 0$.

II. NON-INTERACTING LIMIT

We first consider briefly the noninteracting problem $\varepsilon_i = -U/2 = 0$ which, although rather trivial by itself, generates two inherent energy scales that control the subsequent evolution of single-particle properties with interaction strength. For $U = 0$ the (causal) single-particle impurity Green function $G^0_i(\omega) = \text{Re} G^0_i(\omega) - i\text{sgn}(\omega)\pi D^0_i(\omega)$ is given by

$$
G^0_i(\omega) = \left[ z - \Delta(\omega) \right]^{-1} \tag{2}
$$

with $z = \omega + i0^+\text{sgn}(\omega)$ and $\Delta(\omega) = \Delta_R(\omega) - i\text{sgn}(\omega)\Delta_I(\omega)$ the hybridization function, $\Delta(\omega) = \sum_k |V_{i\downarrow}|^2/(z - \varepsilon_k)$. We are interested in the narrow-band case, meaning $D \gg \Delta_0 = \Delta_I(\omega = 0)$ with $D$ the host bandwidth. The physics of the model is naturally rather insensitive to the precise form of the hybridization. We thus take $\Delta_I(\omega)$ to consist of a single flat band of intensity $\Delta_0$, ranging from $-D$ to $+D$; so that in total

$$
\Delta(\omega) = \frac{\Delta_0}{\pi} \log \left| \frac{\omega + D}{\omega - D} \right| - i\Delta_0 \text{sgn}(\omega) \theta(D - |\omega|) \tag{3}
$$

where $\Delta_R(\omega)$ follows via Hilbert transformation.

The noninteracting single-particle spectrum consists of two contributions: (i) a low-energy continuum for $\omega \in [-D, +D]$, arising from the non-zero imaginary part of the hybridization; (ii) two poles, one lying above and the other one symmetrically below the continuum. The fraction of spectral weight residing in the poles depends strongly on the bandwidth of the host metal. In the usual wide-band model, $D \gg \Delta_0$, most of the spectral weight is concentrated in the single-particle band, while the poles are exponentially weak and hence irrelevant in practice.

The situation is however radically different in the present narrow-band model, defined by $D \ll \Delta_0$. Here the poles are the most prominent features of the spectrum, suggesting that the narrow host behaves in effect as a single site or level. As this “host site” is coupled to the impurity, a bonding and an anti-bonding orbital form in analogy to the $H_2$ molecule. These orbitals occur at frequencies $\pm \omega_0$ far outside the band, obtained by expanding $\Delta_R(\omega) \sim (2/\pi)\Delta_0 D/\omega$ in the denominator of (3) to yield

$$
\omega_0 = \sqrt{\frac{2\Delta_0 D}{\pi}}. \tag{4}
$$

The pole-weight of each orbital is $q = (2\Delta_0 - \pi D)/(4\Delta_0 - \pi D) \sim 1 + O(D/\Delta_0)$, showing that they carry almost the entire spectral density.

The noninteracting single-particle spectrum is thus characterized by a weak continuum of weight $O(D/\Delta_0)$, ranging over the lowest energy scale $|\omega| \leq D$, and two molecular orbitals carrying most of the spectral intensity. The latter occur at the orbital bonding energy $\omega_0$ which, although much larger than $D$, defines a second low-energy scale $\omega_0 \sim \sqrt{\Delta_0 D} \ll \Delta_0$. Central questions then arising include: how does this low-energy scale evolve with increasing interaction strength, over what range of $U$ does it constitute the dominant low-energy physics of the problem, and when by contrast is the latter dominated by the Kondo effect that one expects to prevail for sufficiently large interactions? It is these questions we aim to address in the following sections.

III. PERTURBATION THEORY

The impurity Green function for the interacting system, $G_i(\omega)$, is related to $G^0_i(\omega)$ by the Dyson equation

$$
G_i(\omega) = \frac{1}{\left[ G^0_i(\omega) \right]^{-1} - \Sigma_i(\omega)}. \tag{5}
$$

This simply defines the interaction self-energy $\Sigma_i(\omega) = \Sigma^0_i(\omega) - i\text{sgn}(\omega)\Sigma^R_i(\omega)$, considered here via perturbation theory (PT) in $U$ about the noninteracting limit. One does not doubt such an approach in principle for, although we are interested in the narrow-band regime, the impurity is coupled to a metallic host and one thus anticipates ubiquitously a Fermi liquid ground state that is perturbatively connected to the noninteracting limit.

PT is of course limited in practice, by the order to which it is taken.

The 1st order (Hartree) contribution to $\Sigma_i$, of $\sum_i \frac{D}{U} \hat{n}_i = U/2$, is cancelled precisely by the bare site-energy $\varepsilon_i = -U/2$. The lowest order process is thus of 2nd order in $U$, whereby a propagating $\sigma$-spin electron generates a particle-hole fluctuation of opposite spin on the impurity. Diagrammatically, it reads
with wavy lines representing the interaction $U$ and left-going (right-going) solid lines representing a free particle (hole) propagator $G_i^\sigma$.}

\begin{equation}
\Sigma_i(\omega) \sim \begin{array}{c}
\sigma \\
\sigma
\end{array}
\end{equation}

A. Particle-hole polarisation propagator

The $-\sigma$-spin particle-hole bubble appearing in (1) stands for the noninteracting polarisation propagator

\begin{equation}
0\Pi(\omega) = i \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} G_i^0(\omega') G_i^0(\omega' - \omega).
\end{equation}

Using the Hilbert transform relation for $G_i^0(\omega)$, a short calculation gives

\begin{equation}
\frac{1}{\pi} \text{Im} \, 0\Pi(\omega) = \theta(\omega) \int_{0}^{+|\omega|} d\omega' D_i^0(\omega') D_i^0(\omega' - \omega) + \theta(-\omega) \int_{-|\omega|}^{0} d\omega' D_i^0(\omega') D_i^0(\omega' - \omega).
\end{equation}

Since $\text{Im} \, 0\Pi(\omega)$ is symmetric with respect to the Fermi level $\omega = 0$, it is sufficient to discuss the first term ($\omega > 0$). It describes particle-hole excitations obtained by transferring an electron from an occupied state below the Fermi level ($\omega' - \omega < 0$) to an unoccupied state above it ($\omega' > 0$). The narrow-band model is dominated by particle-hole excitations between the bonding and the anti-bonding orbital, involving an energy cost of $2\omega_0$, which in $\frac{1}{\pi} \text{Im} \, 0\Pi(\omega)$ translates to pole of weight $\approx \frac{1}{4}$ at $\omega = 2\omega_0$.

In addition, $\text{Im} \, 0\Pi(\omega)$ contains two continua, associated with particle-hole excitations to/from the single-particle band and therefore of small spectral weight. A first continuum arises for $\omega \in [\omega_0, \omega_0 + D]$ (net weight $\mathcal{O}(D/\Delta_0)$), corresponding to electronic transfer between the single-particle band and one of the orbitals. A second appears for low frequencies $|\omega| \leq 2D$ (net weight $\mathcal{O}(D^2/\Delta_0^2)$), arising from particle-hole excitations within the single-particle band. As $D_i^0(\omega)$ is finite at the Fermi level $\omega = 0$, the low-frequency behaviour of the latter contribution is

\begin{equation}
\frac{1}{\pi} \text{Im} \, 0\Pi(\omega) \sim_{|\omega| \rightarrow 0} |\omega| \left[D_i^0(0)\right]^2
\end{equation}

(which is used below to prove Fermi-liquid properties on the lowest energy-scale).

B. Self-energy in 2PT

The self-energy in 2nd order perturbation theory (2PT) is given by (1), which translates to:

\begin{equation}
\Sigma_i(\omega) = U^2 \int_{-\infty}^{+\infty} \frac{d\omega'}{2\pi} 0\Pi(\omega') G_i^0(\omega - \omega')
\end{equation}

In analogy to the above calculation for the polarisation propagator, we use the Hilbert transforms for $0\Pi$ and $G_i^0$ to obtain:

\begin{equation}
\Sigma_i^0(\omega) = \theta(\omega) U^2 \int_{0}^{+|\omega|} d\omega' \text{Im} \, 0\Pi(\omega') D_i^0(\omega - \omega') + \theta(-\omega) U^2 \int_{0}^{-|\omega|} d\omega' \text{Im} \, 0\Pi(\omega') D_i^0(\omega - \omega')
\end{equation}

Again, due to particle-hole symmetry, we may restrict the following discussion to positive frequencies; and $\Sigma_i^0(\omega)$ follows from $\Sigma_i^0(\omega)$ by Hilbert transformation.

In the narrow-band limit, the 2PT self-energy is dominated by the following process: an extra $\sigma$-electron is placed in the empty anti-bonding orbital (energy cost $\omega_0$) and excites an electron of opposite spin from the bonding to the anti-bonding orbital (energy cost $2\omega_0$). In $\Sigma_i^0(\omega)$, this generates a pole of weight $\approx \pi U^2/8$ at $\omega = 3\omega_0$, that gives by far the dominant contribution. Much weaker contributions to $\Sigma_i^0(\omega)$ arise in addition from the extra electron being placed in the single-particle band instead of the orbital, or involve one of the particle-hole continua discussed above. This yields self-energy continua for $\omega \in [2\omega_0, 2\omega_0 + D]$ (net weight $\mathcal{O}(U^2D/\Delta_0)$), $\omega \in [\omega_0, \omega_0 + 2D]$ (net weight $\mathcal{O}(U^2[2D/\Delta_0])^2$), and $|\omega| \leq 3D$ with net weight $\mathcal{O}(U^2[D/\Delta_0]^3)$. The latter results from a convolution, as in (11), of the low-frequency continuum of $\text{Im} \, 0\Pi(\omega) \propto \omega$ (see eq. (1)) and the single-particle band. It leads to $\Sigma_i^0(\omega) \propto \omega^2$ close to the Fermi level $\omega = 0$, corresponding to conventional Fermi liquid behaviour.

C. Spectral evolution in the narrow-band regime.

Numerical results for the impurity spectrum $D_i(\omega) = -\frac{1}{\pi} \text{sgn}(\omega) \text{Im} \, G_i(\omega)$ within 2PT will be given in the following section. Here we develop an approximate, but rather accurate analysis that shows in simple physical terms how the spectrum evolves with interaction strength, particularly on the low-energy scales of primary interest.

As discussed above the self-energy is dominated by poles at $\omega = \pm 3\omega_0$, its continua being negligibly small in the narrow-band regime and vanishing as $D \rightarrow 0$. We thus retain solely the pole contributions, i.e.
for any \( U > U/\omega \) in weak coupling solutions.

For \( \omega \rightarrow 0 \), the low-energy pole \( \omega - \Delta_R(\omega) - \Sigma_R^0(\omega) = 0 \) gives rise to a pole-weight, which is valid for \( |\omega| \gg D \) and its counterpart occurring symmetrically below the Fermi level \( \omega = 0 \). The latter follow from the single-particle pole equation \( \omega - \Delta_R(\omega) - \Sigma_R^0(\omega) = 0 \); insertion of (12) into which, together with the expansion \( \Delta_R(\omega) \sim \omega^2/\omega - \) which is valid for \( |\omega| \gg D \) — yields a biquadratic with solutions

\[
\omega_\pm = \frac{1}{4} \left[ \sqrt{U^2 + (8\omega_0)^2} \pm \sqrt{U^2 + (4\omega_0)^2} \right].
\]

The set of low-frequency poles at \( \omega_- \leq \omega_0 \), with pole weights \( q_- \), have their origin in the molecular orbitals of the non-interacting problem, to which they reduce for \( U/\omega_0 \rightarrow 0 \) where \( \omega_- \rightarrow \omega_0 \) and \( q_- \rightarrow 1/2 \). In addition, for any \( U > 0 \), a second set of poles arise at \( \omega_+ \geq 3\omega_0 \). In weak coupling \( U/\omega_0 \ll 1 \), the latter have negligible pole-weight, \( q_+ \sim (U/\omega_0)^2 \). With increasing \( U \) however, they drain weight from the low-frequency orbital remnants and shift to progressively higher frequencies until, for \( U \gg \omega_0 \sim \sqrt{\Delta_0D} \), they correspond to the Hubbard satellites and overwhelmingly dominate the spectrum: \( \omega_+ \sim U/2 \) with pole-weight \( q_+ \sim 1/2 - O((\omega_0/U)^2) \).

The above pole analysis is exact in the strict limit of vanishing bandwidth \( D \rightarrow 0 \), for fixed \( \omega_0 \sim \sqrt{\Delta_0D} \). Here, the host behaves precisely as a single orbital at the Fermi level \( \omega = 0 \), and the problem reduces to the simple two-site model discussed by Lange\(^2\) and employed by Hofstetter and Kehrein\(^3\) to rationalize their Lanczos-determined spectra for the narrow-band AIM. In this limit the hybridization \( \Delta_1(\omega) \) is a \( \delta \)-function, and its weight

\[
\int_{-\infty}^{+\infty} d\omega \Delta_1(\omega) = 2\Delta_0D = \pi|V_0|^2
\]

relates the bonding energy \( \omega_0 \) (eq. (14)) to the hopping between host and impurity, \( \omega_0 = V_0 \). As pointed out by Lange\(^2\), 2PT is in fact exact in this case, the 4-pole spectrum being given precisely by eq. (13); for \( U \gg \omega_0 \) in particular, the low-energy pole \( \omega_- \) reduces to

\[
\omega_- \sim \frac{6\omega_0^2}{U} = \frac{12\Delta_0D}{\pi U} = \frac{3}{2} J
\]

where \( J = 4V_0^2/\omega_0 \) is the antiferromagnetic exchange coupling between the impurity and the host orbital.

As a “zero-bandwidth” approximation, the two-site limit just discussed is however rather limited as a means to interpret the narrow-band AIM. It is certainly accurate for the high-energy spectral poles \( \omega_+ \) (eq. (13)) that evolve for \( U \gg \omega_0 \) to the Hubbard satellites at \( \omega_+ \sim U/2 \). But it naturally fails both on the lowest energy scale of the bandwidth \( D \) and, relatedly, in capturing the strong coupling behaviour of the low-energy spectral poles at \( |\omega| = \omega_- \); the latter, by definition, can only occur outside the band \( \omega_- > D \), whence eq. (17) suggests a breakdown of the two-site analogy for \( \omega \sim O(D) \) or \( U \sim O(\Delta_0) \).

It is however straightforward to obtain, for all interaction strengths, a uniform description of the spectrum at low energies; where by low energy we mean \( |\omega| \ll \omega_0 \sim \sqrt{\Delta_0D} \), encompassing both the lower-energy poles \( \omega_- \) and the continuum for \( |\omega| < D \). For provided only that \( |\omega| \ll 3\omega_0 \), the self-energy given from (12) reduces to its leading low-frequency expansion \( \Sigma_R^0(\omega) \sim - (1/\omega - 1) \omega \). Hence, for \( |\omega| \ll 3\omega_0 \), the impurity Green function \( G_i(\omega) \) is given from (3), using (3) for the hybridization, by

\[
\Delta_0 \thickapprox -\frac{D}{\Delta_0 Z} \log \left[ \frac{1 + \omega}{1 - \omega} + i \text{sgn}(\omega) \theta(1 - |\omega|) \right]^{-1}
\]

where \( \omega = \omega/D \). This equation may be used to understand the low-energy spectrum for all \( U \). It depends upon the single parameter \( \Delta_0Z/D \), where the \( U \)-dependence of the quasi-particle weight \( Z \) is given explicitly by eq. (13) for 2PT. And the characteristic spectra divide into two distinct regimes, according to whether \( \Delta_0Z/D \gg 1 \) or \( \ll 1 \), as now considered.

1. \( \Delta_0Z/D \gg 1 \).

From eq. (13), \( \Delta_0Z/D \gg 1 \) corresponds to \( U/\Delta_0 \ll 6\sqrt{2}/\pi \approx 5 \). Here the spectral poles, at \( |\omega| = \omega_- \) occur far outside the band. Specifically, expanding \( \log \left| \frac{1 + \omega}{1 - \omega} \right| \sim 2/\omega \) for \( |\omega| \gg 1 \), eq. (18) yields \( \omega_- = \sqrt{\frac{2\Delta_0Z}{\pi U}} \gg 1 \), i.e.

\[
\omega_- = \omega_0 \sqrt{Z}
\]
The essential conclusions above are nonetheless largely independent of 2PT. Eq. (18) amounts to a low-frequency expansion of the self-energy (embodied in the first term) that is quite general, independent of the U-dependence of Z, and valid for \( \frac{D}{\Delta_0 Z} |\omega| \ll 1 \). This by itself is sufficient to infer the two distinct spectral regimes, \( \Delta_0 Z \gg D \) where the spectrum contains low-energy poles at \( \omega^- \) (given in terms of \( \omega_0 \) and \( Z \) by eqs. (18)), and with a continuum for \( |\omega| < D \) that is essentially unrenormalized by interactions; and \( \Delta_0 Z \ll D \) where solely the continuum survives and eq. (18) provides a reasonable description of the Kondo resonance for \( \omega/\Delta_0 \gg 1 \). Further, since 2PT is exact for the two-site limit, we anticipate that it should provide a sound description of the observed Lanzos spectra at least for \( \Delta_0 Z/D \gtrsim 1 \), as considered in the following section.

Before proceeding we comment briefly on the suggestion of Hofstetter and Kehrein that the low-energy spectrum (including the poles) in the narrow-band limit \( D \to 0 \), should be described by a scaling function \( D_1(\omega) \equiv f(\omega = \omega/D) \) where \( f \) is independent of \( D \). Eq. (18) supports this, since from the 2PT result \( \Delta_0 Z/D \sim (\Delta_0/U)^2 \) is independent of \( D \) provided \( U \gg \omega_0 \sim \sqrt{\Delta_0 D} \to 0 \) (which encompasses both the \( \Delta_0 Z/D \gg 1 \) and \( \ll 1 \) regimes). This however is distinct from the one-parameter universal scaling that is characteristic of the strong coupling Kondo regime. The latter arises only for \( \Delta_0 Z \ll D \), where the low-energy spectrum \( D_1(\omega) \equiv f(\omega/\Delta_0 Z) \) but is otherwise independent of any of the bare parameters \( D, \Delta_0 \) or \( U \).

### D. Spectra: numerical results

We turn now to the numerically determined 2PT spectra. Fig. shows the low-frequency behaviour of \( D_1(\omega) \) vs. \( \omega = \omega/D \), for a bandwidth of \( D = 10^{-4} \Delta_0 \) and interaction strength \( U = 0.2 \Delta_0 \). For these parameters \( \Delta_0 Z/D \approx 500 \), safely in the weak coupling regime \( \Delta_0 Z/D \gg 1 \) — albeit ’strong’ coupling in the sense that \( U/\omega_0 \approx 3 \), as manifest in a quasi-particle weight \( Z \approx 0.054 < 1 \) that is far removed from the non-interacting limit where \( Z = 1 \). The spectrum is shown for \( |\omega|/D < 200 \), and we remind the reader that almost all (~95%) of the spectral weight resides in the Hubbard satellites at frequencies as large as \( U/2 = 10^5 D \), which are omitted from the figure.

On the lowest energy scale \( |\omega| < D \) we see the expected continuum of net weight \( \mathcal{O}(D/\Delta_0) \) which, in accordance with the discussion above, is indeed essentially unrenormalized from the non-interacting limit. At the band edges \( \omega = \pm D \), the spectrum vanishes of necessity since the hybridization \( \Delta_R(\omega) \) is singular there. Due to the lowest frequency self-energy continua (§ above), the central continuum acquires side bands ranging from \( D \leq |\omega| \leq 3D \), whose weight remains tiny over the whole range of interactions.
On the next higher energy scale, proportional to the antiferromagnetic coupling $J$, we find the 'orbital remnants' at (eq. (17)) $\omega_0 = 3J/2 = 12\Delta_0 D/(\pi U) \simeq 19D$. These poles are by far the most prominent features of the low-energy spectrum, carrying almost all the spectral weight in this sector, although their absolute weight (eq. (19b)) $q_- = Z/2 \simeq 0.027$ is small since the dominant spectral intensity is carried by the high-energy Hubbard satellites. A third low-energy scale is the molecular bonding energy $\omega_0 \sim \sqrt{\Delta_0 D}$ emerging from the non-interacting limit. It enters the single-particle spectrum via the self-energy continua ($\Sigma$) and yields two sets of weak bands at $|\omega| \simeq \omega_0 \simeq 80D$ and $|\omega| \simeq 2\omega_0 \simeq 160D$, albeit with net spectral weights that render them insignificant in practice.

A comparison of Fig. 1 with the spectrum of an 11+1-site Anderson star, calculated numerically for the same parameters by Hofstetter and Kehrein, with the Lanczos method, shows that 2PT is able to reproduce essentially all relevant energy scales. Good agreement is found in the lowest energy scale $D$, given by the Fermi liquid continuum, and on the high-energy scale $U/2$ for the Hubbard satellites, although 2PT remains somewhat incomplete on the antiferromagnetic scale $J$. Here, instead of the single pole predicted by 2PT at $|\omega| = \omega_0 \simeq 19D$, the Lanczos calculations show two sets of $\delta$-peaks, the first occurring for $|\omega| \simeq 18-21D$ and the second for $|\omega| \simeq 25-26D$. Although it is not clear how these sets will evolve with a larger number of sites in the Lanczos calculations, a structure with at least two features will most likely be preserved in this region. This points to the natural limitations of 2PT, and the need for more sophisticated many-body techniques.

For obvious numerical reasons, the Lanczos method cannot detect any features as weak as the 2PT continua at $\omega_0 \simeq 80D$ and $2\omega_0$. Nevertheless we believe these continua to be robust. They cannot be cancelled by higher order self-energy diagrams since, for any frequency, $\Sigma(\omega) \geq 0$ for all self-energy contributions.

Having discussed the weak coupling regime $\Delta_0 Z/D \gg 1$, we now turn to strong coupling, $\Delta_0 Z/D \ll 1$, and the approach to it. Fig. 2 shows the low-energy $D_i(\omega)$ vs. $\omega = \omega/D$, again for a bandwidth of $D = 10^{-4}\Delta_0$; and for interaction strengths $U/\pi\Delta_0 = 2$, 4 and 6, corresponding respectively to $\Delta_0 Z/D \approx 0.58$, 0.15 and 0.06. In agreement with the analysis of §III C above, and excluding the Hubbard satellites at $\pm U/2$, the spectra in all cases are in practice confined exclusively to the low-frequency continuum $|\omega| < D$, whose persistent Fermi liquid character is manifest in the pinning of the spectra at the Fermi level ($\omega = 0$) to its non-interacting value of $1/\pi\Delta_0$. For the two larger interaction strengths in particular, the Lorentzian character of the 2PT Kondo resonance arising for $\Delta_0 Z/D \ll 1$ is seen clearly.

The results above concur with the Lanczos calculations of Hofstetter and Kehrein, performed at a moderate interaction strength $U/\Delta_0 = 4$. No low-energy poles arose, and the spectrum was found to be governed by a Fermi liquid continuum with a broad resonance centered on the Fermi level and two sharper features at the band edges. As shown by the top curve of Fig. 2, 2PT reproduces this behaviour remarkably well, albeit that it sets in at a somewhat larger interaction strength of $U/\Delta_0 \simeq 6$.

For numerical reasons, the strong coupling Kondo regime $\Delta_0 Z/D \ll 1$ naturally cannot be captured adequately by the Lanczos calculations, and the deficiencies of 2PT in this regime have also been highlighted in §III C. It appears however that 2PT provides a rather reasonable description of the Lanczos results for the narrow-band AIM, and is valid up to interaction strengths $U/\pi\Delta_0$ on the order of 2 or so, a regime of validity that corresponds closely to that found also with 2PT for the normal wide-band ($D = \infty$) model (see eg. Ref. 2).

IV. SELF-ENERGY, AND SKELETON EXPANSION.

Within 2PT the structure of the self-energy for the narrow-band model ($\Delta_0 \gg D$) is rather simple, being dominated by poles at $\omega = \pm 3\omega_0$, each of weight $\pi U/8$ (see eq. (12)). In view of the natural limitations of 2PT however, one might ask what may be inferred more generally about the behaviour of $\Sigma_i(\omega)$, and in particular pole contributions thereto? It is aspects of this issue that we now consider.

The self-energy is effectively defined via the Dyson equation (16) whence, for frequencies $\omega$ where the single-particle spectrum is purely real, $\Sigma_i(\omega)$ is given by

$$\Sigma_i(\omega) = \omega - \Delta_R(\omega) - \frac{1}{X(\omega)}. \quad (22)$$

Here $X(\omega) \equiv \text{Re}G_i(\omega)$ is thus defined for convenience, and is given by the Hilbert transform

$$X(\omega) = 2\omega \int_0^{\infty} \frac{D_i(\omega')}{\omega^2 - \omega'^2} \quad (23)$$

(where particle-hole symmetry has been employed, and a principal value is implicit). As is well known (see also Ref. 1), it follows from eq. (22) that the zeros of $X(\omega)$ correspond to the poles in $\Sigma_i(\omega)$. For weak to moderate interaction strengths ($U/\Delta_0 \lesssim 4$), Hofstetter and Kehrein find that the Lanczos determined $X(\omega) = 0$ for $\omega \sim \mathcal{O}(\omega_0)$ and hence that $\Sigma_i(\omega)$ contains poles at frequencies on the order of $\pm \sqrt{\Delta_0 D}$. This concurs with 2PT, which we have argued ($\Sigma$) to be valid in such a weak coupling domain, where $\Delta_0 Z/D \gtrsim 1$. But what of the strong coupling regime $U \gg \Delta_0$ ($\gg D$), where $\Delta_0 Z/D \ll 1$ and the Kondo effect is well developed? The limitations of the Lanczos technique in this domain have been alluded to above, but the general structure of the Lanczos-determined spectrum $D_i(\omega)$ is in fact sufficient to determine the poles of $\Sigma_i(\omega)$, as now shown.
In strong coupling the single-particle spectrum is found to separate into high- and low-energy parts, \( D_i(\omega) = D_i^H(\omega) + D_i^L(\omega) \); we focus below on \( \omega > 0 \) (by particle-hole symmetry). The high-energy contribution is \( D_i^H(\omega) = q+\delta(\omega - \omega_+). \) It corresponds to the Hubbard satellite, with position \( \omega_+ \sim U/2 \) and pole-weight \( q_+ \sim 1/2. \) By contrast the low-energy continuum \( D_i^L(\omega) \) is non-zero only on the band scale \( |\omega| \leq D, \) is pinned at the Fermi level where \( \pi\Delta_0 D_i(\omega = 0) = 1 \) ubiquitously, and contains a well developed Kondo resonance on the scale \( \omega \sim \Delta_0 Z \ll D. \) From eq. (23) it follows that \( X(\omega) = X_H(\omega) + X_L(\omega), \) given asymptotically by

\[
X_H(\omega) \sim \frac{2q_+}{\omega_+} \sim \frac{4}{U^2} \omega \quad \text{for} \quad \omega \ll U/2 \tag{24a}
\]

\[
X_L(\omega) \sim \frac{\delta}{\omega} \quad \text{for} \quad \omega \gg D \tag{24b}
\]

where \( \delta = \int_0^D d\omega D_i^L(\omega) \) is the integrated weight of the low-energy continuum. From eq. (24) the zeros of \( X(\omega), \) and hence the poles of \( \Sigma_i(\omega), \) thus occur at \( \omega = \pm \omega_P \) given by

\[
\omega_P = \omega_+ \sqrt{\frac{\delta}{2q_+}} \sim \frac{U}{2} \sqrt{\delta} \quad \text{(25)}
\]

(which is self-consistent provided \( D \ll \omega_P \ll U/2 \) as indeed found, see below); the corresponding pole-weight in \( \Sigma_i(\omega), \) given from eq. (22) by \( Q = \pi/|\partial X(\omega)/\partial \omega|_{\omega=\omega_P}, \) is

\[
Q = \frac{\pi \omega_+^2}{4q_+} \sim \frac{\pi U^2}{8} \quad \text{(26a)}
\]

Since \( D_i(\omega) \) is normalized to unity however, the integrated low-energy spectral weight \( \delta = 1 - 2q_+. \) In strong coupling moreover, where \( |2\epsilon_i| = U \gg \Delta_0 \gg D, \) the leading asymptotic behaviour of the high-energy spectral pole-weight \( q_+ \) is in turn readily deduced by taking the limit of constant \( V_k \) and \( D \to 0, i.e. \) by considering fixed \( \omega_0 \sim \sqrt{\Delta_0 D} \) and \( D \to 0, \) which is just the two-site limit for which \( q_+ \sim 1/2 - 18\omega_0^2/U^2 \) (amounting in effect to perturbation theory in \( V_k/U \)). Hence \( \delta \sim 36\omega_0^2/U^2, \) and from eq. (23),

\[
\omega_P = 3\omega_0 \quad \text{(26b)}
\]

Eq. (26b) (with \( Q \) from (20a)) is the result in strong coupling \( U \gg \Delta_0 \) for the poles in \( \Sigma_i(\omega), \) the arguments for it do not depend upon perturbation theory in \( U \) about the non-interacting limit, but the result itself is precisely that arising from simple 2PT, eq. (12). This is salutary, for although 2PT extrapolated to strong coupling produces an inadequate caricature of the Kondo resonance on scales \( \omega \sim O(\Delta_0 Z) \ll D \) (see e.g. §11C), the above arguments suggest that on scales of order \( \omega_0 \sim \sqrt{\Delta_0 D} \) it becomes asymptotically exact in strong coupling. In addition, noting that \( \omega_0 = U \)-independent and that eq. (26b) holds both perturbatively for \( U \lesssim O(\Delta_0) \) and in strong coupling \( U \gg \Delta_0, \) it is clear that any dependence of the poles in \( \Sigma_i(\omega) \) upon \( U \) is at best weak across the entire range of interaction strengths.

### A. Skeleton expansion

There is a second feature of the above analysis to which we would draw attention, namely that the poles in \( \Sigma_i(\omega) \) connect continuously to that characteristic of the atomic limit, \( \Delta_0 = 0 \) (i.e. \( V_k = 0 \)). As \( \Delta_0 \to 0 \) the two poles in \( \Sigma_i(\omega), \) each of weight \( Q = \pi U^2/8 \) and occurring at \( \omega = \pm 3\omega_0 \) with \( \omega_0 \sim \sqrt{\Delta_0 D}, \) coalesce to a single pole at \( \omega = 0 \) with weight \( \pi U^2/4, \) thus producing

\[
\Sigma_i(\omega) = \frac{U^2}{\omega + i0^+} \quad \text{for} \quad \Delta_0 = 0 \quad \text{(27)}
\]

This result, which corresponds to 2PT, is of course well known to be exact in the atomic limit for all \( U > 0, \) a feature that is particular to the particle-hole symmetric case considered.

Hofstetter and Kehrein have considered the behaviour of \( \Sigma_i(\omega) \) for the narrow-band AIM from the perspective of the skeleton expansion, where the exact propagator \( G_i(\omega) \) is inserted into every skeleton diagram contributing to \( \Sigma_i(\omega) \). They point out that the pinning of the single-particle spectrum at the Fermi level (for all \( U \geq 0 \) and any \( \Delta_0 \geq 0 \)) attests to the convergence of the skeleton expansion on the lowest energy scales characteristic of the Fermi liquid continuum. Conversely, following Kehrein, they show that the \( |\omega| \sim O(\omega_0) \) poles in \( \Sigma_i(\omega) \) cannot be explained in any order of the skeleton expansion, which fails to converge for such frequencies. Given the above connection between the poles in \( \Sigma_i(\omega) \) and that endemic to the atomic limit, the latter behaviour is entirely natural, since it is known that the skeleton expansion fails to converge for the atomic limit (and more generally, but in essence equivalently, for an insulator). In view of the above it may be instructive to consider the failure of the skeleton expansion, taking the atomic limit as a paradigm. The essence of the skeleton expansion to any finite order is that it involves a partial infinite-order summation of diagrams obtained from PT in \( U \) (and themselves expressed in terms of the non-interacting propagator \( G_i^0(\omega) \)). As such however, it may fail to include higher-order diagrams that act in large part to cancel those that are included, and this is where the dangers arise.

Consider for example the following diagram, which is 4th order in PT but is included in the class of 2nd order skeletons:
It represents a process creating two particle-hole excitations of spin $-\sigma$ on the impurity site. If the first such pair has not hopped off the impurity when the second pair is created — as is inexorable in the atomic limit — then such processes are formally forbidden by the Pauli principle. They are nonetheless properly cancelled by exchange diagrams arising from the same order in PT, for example:

\[ \sigma \]

However the exchange diagram (29), while arising to the same order in PT as (28), belongs to the class of 4th order skeletons. In this sense it is of higher order, and would not therefore be included if the skeleton expansion was truncated at 2nd order.

Generalizing this reasoning illustrates that the skeleton expansion, if truncated after a certain class, will include specific series of diagrams without necessarily accounting for the corresponding exchange terms, since the latter belong in general to a higher skeleton class. Hence, even for systems where PT in $U$ is known to converge order-by-order, the order-by-order convergence in skeletons may not be taken for granted.

The atomic limit, whose relevance to the narrow-band AIM has been pointed out above, provides a direct example of the latter point. Here $\Sigma_i(\omega)$ is given exactly by 2PT (eq. (28)), i.e. by $\Sigma_i(\omega) = \frac{U^2}{4} G_0^0(\omega)$ (where, trivially, the unperturbed $G_0^0(\omega) = 1/(\omega + i0^+ \text{sgn}(\omega))$). The problem is convergent order-by-order in straight PT, all diagrams contributing to $\Sigma_i(\omega)$ in any given order $n > 2$ of PT summing precisely to zero. Consider by contrast the second-order skeleton expansion, denoted $\Sigma_i^{(2)}$ and obtained from eq. (28) by replacing $G^n$ with the exact $G_i$, to give $\Sigma_i^{(2)}(\omega) = \frac{U^2}{4} \frac{\omega^2}{\omega^2 - (3U/2)^2} \sim \frac{\omega}{9}$. This fails entirely to capture the $\sim 1/\omega$ behaviour of the exact $\Sigma_i(\omega)$ (save trivially for $|\omega| \gg 3U/2$), and that it does so for the essential reasons outlined above is directly evident by recasting $\Sigma_i^{(2)}$ as a functional of $G_i^0$, viz:

\[ \Sigma_i^{(2)}(\omega) = \frac{\frac{U^2}{4} G_i^0(\omega)}{1 - \left( \frac{\frac{U^2}{4} G_i^0(\omega)}{\omega} \right)^2} \]  

Finally, we note that the behaviour described in this section is not specific to the narrow-band AIM, but arises also in the infinite-dimensional Hubbard model at half filling (in which context study of the narrow-band AIM was first motivated). Within IPT as $U$ approaches the critical $U_c$ for the Mott transition from the metallic phase $U < U_c$, the self-energy acquires poles (or strictly, sharp resonances) at finite $\omega$ in a preformed gap; and as $U \rightarrow U_c$ — the pole positions approach the Fermi level $\omega = 0$ (less rapidly than the central Fermi liquid continuum vanishes), and with weights that remain finite. Hence as $U \rightarrow U_c$ — the low-frequency behaviour characteristic of an insulator — $\Sigma_i(\omega) \sim A/(\omega + i0^{+} \text{sgn}(\omega))$ which amounts in essence to that for the atomic limit — is smoothly recovered via IPT. The poles in $\Sigma_i(\omega)$ are thus an integral facet of the Mott transition and, from the discussion above, we believe the success of IPT in capturing it is intimately connected to its ability to recover correctly the atomic limit. By contrast, since the poles in $\Sigma_i(\omega)$ cannot be captured via the skeleton expansion approaches based at heart upon the latter — such as self-consistent perturbation theory — simply fail to uncover the transition.

\[ \text{V. CONCLUSIONS} \]

We have studied in this article the symmetric AIM with a narrow host band, $D \ll \Delta_0$. Simple though it is, second order perturbation theory in $U$ is found to give a rich and relatively complete account of the underlying single-particle dynamics. In particular, and in agreement with recent Lanczos calculations, it leads naturally to two distinct regimes of spectral behaviour according to whether $\Delta_0 Z/D \gg 1$ or $\ll 1$, and whose essential characteristics we have argued to be largely independent of the details of 2PT itself.

We have also shown that 2PT is remarkably robust on energy scales of order $|\omega| \sim \sqrt{\Delta_0 D}$, that reflect the underlying molecular orbitals characteristic of the non-interacting limit. Here we have argued that the 2PT result for the self-energy is correct both perturbatively in weak coupling (by construction), and in the strong coupling limit $U \gg \Delta_0$. Such poles in $\Sigma_i(\omega)$ — which cannot be captured to any order in a skeleton expansion — thus appear to be an essentially $U$-independent characteristic of the narrow-band AIM, and that they are captured by 2PT is in turn closely related to its ability to recover correctly the atomic limit of the model.

The latter comments also illustrate the difficulties that confront any theory which seeks to describe single-particle dynamics of the narrow-band AIM in strong coupling, and on all energy scales. At low energies $\omega \sim \omega_K \ll D$ characteristic of the Kondo resonance, low-order PT in $U$ will naturally not suffice and an intrinsically non-perturbative approach will be needed. And yet for energy scales on the order of $\sqrt{\Delta_0 D} \ll \Delta_0$ the essential result of 2PT must be recovered — which as we have discussed is a delicate matter, since 'obvious' approaches
based on partial infinite-order summation of PT in $U$
are liable to qualitative failure here. While accessible to
numerical techniques such as the numerical renormaliza-
tion group, we do not know of any conventional theo-
retical approach that can encompass these twin dictates.
In a subsequent paper we will however show that a re-
cently developed local moment approach can handle
the problem.

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FIG. 1. Low-frequency 2PT impurity spectrum, for bandwidth $D = 10^{-4}\Delta_0$ and $U = 0.2\Delta_0$, where $\Delta_0 Z/D \gg 1$. Note the logarithmic scale for $D_i(\omega)$, employed for clarity. The Hubbard satellites at $|\omega| \simeq U/2 = 10^3 D$ are not shown. Full discussion in text.

FIG. 2. Low-frequency 2PT impurity spectrum, $\pi\Delta_0 D_i(\omega)$ vs. $\omega/D$, for bandwidth $D = 10^{-4}\Delta_0$ and $U/\Delta_0 = 2\pi$ (top), $4\pi$ (middle) and $6\pi$ (bottom), corresponding respectively to $\Delta_0 Z/D \simeq 0.58$, $0.15$ and $0.06$. The emergence of the Kondo resonance for $\Delta_0 Z/D \ll 1$ is seen clearly. Full discussion in text.