Chebyshev matrix product state approach for spectral functions

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We show that recursively generated Chebyshev expansions offer numerically efficient representations for calculating zero-temperature spectral functions of one-dimensional lattice models using matrix product state (MPS) methods. The main features of this Chebyshev matrix product state (CheMPS) approach are as follows: (i) it achieves uniform resolution over the spectral function’s entire spectral width; (ii) it can exploit the fact that the latter can be much smaller than the model’s many-body bandwidth; (iii) it offers a well-controlled broadening scheme that allows finite-size effects to be either resolved or smeared out, as desired; (iv) it is based on using MPS tools to recursively calculate a succession of Chebyshev vectors \(|\omega_n\rangle\), (v) the entanglement entropies of which were found to remain bounded with increasing recursion order \(n\) for all cases analyzed here; and (vi) it distributes the total entanglement entropy that accumulates with increasing \(n\) over the set of Chebyshev vectors \(|\omega_n\rangle\), which need not be combined into a single vector. In this way, the growth in entanglement entropy that usually limits density matrix renormalization group (DMRG) approaches is packaged into conveniently manageable units. We present zero-temperature CheMPS results for the structure factor of spin-\(\frac{1}{2}\) antiferromagnetic Heisenberg chains and perform a detailed finite-size analysis. Making comparisons to three benchmark methods, we find that CheMPS (a) yields results comparable in quality to those of correction-vector DMRG, at dramatically reduced numerical cost; (b) agrees well with Bethe ansatz results for an infinite system, within the limitations expected for numerics on finite systems; and (c) can also be applied in the time domain, where it has potential to serve as a viable alternative to time-dependent DMRG (in particular, at finite temperatures). Finally, we present a detailed error analysis of CheMPS for the case of the noninteracting resonant level model.

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I. INTRODUCTION

Consider a one-dimensional lattice model amenable to treatment by the density matrix renormalization group (DMRG),1–4 with Hamiltonian \(\hat{H}\), ground state \(|0\rangle\), and ground-state energy \(E_0\). This paper is concerned with zero-temperature spectral functions of the form

\[ A^{BC}(\omega) = \langle 0 | \hat{B} \delta(\omega - \hat{H} + E_0) \hat{C} | 0 \rangle, \]  

(1)

which represents the Fourier transform \(\int \frac{dt}{2\pi} e^{i\omega t} G^{BC}(t)\) of the correlator

\[ G^{BC}(t) = \langle 0 | \hat{B}(t) \hat{C}(0) | 0 \rangle. \]  

(2)

One possible framework for calculating such spectral functions is to expand them in terms of Chebyshev polynomials, as advocated in Ref. 5. Such a Chebyshev expansion offers precise and convenient control of the accuracy and resolution with which a spectral function is to be computed. This is very useful, particularly when broadening the spectral function of a length-\(L\) system, which exhibits finite-size subpeaks with spacing \(\omega_L \sim 1/L\), in order to mimic that of an infinite system. If the latter has structures (e.g., sharp or diverging peaks), which are not yet properly resolved at the scale \(\omega_L\), the broadened version of the finite-size spectral function inevitably bears \(L\)-dependent errors in the vicinity of these structures. Hence, when calculating the finite-size version of these structures for the length-\(L\) system, there is no need to achieve an accuracy beyond that of the expected \(L\)-dependent errors, and having convenient control of this accuracy can significantly reduce numerical costs.

In this paper, we show that Chebyshev expansions offer numerically efficient representations for calculating spectral functions using matrix product state (MPS) methods,5–10 with numerical costs that compare favorably to those of other established DMRG-based approaches. In particular, the Chebyshev MPS approach presented here, to be called CheMPS, allows the above-mentioned control of accuracy and resolution to be imported into the DMRG and MPS arena.

The historically first approach for calculating spectral functions with DMRG is the continued-fraction expansion.11 While this method requires only modest numerical resources, it is limited to low frequencies and it is difficult to produce reliable results with it in the case of continua (however, algorithmic improvements were reported recently12). At present, the most accurate, but also most time-consuming, approaches are (i) the correction-vector (CV) method13–15 and (ii) time-dependent DMRG (tDMRG),17,16–18 in particular, when combined with linear prediction techniques.19–22 Since any new approach must measure up to their standards, let us briefly summarize their key ideas, advantages, and drawbacks.

(i) To calculate \(A^{BC}(\omega)\) using the CV approach, it is expressed as

\[ A^{BC}(\omega) = \langle 0 | \hat{B} | C_{\omega} \rangle, \]  

(3a)

in terms of the so-called correction vector

\[ | C_{\omega} \rangle = \lim_{\eta \to 0} \frac{1}{2\pi} \text{Im} \left[ \frac{1}{\omega - \hat{H} + E_0 + i\eta} \right] \hat{C} | 0 \rangle. \]  

(3b)

The correction vector can be calculated for (finite broadening parameter \(\eta\)) using either conventional DMRG (Refs. 13–15) or variational matrix product state (MPS) methods.23 A major
expresses the frequency domain only at the very end. To this end, one
overview of the material developed in detail in the main part
briefly summarize the structure and main features of such
resolution can be achieved by reducing $\eta$ and sampling
enough frequency points. However, this comes at considerable
costs: first, a separate calculation is required for
every choice of $\omega$ (although, in doing so, results for $|C_\omega\rangle$ from previous frequencies can be incorporated); and second, the
calculation of $|C_\omega\rangle$ involves an operator inversion problem that is
numerically poorly conditioned, ever more so the smaller $\eta$ is.

(ii) An alternative possibility is to use tDMRG to calculate
the time-domain correlator $G^{BC}(t)$, Fourier transforming to
the frequency domain only at the very end. To this end, one
expresses
\begin{equation}
G^{BC}(t) = e^{iE_0t} \langle 0|\hat{B}|\bar{C}_t\rangle
\end{equation}
in terms of the time-evolved state
\begin{equation}|ar{C}_t\rangle \equiv e^{-i\hat{H}t}|\bar{C}_0\rangle
\end{equation}
and uses tDMRG to calculate the latter. Two attractive features
of this strategy are as follows: first, it builds on an extensive
body of algorithmic knowledge for efficiently calculating
time evolution,7,16,17 and, second, a simple linear-prediction
scheme19–22 can be used to extrapolate the time dependence
for short and intermediate time scales to longer
times, thereby improving the quality of results at low frequency
at hardly any additional numerical cost. However, obtaining
reliable results over a sufficiently large time interval can, in
itself, be numerically very expensive, since the time evolution
of the many-body state $|C_t\rangle$ is accompanied by a strong growth
in entanglement entropy. This unavoidably also implies a growth of tDMRG truncation errors.

Note that, in both of the schemes outlined above, significant
(often heroic) amounts of numerical resources are devoted to
calculating a single state $|C_\omega\rangle$ for given $\omega$ or $|\bar{C}_t\rangle$ for given $t$,
as accurately as possible; the overlaps or expectation values of
interest, namely, $\langle 0|\hat{B}|C_\omega\rangle$ for $\langle 0|\hat{B}|\bar{C}_t\rangle$, are only calculated
at the end, in a single, final step after $|C_\omega\rangle$ or $|\bar{C}_t\rangle$ have been fully determined. Actually, these states are calculated
so accurately that they would have been equally suitable for
calculating any other quantity (correlator or matrix element)
involving that state. In a sense, DMRG is asked to work
harder than necessary; it is used to calculate a single state with
“general-purpose accuracy,” whereas the accurate calculation
of a particular expectation value involving that state would have
been sufficient.

The main motivation for this paper is to attempt to reduce
this calculational overhead by employing a representation
of the spectral function that avoids the need for calculating
a single state with such high accuracy and instead allows
numerical resources to be focused directly on the calculation of
the relevant expectation values. This can be achieved by repre-
senting the spectral function via a Chebyshev expansion,5,24,25
the coefficients of which, the so-called Chebyshev moments,
can be calculated recursively using MPS tools. Below, we
briefly summarize the structure and main features of such
an expansion, thereby providing both an introduction and an
overview of the material developed in detail in the main part
of this paper.

The Chebyshev polynomials $T_n(x)$ form an orthonormal set
of polynomials on the interval $x \in [-1,1]$. They are very well
studied mathematically,26–28 and are widely used for function
expansions since they have very favorable convergence prop-
ties. As will be described in detail below, the spectral function
can be represented approximately by a so-called Chebyshev
expansion, which becomes exact for $N \to \infty$, of the following
form:
\begin{equation}A^{BC}_N(\omega) = \frac{2W^*/W_s}{\sqrt{1 - \omega^2}} \left[ g_0 \mu_0 + 2 \sum_{n=1}^{N-1} g_n \mu_n T_n(\omega') \right].
\end{equation}

Here, the Chebyshev moments $\mu_n = \langle 0|\hat{B}|\mu_n\rangle$ are obtained from the Chebyshev vectors $|\mu_n\rangle = T_n(\hat{H})|\bar{C}_0\rangle$, and the $g_n$ are
known damping factors that influence broadening effects.
The primes indicate that the Hamiltonian $\hat{H}$ and frequency $\omega$
were expressed in terms of rescaled and shifted versions $\hat{H}'$
and $\omega'$ in such a manner that an interval $\omega \in [0,W_s]$, which contains
the entire spectral weight, is mapped onto a rescaled band $\omega' \in [-W',W']$ of half-width $W' < 1$.

This representation has several useful features:

(i) It resolves the interval $\omega \in [0,W_s]$ with a uniform
resolution of $\mathcal{O}(W_s/N)$.

(ii) The range of frequencies over which the spectral function
has nonzero weight, say $W_s$ (to be called its spectral width), is often significantly smaller than the many-body
bandwidth of the Hamiltonian, say $W$, as depicted in Fig. 1. By
choosing the effective bandwidth $W_s$ to be of order $W_s$ instead
of $W$, huge gains in resolution are possible.

(iii) A well-controlled broadening scheme, encoded in the
damping factors $g_n$, is available that allows finite-size effects
to be either resolved or smeared out, as desired.

(iv) The Chebyshev vectors $|\mu_n\rangle$ are calculated using a (nu-
merically stable) recursion scheme, which exploits Chebyshev
recurrence relations to calculate $|\mu_n\rangle$ from $\mu_n' = H' T_n-1(\hat{H})$ and $\mu_{n-2}$ [see Eq. (30)]. Thus, the expectation values from which
the spectral function is constructed are built up in a series of
recursive steps [see Eq. (7) below] instead of being calculated
at the end in one final step.

(v) The bond entropy of successive Chebyshev vectors
$|\mu_n\rangle$ is found empirically to remain bounded with increasing
recursion number $n$, thus, the complexity of these vectors
remains manageable up to arbitrarily large $n$. 

FIG. 1. (Color online) (a) Sketch of a spectral function, the
spectral width $W_a$ of which is much smaller than the many-body
bandwidth $W$. Before making a Chebyshev expansion, we rescale the
interval $\omega \in [0,W_s]$, with effective bandwidth $W_s = 2W_a$, onto the
interval $\omega' \in [-W',W']$, shown in (b), with rescaled half-bandwidth
$W' = 1 - \frac{1}{2} \epsilon_s$ and a safety factor $\epsilon_s \simeq 0.025$. 

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we present CheMPS results for the structure factor of a spin-1
the resonant level model used for the error analysis of Sec.V.
An appendix gives a detailed account of CheMPS results for
presents a brief outlook toward possible future applications,
Section VII summarizes our main conclusions, and Sec. VIII

Let us contrast this with the CV or tDMRG approaches: imagine expanding the correction-vector or time-evolved state
in terms of the Chebyshev vectors \(|\tau_n\rangle\), i.e., expressing them as linear combinations of the form

\[
|\tilde{C}\rangle = \sum_{n=0}^{N-1} C_n |\tau_n\rangle, \quad |\tilde{C}'\rangle = \sum_{n=0}^{N-1} C'_n |\tau_n\rangle,
\]

respectively. (The coefficients \(C_n\) and \(C'_n\) are related by Fourier transformation.) Now, the CV or tDMRG approaches, in effect, attempt to accurately represent the entanglement of this entire linear combination using a single MPS. This endeavor is numerically very costly since the entanglement entropy of this linear combination grows rapidly with \(N\). The Chebyshev approach avoids this problem by taking expectation values before performing the sum on \(n\):

\[
\langle 0|\hat{B}|\tilde{C}\rangle = \sum_{n=0}^{N-1} C_n \mu_n, \quad \langle 0|\hat{B}|\tilde{C}'\rangle = \sum_{n=0}^{N-1} C'_n \mu_n.
\]

Thus, the Chebyshev expansion very conveniently organizes the calculation into many separate and, hence, numerically less costly, packages or subunits.

Our paper is organized as follows. We introduce the Chebyshev expansion for spectral functions in Sec. II and discuss its implementation using MPS, including an algorithm for performing a projection in energy, in Sec. III. In Sec. IV, we perform CheMPS results for the structure factor of a spin-\(1/2\) Heisenberg chain, perform a detailed analysis of finite-size effects (see Fig. 5), and compare our results to CV, Bethe ansatz, and tDMRG (see Figs. 4, 6, and 8, respectively). In Sec. V, we perform an extensive error analysis of the CheMPS approach using the quadratic resonant level model, and discuss some salient features of density matrix eigenspectra in Sec. VI. Section VII summarizes our main conclusions, and Sec. VIII presents a brief outlook toward possible future applications, involving time dependence or finite-temperature correlators. An appendix gives a detailed account of CheMPS results for the resonant level model used for the error analysis of Sec. V.

II. CHEBYSHEV EXPANSION OF \(A^BC(\omega)\)

A. Chebyshev basics

Let us start by briefly summarizing those properties of Chebyshev polynomials that will be needed below. We follow the notation of Ref. 5, which gives an excellent general discussion of Chebyshev expansion techniques (although without mentioning possible DMRG and MPS applications).

(vi) Finally, and from the perspective of numerical costs, most importantly, CheMPS efficiently copes with the growth in bond entropy with increasing iteration number that usually limits DMRG approaches. It does so by distributing this entropy over all \(|\tau_n\rangle\), thereby packaging it into manageable units [see (v)]. In particular, when constructing and using the states \(|\tau_n\rangle\), one never needs to know more than three at a time (and after use may delete them from memory). Hence, it is not necessary to combine all information contained in all \(|\tau_n\rangle\) into a single MPS.

Let us start by briefly summarizing those properties of Chebyshev polynomials that will be needed below. We follow the notation of Ref. 5, which gives an excellent general discussion of Chebyshev expansion techniques (although without mentioning possible DMRG and MPS applications).
where the Chebyshev moments $\mu_n$ are given by

$$\mu_n = \int_{-1}^{1} dx f(x) T_n(x).$$  \hspace{1cm} (12)

An approximate representation of order $N$ is obtained for $f(x)$ if only the first $N$ terms (i.e., $n \leq N - 1$) are retained. However, such a truncation, in general, introduces artificial oscillations of period $\sim 1/N$ called Gibbs oscillations. These can be smoothed by employing certain broadening kernels, which, in effect, rearrange the infinite series (11) before truncation. This leads to a reconstructed expansion of the form

$$f_N(x) = \frac{1}{\pi \sqrt{1-x^2}} \left[ g_0 + 2 \sum_{n=1}^{N-1} g_n \mu_n T_n(x) \right],$$  \hspace{1cm} (13)

which (for properly chosen kernels) converges uniformly:

$$\max_{-1 < x < 1} |f(x) - f_N(x)| \xrightarrow{N \to \infty} 0.$$  \hspace{1cm} (14)

The reconstructed series (13) contains the same Chebyshev moments $\mu_n$ as Eq. (12), but they are multiplied by damping factors $g_n$, real numbers with a form that is characteristic of the chosen kernel. Several choices have been proposed, which damp out Gibbs oscillations in somewhat different ways (see Ref. 5 for details). We will mostly employ Jackson damping, given by

$$g_n^J = \frac{(N-n+1) \cos \frac{\pi n}{N+1} + \sin \frac{\pi n}{N+1} \cot \frac{\pi}{N+1}}{N+1}.$$  \hspace{1cm} (15)

This is usually the best choice since it guarantees an integrated error of $O(1/N)$ for $f_N(x)$. When used to approximate a $\delta$ function $\delta(x-\bar{x})$ sitting at $\bar{x} \in I$, Jackson damping yields a nearly Gaussian peak of width $\sqrt{1-\bar{x}^2}/\pi N$. On one occasion, we will also employ Lorentz damping

$$g_n^L = \frac{\sin \left[ \frac{\pi}{2} (1-\frac{n}{N}) \right]}{\sin \lambda},$$  \hspace{1cm} (16)

where $\lambda$ is a real parameter. Lorentz damping preserves analytical properties (causality) of Green’s function and broadens a $\delta$ function $\delta(x-\bar{x})$ into a peak, the shape of which, for the choice $\lambda = 4$ used here (following Ref. 5), is nearly Lorentzian of width $\sqrt{1-\bar{x}^2}/\lambda N$.

To summarize: The order-$N$ Chebyshev reconstruction $f_N(x)$ with Jackson or Lorentz damping with $\lambda = 4$ yields a result that is very close to the broadened function

$$f_N^J(x) = \int_{-1}^{1} d\tilde{x} K_{\eta,J}(x-\tilde{x}) f(\tilde{x})$$  \hspace{1cm} (17)

($X = J, L$) with broadening kernels and widths given by

$$K_{\eta,J}^J(x) = \frac{e^{-x^2/(2\eta^2)}}{\sqrt{2\pi} \eta}, \quad \eta_{N,J} = \sqrt{1 - \bar{x}^2} \frac{\pi}{N},$$  \hspace{1cm} (18a)

$$K_{\eta,L}^J(x) = \frac{\eta'/\pi}{\sqrt{x^2 + \eta^2}}, \quad \eta'_{N,L} = \sqrt{1 - \bar{x}^2} \frac{4}{N}.$$  \hspace{1cm} (18b)

respectively. Thus, $f_N(x)$ resolves the shape of $f(x)$ with a resolution of $O(1/N)$.

For purposes of illustration, Fig. 3(a) shows three Chebyshev reconstructions of a $\delta$ function at $\bar{x} = 0$: without damping, giving Gibbs oscillations; with Jackson damping, yielding a near-Gaussian peak; and with Lorentz damping, yielding a near-Lorentzian peak. Figure 3(b) shows a Jackson-damped Chebyshev reconstruction of a comb of Gaussian peaks $\sum_{\alpha} K_{\eta,J}^J(x-\bar{x}_\alpha)$, the widths $\tilde{\eta}_J$ of which are all equal. It illustrates how increasing $N$ reduces the amount of broadening until the original peak form is recovered for sufficiently large $N$. It also shows that the broadened peak widths depend on the peak positions, reflecting the fact that convolving a Gaussian of width $\tilde{\eta}_J(x)$ with a near Gaussian of width $\eta_{N,\bar{x}}$ [Eq. (17)] produces a near Gaussian of width

$$\eta_a \simeq \sqrt{\tilde{\eta}_J^2 + \eta_{N,\bar{x}}^2}. \hspace{1cm} (19)$$

To evaluate the $T_n(x)$ that occur in Eq. (13), we use the first equality of Eq. (10). Although numerically more efficient methods exist for this purpose, their use becomes advisable only for expansion orders much larger than the $N \lesssim O(10^3)$ that we will need in this work.
B. Rescaling of \( \omega \) and \( \hat{H} \)

To construct a Chebyshev expansion of the spectral function \( A^{BC}(\omega) \) of Eq. (1), we need to rescale and shift\(^5\) the Hamiltonian \( \hat{H} \mapsto \hat{H}' \) and the frequency \( \omega \mapsto \omega' \) in such a way that the spectral range of \( A(\omega) \), i.e., the interval \([0, W]\) within which it has nonzero weight, is mapped into the interval \([-1, 1]\). Rescaled, dimensionless energies and frequencies will always carry primes. As safeguards against “leakage” beyond \([-1, 1]\) due to numerical inaccuracies, we choose the linear map (see Fig. 1)

\[
\omega \in [0, W] \mapsto \omega' \in [-W', W'], \quad W' = 1 - \frac{1}{2} \epsilon_1, \tag{20}
\]

which entails two precautionary measures. First, the \( \omega \) interval is taken to be larger than the requisite \([0, W]\) by choosing the effective bandwidth \( W \) to be larger than the spectral width \( W_1 \); second, the \( \omega' \) interval is taken to be slightly smaller than the requisite \([-1, 1]\) by choosing the rescaled half-bandwidth \( W' \) to be smaller than 1, with a safety factor\(^5\) of \( \epsilon_1 \simeq 0.025 \). To be explicit, we define

\[
\omega' = \frac{\omega}{a} - W', \quad a = \frac{W_1}{2W'}, \tag{21a}
\]

\[
\hat{H}' = \frac{\hat{H} - E_0}{a} - W', \tag{21b}
\]

where \( \hat{H}' \) has ground-state energy \( E'_0 = -W' \). Then, we express the spectral function (1) as

\[
A^{BC}(\omega) = \frac{1}{a} \langle 0 | \hat{B} \delta(\omega' - \hat{H}') | \tilde{C}(0) \rangle \tag{22}
\]

(with \( \omega' = \omega'(\omega) \) and \( \hat{H}' \) given by Eqs. (21)), which by construction has no weight for \( \omega' \notin [-W', W'] \).

One possible choice for \( W \) is to equate it to the width of the many-body spectrum of \( H \), given by \( W = E_{\text{max}} - E_0 \). When using DMRG, \( E_0 \) is usually already known from calculating the ground state \( |0 \rangle \) of \( H \), and \( E_{\text{max}} \) can be found, e.g., by calculating\(^8\) the ground state of \( -H \) (reduced DMRG accuracy relative to usual ground-state calculations is sufficient, since only \( E_{\text{max}} \) is of interest here.)

A disadvantage of the choice \( W_1 = W \) is that the many-body bandwidth \( W \) typically is large (it scales with system size), whereas optimal spectral resolution requires \( W_1 \) to be as small as possible: since an \( \lambda \)th order Chebyshev expansion yields a resolution of \( O(1/N) \) on the interval \([-1, 1]\), its resolution on the original interval \([0, W]\) will be \( O(W/N) \), which evidently becomes better the smaller \( W_1 \). If \( \hat{B} \) and \( \hat{C} \) are single-particle operators, the spectral width \( W_4 \) of \( A^{BC}(\omega) \) is independent of system size and, hence, much smaller than the many-body bandwidth \( W_1 \). In this case, it is advisable to choose \( W_1 \) to be of similar order (though still larger) than \( W_4 \). We will choose \( W_4 = 2W_1 \), which is typically \( \ll W \), as illustrated in 1.

C. Chebyshev expansion in frequency domain

To expand the \( \delta \) function in Eq. (22) in Chebyshev polynomials, we use \( \tilde{f}(x) = \delta(x - \hat{H}') \) with \( x = \omega' \) in Eq. (12), and obtain from Eq. (13) a reconstructed Chebyshev operator expansion of the form

\[
\delta_N(\omega' - \hat{H}') = \frac{1}{\pi \sqrt{1 - \omega'^2}} \left[ g_0 + 2 \sum_{n=1}^{N-1} g_n T_n(\hat{H'}) T_n(\omega') \right].
\]

Inserting this into Eq. (22) for \( A^{BC}(\omega) \) yields the Chebyshev expansion (5), with Chebyshev moments given by

\[
\mu_n = \langle 0 | \hat{B} T_n(\hat{H'}) | \tilde{C}(0) \rangle.
\]

Thus, \( \mu_n \) is a ground-state expectation value of an \( n \)-th order polynomial in \( \hat{H}' \), the construction of which might \textit{a priori} appear to become increasingly daunting as \( n \) increases. Fortunately, this challenge can be dealt with \textit{recursively} by expressing the moments as

\[
\mu_n = \langle 0 | \hat{B} | n \rangle, \quad | n \rangle = T_n(\hat{H'}) | \tilde{C}(0) \rangle,
\]

and calculating the \textit{Chebyshev vectors} \(| n \rangle \) by exploiting the Chebyshev recurrence relations (8). The details of this recursive scheme will be discussed in Sec. III.

D. Chebyshev expansion in time domain

The Chebyshev expansion can also be employed for studying time evolution in general, and the correlator \( G^{BC}(t) \) in particular. To this end, we express the time-evolution operator as

\[
\hat{U}(t) = e^{-i \hat{H} t} = \int_{-1}^{1} d\omega' e^{-i[a(\omega' + W') + E_0]t} \delta(\omega' - \hat{H}')
\]

and insert Eq. (23) (without damping, \( g_n = 1 \)) into the latter. This yields\(^{30,31}\)

\[
\hat{U}_N(t) = e^{-i(E_0 + aW')t} \left[ c_0(t) + 2 \sum_{n=1}^{N-1} T_n(\hat{H'}) c_n(t) \right].
\]

\[
c_n(t) = \int_{-1}^{1} \frac{e^{-i a \omega' t}}{\sqrt{1 - \omega'^2}} \frac{1}{\sqrt{\pi}} \frac{1}{1 + \omega'^2} d\omega' = (-i)^n J_n(at),
\]

Here, \( J_n(at) \) is the Bessel function of the first kind of order \( n \). It decays very rapidly with \( n \) once \( n > at \). Hence, an expansion of given order \( N \) gives an essentially exact representation of \( \hat{U}(t) \) for times up to \( t_{\text{max}} \lesssim \frac{N}{a} \), while \( c_{N-1}(t) \) provides an estimate of the error.

By inserting Eqs. (27) into Eqs. (4) for \( G^{BC}(t) \), we find

\[
G_N(t) = e^{-i a W' t} \left[ \mu_0 J_0(at) + 2 \sum_{n=1}^{N-1} (-i)^n \mu_n J_n(at) \right],
\]

where the Chebyshev moments \( \mu_n \) are again given by Eq. (25). Thus, the Chebyshev expansions of \( G_N(t) \) and \( A^{BC}(\omega) \) are governed by the same set of moments \( \mu_n \), as is to be expected for functions linked by Fourier transformation.

III. MPS EVALUATION OF THE CHEBYSHEV MOMENTS \( \mu_n \)

We now present a recursive scheme for calculating the Chebyshev moments \( \mu_n \). The manipulations described below
were implemented using MPS-based methods, which are very convenient for constructing the states of interest, while matrix product operators (MPOs) simplify the implementation of the shift and rescaling transformation [Eq. (21b)] of the Hamiltonian.

A. Recurrence fitting

To initialize the Chebyshev expansion, we calculate ground state \( |0\rangle \) and ground-state energy \( E_0 \) of \( \hat{H} \), make a specific choice for \( W_0 \) and \( W \), and construct \( \hat{H}' \) according to Eq. (21b). Then comes the main task, namely, the recursive calculation of the moments \( \mu_n \). This is done by starting from

\[
|t_0\rangle = \tilde{C}|0\rangle, \quad |t_1\rangle = \hat{H}'|t_0\rangle
\]

and using the recurrence relation [obtained from Eq. (8)]

\[
|t_n\rangle = 2\hat{H}'|t_{n-1}\rangle - |t_{n-2}\rangle,
\]

which can be implemented using the so-called compression or fitting procedure32 (see Ref. 4, Sec. 4.5.2 for details). It finds fitting error for given MPS dimension \( m \) by variationally minimizing the fitting error

\[
\Delta_{\text{fit}} = \| |t_n\rangle - (2\hat{H}'|t_{n-1}\rangle - |t_{n-2}\rangle) \|^2.
\]

We will call this procedure recurrence fitting. In practice, the variational minimization proceeds via a sequence of fitting sweeps back and forth along the chain. These are continued until the state being optimized becomes stationary, in the sense that the overlap

\[
\Delta_{\varepsilon} = \left| 1 - \frac{\langle t_n | t_n' \rangle}{\| |t_n\rangle \| \| |t'_n\rangle \|} \right|
\]

between the states \( |t_n\rangle \) and \( |t'_n\rangle \) before and after one fitting sweep drops below a specified fitting convergence threshold (typically in the range \( 10^{-6} \) to \( 10^{-8} \)). The maximum expansion order for which \( |t_n\rangle \) is obtained using recurrence fitting will be denoted by \( N_{\text{max}} \).

The MPS dimension \( m \) needed to achieve accurate recurrence fitting turns out to be surprisingly small (see Sec. V for a detailed analysis). For example, \( m = 32 \) sufficed for the antiferromagnetic Heisenberg chain of length \( L = 100 \), discussed in Sec. IV. The reason for this remarkable and eminently useful feature lies in the fact that the Chebyshev recurrence relations contain only two terms on the right-hand side, the addition of which requires only modest computational effort. In contrast, CV or TDMRG typically require much larger \( m \) since they attempt to represent the sum of many states [see Eq. (6)] in terms of a single MPS.

For the special but common case that \( \tilde{B} = \tilde{C} \), Eq. (9) yields a relation between different moments

\[
\mu_n + \nu_n = 2\langle t_n | t_n' \rangle - \mu_{n-\nu}.
\]

This can be used to effectively double the order of the expansion to \( 2N_{\text{max}} \) without calculating any additional Chebyshev vectors, by setting \( n' = n - 1 \) or \( n' = n + 1 \):

\[
\tilde{\mu}_{2n-1} = 2\langle t_n | t_{n-1} \rangle - \mu_1,
\]

\[
\tilde{\mu}_{2n} = 2\langle t_n | t_n \rangle - \mu_0.
\]

We use tildes to distinguish \( \tilde{\mu}_n \) moments calculated in this manner from the \( \mu_n \) moments obtained via Eq. (25). Although they should nominally be identical, in numerical practice, \( \tilde{\mu}_n \) moments are less accurate [by up to a factor of 5 in Fig. 9(c) below] since they depend on two Chebyshev vectors, whereas \( \mu_n \) moments depend on only one. Our Chebyshev reconstructions thus generally employ the \( \mu_n \) moments and, unless stated otherwise, \( \tilde{\mu}_n \) moments are used only for results requiring \( N_{\text{max}} \leq n < 2N_{\text{max}} \).

B. Energy truncation

We have argued above that, in order to optimize spectral resolution, it may be desirable to choose the effective bandwidth \( W_0 \) to be smaller than the full many-body bandwidth \( W \). If this is done, however, it is essential to include an additional energy truncation step into the recursion procedure to ensure that each \( |t_n\rangle \) remains free from “high-energy” components, i.e., \( \hat{H}' \) eigenstates with eigenenergies \( E_{n} > 1 \), which fall outside the range \([-1,1]\) that is admissible for arguments of Chebyshev polynomials. If \( W_0 < W \), numerical noise causes the state \( |t_n\rangle \) to contain such high-energy contributions in spite of the precautionary measures described after Eq. (20) because the application of \( \hat{H}' \) to \( |t_{n-1}\rangle \) in Eq. (30) entails a DMRG truncation step, which is not performed in the eigenbasis of \( \hat{H}' \). If such high-energy components were fed into subsequent recursion steps, the norms \( \| |t_n\rangle \| \) of successive Chebyshev vectors would diverge rapidly (as would the resulting moments \( \mu_n \) because this effectively amounts to evaluating Chebyshev polynomials \( T_n(x) \) for \( |x| > 1 \), where \( |T_n| > 1 \) [see Fig. 2(b)]).

As a consequence, after obtaining a new state \( |t_n\rangle \) from Eq. (30), we take the precautionary measure of projecting out any high-energy components that it might contain before proceeding to the next \( |t_{n+1}\rangle \). This can be done by performing several energy truncation sweeps. During an energy truncation sweep, we focus on one site at a time, perform an energy truncation in a local Krylov basis constructed for that site, and then move on to the next site. Shifting the current site is accomplished by standard MPS means, without any truncation, as a DMRG truncation would counteract the energy truncation. (As a consequence, an energy truncation in terms of two-site sweeps has not been implemented.)

The truncation must take place in the energy eigenbasis of the Hamiltonian \( \hat{H}' \). Of course, its complete eigenbasis is not accessible, thus, we build a Krylov subspace of dimension \( d_K \) within the effective Hilbert space at every site. Alternatively, energy truncation can also be performed in the bond representation \( |\psi\rangle = B_{\psi}|t_1\rangle|t_2\rangle \). In this Krylov subspace, the effective Hamiltonian \( \hat{H}_K' \) of dimension \( d_K \) can be fully diagonalized and so we can construct a projection operator to project out all eigenstates with energy bigger than some energy truncation threshold \( \varepsilon_P \). The choice of this threshold depends on the choice of \( W_0 \). We have found the combination \( W_0 = 2W_0 \) and \( \varepsilon_P = 1.0 \) to work well (but other choices, involving, e.g., smaller \( W_0 \) and larger \( \varepsilon_P \) would be possible, too.)

In the following, we describe the procedure just outlined in more detail for a single site using standard MPS nomenclature. Let the effective local Hilbert space for this site be spanned
TABLE I. List of CheMPS parameters that control various algorithmic tasks, influencing their numerical costs and the quality of results.

| Parameter | Recommended value | Description | Task       |
|-----------|-------------------|-------------|------------|
| $W_e$     | $2W_A$ (or $W$)   | Effective bandwidth with (or without) energy truncation | Rescaling of $H$ |
| $\epsilon_i$ | 0.025       | Safety offset in rescaled half-bandwidth: $W' = 1 - \frac{1}{4}\epsilon_i$ |            |
| $m$       | $10^{-6}, \ldots, 10^{-8}$ | MPS dimension | Recurrence fitting |
| $d_K$     | 30                | Krylov subspace dimension | Energy truncation |
| $n_S$     | 10                | Number of sweeps |            |
| $\epsilon_P$ | 1.0          | Energy truncation threshold (in rescaled units) |            |
| $N$       | Depends on system size | Order of expansion, broadening | Spectral reconstruction |
| $g_n$     | $g_n^*$          | Choice of damping factors |            |

by the left, local, and right basis vectors $|l\rangle$, $|\sigma\rangle$, and $|r\rangle$, and expand the Chebyshev vector $|\psi\rangle = |\alpha\rangle$ in this basis:

$$|\psi\rangle = \sum_{l,\sigma} A_l^{\sigma}|l\rangle|\sigma\rangle|r\rangle.$$  

To construct a projection operator $P$ that projects out the high-energy components for this site $|\psi\rangle \mapsto P|\psi\rangle$, one may proceed as follows.

First, build a Krylov subspace of dimension $d_K$ within span$\{|l\rangle|\sigma\rangle|r\rangle\}$ and calculate the matrix elements of $\hat{H}'$ within it (no truncation necessary):

$$|\tilde{l}\rangle = (\hat{H}')^{-1}|l\rangle, \quad i = 1, \ldots, d_K$$

orthonormalize via Gram-Schmidt,

$$|\tilde{l}\rangle \mapsto |l\rangle$$

Next, fully diagonalize $\hat{H}'$ to obtain all eigenenergies $\epsilon'_a$ and eigenvectors $|e_a\rangle$:

$$\hat{H}'|e_a\rangle = \epsilon'_a|e_a\rangle$$

Then, construct the projection operator

$$P = \mathbb{I} - \sum_{a,|e_a\rangle,|e_a\rangle} |e_a\rangle\langle e_a|$$

for a certain energy threshold $\epsilon_P$ and apply it:

$$|\psi\rangle \mapsto P|\psi\rangle.$$  

Performing this procedure once for every site of the chain constitutes a truncation sweep. The state obtained after several truncation sweeps, say $|I_n\rangle_\tau$, is stripped from the unwanted high-energy components of $|I_n\rangle$, as well as possible within a Krylov approximation. After fitting and truncation have been completed, the resulting (unnormalized) state $|I_n\rangle_\tau$ is renamed $|I_n\rangle$, used for calculating $\mu_n$, and fed into the next recursion step.

To quantify the effects of energy truncation, we consider two measures of how much $|\mu_n|$ changes during truncation. First, for a given truncation sweep, we define the average truncated weight per site (averaged over all sites) by

$$N_t^{\text{sweep}} = \frac{1}{L} \sum_k \sum_{a,|e_a\rangle,|e_a\rangle} \langle e_a^k|\psi\rangle^2,$$

where $|e_a^k\rangle$ are the vectors constituting the projector of Eq. (38) at site $k$. Second, we define the truncation-induced state change by

$$\Delta_n = \| |I_n\rangle_\tau - |I_n\rangle \|^2.$$  

The numerical costs for energy truncation are as follows: The cost for the steps in Eqs. (36) are $O(d_K^2 m^3 d^2 D_H)$, where $m$ is the MPS dimension, $d$ is the size of the local site basis, and $D_H$ is the matrix product operator dimension of $\hat{H}'$. The diagonalization of $\hat{H}'^K$ is of $O(d_K^4)$, where $d_K$ is theoretically bounded by $m^2 d$. In our experience, the purpose of the energy truncation, which is solely to eliminate high-energy contributions, is well accomplished already for a relatively small Krylov subspace dimension of $d_K = 30 \ll m^2 d$. An overview of all the parameters relevant for CheMPS is given in Table I. Where applicable, it also lists the values that we found to be optimal. A detailed error analysis, tracing the effects of various choices for these parameters, will be presented in Sec. V.
IV. RESULTS: HEISENBERG ANTIFERROMAGNET

To illustrate the capabilities and power of the proposed CheMPS approach, this section presents results for the spin structure factor of a one-dimensional spin-\(\frac{1}{2}\) Heisenberg antiferromagnet (HAFM) and compares them against results obtained from CV and iDMRG approaches.

A. Spin structure factor

We study the spin-\(\frac{1}{2}\) HAFM for a lattice of length \(L\):

\[ \hat{H}_{\text{HAFM}} = J \sum_{j=1}^{L-1} \mathbf{S}_j \cdot \mathbf{S}_{j+1}, \]

where \(\hat{S}_j\) denotes the spin operator at site \(j\). We choose \(J = 1\) as unit of energy throughout this section. This model exhibits SU(2) symmetry, which has been exploited in our calculations; accordingly, all MPS dimensions noted for the HAFM are to be understood as the number of SU(2) (representative) states being kept. To account for the open boundary conditions, we define spin-wave operators as

\[ \hat{S}_k = \sqrt{\frac{2}{L+1}} \sum_{j=1}^{L} \sin(jk) \hat{S}_j \]

with quasimomentum \(k = \pi n / (L + 1), n = 1, \ldots, L.\) [When displaying numerical results for \(k = \pi n / 2\) below, we mean \(k = \pi n / (L + 1)\) or \(\pi (L/2 + 1)/(L + 1)\), respectively, choosing \(L\) even throughout.] The spin structure factor (spectral function) we are interested in is given by

\[ S(k, \omega) = \mathcal{A}^{N}_{\pi/2} \hat{S}_k (\omega), \]

It is known from exact solutions that the dominant part of the spin structure factor stems from two-spinon contributions, bounded from below and above by

\[ \omega_1 = \frac{\pi}{2} \left| \sin k \right| \quad \text{and} \quad \omega_2 = \pi \left| \sin \frac{k}{2} \right|. \]

(45)

(For the exact solution of an infinite system, \(k\) refers to the true momentum, not quasimomentum.) Moreover, for an infinite system, \(S(k, \omega)\) is known to diverge as

\[ S(k, \omega) \sim [\omega - \omega_1]^{-\frac{1}{2}} \sqrt{\ln [1/(\omega - \omega_1)]} \quad \text{for} \quad k \neq \pi, \]

\[ S(\pi, \omega) \sim \omega^{-1} \sqrt{\ln(1/\omega)} \]

as \(\omega\) approaches the lower threshold \(\omega_1\) from above. This divergence reflects the tendency toward staggered spin order of the ground state of the Heisenberg antiferromagnet. It poses a severe challenge for numerics, which always deals with systems of finite size, and hence will never yield a true divergence. Instead, the divergence will be cut off at \(\omega - \omega_1 \simeq 1/L\), yielding a peak of finite height

\[ \max S(k, \omega) \sim [L \ln L]^{\frac{1}{2}} \quad \text{for} \quad k \neq \pi, \]

\[ \max S(\pi, \omega) \sim L [\ln L]^{\frac{1}{2}}. \]

Thus, the best that one can hope to achieve with numerics is to capture the nature of the divergence as \(\omega\) approaches \(\omega_1\) before it is cut off by finite size, or the scaling of the peak height with system size.

Equation (45) gives a good guide for choosing \(\omega_1\). We found the choices \(W_0 = 6.3 \approx 2\pi\) and \(\epsilon_1 = 0.025\) to work well for all \(k\) and have used them for all figures (4 to 6) of this section. As consistency checks, we verified that the resulting \(S(k, \omega)\) is essentially independent of \(W_0\) and that it agrees with a calculation that included the full many-body bandwidth (\(W_0 = W\)).

To have an accurate starting point for all calculations, we used throughout a ground state obtained by standard DMRG with MPS dimension \(m = 512\). From expansion order \(n = 1\) onward, it turned out to be sufficient to represent all Chebyshev vectors \(|u_n\rangle\) using a surprisingly small MPS dimension of \(m = 32\), or \(m = 64\) for some results involving very large iteration number, as indicated in every figure. (In retrospect, this implies that, for the ground state too, a much smaller \(m\) would have sufficed.) We have verified that the structure factor \(S(k, \omega)\) is well converged w.r.t. \(m\) nevertheless. Detailed evidence for this claim will be presented below. However, already at this stage it is worth remarking that the ability of CheMPS to get good results with comparatively small \(m\) values is perhaps the single most striking conclusion of our work. This will be discussed in detail below.

B. Comparison to CV

We begin our discussion of CheMPS results by comparing them to those of CV calculations, which are known to be very accurate, although also computationally expensive. The CV method involves a broadening parameter \(\eta\) and broadens \(\delta\) functions into Lorentzian peaks of width \(\eta\). This can be mimicked with CheMPS by using Lorentz damping (with \(\lambda = 4.0\)) since this also produces Lorentzian broadening, representing a \(\delta\) function \(\delta(\omega' - \omega)\) by a near-Lorentzian peak, albeit with a frequency-dependent width \(\eta N_{\omega'} = \sqrt{1 - \omega^2 \lambda^2} / N\) (see Sec. II A and 3). To compare CheMPS results with CV results at given \(\eta\), we thus identify \(\eta = a \eta_N\), where \(a\) is the scaling factor from Eqs. (21) and \(\bar{\omega}\) is taken to be the rescaled and shifted version of the frequency \(\omega_{\text{max}}\) at which the peak reaches its maximum. Thus, we set the expansion order used for reconstruction to

\[ N = \frac{4a}{\eta} \sqrt{1 - (\omega_{\text{max}}/a - W)^2}. \]

Figure 4 shows such a comparison for the structure factor \(S(\pi/2, \omega)\) of a \(L = 100\) Heisenberg chain. We used two choices of \(\eta\) that are large enough to avoid finite-size effects, namely, \(\eta = 0.1\) and 0.05, and set \(W_0 = \pi / 2\) [cf. \(\omega_1\) of Eq. (45)]. We used MPS dimensions of \(m_{\text{CV}} = 1000\) or \(m_{\text{CV}} = 32\) for CV or CheMPS calculations, respectively. (Our choice for \(m_{\text{CV}}\) aimed for achieving highly accurate CV results; for \(\eta = 0.05\), this required \(m_{\text{CV}} = 1000\), but for \(\eta = 0.1\), a slightly smaller value for \(m_{\text{CV}}\) would have sufficed.) We find excellent agreement between the two approaches without adjusting any free parameter since \(N\) is fixed by (48). For example, for \(\eta = 0.05, N = 255\), the relative error is less than 3\% for all \(\omega\).

Since this level of agreement is obtained using \(m_{\text{Che}} \ll m_{\text{CV}}\), we conclude that CheMPS with Lorentz damping gives results,
the accuracy of which is comparable to those of CV, at dramatically reduced numerical cost. Indeed, for $\eta = 0.05$, the calculation of the entire CheMPS spectral function was 25 times faster than that of a single CV data point and took up 21 hours on a 2.6-GHz single-core Opteron CPU.

**C. Finite-size effects**

Let us now analyze the role of finite system size. To this end, it is, of course, important to understand broadening effects in detail. The fact that CheMPS offers simple and systematic control of broadening via the choice of the expansion order (and damping factors), as will be illustrated below, is very convenient and may be regarded as one of its main advantages.

Figure 5(a) shows CheMPS results for the spin structure factors $S(k,\omega)$ of four different momenta $k$, calculated for $L = 100$ using Jackson damping. They were reconstructed using the largest expansion order, say $N_L$, that does not yet resolve finite-size effects, a choice that will be called optimal broadening. Each curve shows a dominant peak, and we are interested in finding its intrinsic shape $S^{\text{int}}(k,\omega)$ in the continuum limit of an infinitely long chain ($L \to \infty$). Thus, the following general question arises: Under which conditions will a spectrum calculated for finite system size $L$ and reconstructed with finite expansion order $N$, say, $S_N^L(\omega)$, correctly reproduce the desired continuum spectrum $S^{\text{int}}(\omega)$? The general answer, of course, is that the optimally broadened spectrum should have converged as a function of $L$, i.e., the shape of $S_N^L(\omega)$ should not change upon increasing $L$. However, for a spectrum with an intrinsic divergence, such as Eq. (46), the peak’s height will never saturate with $L$; at best, one can hope to observe $L$ convergence of the shape of its tail and the proper scaling of its height Eq. (47).

To illustrate the nature of finite-size effects and the role of $N$ in revealing or hiding them, Fig. 5(b) shows $S(\pi,\omega)$ for $L = 100$ and several values of $N$, both smaller and larger than $N_L$. As $N$ is increased and the effective broadening $\eta_N \simeq \mathcal{O}(W_L/N)$ decreases, the main peak of the initially very broad and smooth spectral function becomes sharper. Optimal broadening in Fig. 5(b) corresponds to $N_L \simeq 70$, beyond which additional “wiggles” emerge. These develop, with beautifully uniform resolution, into dominant subpeaks as $N$ is increased further. The discrete subpeaks reflect the quantized energies of spin-wave excitations in a finite system. With sufficiently high resolution [$N = 999$ in Fig. 5(b)], numerous additional minor subpeaks emerge, but their weight is very small compared to that of the dominant subpeaks. This fact is important since it implies that the structure factor of a finite-size system is exhausted almost fully by the set of dominant subpeaks, with very small intrinsic widths.

We have checked that there are $\mathcal{O}(L)$ dominant subpeaks within the spectral bandwidth of $S(k,\omega)$. Correspondingly, the average spacing between dominant subpeaks, to be called the finite-size energy scale $\omega_L$, is proportional to $1/L$ [Figs. 5(c) and 5(d)]. The weight of each subpeak decreases similarly, ensuring that the total weight in a given frequency interval converges as $L \to \infty$. The inverse subpeak spacing $\hbar/\omega_L$ corresponds to the Heisenberg time, i.e., the time within which a spin-wave packet propagates the length of the system.

Figures 5(e) and 5(f) illustrate two slightly different broadening strategies. In Fig. 5(e), $L$ is increased for fixed $N$: the distinct subpeaks increasingly overlap, resulting in a smooth spectral function once $\omega_L$ drops below $\eta_N$. In Fig. 5(f), optimal broadening is used ($\eta_N$ just larger than $\omega_L$; now, no subpeaks are visible and the $L$ evolution of the main peak is revealed with better resolution).

In both Figs. 5(e) and 5(f), the peak height shows no indications of converging with increasing $L$. [The same is true for the data of Fig. 5(a).] This reflects the intrinsic divergence of the peak height expected from Eq. (46). Figures 6(a) and 6(b) contain a quantitative analysis of this divergence for $S(\pi,\omega)$ and $S(\pi/2,\omega)$, respectively. The shape of the divergences for an infinite system are shown by the thick solid lines, representing exact Bethe ansatz results from Ref. 38. Thin dashed lines show results from tDMRG from Ref. 22 for $L = 100$, and thin solid lines show CheMPS results for several system sizes between $L = 50$ and 300. For CheMPS spectral reconstruction, we determined the expansion order $N_{300}$ that ensures optimal broadening for $L = 300$, and used a fixed ratio of $N/L = N_{300}/300$ for all curves [namely, 0.42 or 0.67 for Figs. 4(a) and 4(b), respectively]. CheMPS (for $L = 300$) and tDMRG reproduce the peak’s tail and flank well, but clearly and expectedly are unable to produce a true divergence at the lower threshold frequency. Nevertheless, the insets show that the manner in which the CheMPS peak heights increase with $L$ is indeed consistent with Eq. (46). (For the limited range of available system sizes, however, a reliable distinction between $L\ln(L))^{1/2}$, $[L\ln(L)]^{1/2}$, or $L$ behavior is not possible.)

It is also possible to determine the lower threshold frequency $\omega_L$ rather accurately from the CheMPS results by doing an $1/L$ extrapolation. We illustrate this in 6(b) by extrapolating...
the frequencies at which \( S(\pi/2,\omega) = 0.1 \) (triangles). Since the data exhibit a slight curvature when plotted against \( 1/L \) [see lower inset of 6(b)], they were fitted using a second-order polynomial in \( 1/L \). Extrapolating the fit to \( 1/L = 0 \) yields \( \omega\eta = 0.496\pi \) (marked by a square), in good agreement with the prediction \( \omega\eta = \pi/2 \) from Eq. (45).

D. Discrete representation of spectral function

In both Figs. 5(f) and 6, the right flank of the peak still bears signatures of overbroadening: the curve for a given \( L \) lies above those for larger \( L \) (before bending over toward its peak), and all curves lie significantly above the exact Bethe ansatz curve (dashed line). One way of reducing this broadening would be to simply increase \( L \), but this is numerically costly. Clearly, alternative strategies for reducing finite-size effects would be desirable. One such scheme, involving linear prediction in the time domain, will be discussed in the next subsection. Here, we present another scheme, which exploits the ability of CheMPS to accurately resolve finite-size peaks.

The origin of overbroadening is clear: When neighboring subpeaks are broadened enough to overlap, weight is inevitably transferred from large peaks to smaller peaks. This effect is negligible only in the limit \( L \to \infty \), where the subpeak spacing becomes negligible. To avoid overbroadening for a finite-\( L \) system, one thus has to analyze spectra for which \( N \) is large enough that subpeaks do not overlap significantly, such as that shown in Fig. 5(b).

To be concrete, let us represent the true, discrete spectrum of a system of size \( L \) by a sum of peaks, enumerated by a counting index \( \alpha \), with position \( \Omega_\alpha \), width \( \eta_\alpha \), weight \( W_\alpha \), and Gaussian shape \( K^J \) [cf. Eq. (18a)]:

\[
S^J(k,\omega) \simeq \sum_\alpha W_\alpha K^J_{\eta_\alpha}(\omega - \Omega_\alpha). \tag{49}
\]

Its Chebyshev reconstruction with Jackson damping, say, \( S^J(k,\omega) \), will have the same form, except that the peaks will be broadened to have widths \( \eta_\alpha = (\eta_\alpha^2 + \eta^{S,J}_{\alpha,\alpha})^{1/2} \) as explained before Eq. (19). If \( N \) is large enough, the broadened peaks will
The discrete peaks suggest a natural partitioning of the frequency spectrum into intervals \( I_\alpha \): Each contains one peak of weight \( W_\alpha \) at position \( \Omega_\alpha \), extends halfway to the next peaks at \( \Omega_{\alpha+1} \) on either side, and has width \( \Delta_\alpha = (\Omega_{\alpha+1} - \Omega_\alpha)/2 \). The first interval above the lower spectral threshold \( (\omega_1) \) is defined slightly differently: \( I_1 \) has lower bound \( \omega_1 \) and width \( \Delta_1 = (\Omega_1 + \Omega_2)/2 - \omega_1 \).

Now, to produce a smooth curve devoid of finite-size effects, the subpeaks must be broadened until they overlap substantially. However, if the weights in two neighboring intervals differ, say, \( W_\alpha > W_{\alpha+1} \), such broadening inevitably transfers weight from interval \( I_\alpha \) to \( I_{\alpha+1} \), resulting in overbroadening.

Such overbroadening can be avoided by constructing a discrete representation of the spectral function \( S_{\text{dis}}(k, \Omega_\alpha) \), defined by the set of coordinates

\[
\{(\Omega_\alpha, S_\alpha) \mid S_\alpha = S_{\text{dis}}(k, \Omega_\alpha) = W_\alpha/\Delta_\alpha . \}
\]

The identification of \( S_\alpha \) with \( W_\alpha/\Delta_\alpha \) follows from applying the definition of a spectral function, namely, spectral weight per unit frequency interval, to the interval \( I_\alpha \).

Figure 7 shows the resulting discrete data points for four different system sizes. Remarkably, they all fall onto the same curve, which agrees well with the Bethe ansatz result (dashed line). In particular, the first two or three data points for each \( L \) lie right on top of the Bethe ansatz curve [dashed line, see Fig. 7, left inset], beautifully mapping out the true shape of the spectral function down to the lowest discrete excitation frequency \( \Omega_\alpha \) that exists for that \( L \). Evidently, the discrete spectral function is completely free from broadening artifacts, in marked contrast to the optimally

still be clearly separated (as for \( N = 999 \) or 250 in Fig. 5). By fitting each peak (separately, one by one) to a Gaussian, one can determine its position \( \Omega_\alpha \), weight \( W_\alpha \), and effective width \( \eta_\alpha \) and deduce the intrinsic width via \( \eta_\alpha = (\eta_0^2 - \eta_{\Omega,\alpha}^2)^{1/2} \). We find (not shown) that the intrinsic width grows with increasing frequency \( \Omega_\alpha \). This implies, not unexpectedly, that higher-lying spin-wave excitations have shorter lifetimes. However, it also implies that higher-lying peaks eventually start to overlap, so that the analysis to be described below is feasible only for a limited number of low-lying peaks.

FIG. 6. (Color online) Comparison of CheMPS, Bethe ansatz, and tDMRG + prediction for HAFM structure factors with (a) \( k = \pi \) and (b) \( k = \pi/2 \). Dashed lines: Bethe ansatz results for \( L = \infty \), from Ref. 38. Dashed-dotted lines: tDMRG results, from Ref. 22. Other lines show CheMPS results for \( L = 50, 100, 200, \) and 300, reconstructed using a fixed ratio of \( N/L \), namely, 0.42 for (a) and 0.67 for (b). Circles mark Chebyshev peak maxima, also for \( L = 66, 150, \) and 250, for which no curves are shown. The lower inset in (a) zooms into the peak region using a linear scale, illustrating overbroadening. The upper insets of (a) and (b) show the peak heights vs \( L \), together with a fit to the Bethe ansatz expectation from Eq. (46) (dashed line) or to a straight line (solid line). In (b), triangles mark Chebyshev peak maxima, also for \( L = 50, 100, 150, \) and 250, for which no curves are shown. The lower inset in (a) zooms into the peak region using a linear scale, illustrating overbroadening.

FIG. 7. (Color online) Discrete representation [Eq. (50)] of the structure factor \( S_\alpha = S_{\text{dis}}(k, \Omega_\alpha) \) (symbols) for five different system sizes. (The lower panel uses an enlarged vertical scale to zoom in on the tail region.) For comparison, the Bethe ansatz result (dashed line) and two optimally broadened spectra, for \( L = 400 \) and 200 (solid lines), are also shown. Left inset: Zoom to low frequencies, showing that the discrete data completely avoid overbroadening, in contrast to the optimally broadened spectra. Right inset: The log-log version of main plot. The frequency range does not extend low enough to be able to uncover the pure asymptotic predicted by Eq. (46b).
broadened curves shown for \( L = 200 \) and 400 (solid lines) [compare also Fig. 5(f)]. This advantage comes at the price of specifying the spectral function only at discrete points, not via a continuous curve. However, for a system of finite size, such discreteness is fundamentally unavoidable. The good news is that the continuum curve \( S(\pi/2, \omega) \) is evidently well mimicked by the discrete representation \( \{\Omega_{\omega}, S_{\omega}\} \), and that CheMPS allows the latter to be determined in a straightforward fashion for system sizes well beyond what can be done with exact diagonalization. We are not aware of any other numerical many-body method capable of doing so for system sizes as large as those considered here.

For larger frequencies, the scatter of the discrete data w.r.t. the Bethe ansatz curve increases, reflecting the fact that sub-peaks begin to overlap there, making the extraction of discrete data increasingly difficult. However, this is not a serious concern since, in this frequency regime, optimal broadening is able to produce smooth spectra in good agreement with Bethe ansatz anyway.

To conclude this subsection, let us summarize the two main results of our finite-size analysis. The first concerns physics: For a chain of finite chain of \( \mathcal{O}(L) \) sharp sub-peaks, the spacing and weight of which scale as \( 1/L \). The second concerns methodology: CheMPS very conveniently allows this structure to be revealed or hidden by simply choosing \( N \) appropriately. Moreover, it can exploit information on the positions and weights of the discrete sub-peaks to largely eliminate broadening artifacts.

E. Comparison of tCheMPS to tDMRG

Another possible scheme for reducing finite-size effects is to work in the time domain using linear prediction, as shown in Ref. 22 for the HAFM. The idea is to calculate the Fourier transform of \( S(k, \omega) \), namely,

\[
S(k, t) = \sum_{x=1}^{L} e^{ik(x-x')} \langle \hat{S}_x(t) \hat{S}_{x'}(0) \rangle ,
\]

with \( x' \) chosen near the middle of the chain and \( t \) chosen small enough that the spin excitation created at \( x' \) does not reach the edge of the system within \( t \). The function \( S(k, t) \) thus obtained will contain only weak finite-size effects. It is then extrapolated to larger times via linear prediction techniques,\(^{19-22}\) exploiting the fact that momentum excitations typically exhibit damped harmonic dynamics, the time dependence of which can be extrapolated quite accurately. Since the extrapolated function extends to very large times, its Fourier transform yields good spectral resolution at low frequencies\(^{19}\) (with an accuracy that depends on that achieved during linear prediction).

In Ref. 22, the input correlator needed for linear prediction, \( S(k, t) \), was calculated using tDMRG. (Two examples of the resulting spectra are included in our Fig. 6.) We note that \( S(k, t) \) can also be calculated using CheMPS in the time domain, to be called tCheMPS. Indeed, the numerical cost for calculating \( S(k, t) \) by evaluating the requisite correlators \( \langle \hat{S}_x(t) \hat{S}_{x'}(0) \rangle \) via Eq. (28) is essentially the same as calculating its Fourier transform \( S(k, \omega) \) via Eq. (23) since the corresponding Chebyshev moments \( \mu_p \) can be calculated using the same recursion scheme. In fact, if one defines \( \hat{S}_x \) in Eq. (43) using a pure exponential \( e^{ix} \) instead of a sin function, the Chebyshev moments needed for \( S(k, t) \) are simply linear combinations of those of \( S(k, \omega) \).

To gauge the accuracy of tCheMPS, we have calculated \( S(\pi/2, t) \) using both tCheMPS and tDMRG. Figure 8(a) compares the results, and 8(b) characterizes the differences. We view the tDMRG results as benchmark because, for the times of interest, we have checked them to be well converged [with errors \( \lesssim 10^{-3} \) for \( t < 50 \), see 8(b), dashed-dotted line]. As expected, the agreement between tCheMPS and tDMRG is better for larger \( m \). The differences are very small, but grow with time, from being (for \( m = 64 \) below \( 10^{-3} \) for \( t \lesssim 10 \) to around \( 10^{-2} \) for \( t \simeq 30 \), beyond which finite-size effects start to appear.

More generally, the results of Fig. 8 illustrate that CheMPS offers a viable route to time evolution for situations where extreme accuracy is not required. Further comments on this prospect are included in the outlook, Sec. VII.

V. ERROR ANALYSIS

The convergence properties of a Chebyshev expansion are mathematically well controlled and understood [see Eq. (14)], provided that the Chebyshev moments \( \mu_p \) are known precisely. Their evaluation via CheMPS, however, introduces various sources of numerical errors. This section is devoted to an analysis of these errors. In particular, we seek to determine appropriate choices for the control parameters associated with the various CheMPS tasks listed in Table 1. We perform this analysis mostly for a resonant level model (RLM), describing three local levels coupled to a fermionic bath. This model is introduced and discussed in the Appendix, which, for the sake of completeness, also includes CheMPS expansions of the corresponding spectral functions. However, the details presented there are not needed for the following discussion.
For the RLM, on the one hand, the CheMPS evaluation of the \( \mu_n \) is feasible to arbitrarily high orders, and on the other, exact diagonalization (to be denoted by subscript or superscript ED) of the single-particle Hamiltonian allows both the spectral function and the Chebyshev moments \( \mu_n \) to be found exactly. We use the RLM parameters specified in the Appendix throughout and focus mainly on the properties of one of its correlators \( A_{ij} \) (without displaying corresponding subscripts and superscripts), which is defined in Eq. (A2) and the behavior of which is representative for that of \( A_{ij} \).

A. Definition of error measures

We will analyze both \( \mu_n \) and \( \bar{\mu}_n \) moments, calculated from Eqs. (25) and (34), respectively. The differences between CheMPS and ED can be quantified by the error measures

\[
\delta_n^{\text{ED}} = |\mu_n^{\text{CheMPS}} - \mu_n^{\text{ED}}|, \quad n < N_{\text{max}} \\
\delta_n^{\text{ED}} = |\bar{\mu}_n^{\text{CheMPS}} - \bar{\mu}_n^{\text{ED}}|, \quad n < 2N_{\text{max}}.
\]

Moreover, to characterize the accuracy of CheMPS moments without referring to exact results, we also consider

\[
\delta_n^{\text{Che}} = |\mu_n^{\text{CheMPS}} - \bar{\mu}_n^{\text{CheMPS}}|, \quad n < N_{\text{max}}.
\]

We will also use cumulative versions of these, namely,

\[
\Delta^{\text{ED}} = \sqrt{\sum_{n=0}^{N_{\text{max}}-1} (\delta_n^{\text{ED}})^2}, \quad (53a)
\]

\[
\bar{\Delta}^{\text{ED}} = \sqrt{\Delta^{\text{ED}}^2 + \sum_{n=N_{\text{max}}}^{2N_{\text{max}}-1} (\delta_n^{\text{ED}})^2}. \quad (53b)
\]

\[
\bar{\Delta}^{\text{Ch}} = \sqrt{\sum_{n=0}^{N_{\text{max}}-1} (\delta_n^{\text{Che}})^2}. \quad (53c)
\]

Furthermore, we also introduce an integrated error measure for undamped spectral functions (using Jackson damping would yield qualitatively similar error measures):

\[
\Delta^A = \sqrt{\int_0^\infty d\omega A^2(N_{\text{max}}) - A^2(\infty)^2}. \quad (54)
\]

Here we use \( \pm \) for \( A^2(\pm\omega) \) spectra proportional to \( \theta(\pm\omega) \) [see Eq. (A2)] and employ \( \mu_n \) moments for \( n < N_{\text{max}} \) and \( \bar{\mu}_n \) moments for \( N_{\text{max}} < n < 2N_{\text{max}} \), during spectral reconstruction. [Note that \( \Delta^{\text{ED}} \) of Eq. (53b) was constructed to reflect this combination of \( \mu_n \) and \( \bar{\mu}_n \).]

B. Comparison of CheMPS and ED moments

Figure 9 contains the results of our comparison of CheMPS and ED moments for a fixed set of CheMPS parameters, stated in the figure legend. Figures 9(a) and 9(b) show Chebyshev moments \( \mu_n \) and \( \bar{\mu}_n \) and Figs. 9(c) and 9(d) show the \( n \)-dependent error measures \( \delta_n^{\text{ED}} \), \( \delta_n^{\text{Che}} \), and \( \delta_n^{\text{Che}} \). From Fig. 9(c), we note several points: (i) For \( n \leq N_{\text{max}} \), the \( \mu_n \) moments from CheMPS and ED agree to within about 1%; this illustrates that CheMPS is able to generate rather accurate results for several hundred moments at modest computational costs. (ii) \( \mu_n \) moments are more accurate than \( \bar{\mu}_n \) moments; the reason is that each \( \mu_n \) moment depends on only one Chebyshev vector, whereas each \( \bar{\mu}_n \) moment depends on two.

FIG. 9. (Color online) Comparison of CheMPS and ED results for Chebyshev moments of the RLM spectral function \( A^{ij} \). (a), (b) show \( \mu_n \) and \( \bar{\mu}_n \) moments [Eqs. (25) and (34)] and (c), (d) show the \( n \)-dependent error measures \( \delta_n^{\text{ED}} \), \( \delta_n^{\text{Che}} \), and \( \delta_n^{\text{Che}} \) [Eqs. (52)], plotted in (a), (c) for \( n < N_{\text{max}} = 200 \) and in (b), (d) for \( N_{\text{max}} < n < 2N_{\text{max}} \). In (b), the increase in moment magnitude starting around \( n \approx 250 \) marks the onset of resolving finite-size structure in the spectral function. (e), (f) show the cumulative error measures \( \Delta^{\text{ED}} \), \( \Delta^{\text{Che}} \), \( \bar{\Delta}^{\text{Che}} \) [Eqs. (53)], and \( \Delta^A \) [Eq. (54)] for various combinations of the MPS dimension \( m \), the number of energy truncation sweeps \( n_s \), and the Krylov subspace dimension \( d_K \).
[Note, though, that if spectral reconstruction is performed by employing both \[\text{Eq. (41)}\], as functions of recursion number \(N\), but \(\Delta'_{\text{tr}}\) more strongly so since recurrence fitting is a strictly variational procedure, whereas energy truncation is not. (b) \(\Delta'_{\text{tr}}\) as function of \(n\) and (c) the average truncated weight per site \(\Delta_w^{\text{sweep}}\) (for \(n = 20\)) as function of truncation sweep number \(k\). Both (b) and (c) show results for four choices of Krylov subspace dimension \(d_K\), the \(d_K\) dependence of which saturates beyond \(d_K = 30\).

C. Errors induced by recurrence fitting and energy truncation

To better understand the error dependence on \(m, d_K\), and \(n_S\) observed in points (iv) to (vi) of Sec. V B above, let us analyze in more detail the errors generated during recurrence fitting (Sec. III A) and the energy truncation (Sec. III B). The error incurred when constructing \(|t_n\rangle\) from \(|t_{n-1}\rangle\) and \(|t_{n-2}\rangle\) using recurrence fitting is characterized by the relative fitting error \(\delta_{n_{\text{fit}}} = \Delta_{n_{\text{fit}}} / \| |t_n\rangle \|^2 \) [Eq. (31)]. The effect of projecting out high-energy states using energy truncation \(|t_n\rangle \rightarrow P_k |t_n\rangle\) can be characterized by the average truncated weight per site during one truncation sweep \(\Delta_w^{\text{sweep}}\) [Eq. (40)], and by the relative truncation-induced state change \(\Delta'_w = \Delta_{w_{\text{tr}}} / \| |t_n\rangle \|^2 \) [Eq. (41)]. The latter measures intended changes in the state due to the truncation of high-energy weight, but also incorporates the effects of unavoidable numerical errors.

These quantities are analyzed in Fig. 10 in dependence on \(m, d_K\), and \(n_S\). Continuing our list of observations from the previous subsection, we note the following additional features: (vii) Both \(\Delta_{n_{\text{fit}}}^{\text{tr}}\) and \(\Delta'_w\) are smaller than 1% already for \(m = 32\) [Fig. 10(a)], in accord with similar error margins for \(\delta_{n \text{ED}}\) in Fig. 9(c). (viii) Both \(\Delta_{n_{\text{fit}}}^{\text{tr}}\) and \(\Delta'_w\) decrease with increasing \(m\), but \(\Delta'_w\) does so more slowly, and its decrease seems to saturate beyond \(m = 64\). This implies that \textit{energy truncation is the main limiting factor for CheMPS}. The reason is that the intended purpose of energy truncation, namely, to strip \(|t_n\rangle\) from its high-energy components, modifies it in a way so that the errors can not be reduced to arbitrarily small values. Indeed, this is illustrated by the following two points: (ix) While both \(\Delta_{n_{\text{fit}}}^{\text{tr}}\) and \(\Delta'_w\) initially decrease with increasing Krylov subspace dimension \(d_K\), the decrease saturates for \(d_K \gtrsim 30\) [Figs. 10(b) and 10(c)]. (x) While \(\Delta'_w\) initially decreases with the number of sweeps \(n_S\), the decrease saturates already for \(n_S \lesssim 10\) [Fig. 10(c)]. Qualitatively, the behavior shown in Fig. 10(c) is robust. (However, the choices of other CheMPS control parameters do influence its quantitative...}
details, such as the $d_K$ beyond which $N_{\text{sweep}}^*$ becomes $d_K$ independent. The lack of saturation of $N_{\text{sweep}}^*$ with $n_g$ implies that there is no automatic stopping criterion for truncation sweeps. Instead, the choice of $n_g$ can be optimized as described in Sec. V B, where we already concluded that taking $n_g$ much larger than 10 actually deteriorates the results.

When no exact results are available for comparison, the only relevant error measures among all those listed in Eqs. (52) and (53) are $\delta^\text{Ch}$ and $\Delta^\text{Ch}$. Nevertheless, Figs. 9(a)–9(d) show that these measures provide a reasonable estimate of the actual errors compared to the exact solution since the magnitudes of $\delta^\text{Ch}$ and $\Delta^\text{Ch}$ are comparable. Moreover, Figs. 9(e) and 9(f) show that the cumulative error measures $\Delta^\text{Ch}$ and $\Delta^\text{ED}$ reveal the same trends for their dependence on CheMPS parameters such as $d_K$ and $n_g$. Hence, $\delta^\text{Ch}$ and $\Delta^\text{Ch}$ may be used as measures for optimizing CheMPS parameters and estimating the errors of the final results.

Of course, truncation-induced errors can be avoided by simply using the full bandwidth $W_e = W$, for which no truncation is necessary. However, in our experience, the gain in resolution obtained by using, instead, an effective bandwidth $W_e \ll W$ outweighs the small loss in accuracy incurred by the necessity to then perform energy truncation.

VI. DENSITY MATRIX SPECTRA

The effects of energy truncation can be understood in more detail by considering the reduced density matrix

$$\rho_n = \text{Tr}_{\text{aux}}[|n\rangle\langle n|],$$

(55)

where the trace is over one half of the chain. Let us analyze the $n$ dependence of the spectrum of its eigenvalues, say, $\rho_n(i)$. It can be used to quantify the entanglement encoded in $|n\rangle$ via the associated entanglement or bond entropy

$$S_n^{\text{b}} = -\sum_i \rho_n(i) \ln[\rho_n(i)].$$

(56)

Figure 11 shows such density matrix spectra for both the RLM [panels (a) and (b)] and the HAFM [panels (c) and (d)] calculated using both the full many-body bandwidth $W_e = W$ [panels (a) and (c)] and a smaller effective bandwidth $W_e$ [panels (b) and (d)]. The $n = 0$ line in all panels shows the eigenvalue spectrum $\rho_0(i)$, which reflects the entanglement encoded in $|0\rangle = \hat{C}|0\rangle$ at the start of the recursion procedure. In principle, one would expect the entire spectrum of density matrix eigenvalues $\rho_n(i)$ to shift or rise to higher values as $n$ increases since multiplying $|n\rangle$ by $\hat{H}$ when calculating $|n\rangle$ [cf. Eq. (30)] generates entanglement entropy. Such a spectral rise with increasing $n$ is indeed observed in all four panels of Fig. 11, but the rise eventually saturates for sufficiently large $n$. The speed of the initial stages of the rise differs from panel to panel. For the density matrix spectra calculated without energy truncation [Figs. 11(a) and 11(c)], the initial rise is rather slow, in particular for the RLM [11(a), where the rise is preceded by a slight initial decrease], reflecting the lack of strong correlations of this model. In contrast, for density matrix spectra calculated with energy truncation [Figs. 11(b) and 11(d)], the initial rise is very rapid, and its subsequent saturation sets in at quite small $n$ (of order 20 to 30). Thus, energy truncation evidently has the effect of increasing entanglement entropy. The reason is that the latter is calculated in a different basis (the eigenbasis of $\rho_n$) than that used to perform energy truncation (the local eigenbasis of $\hat{H}'$).

According to 11(d), the small MPS dimension of $m = 32$ used for the HAFM in Fig. 5(a) in effect amounts to discarding the contributions to the reduced density matrix of all states with weight below a threshold of around $10^{-3}$. This threshold is rather large compared to typical DMRG calculations, where characteristic truncation errors lie in the range $10^{-6}$ to $10^{-8}$. It is remarkable that CheMPS is nevertheless able to give rather accurate results (such as reproducing CV results obtained using $m_{\text{CV}} = 1500$).

This efficiency appears to be an intrinsic feature of CheMPS, arising from the recursive manner in which the Chebyshev vectors $|n\rangle$ are constructed. Evidence for this conclusion is presented in Fig. 12(a), which shows the bond entropy $S_n^{\text{b}}$ associated with $|n\rangle$ as a function of recursion number $n$. Remarkably, the bond entropy shows no tendencies toward unbounded growth, even up to values as large as $n = 2000$. Quite to the contrary, although the bond entropy increases somewhat when increasing $m$ from 32 to 128 (with $W_e = 6.3$), for either case it tends to decrease with recursion number $n$, and similarly for the choice $W_e = W$ without energy truncation. All of this is very encouraging since it indicates that $n$ can be increased, apparently at will, without incurring any runaway growth of DMRG truncation errors. The reasons for this fact will be recapitulated in the summary below.

For comparison, Fig. 12(b) shows the bond entropy $S_n^{\text{b}}$ of a TDMRG calculation of the time evolution of $|\psi(t)\rangle = e^{-i\hat{H} t} |\psi(0)\rangle$. This entropy is, overall, smaller than the $S_n^{\text{b}}$ of the Chebyshev vectors because the initial state for the time evolution involves an excitation at only one site, whereas the starting state for the CheMPS recursion involved a linear combination of local excitations $\hat{S}_k|0\rangle$ [see Eq. (43)]. The most striking difference between $S_n^{\text{b}}$ and $S_n^{\text{b}}$, however, is that the former shows no trend to increase with $n$, whereas...
the dotted line is from a calculation with a reduced $m$ vectors $|v\rangle$ be necessary. (b) $S$ is Chebyshev expansion and MPS technology. To summarize dimensional quantum lattice models using a combination of for calculating zero-temperature spectral functions of one-

the latter does with $t$. The increase in $S^b$ occurs in spurts, which happen each time a spin wave gets reflected from one of the ends of the system, at which point more numerical resources are required to keep track of the superposition of the ends of the system, after which the increase in $S^b$ is lost due to truncation. The red arrow marks the expansion order roughly necessary to reach the time $t = 85$ using the $t$CheMPS technique for $W = 6.3$; here $N_{c,35} = 271$. To reach the same time using $W_s = W = 68.8$, an order of expansion of $N_{c,35} = 2961$ would be necessary. (b) $S^b$ is shown for two choices of the truncation error $\epsilon_p$. 

the increase in $S^b$ was not severe and remained completely under control (staying below $S^b$ throughout). Nevertheless, we do believe that the contrast between Figs. 12(a) and 12(b), showing a nonincreasing trend for $S^b$ versus an increasing trend for $S^b$, is striking and significant. It suggests that, for situations that feature strong entanglement growth with time, $t$CheMPS might be a promising alternative to $t$DMRG.

VII. SUMMARY

In this paper, we have described CheMPS as a method for calculating zero-temperature spectral functions of one-dimensional quantum lattice models using a combination of a Chebyshev expansion and MPS technology. To summarize our analysis, we would like to highlight what we believe to be the two most important features of CheMPS, namely, its efficiency and its control of spectral resolution.

Efficiency. The first main feature is that CheMPS provides an attractive compromise between accuracy and efficiency. It is capable of reproducing correction-vector results in the frequency domain and $t$DMRG results in the time domain with comparably modest numerical resources. In particular, surprisingly small values for the MPS dimension of $m$ are sufficient, even for obtaining spectral resolution high enough to resolve finite-size effects in great detail. (For example, $m = 32$ sufficed for the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model.) This remarkable efficiency, which we had not anticipated when commencing this study, appears to be a consequence of several factors: (i) CheMPS does not suffer from a runaway growth of DMRG truncation error with increasing $n$ because the information needed to construct the spectral function with a specified accuracy, say $O(1/N)$, is not encoded in a single state, but uniformly distributed over $N$ distinct Chebyshev vectors $|v\rangle$. (ii) These can be determined from Chebyshev recurrence relations involving only three terms, so that it is never necessary to accurately represent the sum of more than two MPS. (iii) Moreover, these recurrence relations are numerically stable, i.e., the inaccuracies in the calculation of Chebyshev vectors $|v\rangle$ do not cause the Chebyshev expansion to diverge. (iv) Finally, the accuracy needed for each $|v\rangle$ is set by that needed for $W_s = W_{1,2}$ using the $t$CheMPS technique for $W = 6.3$; here $N_{c,35} = 271$. To reach the same time using $W_s = W = 68.8$, an order of expansion of $N_{c,35} = 2961$ would be necessary. (b) $S^b$ is shown for two choices of the truncation error $\epsilon_p$.

For spectral functions with a finite spectral width $W_s$ (which is typically much smaller than the many-body bandwidth $W$), CheMPS offers a further attractive feature for enhancing efficiency: one may use an “effective bandwidth” $W_s$ of order $W_s$ (we typically take $W_s = 2W_s$), which enhances spectral resolution by a factor $W/W_s$, at the cost of requiring additional energy truncation sweeps. The latter are not necessary if one takes $W_s = W$, but then considerably higher expansion orders are necessary to achieve comparable resolution. In our experience, the benefits of enhanced resolution offered by the choice $W_s = 2W_s$ outweigh the costs of energy truncation.

Control of spectral resolution. The second main feature of CheMPS is that it offers very convenient control of the accuracy and resolution of the resulting spectral function by simply adjusting the expansion order $N$. This is particularly useful for studying finite-size effects, as exemplified in Fig. 5. On the one hand, Fig. 5(b) shows very strikingly that the structure factor of an HAFM chain of finite length is dominated by a set of discrete subpeaks, which may be associated with the quantized eigenenergies of spin-wave excitations in a finite system. CheMPS allows the energies and weights of these excitations, and their dependence on $L$, to be determined with unprecedented accuracy and ease by simply increasing $N$ until the peaks are well resolved. On the other hand, Fig. 5(f) shows that the limit $L \to \infty$ may be mimicked by choosing $N$ just small enough that the finite-size subpeaks are smeared out. Although the peak shape thus obtained is slightly overbroadened [see inset of Fig. 5(f)], this overbroadening can be eliminated completely (see Fig. 7) by using a discrete representation of the spectral function that uses the energies...
and the weights of the discrete subpeaks as input. The ability to fully eliminate over-broadening effects even for very large many-body systems is, to the best of our knowledge, a unique feature of CheMPS.

On a technical level, the implementation of CheMPS requires only standard MPS techniques, such as the addition of different states and the multiplication of operators. For energy truncation, single-site sweeping needs to be set up with a new kind of local update, as described in III B. However, this procedure is not too different from other known local update prescriptions and can be implemented with modest programming effort.

VIII. OUTLOOK

Regarding future applications of CheMPS, two directions for further methodological development appear particularly promising, namely, time dependence and finite temperature. A few comments are due about each.

Time dependence. While the good agreement between tCheMPS and tDMRG reported in 8 is encouraging, a detailed analysis of tCheMPS should be performed to understand the nature of its error growth with time, and to explore under which conditions, if any, tCheMPS offers competitive advantages relative to tDMRG. On the one hand, tDMRG has the advantage that highly efficient Krylov methods can be used to optimize the evaluation of $e^{-i\hat{H}t}\ket{\psi(t)}$ w.r.t. the state $\ket{\psi(t)}$ being propagated; however, its numerical costs increase rapidly if $\ket{\psi(t)}$ contains a broad spectrum of excited states. On the other hand, CheMPS has the advantage (i) that the Chebyshev expansion of the operator $e^{-i\hat{H}t}$ can be applied with equal accuracy to every state in the Hilbert space, in particular, also highly excited ones. Moreover, (ii) very large evolution times might be achieved more easily with tCheMPS than tDMRG since the former represents $\ket{\psi(t)}$ as a sum over many Chebyshev vectors [see Eq. (6)], thereby being potentially less susceptible than tDMRG to the growth of truncation errors (as discussed in the Introduction, and exemplified in 12). We expect that, for some applications, (i) and/or (ii) may offer advantages for CheMPS over tDMRG, e.g., for calculating quantum quenches starting from strongly nonequilibrium initial states, but leave a detailed investigation to the future.

Finite temperature. The fact that CheMPS uniformly resolves the entire energy spectrum of $\hat{H}$ suggests that it should be particularly suited for calculating the spectral functions $A_T^{BC}(\omega) = \frac{1}{Z} \int d\omega \ e^{-\beta\omega} \rho^{BC}(\omega, \omega + \tilde{\omega})$ (59a) by introducing the density of matrix elements

$$\rho^{BC}(\omega, \omega) = \text{Tr}[\delta(\omega - \hat{H}) \ B \delta(\omega - \hat{H}) \ C] (59b)$$

Then, Chebyshev expand the $\delta$ functions in Eqs. (59b) and (59b) using Eq. (23) (after suitably rescaling Hamiltonian and frequencies). The resulting Chebyshev expansions will contain moments of the form

$$\mu_{nn}^{\omega} = \text{Tr}[\hat{T}_n(\hat{H})], \quad (60a)$$

$$\mu_{nn}^{\omega, \omega}^{\omega} = \text{Tr}[\hat{T}_n(\hat{H}) B \hat{T}_n(\hat{H}) C]. \quad (60b)$$

We now note that this framework is very well suited for an MPO implementation, which would consist of three steps: (i) Using Chebyshev recurrence relations, recursively construct and store MPO representations for each operator $\hat{T}_n(\hat{H})$; we expect (based on our experience with the Chebyshev vectors $|t_n\rangle$) that this should be possible without runaway costs in numerical resources since the construction of $\hat{T}_n(\hat{H})$ requires only $\hat{H}^{\hat{T}_{n-1}}(\hat{H})$ and $\hat{T}_{n-2}(\hat{H})$. (ii) Calculate the moments in Eqs. (VIII) by evaluating the traces, which is straightforward in the context of MPS and MPO. (iii) Insert the resulting moments into the reconstructed Chebyshev expansions for $\rho(\omega)$ and $\rho^{BC}(\omega, \omega)$, and finally evaluate the integrals Eqs. (58a) and (59a). Note the economy of exact diagonalization41,42 and Monte Carlo43 methods, and similar developments have been pursued within the context of exact diagonalization41,42 and Monte Carlo43 methods, and Chebyshev expansions should also be useful in combination with tensor network methods for two-dimensional quantum lattice models.

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Appendix: Resonant Level Model

This appendix introduces the fermionic resonant level model that was used for the error analysis of Sec. V and presents CheMPS results for its spectral functions. The RLM is defined by the following Hamiltonian:

\[ \hat{H}_{RLM} = \sum_{i=1}^{n_d} \varepsilon_i \hat{d}_i^{\dagger} \hat{d}_i + \sum_{i=1}^{n_d} \lambda_i \sum_{k=1}^{L_b} (\hat{d}_k^{\dagger} \hat{c}_k + \text{H.c.}) + \sum_{k=1}^{L_b} \varepsilon_k \hat{c}_k^{\dagger} \hat{c}_k. \]  

(A1)

It describes a set of \( n_d \) discrete, “local” noninteracting fermion levels with energies \( \varepsilon_i \) that hybridize with strengths \( \lambda_i \) with a band of \( L_b \) fermion levels with energies \( \varepsilon_k \) assumed uniformly spaced within the interval \([−W_b, W_b]\). We choose \( W_b = 1 \) as unit of energy throughout this section. We will parametrize the hybridization strengths \( \lambda_i \) in terms of the associated level widths \( \Gamma_i = \pi \frac{\lambda_i}{L_b} V^2 \).

The spectral function \( A_{ij}(\omega) \equiv A_{ij}^+(-\omega) + A_{ij}^{-}\) has two contributions,

\[ A_{ij}^+(\omega) \equiv A^{d_j^{\dagger} d_i}(\omega), \quad A_{ij}^{-}(\omega) \equiv A^{d_i d_j}(\omega), \]  

(A2)

describing particle and hole excitations, which, at \( T=0 \), are proportional to step functions \( \delta(\pm \omega) \) that vanish for \( \omega < 0 \) or \( > 0 \), respectively. Since the RLM Hamiltonian is quadratic, the problem can be solved by diagonalizing the single-particle problem. In the continuum limit \( L_b \to \infty \), this yields the following exact expression for the spectral function \( A_{ij}^{-}\) for \( \omega < D_b = 1 \):

\[ A_{ij}^{-}(\omega) = \lim_{\eta \to 0^+} -\frac{1}{\pi} \Im \left( \omega + i \eta - \Gamma_j - \Delta(\omega) \right)^{-1} \delta_{ij}, \]

\[ \Gamma_{ij} = \varepsilon_i \delta_{ij}, \quad \Delta(\omega) = \frac{1}{\pi} \sqrt{\Gamma_i \Gamma_j} \ln \left( \frac{\omega - D_b}{\omega + D_b} \right) - i \pi , \]  

(A3)

where \( \Gamma \) and \( \Delta \) are matrices of dimension \( n_d \times n_d \). The Chebyshev moments \( \mu_n \) for the finite system of length \( L_b \) can also be found exactly by evaluating the expectation values [Eq. (24)], using the (numerically determined) exact single-particle eigenstates of \( \hat{H} \).

The Hamiltonian (A1) corresponds to a “star geometry” since each local level couples to every band level. For the purposes of using CheMPS, however, it needs to be transformed to a “chain geometry” of the form

\[ \hat{H}_{RLM} = \sum_{i=1}^{n_d} \varepsilon_i \hat{d}_i^{\dagger} \hat{d}_i + \sum_{i=1}^{n_d} \frac{2 \Gamma_i}{\pi} (\hat{d}_i^{\dagger} \hat{f}_1 + \text{H.c.}) + \sum_{\ell=1}^{L_b-1} \lambda_{\ell} \hat{f}_\ell^{\dagger} \hat{f}_{\ell+1} + \text{H.c.}. \]  

(A4)

This can be achieved by using Lanczos tridiagonalization of the band part of the Hamiltonian, thereby determining the hopping coefficients \( \lambda_{\ell} \).

Starting from Eq. (A4), we have used CheMPS to calculate the diagonal components \( A_{ij} \) of the RLM spectral function for a model with \( n_d = 3 \) local levels. In contrast to Sec. IV C, our interest here is not in analyzing finite-size effects, but in determining how the CheMPS parameters need to be adjusted to recover the exact continuum function \( A_{ij}^+ \) of Eq. (A3). Thus, we purposefully chose a set of model parameters leading to three well-separated peaks of slightly different widths, taking \( \varepsilon_j \in [-0.5,0.1,0.6] \) and \( \Gamma_j \in [0.04,0.06,0.03] \), and chose the number of band levels \( L_b = 101 \) large enough so that the finite-size spacing \( \omega_{Lb} \simeq 1/L_b = 0.01 \) is somewhat smaller than the smallest peak width \( \Gamma_3 \). By choosing the expansion order for each curve such that the effective broadening lies in the window between the finite-size spacing and the intrinsic peak width \( \omega_{Lb} < \eta N < \Gamma_j \), it should be possible to reveal the shape of \( A_{ij}^+ \) quite accurately without yet resolving finite-size subpeaks (although traces of the latter might show up for \( A_{ij} \), for which this window is small). To this end, we used the following criterion for choosing \( N \) when reconstructing \( A_{ij}^+ \): the effective broadening \( \eta N \) was taken as large as possible without lowering the peak height significantly below that of \( A_{ij}^+ \) (this corresponds to choosing \( \eta N \ll \Gamma_j \)).

The results of these calculations are summarized in Fig. 13; all spectra shown there were obtained by performing separate expansions for the positive and negative branches \( A_{ij}^{-}(\omega) \) (with one exception, noted below).

Figures 13(a1)–13(g1) were calculated using an effective bandwidth of \( W_e = 2.0 \) (with \( \varepsilon_i = 0.025 \)) for each branch, corresponding to roughly twice the spectral width of each branch, which is of order of the single-particle bandwidth \( W_A \simeq W_b = 1 \). For this choice, an MPS dimension of merely \( m = 32 \) was found to suffice for accurate recurrence fitting. Figure 13(a1) illustrates a number of points: (i) By choosing \( \eta N \) according to the above criterion of recovering the correct peak height, excellent agreement with the continuum limit \( A^\infty \) of Eq. (A3) is obtained over most of the frequency range. (ii) This is the case both with and without Jackson damping (thin black or blue lines, respectively), but, with Jackson damping, higher expansion orders are needed to obtain the correct peak heights since Jackson damping induces some artificial broadening [by a factor of \( \eta N \), see Eq. (18a)]. (iii) Small oscillations remain in some frequency ranges [see Figs. 13(b1)–13(g1) for zooms]. These stem from three sources: finite-size subpeaks, numerical inaccuracies, and step-function artifacts near \( \omega = 0 \) [cf. points (iv), (vi), and (viii) below, respectively]. (iv) For the spectrum with the narrowest peak \( A_{33} \), the window between \( \omega_{Lb} \) and \( \Gamma_3 \) is so small that the criterion of reproducing the continuum peak height implies that small finite-size subpeaks remain visible [see Figs. 13(e1)–13(g1) for zooms]. (v) In contrast, such oscillations are almost entirely absent for the broadest peak \( A_{22} \) [see Figs. 13(d1) and 13(e1)] since its width \( \Gamma_2 \) is somewhat larger than \( \omega_{Lb} \).

To illustrate the effect of energy truncation, Figs. 13(a2)–13(g2) show the same spectral functions as Figs. 13(a1)–13(g1), but now setting \( W_e = W_b \), the full many-body bandwidth (here \( = 52.3 \)), so that no energy truncation is needed. This allows us to make some additional instructive observations: (vi) Using the full bandwidth yields results of higher quality, in that numerical artifacts are significantly weaker (except near \( \omega = 0 \) [compare Figs. 13(d2)–13(g2)]...
and 13(d1)–13(g1)]. The reason is that energy truncation constitutes CheMPS’s dominant source of error (as shown in Sec. V below); its avoidance thus yields more precise Chebyshev moments $\mu_n$, especially for $n > N_{\text{max}}$. (vii) However, this improvement is numerically expensive: the increased effective bandwidth necessitates larger expansion orders $N$, which in turn require a higher MPS dimension $(m = 128)$. (viii) For the present model, it was possible to calculate several thousand moments without encountering numerical instabilities; this illustrates the fact that the Chebyshev recurrence relations are numerically stable.

Finally, let us address (ix) the wiggly artifacts near $\omega = 0$. They reflect the fact that CheMPS was separately applied to the positive and negative branches of the spectral function $A^\pm(\omega)$, shown in zooms in Figs. 13(b) and 13(c), respectively. These are proportional to step functions $\theta(\pm\omega)$, and hence abruptly dip to zero for $\omega < 0$ or $> 0$, respectively. The wiggly artifacts correspond to Gibbs oscillations decorating these sharps dips. This problem can be avoided by performing a single Chebyshev expansion of the sum $A^+(\omega) + A^-(\omega)$, which is a smooth function and leads to the perfectly smooth long-dashed line in Figs. 13(b) and 13(c). This improvement comes at roughly twice the numerical cost since it requires a doubling of the spectral range to $\omega \in [-W_A, W_A]$. This implies a slight but obvious modification of the transformations from $\omega$ to $\omega'$ and from $H$ to $H'$ to account for the shifted range of $\omega$; a doubling of $W_A$ and, hence of the expansion order $N$, required to achieve a specified resolution.

The main conclusions from our CheMPS calculations for the RLM are as follows: The strategy of using twice the spectral width as effective bandwidth ($W_\epsilon = 2W_A$) and performing energy truncation [Fig. 13(a)] is a satisfactory compromise between efficiency (only a few hundred Chebyshev moments are needed) and accuracy (for which energy truncation is the main limiting factor). If desired, better results can be obtained by using the full bandwidth ($W = W_A$) and thus avoiding energy truncation, albeit at the cost of significantly increasing the required expansion order by the factor $W/2W_A$. Nevertheless, the calculation of Chebyshev moments $\mu_n$ with very large $n$ is feasible due to the remarkably numerical stability of Chebyshev recurrence relations.

FIG. 13. (Color online) Diagonal spectral functions $A_{jj}(\omega)$ of a three-level RLM. Thick solid lines show the continuum limit $A^\infty_{jj}(\omega)$ from (A3). Dashed and dashed–double-dotted lines show CheMPS results $A^0_{jj}$ or $A^\infty_{jj}$, with or without Jackson broadening, respectively, calculated for $L_b = 101$ band levels. For each spectrum, the effective broadening $\eta_n$ was taken as large as possible without lowering the peak height significantly below that of $A^\infty_{jj}$. In (a1)–(g1), we used an effective bandwidth of $W_\epsilon = 2.0$ and, in (a2)–(g2), the full many-body bandwidth $W = 52.3$. The latter requires significantly larger expansion orders, but exhibits less numerical inaccuracies [compare (b1)–(g1) and (b2)–(g2)], which represent zooms of the rectangles indicated in (a1) and (a2), respectively. (b), (c): Gibbs oscillations arise if $\omega < \omega_L$ and (d), (e): Gibbs oscillations arise if $\omega > \omega_L$. (f) and (g): $A^\infty_{33}$ shows small but distinct finite-size wiggles because the main peak is so sharp and narrow that recovering its height fully requires an $\eta_n$ so small that it is comparable to $\omega_L$. The main conclusions from our CheMPS calculations for the RLM are as follows: The strategy of using twice the spectral width as effective bandwidth ($W_\epsilon = 2W_A$) and performing energy truncation [Fig. 13(a)] is a satisfactory compromise between efficiency (only a few hundred Chebyshev moments are needed) and accuracy (for which energy truncation is the main limiting factor). If desired, better results can be obtained by using the full bandwidth ($W = W_A$) and thus avoiding energy truncation, albeit at the cost of significantly increasing the required expansion order by the factor $W/2W_A$. Nevertheless, the calculation of Chebyshev moments $\mu_n$ with very large $n$ is feasible due to the remarkably numerical stability of Chebyshev recurrence relations.
It was shown very recently (Ref. 46) that the performance of the continued-fraction approach can be substantially improved by iteratively calculating its expansion coefficients using an adaptive Lanczos-vector method.

In principle, the Lanczos algorithm also provides the maximal eigenvalue. However, in DMRG, the Lanczos gets restarted at every site with the currently known ground state and, thus, the return maximal energy will no longer approach $E_{\text{max}}$ as the ground state converges.

Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables, edited by M. Abramowitz and I. A. Stegun (Dover, New York, 1970).

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