Efficient DMFT impurity solver using real-time dynamics with Matrix Product States

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We propose to calculate spectral functions of quantum impurity models using the Time Evolving Block Decimation (TEBD) for Matrix Product States. The resolution of the spectral function is improved by a so-called linear prediction approach. We apply the method as an impurity solver within the Dynamical Mean Field Theory (DMFT) for the single and two-band Hubbard model on the Bethe lattice. For the single band model we observe sharp features at the inner edges of the Hubbard bands. A finite size scaling shows that they remain present in the thermodynamic limit. We analyze the real time-dependence of the double occupation after adding a single electron and observe oscillations at the same energy as the sharp feature in the Hubbard band, indicating that they correspond to a long-lived, coherent superposition of eigenstates with different occupations. For a two-band Hubbard model we observe distinct features in the Hubbard bands, which are not visible in standard quantum Monte Carlo DMFT and which we interpret as multiplets originating from Hund’s exchange.

I. INTRODUCTION

The field of strongly correlated materials has experienced vast growth during the last three decades. Electronic correlations pose a particular challenge for theory, and many phenomena such as high-temperature superconductivity have eluded a proper understanding to this day. A correlation phenomenon that is non trivial but nonetheless fully understood is the Kondo effect [1, 2]. The Kondo model and its cousin, the Anderson impurity model, are not only relevant for its original purpose, i.e., for magnetic impurities in solids, but also for quantum dots [3] and even for bulk materials. For the latter, dynamical mean-field theory (DMFT) [4–6] maps a bulk lattice model onto the self-consistent solution of an Anderson impurity model and includes in this way a major part of electronic correlations, namely the local ones.

Strong electronic correlations make the computational cost of directly solving the Schrödinger equation prohibitively large, and advanced numerical methods, often approximate ones, are in many cases the only viable option. At the forefront of these methods lie the Quantum Monte-Carlo (QMC) technique [7, 8], the Numerical Renormalization Group [9, 10], the Density Matrix Renormalization Group (DMRG) [11, 12], cluster approaches like Cluster Perturbation Theory [13] and the Variational Cluster Approach [14] and DMFT [4, 6]. All these methods have their strengths and weaknesses. QMC gives formally the exact solution, but is in practice plagued by statistical errors and the sign-problem. The NRG excels at capturing the low-energy physics, but has a hard time to resolve high-energy features in the spectrum and is restricted to impurity problems. The DMRG can treat both the low- and high-energy scale on equal footing, but is best suited for 1-dimensional (1d) models. Methods for higher dimensional (d>1) problems are scarce. One of the most promising among these is the DMFT [5] which becomes exact in the limit d→∞ [4] and which yields an approximation for the finite dimensional lattice. The key quantity of DMFT is the local lattice spectral function \( A(\omega) \) which is calculated self-consistently. The framework of DMFT is readily established [5], but the actual solution of the DMFT equations is complicated: it involves the calculation of the spectral function of an interacting impurity system which even for single band models is highly non-trivial, and the complexity grows quickly with the number of considered bands (i.e. impurity orbitals). Many different approaches have been proposed to tackle the problem. The most common ones are QMC [8, 15–19], exact diagonalization (ED) [20–22], and NRG [23–26]. QMC can efficiently handle multiple bands, but when formulated in imaginary time, it lacks high resolution of the spectral function. This is mainly attributable to the ill-conditioned analytic continuation from imaginary to real frequencies. Based on the work in Refs. [27–28], the QMC method has recently been extended to the calculation of real-frequency spectra using bold line methods [29, 30] (see Refs. [31, 32] and references therein). The analytic continuation is then traded for the introduction of a sign-problem. ED naturally works with real energies, but it is severely limited by the number of possible sites. This again reduces the spectral resolution considerably. Recently, two extensions to the ED method have been put forward [22, 23] which increase the possible resolution of the spectral function [33]. The NRG on the other hand, being designed for impurity problems,
achieves very good spectral resolution at small energies. But due to a necessarily logarithmic discretization of the bath density of states (DOS), high energy features of the bath are increasingly hard to resolve, which is also likely to affect the fixed point of the DMFT-iteration. In addition, NRG has an intrinsic exponential growth of complexity with the number of bands of the underlying lattice model. More than two bands have so far been unfeasible. The DMRG on the other hand offers several ways to be used as an impurity solver within the DMFT. One possible way is to employ the dynamical DMRG (DDMRG) to obtain the DMFT-spectral function. By employing a Suzuki-Trotter approach, but it can be carried out without the need of explicitly adding states. By employing a Suzuki-Trotter decomposition it can easily be parallelized and is therefore hindered by the fact that one has to perform a separate DMRG run for each frequency and to perform the inversion of an ill-conditioned system of linear equations, which can become very time consuming. Recently, the Chebyshev expansion technique has been proposed by some of us as an impurity solver for DMFT. Advantages are that it works at zero temperature, that no inversion problem has to be solved, and that the spectral function can be calculated with uniform resolution and high precision for all \( \omega \) in a single run. This reduces computational costs considerably, but on the other hand it is not straightforward to parallelize the method. In the present work we propose to employ the Time Evolving Block Decimation (TEBD) for Matrix Product States (MPS) to compute the spectral function. We combine it with a so called linear prediction technique to improve on the spectral resolution. Our method shares the advantages of the Chebyshev approach, but it can be carried out without the need of explicitly adding states. By employing a Suzuki-Trotter decomposition it can easily be parallelized and is therefore both a very precise and very efficient method. We apply it as a DMFT impurity solver for the single and the two band Hubbard model on the \( z \to \infty \) Bethe lattice.

II. MODELS

A. One-band Hubbard Model

The central ingredient in DMFT is the iterative calculation of the spectral function \( A_{\text{imp}}(\omega) = \langle \Phi_0 | c_0(\omega - H) c_0^\dagger c_0^\dagger \phi_0 \rangle \) of an impurity model, here a Single Impurity Anderson Model (SIAM)

\[
H = \varepsilon_f \sum_{\sigma} n_{0\sigma} + U n_{0\uparrow} n_{0\downarrow} + \sum_{\kappa \neq 0,\sigma} \varepsilon_\kappa n_{\kappa\sigma} + \sum_{\kappa \neq 0,\sigma} V_\kappa c_{0\uparrow}^\dagger c_{\kappa\sigma}^\dagger + h.c. \tag{1}
\]

Here, \( c_{0\sigma}, c_{0\sigma}^\dagger \) are fermionic annihilation and creation operators at the impurity site, \( U \) and \( \varepsilon_f \) are the interaction and the local potential of the underlying lattice model, i.e. the single band Hubbard model, and \( \varepsilon_\kappa \) and \( V_\kappa \) are variational parameters which are optimized during the DMFT cycles (see below). We assume a spin-symmetric coupling \( V_\kappa \) and bath-dispersion \( \varepsilon_\kappa \).

Greens and spectral functions can be calculated from the real time evolution and subsequent Fourier transformation of

\[
A_{\text{imp}}(t) = \frac{1}{2\pi} \langle \Phi_0 | c_0(t), c_0^\dagger(0) \rangle \phi_0 \tag{2}
\]

to

\[
A_{\text{imp}}(\omega) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dt e^{-i\omega t} A_{\text{imp}}(t). \tag{3}
\]

Here \( c_0(t) \) is given in the Heisenberg picture, and \( \phi_0 \) is a non-degenerate ground state at zero energy. Due to the hermiticity of \( H \), the function \( A_{\text{imp}}(\omega) \) is real and normalized to unity. One way to obtain \( A_{\text{imp}}(\omega) \) is to calculate the two quantities

\[
G^> (t) \equiv \langle \Phi_0 | c_0 e^{-i H t} c_0^\dagger | \Phi_0 \rangle \tag{4}
\]
\[
G^< (t) \equiv \langle \Phi_0 | c_0^\dagger e^{i H t} c_0 | \Phi_0 \rangle
\]

for \( -\infty < t < \infty \) and Fourier-transform them. Using

\[
(G^>(t))^* = G^<(\overline{t}) \tag{5}
\]
\[
G^< (t) = (G^>(t))^* \tag{6}
\]

where the second line is valid only at particle hole symmetry, the spectral function can be expressed as

\[
A_{\text{imp}}(\omega) = \frac{1}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dt \left( G^< (t) + G^< (-t) \right) e^{-i\omega t}
\]

\[
= \frac{2}{(2\pi)^{1/2}} \int_{-\infty}^{\infty} dt G^< (t) e^{-i\omega t}. \tag{6}
\]

To obtain the spectral function at particle-hole symmetry, we thus only need to calculate \( G^> (t) \) for \( t > 0 \), as the real part of \( G^> (t) \) is even in \( t \).

B. Two-band Hubbard Model

The most promising feature of the method is its applicability to multi-band systems. We will demonstrate this by applying it as an impurity solver for the symmetric two-band Hubbard model on the Bethe lattice. Under the assumption that the bath is spin symmetric the resulting effective impurity model assumes the form

\[
H = \sum_{m \sigma} \varepsilon_m n_{m\sigma} + U \sum_{m \sigma} n_{m\uparrow} n_{m\downarrow} + U' \sum_{m \sigma} n_{m\uparrow} n_{m\downarrow}
\]

\[
+ (U' - J) \sum_{m \sigma} n_{m\uparrow} n_{m\downarrow} - J \{ c_{0\uparrow}^\dagger c_{0\uparrow} c_{0\downarrow}^\dagger c_{0\downarrow} + h.c. \}
\]

\[
- J \{ c_{0\uparrow}^\dagger c_{0\downarrow} c_{0\downarrow}^\dagger c_{0\uparrow} + h.c. \} + \sum_{m \kappa \sigma} (V_{m\kappa\sigma} c_{m\kappa\sigma}^\dagger + h.c.)
\]

\[
+ \sum_{m \kappa \sigma} \varepsilon_{m\kappa} n_{m\kappa \sigma}. \tag{7}
\]
with $U' = U - 2J$, and $J = U/4$. Here, $c_{m\sigma}$ is a fermionic annihilation operator of the correlated orbital $m \in \{0, 1\}$ at the impurity site, $n_{m\sigma}$ are the corresponding particle number operators, and $\epsilon_{m\sigma}$ and $\nu_{m\sigma}$ are the bath-electron annihilation and particle number operators for $\kappa \geq 1$, respectively. Note that all spin-flip and pair-hopping terms are included.

### III. METHODS

#### A. Dynamical mean field theory

In this paper we address the single- and two-band Hubbard model on the $z \rightarrow \infty$ Bethe lattice. This is convenient for two reasons: (i) the DMFT yields exact results in this case, and (ii) the DMFT self-consistency scheme is especially simple. The quantity of genuine interest in DMFT is the local lattice spectral function $A_{\text{lat}}(\omega)$ of an interacting, $d$-dimensional lattice problem (e.g., the Hubbard model on the Bethe lattice). At convergence it is identical to the impurity spectral function $A_{\text{imp}}(\omega)$. The basic idea of DMFT is to mimic the effect of the interacting lattice surrounding a given site by a suitably chosen bath of free electrons. Interacting lattice sites and surrounding bath yield an impurity problem described by Eq. (1) or Eq. (7). The bath can be represented by the hybridization function $\Delta_m(\omega) = \sum_{\nu} \frac{V_{mn}}{\omega - \epsilon_m - \nu}$, with an imaginary part $\Delta_m(\omega) \equiv -\frac{1}{\pi} \text{Im} \Delta_m(\omega) = \sum_{\nu} |V_{mn}|^2 \delta(\omega - \epsilon_m)$. The general outline of the DMFT cycle is as follows: For each correlated orbital $m$ on the impurity site we initially guess a $\Delta_m(\omega)$, where $n$ is an iteration index. A set of SIAM parameters $V_{mn}$ and $\epsilon_{mn}$ is then obtained by discretizing $\Delta_m(\omega)$ as described in Ref. [9]. We use a discretization scheme linear in energy in this work. The method can deal with any discretization. After the discretization the system has a linear chain geometry

$$H = \sum_{m\sigma} \epsilon_{m\sigma} n_{m\sigma} + \sum_{m\sigma} \frac{U}{2} n_{m\sigma} n_{m\sigma} + \sum_{m\sigma} \frac{t_{mi} c_{m\sigma}^\dagger c_{m+1i\sigma} + h.c.}{2} + \sum_{m\sigma} \epsilon_{m\sigma} n_{m\sigma}$$

with only nearest neighbor hopping $t_{mi}$ and local potentials $\epsilon_i$. The number of discretization parameters corresponds to the chain length $N$. Using an impurity solver we calculate the impurity spectral function $A_{\text{imp}}(\omega)$ of Eq. (8), from which one obtains the new

$$\tilde{\Delta}_{m}^{n+1}(\omega) = \frac{D^2}{4} (\alpha A_{\text{imp}}^n(\omega) + (1 - \alpha) A_{\text{imp}}^{n-1}(\omega))$$

with a mixing parameter $\alpha \in [0, 1]$ that can be adjusted for better convergence. Here, $2D$ is the bandwidth of the non-interacting spectral function of the Bethe lattice. In the following, all results are given in units of $D$. $\tilde{\Delta}(\omega)$ is then again discretized, and the loop is iterated upon convergence, i.e., until

$$A_{\text{imp}}^{n+1}(\omega) = A_{\text{imp}}^n(\omega) = A_{\text{lat}}^{n}(\omega) \equiv A_{\text{lat}}(\omega).$$

For our calculations we impose particle-hole symmetry which results in $\epsilon_{m\sigma} = 0$ in Eq. (8).

For the two-band Hubbard model we focus on the symmetric model in which at $U/D = 0$ both bands have the same bandwidth $D$. For the discretization we use a symmetric setup with two DMFT-baths of lengths $N_1 = N_2$.

The two-band model has been frequently investigated in the past [25, 31, 53]. Like the single band model it exhibits a MI transition at a finite $U_c/D \approx 2.2$, for $J = U/4$ [25].

Using the NRG as an impurity solver [25], it has been observed that a finite $J$ leads to a strong renormalization of the Kondo temperature and hence affects the MI transition. Obtaining accurate results, especially for the high energy features of the Hubbard bands remains a challenging problem.

#### B. Time Evolving Block Decimation

The essential task of the impurity solver in DMFT is to calculate the greater (or lesser) Greens function $G^<(t) = \langle \Phi_0 | c_{0\uparrow}^\dagger c_{0\downarrow}^\dagger | \Phi_0 \rangle$. We achieve this by calculating the ground state $| \Phi_0 \rangle$ using the DMRG and subsequently employ the Time Evolving Block Decimation (TEBD) [46, 47] to evolve $c_{0\uparrow}^\dagger | \Phi_0 \rangle$ forward in time. We use a second order Trotter breakup with $\Delta t D = 0.00625$, and measure $G^>(t D)$ every 25 Trotter steps in the single-band and every 15 full Trotter steps in the two-band model, i.e. $t_n D = 0.15625 \ n$ (single-band) $t_n D = 0.09375 \ n$ (two-band), $n \in \{0, \ldots, N_{t,\text{max}} - 1\}$. We then apply the linear prediction method (see below) to extrapolate 10000 further points. In the single-band case we also employ an unfolding procedure to separate the spin degrees of freedom of the electrons into a left chain containing up spins and a right chain containing down spins which is computationally more efficient. A decoupling for three- and more band DMFT can be carried out in a similar spirit with multiple chains connected at the impurity site in a star-like geometry, where every chain carries a band and spin index. In the TEBD, only a limited number $\chi$ of Schmidt-states $| \lambda \rangle$ and Schmidt-values $\lambda_n$ can be kept at a certain bond connecting two sites, which is the major approximation of the method. The error of a single time step can be quantified by the truncated weight [12, 47]

$$\epsilon_{tw} = 1 - \sum_{\alpha = \chi + 1}^\infty \lambda_n^\alpha$$

obtained after truncating the state down to a matrix dimension $\chi$, where $d$ is the local Hilbert space dimension. In our implementation of the TEBD, after every time
step the matrix dimension is reduced just enough to obtain the prespecified $c_{\text{trunc}}$. Additionally, we set a hard limit of $\chi = 500$ or 750 for the maximum matrix dimension.

C. Linear Prediction

The so-called linear prediction technique [45, 49, 50, 54] is a very simple and powerful method for the extrapolation of time series. It amounts to describing the solution of time series. It amounts to describing the time series as a sum of many exponentials or, equivalently, the spectrum as a sum of many Lorentzians. On the basis of $N_{t,\text{max}} \equiv 2N_t$ calculated data points $\{x_i\}$, $1 \leq i \leq 2N_t$ at equidistant times $t$, one predicts data points for $t_n, n > 2N_t$ as a linear combination of the first $N_t$ data points:

$$x_n \approx \tilde{x}_n \equiv -\sum_{j=1}^{N_t} a_j x_{n-j}. \quad (12)$$

One obtains the optimal $\{a_j\}$ by minimization of a cost function

$$F = \sum_{n=N_t+1}^{2N_t} |\tilde{x}_n - x_n|^2, \quad (13)$$

which yields

$$Ra = -r, \quad (14)$$

$$R_{ij} = \sum_{n=N_t+1}^{2N_t} w_n x_{n-i}^* x_{n-j}, \quad r_i = \sum_{n=N_t+1}^{2N_t} w_n x_{n-i}^* x_n,$$

for $1 \leq i, j \leq N_t$. Eq. (14) is inverted using a pseudo-inverse with cutoff $\delta$. Data points at $N_t + k (k > 0)$ can then be predicted from

$$\tilde{x}_{N_t+k} = \sum_{n=0}^{N_t} \left[ M^k \right]_{1,n} x_{N_t+1-n}, \quad (15)$$

with

$$M = \begin{pmatrix} -a_1 & -a_2 & -a_3 & \ldots & -a_{N_t} \\ 1 & 0 & 0 & \ldots & 0 \\ 0 & 1 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & 1 & 0 \end{pmatrix}.$$  

All spectral functions have been obtained by predicting 10000 further data points on top of $N_{t,\text{max}}$ computed data points. Due to the exponential dependence of $M$ in Eq. (15), any eigenvalue $\lambda$ of $M$ that is larger than unity has to be either renormalized to unity or set to zero, in order to avoid divergence in the prediction [45, 50]. The interplay of $\delta$ and the eigenvalue rescaling is investigated in more detail in the appendix. There we show that zeroed eigenvalues yield better results.

The linear prediction algorithm has two parameters $N_{t,\text{max}}$ (“time window”) and $\delta$ (pseudo-inverse cutoff). From analysis of the dependence of the DMFT-fixed point on these parameters (see appendix), we found $N_{t,\text{max}} = 350$, and $\delta = 10^{-6}$ or smaller, in conjunction with setting large eigenvalues of the prediction matrix to 0, to yield good results. Unless stated otherwise, these parameter values were used to obtain the results in this paper.

IV. RESULTS

To verify our approach we benchmarked our results for the impurity spectral function of a SIAM with results of the dynamical DMRG [55], to our knowledge the most precise data available (see appendix), and found excellent agreement. In the following we present our results for the one and two-band Hubbard model.

A. One-band Hubbard model

We start by applying our method to DMFT for the single-band Hubbard model on the Bethe lattice for interaction strengths $U/D = 1.0$ and $U/D = 2.0$ in the metallic region and $U/D = 3.2, 3.4$ and $3.6$ in the insulating region, for $D = 0.25$. We use $N_{t,\text{max}} = 200$. Fig. 1(a) and (b) show the results for $U/D = 1.0$ and $2.0$ (red solid lines). At $U/D = 2.0$, distinct features at the inner edges of the Hubbard satellites start to emerge, as has been observed in previous DDMRG [55, 59] and NRG [21] studies, in QMC calculations [30] as well as in MPS calculations with Chebyshev moments [45], and recently also in advanced ED calculations [22, 23, 33]. For comparison we show results obtained with the Chebyshev expansion technique [45] (black dash-dotted lines), which are compatible with our present results. For values of $U/D = 3.2, 3.4$ and $3.6$ we plot results in Fig. 1(c). In contrast to Fig. 1(a) and (b), we use a mixing parameter of $\alpha = 0.3$ in Fig. 1(c), which yields a smoother convergence to the insulating solution. If no mixing is applied, the spectra alternate between an insulating and a metallic solution with a tiny quasi-particle weight. This effect is particularly strong at $U/D = 3.2$ close to the transition and is also enhanced when increasing $N_{t,\text{max}}$ or decreasing $\delta$, which we attribute to Trotter and truncation effects in the time series. We note that in Fig. 1(c) there is some small residual spectral weight left in the gap region (of the order of $10^{-3}$).

B. Sharp peaks in the Hubbard bands

We proceed to study the metallic state in the coexistence region $U_{c1}/D \leq U/D \leq U_{c2}/D$, where $U_{c1}/D \approx 2.38$, and $U_{c2}/D \approx 3.0$ [55]. For such $U/D$, the narrowing
FIG. 1: (a) and (b): DMFT spectral function of the half-filled Hubbard model on the Bethe lattice for $U/D = 1.0, 2.0$ ($N = 120, N_{t,max} = 200, \chi = 500, \epsilon_{tw} = 10^{-10}$) as obtained from TEBD (red solid line). For comparison we plot results obtained using the Chebyshev expansion method [45] (black dash-dotted line). (c) DMFT spectral functions in the insulating phase for $U/D = 3.2, 3.4, 3.6$. For better convergence we used the modified update scheme with $\alpha = 0.3$ in (c). Other parameters as in (a) and (b).

FIG. 2: DMFT spectral function for $U/D = 2.4$, comparing three different computational parameter sets $\chi$ and $\epsilon_{tw}$ ($N = 150$). The spectral function shows the quasiparticle peak at $\omega/D = 0$ and two broad Hubbard bands at $\omega/D \approx \pm U/2D$. Additionally, at the inner edges of the Hubbard band we observe a sharp feature. Insets: closeups of the sharp peak at the inner side of the Hubbard bands (left) and the quasi-particle peak (right).

In Fig. 2, we present $A(\omega)$ for $U/D = 2.4$ and a chain length of $N = 150$ sites. We clearly observe a separation of energy-scales into a sharp resonance at $\omega/D = 0$ and two broad Hubbard satellites at $\omega/D \approx \pm U/2D$, decorated with two sharp features at the inner edges of the Hubbard peaks. The insets are closeups on the sharp side peak of the left Hubbard satellite (left) and the quasi-particle peak (right). The pinning of the height of the Kondo-resonance is fulfilled to good accuracy. In Fig. 2 we analyze the convergence of the results with increasing precision of the MPS calculations. The latter is governed by the truncation error $\epsilon_{tw}$, related to the MPS matrix-dimension $\chi$, which bounds the number of Schmidt states kept at each bi-partition during the simulation. Fig. 2 shows results for three different simulations. With increasing precision we initially observe a sharpening of the Hubbard side-peaks. From the plot we conclude that using $\chi = 500, \epsilon_{tw} = 10^{-10}$ already yields converged results. A slight decrease of the quality of the pinning criterion is most likely related to linear prediction inaccuracies.

A second important parameter is the chain length $N$, which is directly related to the number of discretization points of the bath spectral function. In Fig. 3(a) we present DMFT-spectra for $U/D = 2.4$ and different system sizes $N = 150 \ldots 240$, with $\chi = 500$ or $750$ and $\epsilon_{tw} = 10^{-10}$. With increasing system size $N$, we observe a shift of the Hubbard side-peak position towards smaller $|\omega/D|$ (left inset Fig. 3), as well as a reduction of its height [38, 39]. A similar reduction is observed in the height of the quasi-particle peak (right inset in Fig. 3), in violation of the pinning criterion. The fact that the spectra still converge to a metallic solution hints that the exact pinning is not crucial for DMFT; it is rather the weight of the resonance which appears to count. We note that the spectral height at $\omega/D = 0$ is the quantity which is most susceptible to small errors in the large time evolution in our method, more so than the spectrum at other frequencies.

In Fig. 3(b) to (e) we display a finite size scaling of the side peaks, which demonstrates that they remain present in the infinite size limit. Fig. 3(b) shows a finite size scal-
FIG. 3: (a) Spectral function of converged DMFT cycles at $U/D = 2.4$ for different chain lengths $N = 150, 170, 200, 240$, ($\chi = 500, 750, \epsilon_{tw} = 10^{-10}$). Insets are closeups of Hubbard bands (left) and quasi-particle peak (right). Below: Finite size scaling with respect to $N$ of (b) the height of the inner side peak, (c) the position of the inner side peak, (d) minimum of the inner side peak and (e) area between the dashed black line and inner side peak in (a).

The height of the side peak (the exponent 3.2 was found to map the data to a straight line), and (c) a scaling of its position. In panel (d) we present a finite size scaling of the minimum to the left of the left side peak. Finally panel (e) shows a scaling of an approximate measure of the area of the side peak, namely the area between the left side peak and a straight line through the local minimum, tangent to spectrum at the global minimum (see dashed black line in the lower Hubbard band of the main panel in Fig. 3(a)). Since the height of the central peak is also size-dependent, the exact properties of the side peaks are likely to change with higher precision of the calculations. The important point is that they converge to finite values, i.e. the side peaks remain present in the thermodynamic limit.

FIG. 4: Spectral function for $U/D = 2.8, (N = 200, \chi = 750, \epsilon_{tw} = 10^{-10})$. Right inset: Increasing $U/D = 2.4, 2.6, 2.8$ we observe a narrowing of the quasi-particle peak. The sharp peaks at the inner side of the Hubbard bands get more pronounced and are shifted towards smaller $|\omega/D|$ (left inset). In the region between the quasi-particle peak and the Hubbard bands, the spectral weight is largely suppressed leading to the developing of a gap (or actually a pseudo-gap) with increasing $U/D$ (compare to Fig. 2).

With increasing $U/D$, the quasi-particle peak is expected to narrow until it vanishes at $U_{c2}/D \approx 3.0$. In the main panel of Fig. 4 we show results for $U/D = 2.8$. The right inset tracks the evolution of the quasi-particle peak for $U/D = 2.4, 2.6$ and 2.8. As expected, its weight is strongly reduced upon increasing $U/D$. The Hubbard side-peak (left inset) is visibly shifted towards smaller
to oscillate at a different frequency $\omega/D = 0.63 \pm 0.02$. The energy of this oscillations matches the energy of the side-peak at $\omega/D \approx 0.65$ almost perfectly.

$P_0$ on the other hand rises from exactly 0 to a small finite value, of about the same magnitude as $P_{1\downarrow}$ (see Fig. 5) and shows oscillations with the same frequency as $P_{1\downarrow}$ but shifted almost exactly by a phase of $\pi$ as compared to $P_{1\downarrow}$. The oscillation in $1 - P_1$ are essentially in phase with those of $P_{1\downarrow}$.

Fig. 6 shows the same analysis, but in the insulating phase for $U/D = 3.4$. In this case we solely observe oscillations corresponding to the Hubbard bands; a long lived oscillation is not present, which means that in frequency space only the metallic solution has a sharp feature, in agreement with our DMFT spectra above.

Quite generally an oscillation can be associated with a superposition of two eigenstates with an energy difference corresponding to the oscillation frequency. Adding an electron at time $tD = 0$ to the strongly correlated ground state of the one-band Hubbard model means, if Fourier-transformed to energies, that we will obtain a superposition of eigenstates from all energies. At different energies above the Fermi energy we have three distinct features: the central resonance around $\omega/D = 0$, the sharp side-peak at $\omega/D \approx 0.65$ and the broad upper Hubbard band. Unless matrix elements vanish, we will hence have a superposition of states belonging to these energies. Due to the large imaginary part of the self energy of the Hubbard band (see above), this part of the superposition will decohere on short time scales. After this short time, we will remain in a long lived superposition of states belonging to two sharp features, the central Kondo peak and the sharp resonance at the inner side of the Hubbard bands. This leads to the observed oscillations and the frequencies in Fig. 5.

D. Two-band Hubbard model

Finally in Fig. 7(a) we show first results for a two-band Hubbard model on the Bethe lattice for an interaction strength $U/D = 1.6$ and Hund’s coupling $J/D = 0.4$ close to the Mott phase [25]. We compare two different chain lengths and two different $N_{t,\text{max}}$ in order to get an estimate of the accuracy of our results. In both cases we observe distinct features in the Hubbard satellites. However, the spectra are still not converged in the system size, and pinning is not yet satisfied. Fig. 7(b) compares our results with ones we obtained using a continuous-time QMC method to solve the two-orbital impurity problem. For the QMC, we employed a hybridization expansion algorithm in matrix form as implemented in the TRIQS package [47, 48, 50]. This allows us to perform calculations for the full rotationally-invariant Hamiltonian Eq. (7) at low temperatures, $\beta D = 500$. The imaginary-time spectra of QMC have been continued to the real frequency axis using a stochastic Maximum-Entropy method [57] and alternatively Padé approxi-
FIG. 7: (a) DMFT spectral function for a two-band Hubbard model on the Bethe lattice for \( U/D = 1.6 \) and \( J/D = 0.4 \). We test the numerical accuracy by using two different bath chain-lengths, \( N_1 = N_2 = 60, 90 \), and linear prediction windows, \( N_{t,max} = 160, 230 \) (other parameters: \( \chi = 500 \), \( \epsilon_{tw} = 10^{-8} \)). (b) Comparison of the DMFT spectral function obtained from TEBD (red solid) with QMC + Maxent (blue dash-dotted) and QMC + Padé (black dashed). QMC data are obtained for \( \beta = 500 \).

The qualitative agreement of the position of the Hubbard bands is satisfactory. The features in the Hubbard satellites which are seen in the TEBD results, however, are completely absent in both analytically continued spectra. From the solution in the atomic limit, we know that there is a multiplet splitting of the Hubbard bands due to Hund’s exchange. Hence, we expect this natural splitting to be responsible for the Hubbard band sub-structure in Fig. 7.

V. CONCLUSIONS

We applied the Time Evolving Block Decimation (TEBD) algorithm to construct an impurity solver for dynamical mean-field theory for the single- and two-band Hubbard models on the \( \omega \to \infty \) Bethe lattice. Our method is parallelizable [58] and scalable to multi-band impurity systems. It works directly at zero temperature and real frequency, without the need for analytic continuation and it produces very accurate results as an impurity solver with high resolution at all frequencies. We applied our method to DMFT for the single band Hubbard model, where we confirm the existence of a sharp feature at the inner edges of the Hubbard bands due to Hund’s exchange. Hence, we expect this natural splitting to be responsible for the Hubbard band sub-structure in Fig. 7.

We tested the validity and precision of our method as an impurity solver for the case of the single impurity Anderson model at parameters for which results are available from the most precise technique to date, namely

VI. APPENDIX

A. Benchmark

We tested the validity and precision of our method as an impurity solver for the case of the single impurity Anderson model at parameters for which results are available from the most precise technique to date, namely

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FIG. A1: Comparison of TEBD-computed spectral function with results obtained from Dynamical DMRG calculations \[45, 55\] for a single impurity Anderson model with \( U/\Gamma = 6.0 \) and a hybridization strength \( \Gamma = \pi V^2 \rho(0) = 0.5 \) (\( N = 120, \chi = 500, \epsilon_{tw} = 10^{-10} \)).

\[
\begin{align*}
\pi A(\omega) &= \frac{2}{\gamma} \sqrt{D^2 - \omega^2} \\
\omega/D &= -3, -2, -1, 0, 1, 2, 3
\end{align*}
\]

FIG. A2: Influence of linear prediction parameters on spectral functions. We show results obtained with different pseudo-inverse cutoffs \( \delta \) and different treatment of large eigenvalues. The linear prediction was done on data obtained from a converged DMFT run with \( U/D = 2.8, N = 120, N_{t,max} = 350, \chi = 500, \epsilon_{tw} = 10^{-10}, \delta = 10^{-4} \). \( \delta \) was varied after the DMFT had converged. Results at \( \delta < 10^{-6} \) are the same as for \( \delta = 10^{-6} \).

\[
\begin{align*}
\pi A(\omega)/D &= 0.5, 0.75, 1, 1.5, 2, 2.5 \\
\omega/D &= -4, -2, 0, 2, 4
\end{align*}
\]

B. Parameter studies for prediction

Here we present more detailed results on the influence of the prediction parameters \( \delta \) and the number of measured data points \( N_{t,max} \). In Fig. A2 we show a DMFT-spectrum with \( U/D = 2.8, N = 120, \chi = 500, N_{t,max} = 350, \delta = 10^{-4} \) and large eigenvalues normalized to unity (black solid line). It is instructive to take these converged results and from the data of the last iteration calculate the spectral function with different pseudo-inverse cutoffs \( \delta \) and different treatment of large eigenvalues. We see that setting eigenvalues to unity tends to produce an overshoot at \( \omega/D = 0 \), whereas results with zeroed eigenvalues are stable and converged at \( \delta \leq 10^{-6} \). This behavior remains the same when doing full DMFT cycles. For eigenvalues rescaled to unity we also observe that for small \( \delta < 10^{-6} \) the prediction can pick up errors due to truncation and Trotter breakup, leading to artificial structures in the spectral functions. We conclude that converged results can best be obtained by setting large eigenvalues to zero and choosing \( \delta \leq 10^{-6} \).

In Fig. A3 we analyze the effect of \( N_{t,max} \) on the fixed point of the DMFT iterations for \( U/D = 2.8, \chi = 500 \) and \( \epsilon_{tw} = 10^{-10} \). We take \( N = 150, \) large enough to use different \( N_{t,max} \) without getting reflections from the boundaries of the system, which would spoil the linear prediction. We observe a very slight non-monotonic behavior of the Hubbard side peak height as well as the peak
position (left inset). The quasi particle peak height shows the same non-monotonic behavior (right inset). We attribute this behavior to truncation and Trotter effects, which become stronger for increasing $N_{t,max}$, also confirmed by tiny artificial structures in the pseudo-gap region for $N_{t,max} = 450$. The dependence of the fixed point on $N_{t,max}$ is very small. Using a large $N_{t,max} = 450$ does not improve systematically on the results, hence for computational efficiency we use $N_{t,max} = 350$ in the main paper.