Chebyshev approach to quantum systems coupled to a bath

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We propose a new concept for the dynamics of a quantum bath, the Chebyshev space, and a new method based on this concept, the Chebyshev space method. The Chebyshev space is an abstract vector space that exactly represents the fermionic or bosonic bath degrees of freedom, without a discretization of the bath density of states. Relying on Chebyshev expansions the Chebyshev space representation of a bath has very favorable properties with respect to extremely precise and efficient calculations of groundstate properties, static and dynamical correlations, and time-evolution for a great variety of quantum systems. The aim of the present work is to introduce the Chebyshev space in detail and to demonstrate the capabilities of the Chebyshev space method. Although the central idea is derived in full generality the focus is on model systems coupled to fermionic baths. In particular we address quantum impurity problems, such as an impurity in a host or a bosonic impurity with a static barrier, and the motion of a wave packet on a chain coupled to leads. For the bosonic impurity, the phase transition from a delocalized electron to a localized polaron in arbitrary dimension is detected. For the wave packet on a chain, we show how the Chebyshev space method implements different boundary conditions, including transparent boundary conditions replacing infinite leads. Furthermore the self-consistent solution of the Holstein model in infinite dimension is calculated. With the examples we demonstrate how highly accurate results for system energies, correlation and spectral functions, and time-dependence of observables are obtained with modest computational effort.

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I. INTRODUCTION

The calculation of spectral or dynamical properties of quantum systems, expressed through spectral functions or captured in the time evolution of a wave function, is one of the most important and most promising applications of modern numerical techniques in theoretical physics or chemistry. For many purposes, approximation free techniques that allow to calculate numerically exact results for arbitrary Hamiltonians on large Hilbert spaces are of interest. One of the most powerful tools in this context are techniques based on Chebyshev expansions, like the kernel polynomial method (KPM), which yield results of high accuracy with modest computational effort. Chebyshev techniques often outperform the Lanczos algorithm with respect to accuracy and efficiency, and are applicable to problems that are beyond the reach of matrix diagonalization. In this article we propose an extension of Chebyshev techniques that considerably enlarges their field of applications. Possible new applications we have in mind include (i) damping and decoherence in quantum systems coupled to an environment like a bosonic heat bath, (ii) transport through quantum systems coupled to fermionic baths, (iii) the solution of quantum impurity models, (iv) non-equilibrium dynamics of mesoscopic devices coupled to leads, and in general, (v) the calculation of static and dynamical correlation functions or time propagation in these physical situations, (vi) the combination with diagrammatic Green function techniques, (vii) the treatment of degrees of freedom with non-trivial dynamics like phonons with dispersion.

We concentrate here on a situation for which the development of ideas is particularly clear: A quantum system coupled to a fermionic bath. The bath serves as a reservoir for fermions, which can hop from the bath to the quantum system and back. The standard example is that of a mesoscopic system contacted with leads. For a single quantum dot, the appropriate model is the famous Anderson model for the Kondo effect, which describes an impurity site with Coulomb interaction embedded in a host of non-interacting electrons. This model also arises in dynamical mean-field theory (DMFT) where the solution of an Anderson model in dependence on a host spectral function is a central issue.

In all these cases the quantum system allows for many-particle interactions, which give rise to non-trivial correlations. For their description one has to rely on several correlation functions whose calculation requires the full apparatus of many-body theory. In the numerical calculation we have to deal with complicated objects like a Fock space of many fermions. Due to the coupling between the quantum system and the bath, further correlations between the quantum system and the bath develop. As a consequence one cannot separate the degrees of freedom of the quantum system and of the bath, but must treat their evolution in parallel. However, the bath consists of non-interacting fermions, and is entirely described by single-particle spectral functions, as no correlations exist in absence of coupling to the quantum system. Plainly spoken, we do not need to describe all details of the bath, but only how its presence influences the dynamics of the quantum system. It is important to exploit this simplification to make a calculation possible. Trivial as this point may seem, it is not easily incorporated into a numerical calculation. The numeri-
The article is organized as follows. In Sec. III we introduce the CS, and explain in Sec. IV the implementation of the CSM for the example of an impurity embedded in a host. In Sec. V we derive an important property of the CS and discuss its practical relevance. Sec. VI describes how self-consistent calculations are performed in CSM, and Sec. VII demonstrates how the concurrent dynamics of a quantum system and a bath, when degrees of freedom evolve in parallel, is accounted for. This provides the basis for the study of the phase transition for a bosonic impurity in Sec. VIII and to the self-consistent solution of the Holstein model within DMFT in Sec. VIIA. In Sec. IX we address the time evolution of a wave packet on a long chain with different boundary conditions realized by CSM. We summarize in Sec. X and point out possible future advancements of CSM. In the Appendices, we provide a short account of technical aspects of Chebyshev expansions and KPM, and the derivation of some mathematical results used in the text.

II. CHEBYSHEV EXPANSIONS AND THE KERNEL POLYNOMIAL

The recurrent theme of this article is the expansion of a spectral function in a series of Chebyshev polynomials. To make the article self-contained we add an appendix on technical issues of Chebyshev expansions and KPM (App. A). For a more detailed exposition, we refer the reader to the recent review Ref. [3] and references cited therein.

The Chebyshev polynomials $T_n(x)$ are defined by the two-term recurrence

$$
T_0(x) = 1, \quad T_1(x) = x, \quad T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x),
$$

which is equivalent to $T_n(x) = \cos(n \arccos x)$. The Chebyshev polynomials are mutually orthogonal on the interval $[-1, 1]$ with respect to the scalar product given by the weighting function $(1 - x^2)^{-1/2}$, obeying the relations

$$
\int_{-1}^{1} T_m(x)T_n(x) \sqrt{1 - x^2} dx = \begin{cases} 
1, & n = m = 0 \\
\frac{1}{2} \delta_{mn}, & n, m \neq 0
\end{cases}
$$

Eq. (2) implies that the Chebyshev polynomials form an orthogonal basis for functions defined on the interval $[-1, 1]$. To expand a spectral function, defined as

$$
A(\omega) = \langle \psi |(\omega - H)|\psi \rangle = -\frac{1}{\pi} \lim_{\eta \to 0^+} \text{Im} \langle \psi |(\omega + i\eta - H)^{-1}|\psi \rangle
$$

to some Hamiltonian $H$ and vector $|\psi\rangle$, in a series of Chebyshev polynomials it must therefore vanish outside $[-1, 1]$. This can be achieved by re-scaling the Hamiltonian $H$ as $H = p\tilde{H} + q$, where $p, q$ is chosen in such a way that all eigenvalues of $\tilde{H}$ lie in $[-1, 1]$, or equivalently...
\[ |\hat{H}| < 1. \] After a corresponding variable substitution \( x = (\omega - q)/p, \) the Chebyshev expansion for \( A(\omega) \) reads
\[
A(\omega) = \frac{1}{p} \sum_{n=1}^{\infty} \frac{\mu_n}{1 - x^2} T_n(x),
\]
for \( A(\omega) \) on the interval \([\omega_{\text{min}}, \omega_{\text{max}}]\) with \( \omega_{\text{min}} = -p + q, \omega_{\text{max}} = p + q. \) Comparing this expansion to the definition (3), and using the orthogonality relation (2), we find that the coefficients in this series – the Chebyshev moments – are given by
\[
\mu_n = \int_{-1}^{1} T_n(x) A(px + q) dx = \langle \psi | T_n(\hat{H}) | \psi \rangle.
\]
We will assume in the following that any Hamiltonian is constructed from a truncated series, taking the first \( n \) terms. The calculation of the moments therefore requires (i) to apply \( \hat{H} \) to a vector, i.e. to perform matrix-vector multiplication if \( \hat{H} \) is explicitly given as a matrix, and (ii) to evaluate a scalar product of two vectors.

In any practical application only a finite number \( N \) of moments can be calculated, and \( A(\omega) \) has to be reconstructed from a truncated series, taking the first \( N \) terms in Eq. (5). The reconstruction of \( A(\omega) \) from such a finite series is the issue of KPM (see App. A). High resolution of \( A(\omega) \) is already obtained with a fairly small number of moments, thus allowing for accurate calculations with moderate demands on computational time or memory. The resolution of KPM scales linearly with \( N. \) It is usually much better than for the Lanczos (Recursion) Method\textsuperscript{11,12,13}, and can be unrestrictedly increased without problems.\textsuperscript{5}

III. THE GENERAL SCHEME

A coupled quantum system and bath is generally described by a Hamiltonian of the form\textsuperscript{6,14}
\[
H = H_S + H_L + H_B.
\]
\( H_S \) and \( H_B \) denote the Hamiltonian for the quantum system and the bath, respectively, and \( H_L \) describes the coupling between system and bath. Without coupling, for \( H_L = 0, \) the degrees of freedom of the quantum system and the bath evolve independently, i.e. \( H_S \) and \( H_B \) commute. We restrict ourselves in this article to situations with a single spinless fermion. This allows to introduce the CS without a discussion of complications inherent to many-fermion physics. The CSM can be extended to finite fermion density, or the inclusion of spin degrees of freedom, with the same implementation of a CS as given in this article. We return to that issue in Sec. IX.

Since the bath consists of non-interacting fermions, \( H_B \) is a bilinear Hamiltonian
\[
H_B = \sum_{\alpha\beta} (H_B)_{\alpha\beta} f_{\alpha}^\dagger f_{\beta},
\]
where \( f_{\alpha}^\dagger \) are fermionic operators for the bath degrees of freedom. The indices \( \alpha, \beta \) can denote e.g. an arbitrary set of orbitals, sites of a lattice, or, if \( (H_B)_{\alpha\beta} \) is diagonal, the eigenstates of \( H_B. \) A change of indices corresponds to a unitary transformation of the matrix \((H_B)_{\alpha\beta}\). The system Hamiltonian \( H_S \) can be of arbitrary form, involving any type of interaction. We do not specify \( H_S \) now, and discuss examples for various different \( H_S \) later.

More can be said about the coupling term \( H_L. \) In general, the bath is in contact to one (or a few) site(s) of the quantum system, say site 0 with fermionic operator \( c_0^\dagger. \) Fermions hop from this site to the bath, and back. The appropriate choice for \( H_L \) is
\[
H_L = \sum_{\alpha} t_{\alpha} (c_{\alpha}^\dagger f_0 + f_0^\dagger c_{\alpha}) \quad (t_\alpha \in \mathbb{R}),
\]
or a sum of terms of this form. It is convenient to introduce a fermionic operator \( d^{\dagger} \) by
\[
d_\alpha^\dagger = \sum_{\alpha} a_{\alpha} f_{\alpha}^\dagger, \quad a_{\alpha} = t_\alpha/(\sum_{\alpha} t_{\alpha}^2)^{1/2}.
\]
As \( \sum_{\alpha} a_{\alpha}^2 = 1, \) the fermionic anticommutator relation \( \{d, d^\dagger\} = 1 \) is fulfilled. With the introduction of \( d^{\dagger}, \) \( H_L \) acquires the form of a hopping term between two sites,
\[
H_L = V (c_0^\dagger d + d^\dagger c_0), \quad V = (\sum_{\alpha} t_{\alpha}^2)^{1/2}.
\]

Depending on the meaning of indices in Eq. (7), \( d \) can denote a concrete orbital or a site in a lattice, or just an abstract linear combination of \( f-\)operators. If we think of a mesoscopic system contacted to a lead, then \( c_0^\dagger \) and \( d^{\dagger} \) denote operators for the contact point in the system and lead, respectively.

We define the bath spectral function \( A_B(\omega) \) as the spectral function of the \( d \)-orbital,
\[
A_B(\omega) = \langle \text{vac} | d^\dagger \delta(\omega - H_B) d^\dagger \text{vac} \rangle
\]
where \( |\text{vac}\rangle \) is the bath vacuum, i.e. \( d^\dagger \text{vac} = 0. \) Remember that we study situations with a single fermion. For finite fermion density, we had to consider both the particle and hole part of the spectral function, and to account for Pauli blocking.

After the transformation (9), the bath occurs in the calculation of correlation functions for the quantum system only through the spectral function \( A_B(\omega) \) and the coupling strength \( V. \) The precise coefficients in Eqs. (7), (8) do not occur. In this sense, all Hamiltonians (6) with the same \( A_B(\omega), \) \( V, \) but potentially different \( H_B, H_L, \) are equivalent. Often the problem under
study is defined in this way, by specifying $A_B(\omega)$ and $V$, without an explicit representation of $H_B$ or $H_L$, as in Eqs. 1, 8 at hand.

Given such a problem, how can it be accessed within numerically exact techniques like Lanczos or KPM? Since these techniques need the Hamiltonian $H$ explicitly given, it seems inevitable to use an explicit representation of $H_B$ in the form 14. One possible way to obtain such a representation is to discretize $A_B(\omega)$ by a finite number of $\delta$-peaks, as

$$A_B(\omega) \approx \sum_\alpha w_\alpha \delta(\omega - \epsilon_\alpha). \quad (12)$$

This approximation translates to $H_B = \sum_\alpha \epsilon_\alpha f_\alpha^\dagger f_\alpha$, and $d^\dagger = \sum_\alpha w_\alpha^{1/2} f_\alpha^\dagger$. A calculation then relies on our ability to construct a good approximation (12). This poses certain questions: How to choose the positions $\epsilon_\alpha$ of peaks, how to choose their weights $w_\alpha$, and how many of them are needed to approximate $A_B(\omega)$ sufficiently well? When is an approximation to $A_B(\omega)$ sufficiently good, and what is the precise meaning of “approximation” in Eq. (12)? Is there an optimal way to choose $\epsilon_\alpha$, $w_\alpha$ for a given number of peaks? While the result of a calculation for the quantum system does not depend on the precise form of $H_B$, it does depend on the approximation for $H_B$ or $A_B(\omega)$.

How can we control this dependence? There is no definite answer to these questions, and the need to discretize $A_B(\omega)$ is quite unsatisfactory. Our new proposition, the use of the CS in the CSM, avoids the discretization of $A_B(\omega)$. It works without a representation of $H_B$ in the form 14, but addresses $H_B$ only via the spectral function $A_B(\omega)$.

The central ingredient of CS(M) is a representation of $H_B$ related to the Chebyshev expansion of $A_B(\omega)$. To obtain this representation, define the Chebyshev vectors

$$|n\rangle = T_n(H_B)d^\dagger|\text{vac}\rangle \quad (13)$$

for $n \geq 0$. These vectors are neither normalized nor orthogonal. We need only the scalar products

$$\langle 0|n \rangle = \langle \text{vac}|d^\dagger T_n(H_B)|\text{vac}\rangle = \mu_n^B, \quad (14)$$

where $\mu_n^B$ is the $n$th Chebyshev moment of the bath spectral function $A_B(\omega)$, according to the expansion 14. The Chebyshev vectors span a Hilbert space $H_c$, the CS. By definition, $H_c$ is a subspace of the Fock space for the bath operators $f^{(1)}$, but we refer to the Chebyshev vectors only as abstract vectors, whose possible representation in terms of the $f^{(1)}$ is irrelevant.

From the recurrence relation 14 it follows that the operation of $H_B$ on $H_c$ is given by

$$H_B|n\rangle = \begin{cases} |1\rangle, & n = 0 \\
                             (1/2)(|n-1\rangle + |n+1\rangle), & n \neq 0. \end{cases} \quad (15)$$

Since $|n\rangle$ is a one-fermion state, $d|n\rangle$ is proportional to $|\text{vac}\rangle$. Together with the definition of $\mu_n^B$ this yields

$$d^\dagger|n\rangle = d^\dagger T_n(H_B)d^\dagger|\text{vac}\rangle = \mu_n^B|\text{vac}\rangle \quad (16)$$

and

$$d^\dagger d|n\rangle = d^\dagger d^\dagger T_n(H_B)d^\dagger|\text{vac}\rangle = d^\dagger|\text{vac}\rangle d^\dagger T_n(H_B)d^\dagger|\text{vac}\rangle = \mu_n^B|\text{vac}\rangle \quad (17)$$

The reader should note that in these equations the only parameters are the Chebyshev moments $\mu_n^B$ of the spectral function $A_B(\omega)$.

Eqs. 14–17 constitute the basis of our CS approach. What we have achieved is that $H_B$ is put into a form that makes no reference to a representation like 7. Still, $H_B$ is given as a Hamiltonian acting on a Hilbert space. This is a very useful form for $H_B$, which can be used within numerically exact techniques like Lanczos or KPM and avoids discretization of $A_B(\omega)$.

IV. A FERMIonic SITE EMBEDDED IN A HOST

We illustrate the use of the CS(M) with the example

$$H = -\Delta d^\dagger d + H_B \quad (18)$$

of an unperturbed system $H_B$ with a perturbation $-\Delta d^\dagger d$. This is the Hamiltonian of a single site in a sea of non-interacting fermions, like an impurity embedded in a host or lattice. Note that this example is not of the form 6, as it deals with a site embedded in the bath, while in Eq. 6 and later examples fermions leave the bath by hopping to the quantum system.

Our goal is to calculate the spectral function

$$A(\omega) = \langle \text{vac}|d\delta(\omega - H) d^\dagger|\text{vac}\rangle \quad (19)$$

to give $A_B(\omega)$ and $\Delta$ within CSM, i.e. using KPM with the Eqs. 14–17 for the CS. We can compare the results to the exact result

$$G(z) = [G_B(z)^{-1} + \Delta]^{-1} \quad (20)$$

for the corresponding Green functions

$$G_B(z) = \langle \text{vac}|d|z - H_B(\omega)\rangle^{-1}d^\dagger|\text{vac}\rangle. \quad (21)$$

To obtain the Chebyshev moments $\mu_n(\omega)$, we have to recursively calculate the vectors $T_n(H)d^\dagger|\text{vac}\rangle$ according to Eq. 14. The calculation proceeds in the space $H_c$, and each vector is given as a linear combination of Chebyshev vectors $|n\rangle$. With $H_B$ according to 15 and $\Delta d^\dagger d$ according to 17, $H$ is represented by the matrix

$$H_{mn} = \frac{1}{2} \begin{pmatrix} -2\Delta \mu_0^B & 1 - 2\Delta \mu_1^B & -2\Delta \mu_2^B & -2\Delta \mu_3^B & \ldots \\ 2 & 0 & 1 & 0 & \ldots \\ 0 & 1 & 1 & 0 & \ldots \\ \vdots & \vdots & \ddots & \ddots & \ddots \end{pmatrix} \quad (22)$$
with $H|m\rangle = \sum_m (H)_{mn} |m\rangle$. Note that $(H)_{mn} \neq \langle m|H|n\rangle$, because the Chebyshev vectors are not orthogonal. Especially, $(H)_{mn}$ is not symmetric. Nevertheless, $H$ is hermitian by definition (an explicit calculation is given in App. C).

Starting with the vector $|0\rangle = d^\dagger|\text{vac}\rangle$, in any step of the Chebyshev iteration we apply $H$ according to (22) to obtain the vector $T_n(H)|0\rangle$ from previous vectors $T_{n-1}(H)|0\rangle$, $T_{n-2}(H)|0\rangle$. The moment $\mu_n$ is finally obtained from the scalar product $\langle 0|T_n(H)|0\rangle$ according to Eq. (13). During the iteration the index of any vector $|n\rangle$ is increased at most by one in Eq. (22), and the vector $T_n(H)|0\rangle$ is a linear combination of Chebyshev vectors $|m\rangle$, with $m \leq n$. The $n^{th}$ Chebyshev moment $\mu_n$ of $A(\omega)$ is therefore obtained from the first $n$ Chebyshev moments $\mu^n_0, \ldots, \mu^n_n$ of $A(\omega)$. We have thus devised a computational scheme to map $n$ moments of a given spectral function $A_B(\omega)$ to one part $H_B$ of $H$ to $n$ moments of a spectral function $A(\omega)$ to the full Hamiltonian $H$ without resorting to an explicit representation (2) of $H_B$ in an orthonormal basis $f^\lambda_n$. This is the essence of CSM.

Note that only spectral functions $A_B(\omega)$, $A(\omega)$ occur in the calculation. The ‘missing’ real part of the corresponding Green function, which is needed in Eq. (20), is implicitly accounted for by causality relations preserved in the calculation. As shown in Ref. 3, we can obtain the Green function $G(\omega)$ from moments $\mu_n$ of the spectral function $A(\omega)$ without invoking Kramers-Kronig-relations.

A. Scaling of $H$ and $H_B$

We have so far omitted the scaling of $H$ and $H_B$ to the interval $[-1,1]$. To determine the scaling of $H_B$ we must choose a scaling interval $I_B$ that contains the domain of non-zero values of $A_B(\omega)$, i.e. $A_B(\omega) = 0$ for $\omega \not\in I_B$ (cf. Sec. II). For $I_B = [\omega_{\text{min}}, \omega_{\text{max}}]$, the scaling factors

$$r = (\omega_{\text{max}} - \omega_{\text{min}})/2, \quad s = (\omega_{\text{max}} + \omega_{\text{min}})/2$$

(23) give the scaling $H_B = r \tilde{H}_B + s H_B$. The smaller $I_B$, the higher is the resolution of $A_B(\omega)$ for a given number of moments. Similarly, we choose a scaling interval $I$ with $A(\omega) = 0$ for $\omega \not\in I$. With scaling factors $p, q$ determined from $I$ as before, we find for the scaling of $H$

$$\tilde{H} = \frac{1}{p} (H - q) = -\frac{\Delta}{p} d^d d + \frac{r}{p} \tilde{H}_B + \frac{s - q}{p}$$

(24)

It is straightforward to introduce the scaling factors into Eqs. (15), (16), and the matrix form (22).

Since we do not know $A(\omega)$ in advance, we have to rely on estimates for $I$. For Eq. (18), the term $-\Delta d^d d$ has eigenvalues 0 and $-\Delta$. It follows that any $I$ with $I \supset I_B \cup (I_B - \Delta)$ is a possible choice. Similar estimates can be obtained in other situations. Alternatively we can determine the minimal and maximal eigenvalue of $H$ by the Lanczos algorithm (cf. Sec. VIII). Note that precise knowledge of the minimal or maximal eigenvalue of $H$ is not necessary, but any bound works. It often suffices to obtain an estimate from operator norms. A factor of the order of two in the scaling is tolerable for most practical purposes. The resolution of CSM – or KPM – still compares quite favorably to the resolution of other techniques. The possible loss of resolution for a too large $I$ can be compensated for by increasing the number of moments in the calculation. We show in Sec. IV that we can even increase the resolution for $A(\omega)$ without increasing the number of moments for $A_B(\omega)$.

The reader should be reminded that the need to consider scaling is the price one has to pay for the high resolution of the Chebyshev technique – this is certainly no drawback of the method. Interestingly, there are situations where the divergence of moments for wrong scaling can be used to our advantage: We will exploit it below to determine the groundstate energy of $H$.

Now consider the case $\Delta = 0$ in Eq. (18). We know that then $A(\omega) = A_B(\omega)$. With scaling intervals $I \supset I_B$, the moments $\mu_n$, $\mu_n^B$ of these two identical functions are different since $I \not\supset I_B$. We can use CSM to calculate the $\mu_n$, reproducing $A_B(\omega)$ on the larger interval $I$ (see next subsection). Now assume that we choose $I_B$ much larger than necessary. In principle, a possible scaling interval $I$ for $H$ might then be smaller than $I_B$, i.e. $I \subset I_B$. Will CSM then reproduce the spectral function $A_B(\omega)$, respectively its moments, on the smaller interval $I$?

The answer is no: The interval $I$ must always be larger than $I_B$, i.e. $I \supset I_B$. Then, and only then, the Chebyshev iteration for $\Delta = 0$, and $H = H_B$, is stable in the space $H_e$. This can be understood from the fact that $H_B$ acts within $H_e$ like an operator with unity norm: The column sums of the matrix (22) for $\Delta = 0$ are unity, and the first column has a single unity entry. Note that this is a statement about the norm of $H_B$ as a matrix, and not with respect to the scalar product of Chebyshev vectors. If now $I \supset I_B$, then $r/p > 1$, and $\|\tilde{H}\| > 1$ in Eq. (24). Then, the coefficients in front of the Chebyshev vectors $|n\rangle$ diverge during the iteration, while the weights $\mu_n^B$ decay with the same rate. Each moment $\mu_n$ is a sum of products of coefficients and moments $\mu_n^B$. Within exact arithmetics the correct moments $\mu_n$ would be reproduced. In finite precision arithmetics however, numerical round-off errors entirely ruin the output. On the contrary, for $I \supset I_B$, the recursion is perfectly stable, up to any number of moments. This is an important point to be aware of.

B. Numerical results

We now show results from CSM for the model defined in Eq. (18). We start with a semi-circular spectral function

$$A_B(\omega) = \frac{8}{\pi W^2} \sqrt{W^2/4 - \omega^2}, \quad |\omega| \leq W/2,$$

(25)
realized e.g. as the density of states in a Bethe lattice. W is the band width. The first test of CSM is the calculation of $A(\omega)$ for $\Delta = 0$. The figures displays the region around the lower band edge $\omega = -W/2$, for curves with $N = 2^{10}, 2^{13}, 2^{16}$ Chebyshev moments, the exact result, and a curve with Lorentzian broadening $\eta/(\omega^2 + \eta^2)$ to $\eta = 5 \times 10^{-3}$. The latter curve illustrates the typical quality of results from the Lanczos Recursion Method. With $N = 2^{10}$ Chebyshev moments the exact curve is much better reproduced than with Lorentzian broadening. The inset shows the full curve, whose deviation from the exact result is below linewidth on this scale. The curve for $N = 2^{16}$ lies on top of the exact result even in magnification of the band edge, and demonstrates that CSM can achieve arbitrary precision.

We expect strongest deviations from the numerical result to Eq. (25) close to the band edges, where the spectral function behaves like a square root. For $N = 2^{10}$ moments, the absolute deviation $|A^n(\omega) - \bar{A}^n(\omega)|$ between numerical ($A^n(\omega)$) and exact ($\bar{A}^n(\omega)$) spectral function is smaller then $6 \times 10^{-2}$ at the band edge, and smaller than $5 \times 10^{-5}$ over the remaining 90% of the band. The cumulative deviation $\int |A^n(\omega) - \bar{A}^n(\omega)| d\omega$ is below $10^{-4}$. Notably, the resolution is much higher than for other methods, e.g. using the Lanczos Recursion Method with Lorentzian broadening of the spectral function. Note also that the two-fold Chebyshev recursion – once for the moments of $A_B(\omega)$, once for $A(\omega)$ – is perfectly stable for any number of moments. The calculation of many thousands of Chebyshev moments is no problem, allowing for unprecedented resolution.

To further test the accuracy of our approach we calculate the groundstate energy $E_0(\Delta)$ of an impurity in an infinite chain (1d), square (2d), cubic (3d) tight-binding lattice, and for the semi-circular density of states in Eq. (25) (see Fig. 3). For sufficiently large $\Delta$ a bound state at the impurity exists, with energy outside the band of continuum states, i.e. $E_0(\Delta) < -W/2$. In 1d and 2d, a bound states exists for any $\Delta > 0$, while in 3d and for the semi-circular density of states a bound state exists above a critical value $\Delta_c$. In Fig. 4 we show the impurity spectral function for $\Delta \neq 0$. $A(\omega)$ has a $\delta$-peak at $\omega = E_0$ if $\Delta > \Delta_c$. Even if the peak is very close to the band edge it can be resolved within CSM by increasing the number of moments $N$.

To find $E_0(\Delta)$ within CSM, we exploit the possible divergence of moments in the Chebyshev recursion. We initially choose a scaling interval $I = [\omega_{\text{min}}, \omega_{\text{max}}]$ for $H$ so large that moments do not diverge. Then we vary $\omega_{\text{min}}$. If the moments diverge, $E_0 < \omega_{\text{min}}$, otherwise $E_0 \geq \omega_{\text{min}}$. Using e.g. a bisection algorithm on $\omega_{\text{min}}$ we can calculate $E_0$ to high precision. The computational effort for Fig. 3 is independent of the lattice dimension, as only a fixed number of moments enter the calculation. The most demanding case here is indeed 1d, as the spectral function diverges at the band edge. Despite this particular complication, the results are extremely accurate already for $N = 2^{10}$ moments.

For our example, $E_0$ is the groundstate energy of a single particle, i.e. the smallest energy with $A(E_0) \neq 0$. The weight $A(E_0)$ can be arbitrarily small. From Eq. (20), we see that $A(\omega) \neq 0$ whenever $A_B(\omega) \neq 0$. Within the numerics the domain of non-zero values of $A_B(\omega)$ is fixed by the scaling interval $I_B = [\omega_{\text{min}}, \omega_{\text{max}}]$. We also know
moments of \( F \) or \( \Delta \)

\[
N \text{ continuum states (cf. Fig. 3). The deviation of the curves with scaling intervals are circular for this } \Delta, \text{ a less than } 10^{-4} \text{ obtain the results shown is small – a calculation for provides highest accuracy. The computational effort to change } N \mid n = \text{lem occurs. Note that the situation is different at finite } \omega, \text{ especially for } \Delta \text{ min}. \text{ Therefore } \omega < \text{min } B \text{ min} \text{, discrete energy levels in the truncated bath Hamiltonian } H_B \text{ are resolved. Even } N \gg M \text{ does not lead to erroneous results as a negative spectral function. In particular, the CSM is perfectly stable for arbitrary } N \text{ and } M. \]

Using \( M < N \) moments of \( A_B(\omega) \) in the calculation is equivalent to working with a truncated bath Hamiltonian \( H_B^M \) on the \( M \)-dimensional subspace \( \mathcal{H}_c^M \) of \( \mathcal{H}_c \) that is spanned by vectors \([0], \ldots, [M - 1])\). The matrix of \( H_B^M \), with \( H_B^M(n) = \sum_m (H_B^M)_{mn} |m| \), is according to Eq. (15) the tridiagonal \( M \times M \)-matrix

\[
(H_B^M)_{mn} = \frac{1}{2} \begin{pmatrix}
0 & 1 & & & \\
2 & 0 & 1 & & \\
& 1 & 0 & 1 & \\
& & \ddots & \ddots & \ddots \\
& & & 1 & 0 \\
& & & & 1
\end{pmatrix}.
\]

We show in App. B that the characteristic polynomial of \( (H_B^M)_{mn} \) is

\[
\det[x - (H_B^M)_{mn}] = 2^{-(M-1)} T_M(x).
\]

The \( M^{th} \) Chebyshev polynomial \( T_M(x) = \cos(M \arccos x) \) has \( M \) distinct real roots \( x_j = \cos \left( \frac{j \pi}{M} \right) \) for \( j = 1, \ldots, M \). It follows that \( (H_B^M)_{mn} \) has \( M \) distinct real eigenvalues, hence \( H_B^M \) is a diagonalizable \( M \times M \)-matrix with real eigenvalues \( x_j \). The position of the discrete energy levels resolved for \( N \gg M \) in Fig. 4 is determined by the \( x_j \). We discuss in

V. PROPERTIES OF THE TRUNCATED CHEBYSHEV REPRESENTATION OF \( H_B \)

In the examples of the previous section we calculate \( N \) moments of \( A(\omega) \) from the same number of moments of \( A_B(\omega) \). Calculations can also be performed for a different number of moments of \( A_B(\omega) \), say \( M \). For \( M \geq N \), the moments of \( A(\omega) \) do not change and the calculation is exact, as we noted above. For \( M < N \) however, the calculation is approximate and its result depends on \( M \).

The computational effort for given \( M, N \) scales as \( O(MN) \) for time, and \( O(M) \) for memory: Calculating more moments of \( A(\omega) \) requires only more time, while using more moments of \( A_B(\omega) \) requires more time and memory. It is therefore natural to ask whether we can obtain \( N \) moments of \( A(\omega) \) from fewer moments of \( A_B(\omega) \), especially if we remember that both are calculated with different scaling for \( H \) and \( H_B \). We know that the resolution of a Chebyshev expansion increases linearly with the number of moments, as can be deduced e.g. from the width (standard deviation) \( \sigma = \pi/N \) of the Jackson kernel, see Appendix A. If we demand that the resolution for \( A(\omega) \) and \( A_B(\omega) \) is the same, we obtain the condition \( M/N \geq r/p \), with the scaling \( H = p\tilde{H} + q \), \( H_B = r\tilde{H}_B + s \) as in Eq. (24). As we discussed there, the factor \( r/p \) is always smaller than unity. For the example of the Holstein model in Sec. VIII A, it is easily of the order \( 10^{-1} \).

In Fig. 4 we show \( A(\omega) \) for different ratios \( M/N \). As long as the condition \( M/N \geq r/p \) is fulfilled, we produce an absolutely accurate \( A(\omega) \) from \( M < N \) moments of \( A_B(\omega) \), while the computational effort is considerably reduced. In the worst case, for \( M/N \ll r/p \), discrete energy levels in the truncated bath Hamiltonian \( H_B^M \) are resolved. Even \( N \gg M \) does not lead to erroneous results as a negative spectral function. In particular, the CSM is perfectly stable for arbitrary \( N \) and \( M \).
FIG. 5: (Color online) Similar to Fig. 2, this figure shows the spectral function $A(\omega)$ for semi-circular $A_B(\omega)$ according to Eq. (24), with $W = 1$ and $\Delta = 0$. The scaling intervals are $I_B = [-0.5 + \epsilon]W, (0.5 + \epsilon)W]$ with $\epsilon = 10^{-3}$ and $I = [-2W, 2W]$, i.e. $r/p = 1/4$ in Eq. (24). The calculation is performed for $N = 2^n$ Chebyshev moments of $A(\omega)$ and $M$ moments of $A_B(\omega)$. As long as $M/N \geq r/p$, i.e. here $M \geq 2^6$, the result can not be distinguished from the (numerically exact) curve for $M = N$. For $M = 2^5$, deviations occur at the band edges, and for $M = 2^4$ single spurious peaks are resolved. The inset displays a calculation for $N = 2^{11}$ and $M = 2^4$. Even for this strong mismatch, a perfectly positive spectral function is obtained, resolving $\delta$-peaks at $\omega_j = r\zeta_j + s$ corresponding to the roots $x_j$ of $T_M(x)$ (see text).

App. 1 how the weight of the corresponding peaks can be obtained from the moments $\mu_m$.

VI. LINEAR CHAIN COUPLED TO A BATH

A different example is provided by an electron hopping along a finite chain of length $L$ that is connected to a bath at its ‘right’ end (site $L$). The Hamiltonian

$$H = -t \sum_{i=1}^{L-1} (c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1}) + H_L + H_B$$

has the form of Eq. (6). Here, $c_i^\dagger$ creates an electron at lattice site $i$, and the coupling between chain and bath is $H_L = -t(d_i^\dagger c_L + c_i^\dagger d)$, as in Eq. (10), with $V = -t$. That the bath couples to the $d$-orbital implies that $[c_i^\dagger, H_B] = 0$, but $[d_i^\dagger, H_B] \neq 0$.

In difference to the example in Sec. IV (see Eq. (13)) the particle hops to and from the bath, hence the Hilbert space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_C$ of the problem is the direct sum of the Hilbert space $\mathcal{H}_S$ of the chain and the CSS $\mathcal{H}_C$. A basis of $\mathcal{H}_S$ consists of vectors $|\psi_i\rangle = c_i^\dagger |\text{vac}\rangle$, for the electron at site $i$. The vectors $|\psi_i\rangle$ are orthogonal to the Chebyshev vectors $|n\rangle$. The operation of $H$ is summarized in

$${H|\psi_i}\rangle = -t|\psi_{i+1}\rangle,$$

$${H|\psi_i}\rangle = -t|\psi_{i+1}\rangle - t|\psi_{i-1}\rangle$$

for $i = 2, \ldots, L - 1$,

$${H|\psi_L}\rangle = -t|0\rangle - t|\psi_{L-1}\rangle,$$

$${H|n\rangle} = -t\mu_n^B|\psi_L\rangle + H_B|n\rangle,$$

with the missing equations supplied by Eq. (15).

The calculation of the spectral function $A_{11}(\omega) = \langle \text{vac}|c_1\delta(\omega - H)|c_1^\dagger \text{vac}\rangle$ is the spectral function to the ‘left’ end of the chain in Fig. 1 to given bath spectral function $A_B(\omega)$ proceeds along the lines established in Sec. IV. In contrast to the example (13), where Eq. (13) was used, scalar products with the starting vector $c_1|\text{vac}\rangle$ of the Chebyshev iteration do not involve the $\mu_m^B$.

To make the present example self-consistent we demand that $A_{11}(\omega) = A_B(\omega)$. The self-consistent solution $A_{11}(\omega)$ is the spectral function of a half-infinite chain at its open end, i.e. the semi-circular spectral function from Eq. (20) with $W = 4t$. To obtain the self-consistent $A_{11}(\omega)$ we start with an initial guess for $A_B(\omega)$, e.g. setting $\mu_n^B = 0$ corresponding to $A_B(\omega) = 0$, and calculate the moments $\mu_n$ of $A_{11}(\omega)$. Note that the choice $\mu_n^B = 0$ does not correspond to a spectral function, as the sum rule $\int A_B(\omega)d\omega = \mu_0^B = 1$ is violated. This does not matter for the calculation, and we could obtain the same effect by setting $V = 0$. We start a new calculation taking the $\mu_n$ just calculated as new bath moments $\mu_m^B$, and reiterate this calculation until the moments $\mu_n$, or equivalently $A_{11}(\omega)$, are converged (see Fig. 6).

We found in Sec. IV that we must choose the scaling interval $I$ for $A_{11}(\omega)$ larger than $I_B$ for $A_B(\omega)$. If we start a new iteration with the previously calculated moments $\mu_n$ replacing $\mu_n^B$ we must also replace the interval $I_B$ by $I$, and consequently allow for growing scaling intervals – and corresponding loss of resolution – during the iteration. As an alternative, we keep the interval $I_B$ fixed and rescale $A_{11}(\omega)$ from $I$ to $I_B$ in our implementation. We first construct $A_{11}(\omega)$ on the interval $I$ from the $\mu_n$, then rescale it in $\omega$-space to the interval $I_B$ with a linear transformation $\omega \mapsto (r/p)(\omega - q) + s$ (cf. Eq. 24), and finally feed the moments of this rescaled spectral function as new $\mu_n^B$ back into the calculation. In the rescaling we can check whether we throw away significant weight of $A_{11}(\omega)$ which signals a too small $I_B$. For some examples where we do not know the relevant interval $I_B$ in advance, e.g. for the Holstein polaron (Sec. VII A), we let the program determine a suitable $I_B$ that contains all but negligible weight of $A_{11}(\omega)$. Typically, the interval changes during the first few iterations and then stabilizes with convergence of $A_{11}(\omega)$. The rescaling transformation needs two Fourier transforms (preferentially FFT) for the calculation of the spectral function from the moments and vice versa, and one interpolation for the linear scaling. We use spline interpolation, but for not too few moments everything also works without interpolation.
We discussed in Sec. VII how to calculate with CSM $N$ moments $\mu_n$ from moments $\mu_{m}^B$ for $M < N$, depending on the scaling intervals $I$ and $I_B$. Do we waste part of the numerical results if again only $M < N$ moments $\mu_{m}^B$ are calculated in the rescaling transformation? Obviously not: For a smaller interval less moments are needed to obtain the same resolution. In both directions, via CSM or the rescaling transformation, the number of moments should be related by the estimate $M/N \sim \tau/p$.

The reader should note that the rescaling transformation – which shrinks the $\omega$-interval of the Chebyshev expansion – is a linear transformation of moments $\{\mu_n\} \mapsto \{\mu_n^B\}$. A calculated $\mu_m^B$ depends on every $\mu_n$. In contrast, the CSM of Sec. VII implements for $\Delta = 0$ in Eq. (15) a transformation $\{\mu_n\} \mapsto \{\mu_n^B\}$, that blows up the $\omega$-interval (cf. Fig. 2). An inspection of Eqs. (14), (15) shows that this transformation is also linear. For $\Delta \neq 0$, it ceases to be linear as the $\mu_n^B$ also occur in $H$ itself (cf. Eq. 22), by virtue of Eq. (17). The transformation has the property that each calculated $\mu_n$ depends only on $\mu_m^B$ with $m \leq n$. We now understand a second reason why the Chebyshev iteration has to be unstable for $I_B \not\subseteq I$. If the Chebyshev iteration could be used to shrink the $\omega$-interval – that is for $I \subset I_B$ – every calculated moment $\mu_n$ had to depend on every moment supplied to the calculation $\mu_n^B$, in contradiction to the properties of the recursion.

We discussed in Sec. VII how to calculate with CSM $N$ moments $\mu_n$ from moments $\mu_m^B$ for $M < N$, depending on the scaling intervals $I$ and $I_B$. Do we waste part of the numerical results if again only $M < N$ moments $\mu_m^B$ are calculated in the rescaling transformation? Obviously not: For a smaller interval less moments are needed to obtain the same resolution. In both directions, via CSM or the rescaling transformation, the number of moments should be related by the estimate $M/N \sim \tau/p$.

VII. CONCURRENT DYNAMICS

The general Hamiltonian Eq. (11) operates on a product space $H = H_S \otimes H_B$. $H_S$ ($H_B$) operates on $H_S$ ($H_B$), and $H_L$ links the two spaces. In CSM, $H_B = H_{Bc}$. We can generally write the Hilbert space of $H$ in such a way, with $H_S$ and $H_B$ as Fock spaces, but additional constraints may single out a subspace. In the example of the linear chain with the restriction to a single electron, $H$ is the direct sum of $H_S$ and $H_L$.

Assume that system and bath do not couple, i.e. $H_L = 0$ and $H = H_S + H_B$. As $H_S$ and $H_B$ commute, the spectral function $A(\omega) = \langle \psi|\delta(\omega - H)|\psi\rangle$ to a product state $|\psi\rangle = |\psi_S\rangle \otimes |\psi_B\rangle$ is the convolution of the spectral functions of $H_S$ and $H_B$. Explicitly,

$$A(\omega) = \sum_\alpha |\langle \alpha|\psi_S\rangle|^2 A_B(\omega - \epsilon_\alpha) \ ,$$

where the sum is over eigenstates $|\alpha\rangle$ with eigenvalue $\epsilon_\alpha$ of $H_S$, and $A_B(\omega) = \langle \psi_B|\delta(\omega - H_B)|\psi_B\rangle$. To evaluate this expression we must diagonalize $H_S$ in advance, to obtain its eigenvalues and eigenstates. It is therefore difficult to use Eq. (30) for even moderately complicated $H_S$. Within CSM we calculate $A(\omega)$ without diagonalization of $H_S$. The convolution in Eq. (30) is implicitly performed in course of the Chebyshev iteration. This feature is essential for all situations where system and bath degrees of freedom evolve in parallel.

We want to illustrate this point for the Hamiltonian

$$H_S = -\sqrt{\epsilon_p}\omega_0 (b^\dagger + b)c^\dagger c + \omega_0 b^\dagger b \ ,$$

of a bosonic site, the independent boson model. It is a simple model for electron-phonon coupling of localized electrons, if the bosons ($b^\dagger$) parametrize the elongation of an ion that produces an electric field which shifts the energy of an electron at the site ($c^\dagger$). The groundstate of the bosonic part of $H_S$ in presence of a fermion, to energy $E_0 = -\epsilon_p$, is the coherent state

$$|\text{coh}\rangle = e^{-\epsilon_p^2 / 2} \sum_{n=0}^{\infty} \frac{g^n}{\sqrt{n!}} (b^\dagger)^n |\text{vac}\rangle , \quad g = (\epsilon_p/\omega_0)^{1/2} \ .$$

For $A_B(\omega)$ we assume a semi-circular spectral function as in Eq. (25), and prepare the system in the state $|\psi\rangle = |\text{coh}\rangle \otimes c^\dagger |\text{vac}\rangle$. We calculate the spectral function

$$A(\omega) = \langle |\psi|^2 |\text{d}\delta(\omega - H + E_0) d^\dagger c|\psi\rangle \ .$$

Physically, this corresponds to a sudden excitation of the electron from the bosonic site ($c$-orbital) to a continuum of states given by $H_B$, which is related to X-ray absorption of a localized electron. We know that we should obtain $A(\omega)$ as a sum of semi-circular spectral functions shifted by multiples of $\omega_0$, weighted with the Poissonian distribution of bosons in $|\text{coh}\rangle$. The lowest band is centered at $\epsilon_p$, which is the energy to remove the electron from the bosonic site. In Fig. 7 we show $A(\omega)$ calculated by CSM. The numerical result perfectly agrees with the expected outcome.
In contrast, the calculation of such ‘mixed’ dynamics is nothing changes to the applicability of our approach if that system and bath degrees of freedom do not mix.

\[
\frac{r}{p} \leq W/(n_\omega \mu_\omega) = 0.02.
\]

According to Sec. IV it is sufficient to use about \( M = 160 \) bath moments. The inset displays in magnification, how accurately the semi-circular spectral function is resolved for a single subband.

### VIII. A BOSONIC SITE COUPLED TO A BATH

We assumed in the previous section that \( H_L = 0 \), so that system and bath degrees of freedom do not mix. Nothing changes to the applicability of our approach if this restriction is abandoned, as the next examples show. In contrast, the calculation of such ‘mixed’ dynamics is the intended application of CSM.

Let us combine the example from the previous section with the example from Sec. IV. We get the Hamiltonian

\[
H = -\Delta c^\dagger c - \sqrt{\epsilon_p \omega_\omega_0} (b^\dagger b + b c^\dagger c + \omega_0 b^\dagger b) - t (d^\dagger c + c^\dagger d) + H_B
\]

(34)
of a bosonic impurity (\( c \)-orbital) coupled to a fermionic bath, e.g. a lattice. Note that the impurity site is coupled to the bath via a term \( H_L = -t (d^\dagger c + c^\dagger d) \) as in Eq. (16) or Eq. (28). We could also study a model with an bosonic impurity embedded in a host similar to Eq. (18), but the present form is convenient for the study of the Holstein model (Sec. VII A).

For \( \Delta < 0 \), the impurity is repulsive and acts as a static barrier for electron motion. Two competing mechanism determine the groundstate: On the one hand, the energy of the impurity state is increased by \( -\Delta \), favoring a delocalized groundstate. On the other hand, the formation of a localized polaron at the bosonic impurity lowers the energy of the electron roughly by \( \epsilon_p \). A localized impurity state occurs if the loss in kinetic energy is overcome by the gain in potential energy. We know from Sec. IV that this happens – for an attractive impurity – if \( \Delta \) is larger than a critical \( \Delta_c \). By a rough estimate, we expect here a localized groundstate for \( \epsilon_p \gtrsim \Delta_c - \Delta \).

To address this issue we must calculate the groundstate of the model (35). In Sec. IV B we explained how to determined the groundstate energy \( E_0 \) using Chebyshev expansions, testing for the divergence of Chebyshev moments for different scaling of \( H \). This time we must obtain the groundstate itself, not just its energy, to be able to calculate correlation functions for the degrees of freedom of the bosonic site. To calculate the groundstate we use the Lanczos algorithm. This requires our ability to perform two operations: To apply \( H \) to a vector, and to calculate the scalar product between vectors. For \( H_B \) defined on the CS \( \mathcal{H}_c \), Eq. (13) defines the application of \( H_B \) to a vector, and Eq. (14) (or Eq. (15) in App. A) gives the scalar product. Note that for a successful application of Lanczos the moments \( \mu_n^B \) should be modified by attenuation factors (Eq. (15)), cf. App. A and C.

In Fig. 7 we show the groundstate energy \( E_0 \), the occupation probability \( \langle c^\dagger c \rangle \) and the average number of bosons \( \langle b^\dagger b \rangle \) calculated with the Lanczos algorithm and the CS. As in Sec. IV B the computational effort is independent of the dimension. We used a semi-circular \( A_B(\omega) \) here, for a 3d lattice the results are qualitatively the same. While \( E_0 \) is a smooth function of \( \epsilon_p \), \( \langle c^\dagger c \rangle \) and \( \langle b^\dagger b \rangle \) signal the phase transition from a delocalized electron to a localized polaron at a critical \( \epsilon_p^c \). For \( \omega_0 \to \infty \), \( \epsilon_p^c \) converges to the value \( \Delta_c - \Delta \) of the simple estimate. For \( \omega_0 \to 0 \), the phase transition becomes more pronounced, as a precursor of the first-order transition in the adiabatic limit \( \omega_0 = 0 \). Note that in contrast to the (Holstein) polaron problem, this model has a phase
transition also for finite $\omega_0$.

It is perhaps surprising that the Lanczos algorithm, which constructs an orthonormal basis, works in combination with the CS construction, which is based on non-orthogonal vectors. For $H = H_B$ the Lanczos algorithm constructs an orthonormal basis of $\mathcal{H}_c$ and is equivalent to Gram-Schmidt orthonormalization of the Chebyshev vectors $|n\rangle$. It is known that the Gram-Schmidt procedure is prone to instabilities, namely loss of orthogonality. The same is true for the Lanczos algorithm, which is a problem for the calculation of spectral functions. The calculation of the groundstate however does not require to construct an orthonormal basis of $\mathcal{H}_c$, and loss of orthogonality is not a severe problem. For the model (18) or (34) we can force the Lanczos algorithm to fail, if $\Delta = \epsilon_p = 0$ and $\omega_{\text{min}}^B \ll -W/2$ for the lower bound $\omega_{\text{min}}^B$ of $I_B$. For these parameters, the groundstate is a linear combination of Chebyshev vectors $|n\rangle$ with energy $E_0 > \omega_{\text{min}}^B$, and the Lanczos algorithm will not converge. Remember also the discussion in Sec. VII concerning the calculation of $E_0(\Delta)$ for a single fermion, where we noted that we must guarantee $E_0 < \omega_{\text{min}}^B$. In practice, we never encountered a problem with the Lanczos algorithm in combination with the CS construction. For Fig. 9, Lanczos converges fastest for large $\epsilon_p$, when the groundstate is localized at the impurity site.

### A. Holstein model

The solution of the model (34) is related to the self-consistent solution of the Holstein model within DMFT. The Holstein model is a standard model for electron-phonon-coupling. Its Hamiltonian

$$ H = -t_{ij} \sum_{ij} c_i^\dagger c_j - \sqrt{\epsilon_p \omega_0} \sum_i (b_i^\dagger + b_i) c_i^\dagger c_i + \omega_0 \sum_i b_i^\dagger b_i $$

contains a local coupling of the electron density $(c_i^\dagger c_i)$ to dispersionless optical phonons $(b_i^\dagger b_i)$, in addition to the kinetic energy of electrons modelled by the hopping term, and the kinetic energy of phonons with frequency $\omega_0$. The polaron shift $\epsilon_p$ is the groundstate energy of the model for $t_{ij} = 0$ (cf. Sec. VII).

The solution of the Holstein model, especially for spectral properties, is still a demanding problem (for a recent review see Ref. 10). We successfully used Chebyshev expansions to obtain spectral functions or the optical conductivity for finite systems. Here we use DMFT to relate the Holstein model to the model (34) where a coupling to a bath occurs.

Within DMFT, the $(k$-integrated) spectral function

$$ A(\omega) = \langle \text{vac}|c_\alpha \delta(\omega - H)c_\alpha^\dagger|\text{vac}\rangle $$

is obtained as the self-consistent solution of an impurity model with a single interacting site. For the Holstein model (35), the impurity model is just the model of a single bosonic site (53) for $\Delta = 0$. If we assume a semi-circular density of states for the non-interacting problem, i.e. $A(\omega)$ has the functional dependence of Eq. (25) for $\epsilon_p = 0$, self-consistency is established by $A(\omega) = A_B(\omega)$. For a different non-interacting density of states this relation is more complicated, but the difference is not relevant in our context. We have shown in Sec. VII how a self-consistent calculation is performed. The complicated part of the DMFT calculation, to obtain $A(\omega)$ for the Hamiltonian (34) to given $A_B(\omega)$, is solved by an application of CSM.

In Fig. 9 we show $A(\omega)$ for two sets of parameters. For $\epsilon_p/W = 0.75$, a polaron has formed as a new quasiparticle, which results in several separated bands in $A(\omega)$. We also show the imaginary part of the DMFT selfenergy $\Sigma(\omega)$. In our example, it can be obtained in the form of a Green function

$$ \Sigma(\omega) = \langle \text{vac}|c_b(b(\omega - H_1)^{-1}b^\dagger c_\alpha)|\text{vac}\rangle, $$

where $H_1 = (1 - P_0)H(1 - P_0)$ is projected onto the subspace orthogonal to the boson vacuum $|\text{vac}\rangle$, i.e. $P_0 = |\text{vac}\rangle\langle\text{vac}|$. The projection guarantees that only irreducible diagrams contribute to $\Sigma(\omega)$. We calculate $\Sigma(\omega)$ once $A(\omega)$ is converged. When a polaron has formed, the polaron bands are separated by a pole in $\Sigma(\omega)$. Similar to Fig. 8 a pole close to a band has to be resolved, which requires high resolution. Note that $\text{Im}\Sigma(\omega)$ is zero for the lowest polaron band, where emission of a virtual phonon is energetically forbidden.

In Fig. 10 we show a calculation for a 1d chain. Since DMFT is constructed in the limit of high dimension, only
the basic features of polaron formation in 1d are correctly described. With CSM, this calculation could be extended to a cluster of bosonic sites, using one of the recently developed cluster extensions\textsuperscript{18} of DMFT.

**B. Comparison to the analytical solution**

For the Hamiltonian (34), hence for the DMFT-solution of the Holstein model (35), an explicit solution for the spectral function $A(\omega)$ can be obtained as a continued fraction\textsuperscript{20,21} (CF)

$$A(\omega) = \frac{1}{\omega - t^2 A_B(\omega) - \frac{\epsilon_p \omega_0}{\omega - \omega_0 - t^2 A_B(\omega - \omega_0) - 2 \epsilon_p \omega_0}}. \quad (38)$$

We can construct the CF from a formal Lanczos recursion. The recursion starts with the state $c^\dagger |\text{vac}\rangle$ and consecutively produces the states $(b^\dagger / \sqrt{n!}) c^\dagger |\text{vac}\rangle$, which form an orthonormal basis of the Hilbert space $\mathcal{H}_b$ of the bosonic impurity site. In this basis, the matrix of $H$ (Eq. (34)) is tridiagonal, and $A(\omega)$, which is the $(1,1)$-element of this matrix, can be expressed as a CF.

To treat the coupling to the bath in Eq. (34), we use Eq. (39). If the electron is in the bath, the states of the bosonic site evolve by the Hamiltonian $H_b^\omega = \omega_0 b^\dagger b$. In the $n^{th}$ level of the CF (38), which corresponds to the excitation of $n$ bosons, we must therefore insert $A_B(\omega)$ with energy shift $A_B(\omega - n \omega_0)$.

For this example, the (Lanczos) recursion leading to the CF creates every eigenstate of $\omega_0 b^\dagger b$ one by one. Otherwise, if eigenstates were mixed during the recursion, linear combinations $\sum_n w_n A_B(\omega - n \omega_0)$ would occur instead of $A_B(\omega - n \omega_0)$. The weight $w_n$ had to be determined during the recursion, and depended on the parameters. This is one of the many obstructions that prohibit a generalization of Eq. (38) to other models, e.g. with a cluster of interacting (bosonic) sites or different electron-phonon coupling. Within CSM these considerations are pointless, as its application does not rely on our ability to solve one part of the Hamiltonian prior to the actual calculation. Note also, that the general CS construction allows to calculate the groundstate and correlation functions that cannot be expressed in a form like (38).

**IX. TIME EVOLUTION OF A WAVE PACKET ON A CHAIN COUPLED TO LEADS**

In the preceding sections we used the CS construction for the calculation of spectral properties within CSM. It is an essential advantage of Chebyshev techniques, and the CS construction, that they can be easily adapted to new problems. In this section we treat the time evolution of a wave packet on a chain coupled to leads. To describe the coupling to a lead we can use the CS construction from Sec. III without change.

Within Chebyshev techniques, time evolution of a vector $|\psi(t)\rangle = e^{-iHt}|\psi(0)\rangle$ is determined from the Chebyshev expansion of the time evolution operator\textsuperscript{22}

$$e^{-iHt} = c_0 + 2 \sum_{n=1}^{\infty} c_n T_n(H). \quad (39)$$

The expansion coefficients are given by Bessel functions

$$c_n = \int_{-1}^{1} T_n(x)e^{-ixt} \frac{dx}{\pi \sqrt{1 - x^2}} = (-i)^n J_n(t), \quad (40)$$

where $J_n(t)$ denotes the Bessel function of order $n$. As usually, we omit the scaling of $H$. Since $J_n(t)$ decays rapidly for $n \gg t$, the infinite series can be truncated to obtain $|\psi(t)\rangle$ with high precision. An adequate choice for the number of moments is given by $N \gtrsim 1.5t$.

We apply the Chebyshev time evolution to the propagation of an electron along a chain of length $L$, which is coupled to a bath at site $L$. The chain geometry is identical to the example studied in Sec. III and the Hamiltonian is given by Eq. (25). The calculation of $T_n(H)|\psi(0)\rangle$ proceeds along the lines established in previous sections, and $|\psi(t)\rangle$ is obtained from Eqs. (39), (40).

At $t = 0$, we place a Gaussian wave packet of width $\sigma$ and momentum $K$ centered at site $m_0 = L/2$,

$$|\psi(0)\rangle \propto \sum_m e^{iKm} e^{-(m-m_0)^2/2\sigma^2} c^\dagger_m |\text{vac}\rangle, \quad (41)$$
(we omit normalization here), and let it evolve in time (see Fig. 11). Without a bath, the particle is reflected at the right end of the chain and returns, moving to the left.

We now add a bath to the right end, whose spectral function $A_B(\omega)$ is given by Eq. (25), with $W = 4t$. Since this is the spectral function of a half-infinite chain at its open end, also the full Hamiltonian $H$ describes a half-infinite chain. Physically, the open boundary at site $L$ is removed by coupling to an infinite lead. In contrast to the previous situation, the particle will not be reflected at site $L$, but propagates into the bath (or lead). As the middle panel in Fig. 11 shows, no spurious reflection occurs.

In the Hamiltonian $H$, sites $1 \ldots L$ are explicitly included while sites $\ge L+1$ of the lead are realized through the bath. In this way, we can use our Chebyshev approach to realize ‘transparent boundary conditions’ that mimic an infinite system with a finite number of lattice sites explicitly treated. Transparent boundary conditions are implemented in Refs. 23,24 by a modification of time propagation algorithms like e.g. Crank-Nicholson. Within the CS construction, modified boundary conditions are implemented independently of the actual calculation. For time propagation we use the same Eqs. (14) – (16) as for the calculation of spectral properties. This permits us to use a variety of algorithms, like we used Lanczos algorithm in Sec. VIII. We could also use the CS in combination with Crank-Nicholson, but for the time-independent Hamiltonians considered here Chebyshev time propagation is most efficient.

Transparent boundary conditions correspond to a particular choice for $A_B(\omega)$. We have the freedom to choose any $A_B(\omega)$. For example, if $A_B(\omega)$ is the spectral function of a 300 site chain at its end, and $L = 700$, $H$ describes a chain of length $L + 300 = 1000$. As before, the particle is reflected and returns moving to the left (see bottom panel in Fig. 11 in comparison to the top panel). The point is that the reflecting barrier is now realized through a bath with carefully chosen $A_B(\omega)$, and not by lattice sites 701...L explicitly included in the Hamiltonian. We might call these ‘reflecting boundary conditions’.

For Fig. 12 we slice the chain in two parts which are connected by a bath. Similar to the previous example, the bath shall replace a finite segment of the chain. Since the bath has now two entry points – at its junction to the left and to the right part of the chain –, this example involves off-diagonal bath spectral functions. Let $d_{t/2}^{(1)}$ denote the operators to the two entry points. Following Sec. III we need two different types of Chebyshev vectors $|n_b\rangle = T_n(H_B)d_t^{(b)}|\text{vac}\rangle$ for $b = 1, 2$. Eq. (16) generalizes to $d_{n}\langle n_b\rangle = \mu_{n}^{(b, ab)}|\text{vac}\rangle$, where the four different types of moments $\mu_{n}^{(b, ab)}$ correspond to the four different spectral function characterizing the bath: The diagonal $A_{1,1}^{B}(\omega)$, $A_{2,2}^{B}(\omega)$ for moving into the bath and back, and the off-diagonal $A_{1,2}^{B}(\omega)$, $A_{2,1}^{B}(\omega)$ for moving through the bath. The latter ones give the energy-dependent transmission rate through the bath. Only for non-zero $A_{1,2}^{B}(\omega)$, $A_{2,1}^{B}(\omega)$, the bath connects the two parts of the chain. In Fig. 12 the spectral functions of the bath are those of a finite chain segment. We see how the wave moves into the bath at its left side, passes through and remerges at the right site. The bath perfectly mimics the transmission through a chain segment. As we noted above, we have the freedom to change the behavior by a different choice.
of the bath spectral functions $A^B_{\alpha\beta}(\omega)$.

X. SUMMARY AND OUTLOOK

In this article we introduced the Chebyshev space method (CSM) for the treatment of degrees of freedom with non-trivial dynamics. In our examples the degree of freedom is given by the operator $d^\dagger$ which creates a fermion in a bath, and the dynamics of $d^\dagger$ is specified by a spectral function $A_B(\omega)$. We demonstrated for various examples, how CSM yields extremely accurate results with modest computational effort. For the example in Secs. IV B, VIII the computational effort is even independent of the geometry or dimension.

A particular advantage of the Chebyshev space (CS) construction is that it still provides a Hamiltonian $H_B$ acting on a Hilbert space, albeit it is an abstract space without a direct physical counterpart. We can use this form of $H_B$ in different situations, like in the Lanczos algorithm or for time propagation. We have therefore obtained a numerically exact Hamiltonian treatment of degrees of freedom with non-trivial dynamics, which does not rely on a discretization of spectral functions. To the best of our knowledge, this has been achieved for the first time.

The concept of a CS and an ancillary Hamiltonian $H_B$ acting on this space is very general. It makes no assumption about the Hamiltonian $H_S$ for the quantum system, and can be extended to various problems mentioned in the introduction. We have obtained preliminary results for the Holstein model within cluster extensions of DMFT, but the issue needs further exploration from the physical point of view.

An especially important topic is the extension to interacting fermions at finite density, or to bosonic baths. With a single fermion, the bath is in the vacuum state (vac) if the fermion is removed by application of the operator $d$. This simplification is no longer true for finite fermion density, when adding and removing a fermion creates particle-hole pairs in the bath, which initially was prepared as the particle-hole vacuum (or Fermi sea). We have derived a formalism that deals with particle-hole pairs in the context of CSM. The CS construction is used in this formalism without change. A similar formalism for bosonic baths can be derived. As a first result, this formalism allows for the calculation of the core level spectral function in the X-ray absorption problem. The spectral function can be calculated exactly in this case. It is equivalent to the Anderson model with one immobile spin species, but the extension to the full Kondo problem is much harder. The presentation of this formalism is left for a future publication.

The CS construction can be also used in the context of (diagrammatic) Green function techniques. Any Feynman diagram contains energy-dependent Green functions which represent a degree of freedom with non-trivial dynamics. The difficult task is to sum up a huge number of Feynman diagrams. Note that we can interpret the self-consistent calculation of the Holstein model in Sec. VIII as the exact summation of a certain class of Feynman diagrams. The bosonic impurity model defines a set of skeleton diagrams for this problem, and imposing self-consistency corresponds to replacing bare Green functions (‘thin lines’ in a diagram) by renormalized Green functions (‘thick lines’). In this example, diagrams are selected by a geometric rule, but with some modifications a different selection rule can be implemented. The CSM provides the link between exact numerical techniques for Hamilton operators, and general approximation schemes for Green functions.

In conclusion, we believe that the CSM introduced in this work is a powerful addition to existing numerical techniques in theoretical physics or chemistry. It substantially enlarges the field of applications of Chebyshev techniques and keeps their advantages. The results we obtained in this work are promising for successful applications to more complicated problems, and the possible combination of CSM with other techniques shall prove fruitful. The further development of CSM and its application to the study of physical problems mentioned in the introduction is the subject of current research.

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APPENDIX A: CHEBYSHEV EXPANSIONS AND THE KERNEL POLYNOMIAL

In this article we repeatedly approximate a function $f : [-1,1] \rightarrow \mathbb{R}$ by a finite Chebyshev series

$$f_N(x) = \frac{1}{\pi\sqrt{1-x^2}} \left[ \mu_0 + 2 \sum_{n=1}^{N-1} \mu_n T_n(x) \right], \quad (A1)$$

where the moments $\mu_n$ are given by

$$\mu_n = \int_{-1}^{1} f(x) T_n(x) \, dx. \quad (A2)$$

A central question is how good $f(x)$ is approximated by $f_N$. Functional analysis teaches us that the $f_N$ converge to $f$ in the integral norm

$$\|f(x) - f_N(x)\| = \left[ \int_{-1}^{1} \frac{(f(x) - f_N(x))^2}{\pi\sqrt{1-x^2}} \, dx \right]^{1/2} \quad (A3)$$

corresponding to the scalar product used in (2), provided $\|f(x)\|$ is finite. For practical purposes, this convergence property is too weak, and we demand uniform or at least pointwise convergence. We do not try to resolve the issue of convergence here, but state that for sufficiently smooth $f(x)$ the series $f_N$ will converge uniformly to $f$ on any closed sub-interval of $[-1,1]$ that excludes the end-points $\pm 1$. Convergence at the end-points is of
course spoiled by the divergence of the weighting function \((1 - x^2)^{-1/2}\).

In physical applications, we want to expand spectral functions which are not necessarily continuous, and perhaps contain some \(\delta\)-peaks due to (quasi-) particle states with infinite lifetime. In this case, the series cannot converge uniformly, otherwise its limit \(f\) had to be continuous itself, but the situation is even worse. The infamous Gibbs phenomenon ruins convergence at all: In plain words, the series (A1) fails to converge in the vicinity of a discontinuity, e.g., a jump of the function, instead shows rapid oscillations whose height does not decrease as the number of terms \(N \to \infty\). The Gibbs phenomenon is a severe obstacle for practical applications.

Fortunately, the problem arising from the Gibbs phenomenon is solved for Chebyshev expansions. It is possible to specify, prior to the calculation of the \(\mu_n\), a set of attenuation factors \(g_n\), \(n = 0, \ldots, N - 1\) for every \(N\), such that the modified approximants

\[
\tilde{f}_N = \frac{1}{\pi \sqrt{1 - x^2}} \left[ g_N \mu_0 + 2 \sum_{n=1}^{N-1} g_n \mu_n T_n(x) \right] \quad (A4)
\]

do not show the Gibbs phenomenon but approximate a wide class of functions in a favourable way. Plainly spoken, the attenuation factors damp out high frequency oscillations that otherwise lead to spurious results in the finite series. Instead of a more precise formulation we show an example in Fig. 13. The best choice in many cases are factors \(g_n\) derived from the so-called Jackson kernel (A5), leading to the explicit expression

\[
g_n = \frac{(N - n + 1) \cos \frac{\pi n}{N+1} + \sin \frac{\pi n}{N+1} \cot \frac{\pi n}{N+1}}{N+1}. \quad (A5)
\]

Modifying moments with these attenuation factors is related to convolution with an almost Gaussian peak of width \(\sigma = \pi/N\) (cf. Ref. [2]). An important property of the modification with these attenuation factors is that the modified approximants \(\tilde{f}_N\) are positive whenever the function \(f\) is. This is not true for the unmodified approximants (cf. Fig. 13). Besides Eq. (A5), other suggestions for attenuation factors exist, see Ref. [3] for a different choice in the context of Green functions, with an application in Ref. [4].

Note that the factors \(g_n\) in Eq. (A5) have the property that \(g_n \to 1\) for \(N \to \infty\). We can therefore always use the attenuation factors \(g_n\) without losing information. For functions with discontinuities multiplication with attenuation factors enforces the decay of moments relevant for good approximation properties. For smooth \(f(x)\) the moments itself decay rapidly, and multiplication with the attenuation factors does not change the result for not too small \(N\).

The introduction of attenuation factors is the essence of the kernel polynomial method (KPM). Within KPM resolution for spectral functions is already obtained with a fairly small number of moments, thus allowing for accurate calculations with moderate demands on computational time or memory. The possible resolution is much better than known e.g., from the Lanczos algorithm where peaks are commonly broadened by a Lorentzian function. Furthermore, the resolution of the Chebyshev expansion is uniform over the energy interval, and does not deteriorate towards the center of the spectrum.

**APPENDIX B: DETERMINANTS AND TWO-TERM RECURRENCES**

We formulate a well-known determinant identity related to two-term recurrences. Define, for each \(n\) and given \(a_j, b_j, c_j\), a tridiagonal \(n \times n\)-matrix

\[
A_n = \begin{pmatrix} a_1 & c_1 \\ b_1 & a_2 & c_2 \\ & \ddots & \ddots & \ddots \\ & & a_{n-2} & c_{n-2} \\ & & b_{n-2} & a_{n-1} & c_{n-1} \\ & & & b_{n-1} & a_n \end{pmatrix}. \quad (B1)
\]

Expanding in the last row yields

\[
det A_n = a_n \det A_{n-1} - b_{n-1} c_{n-1} \det A_{n-2}. \quad (B2)
\]
From this relation it follows that the characteristic polynomials \( \chi_n = \det(x - A_n) \) obey the two-term recurrence
\[
\chi_0 = 1, \quad \chi_1 = x - a_1, \\
\chi_{n+1} = (x - a_{n+1})\chi_n - b_n c_n \chi_{n-1}.
\] (B3)

Conversely, for polynomials \( P_n \) defined by a two-term recurrence
\[
P_0 = 1, \quad P_1 = a_1 x, \quad P_n = a_n x P_{n-1} - b_{n-1} P_{n-2},
\] (B4)
this result implies that
\[
P_n = \det\begin{pmatrix}
  a_1 x & d_1 & \\
  c_1 & a_2 x & d_2 & \\
  & c_2 & a_3 x & d_3 & \\
  & & c_3 & a_4 x & \\
  & & & \ddots & \\
\end{pmatrix},
\] (B5)
where \( c_n, d_n \) is chosen in such a way that \( c_n d_n = b_n, \) e.g. for positive \( b_n \) we may choose \( c_n = d_n = \sqrt{b_n}. \) By multiplying the \( j^{th} \) column – or equivalently, \( j^{th} \) row – by \( 1/a_j, \) \( P_n \) can be expressed as the characteristic polynomial of a tridiagonal matrix times a prefactor \( \prod_{j=1}^n a_j. \)

In particular, the Chebyshev polynomials fulfill
\[
T_n(x) = \det\begin{pmatrix}
  x & 1 & \\
  1 & 2x & 1 & \\
  & 1 & 2x & \\
  & & \ddots & \\
\end{pmatrix}.
\] (B6)
Multiplying the second to the last column by \( 1/2, \) we find the result \( T_M(x) = 2^{M-1} \det(x - H_B^M) \) used in the main text.

**APPENDIX C: HERMITICITY OF \( H_B \)**

We first prove that \( H_B \) is hermitian by calculating explicitly that \( H_B \) is equal to its adjoint. The product of two Chebyshev polynomials satisfies the identity \( ^* \)
\[
T_m(x)T_n(x) = (T_{m+n}(x) + T_{m-n}(x))/2.
\] (C1)
For notational convenience, we define here \( T_{-n}(x) = T_n(x). \) It follows for Chebyshev vectors \( |n\rangle = T_n(H_B)|0\rangle \) that
\[
\langle m|n\rangle = (\mu_{m+n}^B + \mu_{m-n}^B)/2,
\] (C2)
where we again define \( \mu_{m,n}^B = \mu_{n,m}^B. \) The scalar product of two vectors \( |a\rangle = \sum_{n=0}^\infty a_n |n\rangle, \) \( |b\rangle = \sum_{n=0}^\infty b_n |n\rangle \) given as linear combinations of Chebyshev vectors is now found as
\[
\langle b|a\rangle = \sum_{m,n=0}^\infty b_m^* a_n (\mu_{m+n}^B + \mu_{m-n}^B)/2.
\] (C3)
Since \( \mu_{m,n}^B = \mu_{n,m}^B, \) with the notational convention adopted above, we have \( \langle a|b\rangle = \langle b|a\rangle^*, \) as it must be (note that the moments are real).

To calculate a scalar product with \( H_B \) we use that
\[
H_B|a\rangle = \frac{1}{2} \sum_{n=0}^\infty a_n (|n-1\rangle + |n+1\rangle),
\] (C4)
where the summand for \( n = 0 \) is \( a_0 (|1\rangle + |1\rangle)/2 = a_0 |1\rangle \) in accordance with Eq. (20). Inserting this equation we find
\[
\langle b|H_B|a\rangle = \frac{1}{2} \sum_{m,n=0}^\infty b_m^* a_n (\langle m|n-1\rangle + \langle m|n+1\rangle)
= \frac{1}{4} \sum_{m,n=0}^\infty b_m^* a_n (\mu_{m+n+1}^B + \mu_{m-n+1}^B)
+ \mu_{m+n+1}^B + \mu_{m-n-1}^B.
\] (C5)
We can condense this equation to matrix-vector form
\[
\langle b|H_B|a\rangle = \frac{1}{4} \sum_{m,n=0}^\infty b_m^* a_n M_{mn},
\]
\[
M_{mn} = \mu_{m+n+1}^B + \mu_{m-n+1}^B + \mu_{m+n+1}^B + \mu_{m-n-1}^B.
\] (C6)
Since \( M_{mn} \) depends only on the sum and difference of \( m, n, \) \( M_{mn} = M_{nm} = M_{m,n}^* \) (the moments are real, and \( \mu_{m,n}^B = \mu_{n,m}^B \) ). It follows that \( \langle b|H_B|a\rangle = \langle a|H_B|b\rangle^* \), and \( H_B \) is hermitian.

We derived the hermiticity of \( H_B \) without imposing any constraint on the moments. This may be a bit puzzling, because the moments should correspond to a non-negative spectral function \( A_B(\omega) \) if \( H_B \) is hermitian. The puzzle is resolved by observing that the scalar product \( \langle C3 \rangle \) has to be positive (semi-) definite. This requirement imposes constraints on the moments that are equivalent to a non-negative \( A_B(\omega) \). To mention one, \( \langle n|n\rangle = (\mu_0^B + \mu_{2n}^B)/2, \) so it must \( \mu_0^B \geq \mu_{2n}^B \). Consider for example \( H_B = 0, \) equivalent to \( A_B(\omega) = \delta(\omega) \). We then have \( \mu_{2n}^B = (-1)^n, \mu_{2n+1}^B = 0, \) i.e. equality holds in this inequality. The scalar product \( \langle C3 \rangle \) is positive semi-definite, but not positive definite, as \( \langle n|n\rangle = 0 \) and \( \langle n|n\rangle = 0 \) for odd \( n \).

We can characterize the properties of the scalar product \( \langle C3 \rangle \) better, if we consider Chebyshev expansions
\[
f(x) = \sum_{m=0}^\infty f_m T_m(x), \quad g(x) = \sum_{m=0}^\infty g_m T_m(x)
\] (C7)
of functions \( f, g : [-1,1] \to \mathbb{R} \), and the associated vectors
\[
|f\rangle = \sum_{m=0}^\infty f_m |m\rangle, \quad |g\rangle = \sum_{m=0}^\infty g_m |m\rangle
\] (C8)
in \( \mathcal{H}_c. \) With Eqs. \( \langle C1 \rangle, \langle I \rangle \) we find for \( A_B(\omega) \) as in Eq. \( \langle I \rangle \)
\[
\int_{-1}^1 T_m(x) T_n(x) A_B(x) dx = (\mu_{m+n}^B + \mu_{m-n}^B)/2,
\]
in \( \mathcal{H}_c. \)
which implies
\[ \int_{-1}^{1} f(x)g(x) A_B(x) \, dx = \langle f | g \rangle. \quad (C9) \]

The scalar product \((C3)\) in \(H\), therefore corresponds to a scalar product of functions \([-1, 1] \rightarrow \mathbb{R}\), given as the integral on the left hand side of this equation. We conclude, that for continuous \(A_B(\omega)\) the scalar product \((C3)\) is positive semi-definite (positive definite) if and only if \(A_B(\omega) \geq 0\) (and \(A_B(\omega)\) does not vanish on an open interval).

We discussed in App. [A] that a truncated, finite Chebyshev expansion of \(A_B(\omega)\) may fail to be positive although \(A_B(\omega)\) is. Positivity of the finite Chebyshev expansion is ensured by using attenuation factors of a positive kernel like in Eq. \((A5)\). To obtain a positive definite scalar product \((C3)\) for a finite Chebyshev expansion we must therefore use modified moments \(\mu_n^B, g_m^B\) instead of unmodified moments \(\mu_n, g_m\). For the Lanczos algorithm, used in Sec. VIII which aims at constructing an orthonormal basis in Krylov-subspaces, positive definiteness of \((C3)\) is crucial. For the calculation of spectral or dynamical properties it is not that essential. But we learned in App. [A] that the modification of moments by attenuation factors never ruins a result. Hence our recommendation is to always modify the moments \(\mu_n^B\) put into the calculation with attenuation factors.

**APPENDIX D: EIGENSTATES OF \(H_B^M\)**

According to App. [B] the characteristic polynomial of \(H_B^M\) (Eq. \((29)\)) is det\([x - (H_B^M)_{mn}] = 2^{-i(M-1)}T_M(x)\). The \(M^{th}\) Chebyshev polynomial \(T_M(x) = \cos(M \arccos x)\) has \(M\) distinct real roots
\[ x_j = \cos \left( \frac{\pi(j-1/2)}{M} \right), \quad j = 1, \ldots, M. \quad (D1) \]

We concluded in Sec. [V] that \(H_B^M\) is diagonalizable with real eigenvalues \(x_j\). The eigenstates of \(H_B^M\) can be given explicitly, using the recurrence \((1)\). The state
\[ |\phi_j\rangle = |0\rangle + 2 \sum_{m=1}^{M-1} T_m(x_j) |m\rangle \quad (D2) \]
is the eigenstate of \(H_B^M\) to eigenvalue \(x_j\), i.e. \(H_B^M |\phi_j\rangle = x_j |\phi_j\rangle\). If we use Eq. \((29)\) to calculate \(H_B^M |\phi_j\rangle\), we find that the term proportional to \(T_M(x_j)\) drops out, because \(x_j\) is a root of \(T_M(x)\). This explains why the roots of \(T_M(x)\) occur as eigenvalues of \(H_B^M\).

Scalar products of the states \(|\phi_j\rangle\) have to be calculated using Eq. \((C3)\). It turns out, that the \(|\phi_j\rangle\) are not orthogonal to each other. Indeed, while \(H_B\) is hermitian, the truncated \(H_B^M\) is not hermitian. If one repeats the calculations leading to Eq. \((C3)\), now with upper summation boundary \(M - 1\) instead of \(\infty\), one finds that a term \(a_{M-1} |M\rangle\) is missing, and the scalar product is not symmetric in \(|a\rangle, |b\rangle\). The mathematical reason that \(H_B^M\) fails to be hermitian, is that \(H_B^M\) is obtained from \(H_B\) via a non-orthogonal projection. Working with a non-hermitian operator could in principle spoil the calculation for \(M < N\). We found in Sec. [V] that this does not happen. By an explicit calculation of the spectral function encoded by \(H_B^M\), we now show that the non-hermiticity of \(H_B^M\) has no (negative) consequences.

As Fig. [5] shows, for \(N \gg M\) CSM resolves \(M\) poles in the spectral function encoded by \(H_B^M\). The position of the poles is determined by \(x_j\), and their weight \(w_j\) can be calculated using the eigenstates \(|\phi_j\rangle\). We first expand the \(0^{th}\) Chebyshev vector \(|0\rangle\) in the \(|\phi_j\rangle\). With the identity
\[ \frac{1}{M} \sum_{j=1}^{M} T_m(x_j) T_n(x_j) = \begin{cases} \frac{1}{2} \delta_{m,n} & , & m, n \neq 0 \\ 1 & , & m = n = 0 \end{cases}, \]
which is a kind of discrete orthogonality relation for Chebyshev polynomials, we find that
\[ |0\rangle = \frac{1}{M} \sum_{j=1}^{M} |\phi_j\rangle. \quad (D4) \]
The coefficients in this linear combination are \(T_0(x_j) = 1\). Now \(\delta(\omega - H_B^M) |\phi_j\rangle = \delta(\omega - x_j) |\phi_j\rangle\), and we obtain
\[ \langle 0 | \delta(\omega - H_B^M) |0\rangle = \sum_{j=1}^{M} w_j \delta(\omega - x_j), \quad (D5) \]
with the weight of each pole given by
\[ w_j = \frac{1}{M} \langle 0 | \delta(\omega - H_B^M) |0\rangle = \frac{1}{M} \left[ \mu_B^0 + 2 \sum_{m=1}^{M-1} T_m(x_j) \mu_m^B \right] \]
\[ = \frac{\pi}{M} \sqrt{1 - x_j^2} A_B(x_j). \quad (D6) \]
The first line in this equation follows from the definition \((D2)\), the second line from comparison with Eq. \((4)\). Here \(A_B(\omega)\) is assumed as an expansion with \(M\) Chebyshev moments, in accordance with the truncation of \(H_B^M\). The weight \(w_j\) of the pole at \(x_j\) is therefore the value of \(A_B(\omega)\) at the position of the pole, weighted by the inverse \((1 - x_j^2)^{1/2}\) of the weighting function for Chebyshev expansions (and with \(1/M\) for \(M\) poles). Using the attenuation factors from Eq. \((A5)\), \(A_B(\omega)\) is positive, which implies that the weight \(w_j\) of each pole is positive. The total weight is
\[ \sum_{j=1}^{M} w_j = \langle 0 | \frac{1}{M} \sum_{j=1}^{M} |\phi_j\rangle = \langle 0 | 0 \rangle = \mu_0^B = 1, \quad (D7) \]
according to the sum rule \(\mu_0^B = \int_{-1}^{1} A_B(x) \, dx = 1\). This result also follows with the explicit expression for \(w_j\) in terms of the \(\mu_m^B\) (first line of Eq. \((D6)\)), and Eq. \((D3)\). If we express \(w_j\) by \(A_B(\omega)\) (second line of Eq. \((D6)\)), we find...
a nice relation to quadrature formulas from numerical integration. In the expression for the total weight
\[ \sum_{j=1}^{M} w_j = \frac{\pi}{M} \sum_{j=1}^{M} \sqrt{1-x_j^2} A_B(x_j), \quad (D8) \]
the right hand side is the formula for Gauss-Chebyshev integration of a function, with abscissas at \( x_j \). Now \( A_B(\omega) \), expanded with \( M \) Chebyshev moments, is a polynomial of order \( M \) times the weighting function \((1-x^2)^{-1/2}\). The Gauss-Chebyshev integration formula is exact in this case, and we find once again
\[ \sum w_j = \int_{-1}^{1} A_B(x)dx = 1. \]

We can finally understand why \( H_B^M \) is non-hermitian using the scalar product Eq. (C9). A state \(|\phi_j\rangle\) corresponds to the function
\[ \phi_j(x) = T_0(x_j)T_0(x) + 2 \sum_{m=1}^{M-1} T_m(x_j)T_m(x) \quad (D9) \]
which is the \( M^{th} \) Chebyshev approximation to \( \delta(x-x_j) \). With a finite number of moments, \( \phi_j(x) \) has finite width. Using Eq. (C9) for the scalar product,
\[ \langle \phi_j|\phi_k \rangle = \int_{-1}^{1} \phi_j(x)\phi_k(x)A_B(x)dx, \quad (D10) \]
we see that the integral is non-zero even for \( j \neq k \), since the two functions \( \phi_j(x), \phi_k(x) \) have finite overlap. The deviation of \( H_B^M \) from hermiticity is therefore an effect of finite resolution of a finite Chebyshev expansion. The larger \( M \), the smaller is the overlap and hence the scalar product. We conclude that in the limit \( M \to \infty \), the states \(|\phi_j\rangle\) are mutually orthogonal, in accordance with hermiticity of \( H_B \) proved in App. [C].

We have obtained two important results in this Appendix. First, despite its non-hermiticity, \( H_B^M \) encodes a positive, normalized spectral function. Using the truncated \( H_B^M \), as in Sec. [X] for \( M < N \), does therefore not lead to erroneous results. Second, we related the CS construction for \( H_B \) to an explicit representation Eq. (7). In particular, Eq. (D10) shows how to obtain from given moments \( \mu_m^B \) a discretization (Eq. (12)) of \( A_B(\omega) \) (the opposite way is given by Eq. (5)). The point is that the CS construction indicates how to discretize a given \( A_B(\omega) \) to prescribed resolution. Within CSM we can work without a discretization anyway. The reader should note that the CS construction is no longer equivalent to the discretization of \( A_B(\omega) \) in the extensions of CSM mentioned in the Summary (Sec. [X]).

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