Sum-Rule Conserving Spectral Functions from the Numerical Renormalization Group

Andreas Weichselbaum and Jan von Delft

Physics Department, Arnold Sommerfeld Center for Theoretical Physics, and Center for NanoScience,
Ludwig-Maximilians-Universität München, D-80333 München, Germany

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We show how spectral functions for quantum impurity models can be calculated very accurately using a complete set of discarded numerical renormalization group eigenstates, recently introduced by Anders and Schiller. The only approximation is to judiciously exploit energy scale separation. Our derivation avoids both the overcounting ambiguities and the single-shell approximation for the equilibrium density matrix prevalent in current methods, ensuring that relevant sum rules hold rigorously and spectral features at energies below the temperature can be described accurately.

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Quantum impurity models describe a quantum system with a small number of discrete states, the “impurity,” coupled to a continuous bath of fermionic or bosonic excitations. Such models are relevant for describing transport through quantum dots, for the treatment of correlated lattice models using dynamical mean field theory, or for the modeling of the decoherence of qubits.

The impurity’s dynamics in thermal equilibrium can be characterized by spectral functions of the type \( \mathcal{A}^{Bc}(\omega) = \int \frac{d\omega}{2\pi} \epsilon(\omega) \rho(\omega) \), with \( \rho(\omega) \) being the density matrix at temperature \( T \) and \( \epsilon(\omega) \) the energy. The Lehmann representation reads

\[
\mathcal{A}^{Bc}(\omega) = \sum_{a,b} \langle b | \hat{C}^\dagger | a \rangle \frac{e^{-\beta E_a}}{Z} \langle a | \hat{B} | b \rangle \delta(\omega - E_{ba}),
\]

where \( Z = \sum_a e^{-\beta E_a} \) and \( E_{ba} = E_b - E_a \), which implies the sum rule \( \int d\omega \mathcal{A}^{Bc}(\omega) = \langle \hat{B} \hat{C} \rangle_T \). In this Letter, we describe a strategy for numerically calculating \( \mathcal{A}^{Bc}(\omega) \) that, in contrast to previous methods, rigorously satisfies this sum rule and accurately describes both high and low frequencies, including \( \omega \approx T \), which we test by checking our results against Fermi-liquid relations.

Our work builds on Wilson’s numerical renormalization group (NRG) method [1]. Wilson discretized the environmental spectrum on a logarithmic grid of energies \( \Lambda^{-n} \) (with \( \Lambda > 1 \), \( 1 \leq n \leq N \rightarrow \infty \)), with exponentially high resolution of low-energy excitations, and mapped the impurity model onto a “Wilson tight-binding chain,” with hopping matrix elements that decrease exponentially as \( \Lambda^{-n/2} \) with site index \( n \). Because of this separation of energy scales, the Hamiltonian can be diagonalized iteratively: adding one site at a time, a new “shell” of eigenstates is constructed from the new site’s states and the \( M_k \) lowest-lying eigenstates of the previous shell (the so-called “kept” states), while “discarding” the rest.

Subsequent authors [2–10] have shown that spectral functions such as \( \mathcal{A}^{Bc}(\omega) \) can be calculated via the Lehmann sum, using NRG states (kept and discarded) of those shells \( n \) for which \( \omega \approx \Lambda^{-n/2} \). Though plausible on heuristic grounds, this strategy entails double-counting ambiguities [5] about how to combine data from successive shells. Patching schemes [9] for addressing such ambiguities involve arbitrariness. As a result, the relevant sum rule is not satisfied rigorously, with typical errors of a few percent. Also, the thermal density matrix (DM) \( \hat{\rho} = e^{-\beta \hat{H}} / Z \) has until now been represented rather crudely using only the single \( N_t \)th shell for which \( T = \Lambda^{-1/2(NT-1)} \) [8], with a chain of length \( N = N_T \), resulting in inaccurate spectral information for \( \omega \approx T \). In this Letter we avoid these problems by using in the Lehmann sum an approximate but complete set of eigenstates, introduced recently by Anders and Schiller (AS) [11].

Wilson’s truncation scheme.—The Wilson chain’s zeroth site represents the bare impurity Hamiltonian \( \hat{H}_0 \) with a set of \( d_0 \) impurity states \( |\sigma_0\rangle \). It is coupled to a fermionic chain, whose \( n \)th site (\( 1 \leq n \leq N \)) represents a set of \( d \) states \( |\sigma_n\rangle \), responsible for providing energy resolution to the spectrum at scale \( \Lambda^{-n/2} \). For a spinful fermionic band, for example, \( \sigma_n \in \{0,1,\ldots,m\} \), hence \( d = 4 \). (Bosonic chains can be treated similarly [10].) The Hamiltonian \( \hat{H} = \hat{H}_N \) for the full chain is constructed iteratively by adding one site at a time, using \( \hat{H}_n = \hat{H}_{n-1} + \hat{h}_n \) (acting in a \( d^2 d_0 \)-dimensional Fock space \( \mathcal{F}_n \) spanned by the basis states \( |\sigma_n \rangle \otimes \cdots \otimes |\sigma_0 \rangle \)), where \( \hat{h}_n \) links sites \( n \) and \( n-1 \) with hopping strength \( \sim \Lambda^{-n/2} \). Since the number of eigenstates of \( \hat{H}_n \) grows exponentially with \( n \), Wilson proposed the following iterative truncation scheme to numerically diagonalize the Hamiltonian: Let \( n_0 \) be the last iteration for which a complete set \( |\sigma_n \rangle \) of kept eigenstates of \( \hat{H}_{n_0} \) can be calculated without truncation. For \( n > n_0 \), construct the orthonormal eigenstates \( |\sigma_n \rangle \) of \( \hat{H}_n \) (the \( n \)th “shell”), with eigenvalues \( E^n_n \), as linear combinations of the kept eigenstates \( |\sigma_{n-1} \rangle \) of \( \hat{H}_{n-1} \) and the states \( |\sigma_n \rangle \) of site \( n \),

\[
|\sigma_n \rangle = \sum_{\sigma_{n-1}} \sum_{a_1 a_2 \ldots a_K} \langle a_1 | \sigma_{n-1} \rangle \langle a_2 | \sigma_{n-1} \rangle \ldots \langle a_K | \sigma_{n-1} \rangle |a_{n-1}\rangle \langle a_n | a_{n-1} \rangle \ldots \langle a_K | a_{n-1} \rangle,
\]

with coefficients arranged into a matrix \( A_{KX}^{[\sigma_n]} \) whose ele-
ments are labeled by $ss'$. The superscript $X = K$ or $D$ indicates that the new shell has been partitioned into "kept" states (say the $M_K$ lowest-lying eigenstates of $\hat{H}_n$) to be retained for the next iteration and "discarded" states (the remaining ones). Since $\hat{H}_n$ acts as a weak perturbation (of relative size $\Delta^{-1/2}$) on $\hat{H}_{n-1}$, the $d$-fold degeneracy of the states $|\sigma_n\rangle \otimes |s\rangle_{n-1}$ is lifted, resulting in a characteristic energy spacing $\Delta^{-n/2}$ for shell $n$. Iterating until the spectrum of low-lying eigenvalues has reached a fixed point (for $n = N$, say), one generates a set of eigenstates $\{|s\rangle_N\}$ with the structure of matrix product states [12] (Fig. 1). The states generated for the last $N$th shell will all be regarded as discarded [11].

Anders-Schiller basis.—Recently, AS have shown [11] that the discarded states can be used to build a complete basis for the whole Wilson chain: the states $\{|s\rangle_N\}$ describing the $n$th shell are supplemented by a set of $d^{N-n}$ degenerate "environmental" states $\{|e_n\rangle = |\sigma_N\rangle \otimes \cdots \otimes |\sigma_{n+1}\rangle\}$ spanning the rest of the chain to construct the set of states $\{|se\rangle_N = |e_n\rangle \otimes |s\rangle_N\}$. These reside in the complete Fock space $\mathcal{F}_N$ of the full chain, spanning $\mathcal{F}_N$ if $n \leq N$. Ignoring the degeneracy-lifting effect of the rest of the chain, these states become approximate eigenstates of the Hamiltonian $\hat{H}_N$ of the full chain ("NRG approximation"),

$$\hat{H}_N|se\rangle_N \approx E^s|se\rangle_N,$$

with eigenenergies independent of the $(d^{N-n})$-fold degenerate environmental index $e_n$. (This will facilitate tracing out the environment below.) By construction, we have $D_n^0|se\rangle_N = \delta_{mn}|se\rangle_N$ and

$$K_m^j|se\rangle^D = \begin{cases} 0, & m \geq n \\ \delta_{e_n,e'_m}|A^{s_{n+1}}|A^{s_n}, & m < n. \end{cases}$$

The discarded states of shell $n$ are orthogonal to the discarded states of any other shell, and to the kept states of that or any later shell. Combining the discarded states from all shells thus yields a complete set of NRG eigenstates of $\hat{H}_n$, the "Anders-Schiller basis," that span the full Fock space $\mathcal{F}_N$ ($\Sigma_n$ henceforth stands for $\Sigma_{n>n_0}$):

$$1^{(d^{N-n})} = \sum_{se} |se\rangle_n^K \langle se| = \sum_{n} \sum_{se} |se\rangle_n^{DD} \langle se|.$$  (5)

Local operators.—Let us now consider a "local" operator $\hat{B}$ acting nontrivially only on sites up to $n_0$. Two particularly useful representations are

$$\hat{B} = \sum_{ss'} \langle ss'| \hat{B}_{Kn}^{[sn]} \rangle^K_n |ss'\rangle^K_n = \sum_{n} \sum_{XX} \hat{B}^{[nn]}_{XX}. \quad (6)$$

The left equality, written $\hat{B} = \hat{B}_{Kn}^{[nn]}$, in brief, represents the operator in the complete basis set $\{|se\rangle_N\}$, with matrix elements known exactly numerically (possibly up to fermionic minus signs depending on the environmental states, but these enter quadratically in correlation functions and hence cancel). The right-hand side (RHS) of Eq. (6) expresses $\hat{B}$ in the AS basis and is obtained as follows: starting from $\hat{B}_{Kn}^{[nn]}$, one iteratively refines the "kept-kept" part of $\hat{B}$ from, say, the $(n-1)^{th}$ iteration in terms of the NRG eigenstates $\{|se\rangle_n\}$ of the next shell, including both kept and discarded states ($X = K, D$),

$$\hat{B}_{Kn}^{[nn-1]} = \sum_{XX} \sum_{ss'} |se\rangle_n^K \langle ss'| \hat{B}_{Kn}^{[nn]} \rangle_{XX} |se\rangle_n^K = \sum_{XX} \hat{B}_{Kn}^{[nn]} \quad (7)$$

thereby defining the operators $\hat{B}_{Kn}^{[nn]}$, with matrix elements $\langle ss'| \hat{B}_{Kn}^{[nn]} \rangle_{XX} = \langle s_{n+1} | A^{s_{n+1}} \cdots A^{s_n} | ss', \rangle_{XX}$. Splitting off all $XX \neq KK$ terms ($DD, KD, DK$) and iteratively refining each $KK$ term until $n = N$, we obtain the RHS of Eq. (6). It has two important features. First, the matrix elements of the time-dependent operator $\hat{B}(t) = e^{-it\hat{H}}\hat{B} e^{it\hat{H}}$, evaluated within the NRG approximation, $\langle ss'| \hat{B}(t) \rangle_{XX} \approx \langle ss'| \hat{B}_{Kn}^{[nn]} \rangle_{XX} e^{-i(E^s_n - E^n)}$, contain differences of eigenenergies from the same shell only, i.e., calculated with the same level of accuracy. Second, by excluding $KK$ terms it rigorously avoids the double-counting ambiguities and heuristic patching rules plaguing previous approaches [2–10].

Thermal averages.—To calculate thermal averages $\langle \cdots \rangle_T = \text{Tr}[\hat{\rho}^{[nn]}]$, we write the full density matrix (FDM) $\hat{\rho} = e^{-\beta \hat{H}}/Z$ using the NRG approximation Eq. (3),

$$\hat{\rho} \approx \sum_{n} \sum_{se} |se\rangle_n^D e^{-\beta E^n_n} \frac{D_n^0}{Z} \langle se| = \sum_{n} w_n \hat{\rho}_{DD}^{[nn]}.$$

where $w_n = \frac{d^{N-n}2^D}{Z}$ and $Z^0 = \sum_{n} e^{-\beta E^n_n}$. The RHS of Eq. (8) expresses $\hat{\rho}$ as sum over $\hat{\rho}_{DD}^{[nn]}$, the density matrix for the discarded states of shell $n$, properly normalized as $\text{Tr}[\hat{\rho}_{DD}^{[nn]}] = 1$, and entering with relative weight $w_n$, with $\sum_n w_n = 1$. Similarly, for spectral functions we have

$$\langle \cdots \rangle_T = \sum_{n} w_n \langle \cdots \rangle_n, \quad \mathcal{A} (\omega) = \sum_{n} w_n \mathcal{A}_n (\omega),$$

where the averages $\langle \cdots \rangle_n$ and spectral functions $\mathcal{A}_n (\omega)$ are calculated with respect to $\hat{\rho}^{[nn]}_{DD}$ of shell $n$ only.

Previous strategies [4–11] for thermal averaging amount to using a "single-shell approximation" $w_n = \delta_{n,N}$ for the density matrix and terminating the chain at a length $N = N_T$ set by $T \approx \Delta^{-1/2(N-1)}$. As a result, spectral features on scales $\omega \ll T$, which would require a longer chain, are described less accurately [see Figs. 2(a) and 2(b)]. Our
novel approach avoids these problems by using the full density matrix (FDM), summed over all shells, letting the weighting function \( w_n \) select the shells relevant for a given temperature yielding a smooth \( T \) dependence [see Fig. 2(c)]. Since \( w_n \) has a peak width of five to ten shells depending on \( \Lambda, \alpha \), and \( M_k \) and peaks at \( n \) values somewhat above \( N_T \) [arrow Fig. 2(b)], spectral information from energies well below \( T \) is retained.

Let us now consider the spectral function \( \mathcal{A}^{BC}(\omega) \), for local operators \( \hat{B} \) and \( \hat{C} \). Equations (4), (6), (8), and (9) can be used to evaluate \( \langle \hat{B}(t)\hat{C}(t) \rangle_n \). Fourier transforming the result we find (sums over \( ss' \) and \( \sigma_n \) implied)

\[
\mathcal{A}^{BC}_n(\omega) = \sum_{m,m_n} \sum_{XX'} \sum_{\sigma} \* \left[ c_{X+}^\dagger \rho_{XX}^{(m)} c_{X'}^\dagger \rho_{XX'}^{(m_n)} \right] \* \delta(\omega - E_{m}^n),
\]

\[
\left[ \rho_{DD}^{(m-n)} \right]_{ss'} = \delta_{ss'} e^{-\beta E_n^m},
\]

\[
\left[ \rho_{KK}^{(m-n)} \right]_{ss'} = [A_{KK}^{\sigma_n\dagger} \ldots A_{KK}^{\sigma_1\dagger} \cdot \rho_{DD}^{(m-n)} \cdot A_{KK}^{\sigma_n} \ldots A_{KK}^{\sigma_1} \cdot]_{ss'}.
\]

Similarly, the static quantity \( \langle \hat{B} \hat{C} \rangle_0 \) equals the first line’s RHS without the \( \delta \) function. The matrix elements \( \rho_{XX}^{(m-n)} \) are given by the second and third lines, together with \( \rho_{KK}^{(m-n)} = \rho_{DD}^{(m-n)} = 0 \). After performing a “forward run” to generate all relevant NRG eigenergies and matrix elements, \( \mathcal{A}^{BC}(\omega) \) can be calculated in a “backward run,” performing a sum with the structure \( \sum_{m>n} \* [C_{\rho}^{\text{red}} B \cdot \delta(\omega - E_m^m)] \* \), starting from \( m = N \). Here \( \rho_{XX}^{(m-n)} \) is the full reduced density matrix for shell \( m \), obtained iteratively by tracing out all shells at smaller scales \( \Lambda^{-n/2} \) (\( n \geq m \)).

Equations (8)–(10) are the main results of our “FDM-NRG” approach. They rigorously generalize Hofstetter’s DM-NRG [8] (which leads to similar expressions, but using \( w_n = \delta_{n,n'} \) and without excluding \( K \) matrix elements), and provide a concise prescription, free from double-counting ambiguities, for how to combine NRG data from different shells when calculating \( \mathcal{A}^{BC}(\omega) \). The relevant sum rule is satisfied identically, since by construction \( \int d\omega \mathcal{A}^{BC}_n(\omega) = \langle \hat{B} \hat{C} \rangle_0 \) holds for every \( n \) and arbitrary temperature and NRG parameters \( \Lambda \) and \( M_k \).

**Smoothing discrete data.**—We obtain smooth curves for \( \mathcal{A}^{BC}(\omega) \) by broadening the discrete \( \delta \) functions in Eq. (10) using a broadening kernel that smoothly interpolates from a log-Gaussian form (of width \( \alpha \)) [2,4] for \( |\omega| \geq \omega_0 \), to a regular Gaussian (of width \( \omega_0 \)) for \( |\omega| < \omega_0 \), where \( \omega_0 \) is a “smearing parameter” whose significance is explained below. To obtain high-quality data, we combine small choices of \( \alpha \) with an average over \( N_z \) slightly shifted discretizations [3] (see [13] for more details).

**Application to Anderson model.**—We illustrate our approach for the standard single-impurity Anderson model (SIAM). Its local Hamiltonian \( \hat{h}_0 = \sum_{\sigma} \epsilon_0 c_{0\sigma}^\dagger c_{0\sigma} + U c_{0\uparrow}^\dagger c_{0\uparrow} c_{0\downarrow} + U c_{0\downarrow}^\dagger c_{0\downarrow} c_{0\uparrow} \), describes a localized state with energy \( \epsilon_0 \), with a Coulomb penalty \( U \) for double occupancy. It is coupled to a Wilson chain \( \sum_{n \neq 0} \lambda_n c_{n+1}^\dagger c_n + \text{H.c.} \), which generates a local level width \( \Gamma \). We calculated \( \mathcal{A}^{<}(\omega) = \mathcal{A}^{c_{0\uparrow}^\dagger c_{0\uparrow}}(-\omega) \), \( \mathcal{A}^{>}(\omega) = \mathcal{A}^{c_{0\downarrow}^\dagger c_{0\downarrow}}(\omega) \) and \( \mathcal{A} = \mathcal{A}^{>} + \mathcal{A}^{<} \). An “improved” version \( \mathcal{A}^{\text{im}} \) thereof can be obtained by calculating the impurity self-energy \( \Sigma(\omega, T) \) [6,13] via FDM-NRG, which is less sensitive to smoothening details and yields more accurate results for the Kondo peak height \( \mathcal{A}_{T=0}(0) \) at zero temperature.

**Sum rules.**—As expected, we find FDM-NRG to be significantly more accurate at lower computational cost.
than NRG or DM-NRG [8,15]. The sum rules
\[ \int d\omega A_{\text{inv}}^{\text{inv}}(\omega) = \langle c_{0\sigma}^\dagger c_{0\sigma} \rangle_T, \quad \int d\omega A(\omega) = 1 \quad (11) \]
hold exactly to 10^{-15} for our discrete data, and to 10^{-4}
after smoothing (due to numerical integration inaccuracies).
Moreover, even for \( M_K \) as small as 256, our results
for \( A_{T=0}(0) \) and \( A_{\text{inv}}^{\text{inv}}(0) \) typically agree to within 2\% and
0.2\%, respectively, with the Friedel sum rule, which
requires \( \pi T A(0) = 2 \). The exact relation
\[ A(\omega) = f(\omega) A(\omega) \quad (f \text{ is the Fermi function}) \]
follows from detailed balance, is likewise satisfied well
(though not rigorously so): the left-hand side of Eq. (11)
typically equals \( \int d\omega f(\omega) A(\omega) \) to better than 10^{-4}.

Low-frequency data.—Because of the underlying loga-
metric discretization, all NRG-based schemes for calcu-
ling finite-temperature spectral functions inevitably
produce spurious oscillations at very low frequencies
\( |\omega| \ll T \). The scale \( \delta_T \) at which these set in can be un-
derstood as follows: the Lehmann sum in Eq. (1) is dominated
by contributions from initial states \( |\omega| \) with energy \( E_\omega \approx T \),
represented by NRG shells with \( n \) near \( N_f \). The charac-
teristic energy scale of these states limits the accuracy obtain-
able for energy differences \( E_\omega \) to accessible final states \( |b\). Thus the scale \( \delta_T \) is set by those shells which con-
tribute with largest weight \( w_n \) to the density matrix.

We analyze this in more detail in Figs. 2(a) and 2(b) by
purposefully choosing the smearing parameter to be un-
conventionally small, \( \omega_0 \ll T \). The resulting spurious os-
cillations are usually smeared out using \( \omega_0 \gtrsim \delta_T \[
Fig. 2(a), thick gray (red) curve], resulting in quantita-
tively accurate spectral functions only for \( |\omega| \gtrsim \omega_0 \approx \delta_T \).
For conventional NRG approaches, the “single-shell” ap-
proximation \( w_n = \delta_{n N_f} \) typically leads to \( \delta_T \approx T \), as can be seen in Fig. 2(a) [dashed (green) line and thin solid
(blue) line]. In contrast, FDM-NRG yields a significantly reduced value of \( \delta_T \approx T/5 \) [Fig. 2(a), black line, and
Fig. 2(b)], since the weighting functions \( w_n \) [inset of Fig. 2(b)] retain weight over several shells below \( N_f \), so that lower-frequency information is included.

Fermi-liquid relations.—To illustrate the accuracy of our
low-frequency results, we calculated \( A_{\text{inv}}^{\text{inv}}(\omega) \) for
\( \omega, T \ll T_K \) for the symmetric SIAM, and made quantita-
tive comparisons to the exact Fermi-liquid relations [14],
\[ A_T(\omega) \approx A_0 \left[ 1 - c \frac{\omega^2}{\pi T} \right] \]
\[ G(T) \equiv \frac{1}{2} \pi T c A_T(\omega) \left( \frac{\partial f}{\partial \omega} \right) \approx A_0 \left[ 1 - c \frac{\omega^2}{\pi T} \right]. \]
Here \( A_0 \equiv 1/\pi T, c = \pi^4/16, \) and the Kondo temperature
\( T_K \) is defined via the static magnetic susceptibility [4]
\( \chi(0)T_0 = 1/4T_K \). Figures 2(c) and 2(d) show the FDM-
NRG data [gray (colored) dots and lines] to be in remarkably
good quantitative agreement with these relations
(black dashed curves). The results for the “conductance”
\( G(T) \), being a frequency integrated quantity obtained by
summing over discrete data directly without the need for
broadening, are more accurate than for \( A_T^{\text{inv}}(\omega) \), and
produce the prefactor \( c \) with an accuracy consistently
within 5\% (until now, accuracies of the order of 10\%–
30\% had been customary). The smoothness of the data in
Fig. 2(c), obtained using temperatures not confined to the
logarithmic grid \( \Lambda^{-n/2} \) [gray vertical lines in Fig. 2(b),
together with the remarkable stability with respect to dif-
ferent \( z \) shifts illustrate the accuracy of our approach.

Conclusions.—Our FDM-NRG method offers a trans-
parent framework for the calculation of spectral functions
of quantum impurity models, with much improved accu-
raty at reduced computational cost. Its results satisfy
frequency sum rules rigorously and give excellent agree-
ment with other consistency checks such as the Friedel sum
rule, detailed balance, or Fermi-liquid relations, including
the regime \( \omega \ll T \).

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Note added.—Just before completion of this work we
learned that Peters, Pruschke, and Anders had followed up
on the same idea [15].

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appendices which give more details. For more information
on EPAPS, see http://www.aip.org/pubservs/epaps.html.
245114 (2006). We recommend this paper for a more
detailed comparison of the new and previous approaches.
APPENDIX

Smoothing Discrete Data:— The FDM-NRG yields the spectral function in the form of a Lehmann sum over discrete δ-functions, which have to be broadened to obtain a smooth function. Ideally, this should be done using a procedure for which the results are independent both of the parameters used for broadening and for discretizing the conduction band.

We calculate the smoothed spectral function using \( A(\omega) \equiv \int d\omega' K(\omega, \omega') A_{\text{raw}}(\omega') \). Here \( A_{\text{raw}}(\omega') = \sum_n w_n A_n(\omega') \) represents the discrete numerical data obtained from Eq. (10), which in practice we collect in binned form, typically using 250 bins per decade in \( \omega' \), so that \( \int d\omega' \) becomes a sum over bins. The raw data is folded with the broadening kernel \( K(\omega, \omega') \), which we choose to be of the following form:

\[
K(\omega, \omega') = L(\omega, \omega') h(\omega') + G(\omega, \omega') [1 - h(\omega')] \quad (14a)
\]

where

\[
L(\omega, \omega') = \frac{\theta(\omega')}{\sqrt{\pi |\alpha|}} e^{-\left(\frac{\omega - \omega'}{|\alpha|}\right)^2} \quad (14b)
\]

\[
G(\omega, \omega') = \frac{1}{\sqrt{\pi |\alpha|}} e^{-\left(\frac{\omega - \omega'}{|\alpha|}\right)^2} \quad (14c)
\]

\[
h(\omega') = \begin{cases}
1, & |\omega'| \geq \omega_0 \smallskip \\
\left|\frac{\omega'}{\omega_0}\right|^{-\gamma}, & |\omega'| < \omega_0
\end{cases} \quad (14d)
\]

The chosen kernel \( K \) constitutes a smooth interpolation, of somewhat arbitrary shape \( h(\omega') \), between a log-Gaussian [2, 4] broadening kernel \( L \) on the one hand, used for all \( \omega' \)-frequencies but the smallest (with \( \omega \) and \( \omega' \) restricted to have the same sign); and a Gaussian broadening kernel \( G \) of width \( \omega_0 \) on the other, used for \( |\omega'| < \omega_0 \) to smoothly connect the regimes of positive and negative frequencies. We choose \( \omega_0 \) to be roughly a factor of 2 smaller than the smallest energy scale in the problem, including the Kondo temperature \( T_K \) (note that by construction in Eq. (14d) the transition to regular Gaussian sets in below \( \omega_0 \)).

The log-Gaussian kernel \( L(\omega, \omega') \) was purposefully chosen to have the following three desirable features:

(i) \textit{Frequency-dependent width:} being Gaussian on a logarithmic scale, on a linear scale its width as function of \( \omega \) is proportional to \( \omega' \). This is needed to deal with the fact that spectral data generated using Wilson’s logarithmic discretization grid is more coarse-grained at large frequencies than at smaller ones.

(ii) \textit{Conservation of weight:} we have \( \int d\omega L(\omega, \omega') = 1 \), ensuring that \( \int d\omega A(\omega) = \int d\omega' A_{\text{raw}}(\omega') \).

(iii) \textit{Conservation of peak height:} for the choice \( \gamma = \alpha/4 \) (adopted henceforth) \( L \) is symmetric under \( \omega \leftrightarrow \omega' \), so that also \( \int d\omega' L(\omega, \omega') = 1 \). This ensures that the logarithmic broadening kernel maps a constant function onto itself (if \( A_{\text{raw}}(\omega') = A_0 \), then \( A_{\text{raw}}(\omega) = A_0 \)), and thus does not change the height of a peak whose width on a logarithmic scale is broader than \( \alpha \). (In this respect our \( L \) differs from that of [2, 4, 15].)

Since choice (iii) implies that our log-Gaussian Kernel, as function of \( \omega \), describes a peak asymmetric w.r.t. \( \omega' \) (shifted by \( \alpha/4 \) on a log scale), on a linear \( \omega \)-scale the broadened data is stretched relative to the raw data by factor \( e^{\alpha/4} \). This effect can be minimized by keeping \( \alpha \) as small as possible. The smoothing of plain NRG data typically requires \( \alpha \sim 1/\sqrt{X} \) (e.g. 0.7 for \( X = 2 \)). However, smaller values (e.g. \( \alpha \leq 0.3 \) or even smaller) can be achieved by using the “z-trick” [3]: collect several (say \( N_z \)) sets of discrete FDM-NRG data, each obtained from a different, slightly shifted logarithmic grid \( \{\Lambda^{n-z}\} \) of discrete frequencies, for \( N_z \) different values of \( z \) between \(-0.5 \) and 0.5, and average the results. The hopping matrix elements along the Wilson chain are recalculated for each \( z \) by carefully tridiagonalizing the underlying logarithmically discretized Hamiltonian.

Self-energy representation:— The accuracy of the results for \( A_{\sigma}(\omega) \) for the Anderson model can be improved by expressing it in terms of the impurity self energy [6]: first, note that \( A_{\sigma}(\omega) = -\text{Im}[G^R_{\sigma}(\omega)]/\pi \), where \( G^R_{\sigma}(\omega) \) is the Fourier transform of \( G^R_{\sigma}(t) = -i\theta(t)\langle c_{t\sigma}(t), c^\dagger_{t\sigma}\rangle \rangle \). An improved version for \( G^R_{\sigma}(\omega) \) can be obtained by expressing it as

\[
G^R_{\sigma}(\omega) = \frac{1}{\omega - \Delta_{\sigma}(\omega) - \Sigma^U_{\sigma}(\omega)} \quad \Sigma^U_{\sigma}(\omega) = U \frac{F^R_{\sigma}(\omega)}{G^R_{\sigma}(\omega)}.
\]

Here \( \Delta_{\sigma}(\omega) \), the \( U \)-independent part of the self energy which characterizes the level’s broadening, can be computed exactly, \( G^R_{\sigma}(\omega) \) is the standard ("non-improved") version of the correlator, and \( F^R_{\sigma}(\omega) \) is the Fourier transform of \(-i\theta(t)\langle [c^\dagger_{t\sigma}(t), c_{t\sigma}] \rangle \). We calculate the imaginary parts of \( G^R_{\sigma}(\omega) \) and \( F^R_{\sigma}(\omega) \) using FDM-NRG from Lehmann representations of the form (10), smoothen the discrete data as described above, Kramers-Kronig transform the smoothed results to obtain their real parts, and finally calculate \( \Sigma^U_{\sigma}(\omega) \). Small wavy features in \( G^R_{\sigma}(\omega) \) and \( F^R_{\sigma}(\omega) \) that reflect the logarithmic discretization grid largely cancel out in the ratio \( \Sigma^U_{\sigma}(\omega) \). Thus, smooth results for \( G^R_{\sigma}(\omega) \) and \( A^R_{\text{raw}}(\omega) \) can be obtained using much less (or even no) z-trick averaging, thus reducing the number of distinct FDM-NRG runs required to get good results. Moreover, since \( \Sigma^U_{\sigma}(\omega \rightarrow 0) \) at \( T = 0 \) is found to approach 0, the self-energy representation also improves the accuracy with which the Friedel sum rule is fulfilled.
Friedel Sum Rule:— The Friedel sum rule \( A(0) = \sin^2(\eta_0 \pi/2)/\pi \Gamma \) is a well known analytic result that is exact at zero temperature and can be used to check our data. Figure 1 shows a comparison of our method for calculating spectral functions to previous methods. As will be seen our method clearly leads to more accurate agreement with the Friedel sum rule for arbitrary parameter combinations. Since we know the dot occupancy \( n_0 \) numerically from our FDM-NRG method, we compare the actual value of our spectral function at \( \omega = 0 \) to the expected value predicted by Friedel sum rule. We do this for our FDM-NRG method, but also for the older versions of plain NRG ('nrg' in Fig. 1 and Hofstetter's DM-NRG ('hof')). In all three cases, the spectral function was calculated using the self-energy representation (Ref [6]) as outlined in the Appendix of our paper.

Panels 1a and 1b show the comparison for the single impurity Anderson model (the same as used in our paper), but here for a whole sweep of the onsite energy \( \epsilon_d \). Figure 1a shows the relative error of \( A(\omega = 0) \) with respect to the value expected from the Friedel sum rule. Figure 1b shows the same data, but normalized with respect to the maximum of the full spectral function. This is just to show that the increase of the error as \( \epsilon_d \) increases from its value \(-0.5\) (the symmetry point of the model) seen in Fig. 1a is due to fact that absolute value of \( A(\omega = 0) \) then becomes smaller, because the dominant peak then shifts increasingly further away from \( \omega = 0 \).

All data in Figure 1 were obtained using exactly the same broadening procedure as described in the attachment to our paper, for the discrete data obtained from the three different methods. The origin of the artificial oscillations in the error for the previous methods ('nrg' and 'hof' in the figure) can be easily understood by looking at the underlying smooth spectral functions that were used to obtain Figs. 1a and 1b. For \( \epsilon_d = -0.5U \) a zoom into the spectral function is shown around \( \omega = 0 \) for FDM-NRG in Fig. 1c and for the other methods in Fig. 1d. The solid lines are the smoothened discrete data, the dashed curves the subsequently improved data using self-energy (Ref [6]). Evidently, the data in Fig. 1d shows problematic artifacts (dips and other oscillations) not present in Fig. 1c.

Of course, the broadening parameters employed here could have been chosen such that the previous methods ('nrg' and 'hof' in the figure) also yield more satisfactory results, in that the data around \( \omega = 0 \) could have been ‘tailored’ to look smoother by using a few crutches such as increased broadening parameter \( \alpha \). However, we did not do that here to emphasize the greatly improved quality of our FDM-NRG approach compared to standard NRG and DM-NRG. Clearly, FDM-NRG gives the best data quality throughout.

FIG. 1: Comparison of the Friedel sum rule of our FDM-NRG to the previous methods of plain NRG ('nrg') and Hofstetter's DM-NRG ('hof'). This is done for the same model parameters as in our paper while sweeping the onsite energy \( \epsilon_d \) (\( \Lambda = 2, M_K = 256, N_c = 8, \alpha = 0.3, U = 0.12, \epsilon_d = -U/2, \Gamma = 0.01, B = 0 \) and \( T_K = 2.210^{-4} \)). Panel (a) Relative error of the Friedel sum rule. Panel (b) Absolute error with respect to maximum peak height of full spectral function \( A_{\text{max}} \). Panels (c) and (d) show a zoom into the spectral function around \( \omega = 0 \) for the symmetric point \( \epsilon_d = -U/2 \) for the methods presented in our paper (panel c) and for the previous methods (panel d), respectively.