

## Adaptive Lanczos-vector method for dynamic properties within the DMRG

P. E. Dargel,<sup>1</sup> A. Honecker,<sup>1</sup> R. Peters,<sup>2</sup> R. M. Noack,<sup>3</sup> and T. Pruschke<sup>1</sup>

<sup>1</sup>*Institut für Theoretische Physik, Georg-August-Universität Göttingen, 37077 Göttingen, Germany*

<sup>2</sup>*Department of Physics, Kyoto University, Kyoto 606-8502, Japan*

<sup>3</sup>*Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany*

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Current widely-used approaches to calculate spectral functions using the density-matrix renormalization group in frequency space either necessarily include an artificial broadening (correction-vector method), have limited resolution (time-domain density-matrix renormalization group with Fourier transform method), or are limited to low-energy properties or single dominant modes (original continued fraction method). Here we propose an adaptive Lanczos-vector method to calculate the coefficients of a continued fraction expansion of the spectral function iteratively. We show that one can obtain a very accurate representation of the spectral function very efficiently, and that one can also directly extract the spectral weights and poles for the discrete system.

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Dynamical quantities such as the local density of states, the single-particle spectral weight, or the dynamical spin or charge correlation functions are of central importance in theoretical and experimental condensed matter physics. Since electrons in solids are interacting quantum objects, a reliable calculation of their properties usually has to resort to numerical approaches. The density-matrix renormalization group (DMRG)<sup>1</sup> is one such algorithm. Within the DMRG, the calculation of dynamical quantities is a considerable challenge. A first attempt by Hallberg was based on a continued fraction expansion (CFE).<sup>2</sup> Subsequently, Kühner and White showed that this approach is suitable, “if only the low-energy part of the correlation function is of interest, or if the bulk of the weight is in one single peak”,<sup>3</sup> and applied the correction vector method,<sup>3,4</sup> which since then has successfully been applied to many model systems.<sup>5,6</sup> However, this approach has the drawback that one needs to introduce an artificial broadening into the spectra, which can be viewed as convolution of the true spectral function with a Lorentzian of width  $\eta$ . As one is eventually interested in the limit  $\eta \rightarrow 0$ , one has to “deconvolute” the spectrum at the end of the calculation. This is, like analytic continuation of Monte-Carlo data, a numerically ill-defined procedure.<sup>6</sup> Furthermore, the calculation of the correction vector at every step of the DMRG is very time-consuming and the frequencies that one can address are limited. Another popular approach to calculating spectral functions is to Fourier-transform time-dependent DMRG data.<sup>7</sup> To obtain good frequency resolution, one has to calculate time-domain data over a long time interval. However, accessing long time scales is limited by either a loss of accuracy due to the approximate nature of the DMRG, or by finite-size effects such as reflections from open ends. A method that can resolve spectral features with high resolution and no artificial broadening is therefore desirable. Here we present an adaptive Lanczos-vector method (ALM) that takes advantage of the CFE used in Ref. 2, but gains efficiency by adapting the basis as in adaptive time evolution.

The spectral function for the operators  $\hat{A}$  and  $\hat{B}$  is  $2\pi i \rho_{\hat{A},\hat{B}}(\omega) = G_{\hat{A},\hat{B}}(\omega + i0^+) - G_{\hat{A},\hat{B}}(\omega - i0^+)$ , where  $G_{\hat{A},\hat{B}}(z)$  denotes the zero-temperature Green’s function. Here we will take  $\hat{B} = \hat{A}^\dagger$ , yielding

$$G_{\hat{A},\hat{A}^\dagger}(z) =: G_{\hat{A},\hat{A}^\dagger}^{(1)}(z) - s \cdot G_{\hat{A}^\dagger,\hat{A}}^{(2)}(z) \quad (1)$$

$$G_{\hat{X},\hat{Y}}^{(1/2)}(z) = \langle \psi_0 | \hat{X} \frac{1}{z \mp (\hat{H} - E_0)} \hat{Y} | \psi_0 \rangle,$$

where  $|\psi_0\rangle$  is the ground state of Hamiltonian  $\hat{H}$ ,  $E_0$  is the ground-state energy, and  $s = +1/-1$  when  $\hat{A}$  is a bosonic/fermionic operator. One of several ways to represent the resolvent in Eq. (1) is the CFE<sup>2,8</sup>

$$G_{\hat{A},\hat{A}^\dagger}^{(1)}(z) = \frac{\langle \psi_0 | \hat{A} \hat{A}^\dagger | \psi_0 \rangle}{z - a_0 - \frac{b_1^2}{z - a_1 - \frac{b_2^2}{z - \dots}}}, \quad (2)$$

with a similar expression for  $G_{\hat{A}^\dagger,\hat{A}}^{(2)}$ . The coefficients  $a_i, b_i$  of this CFE can be calculated using the recursion formula

$$|f_0\rangle = \hat{A}^\dagger |\psi_0\rangle, \quad |f_{n+1}\rangle = H |f_n\rangle - a_n |f_n\rangle - b_n^2 |f_{n-1}\rangle$$

$$a_n = \langle f_n | H | f_n \rangle / \langle f_n | f_n \rangle,$$

$$b_n = \langle f_n | f_n \rangle / \langle f_{n-1} | f_{n-1} \rangle, \quad b_0 = 0, \quad (3)$$

which is essentially the one used in the Lanczos method, but with starting vector  $|f_0\rangle$  replacing a random vector. Thus, we will call the  $|f_i\rangle$  Lanczos vectors in the following. Hallberg<sup>2</sup> used the CFE (2) and the recursion formulae (3) to obtain spectral functions via a multi-target DMRG, i.e., by optimizing the DMRG basis for the ground state and the Lanczos states simultaneously.

The structure of the recursion formula (3) suggests implementing an iterative method to calculate the Lanczos vectors in the DMRG that optimizes the basis for only the three Lanczos vectors needed at each recursion step. One initially calculates the ground state  $|\psi_0\rangle$  of the system to the desired accuracy with the usual DMRG algorithm.

One then performs single finite-system sweeps, simultaneously targeting the additional vectors  $|f_0\rangle$  and  $|f_1\rangle$ , from which one can evaluate  $a_0$ ,  $a_1$ , and  $b_1$ . The recursion proceeds by replacing  $|\psi_0\rangle$ ,  $|f_0\rangle$ , and  $|f_1\rangle$  by  $|f_0\rangle$ ,  $|f_1\rangle$ , and the new vector  $|f_2\rangle$ . At this point, a technical subtlety arises:  $|f_0\rangle$  and  $|f_1\rangle$  cannot be recalculated because there is no longer a condition to optimize them. Instead, we transform the wave function from the previous finite-size DMRG step to the new superblock configuration<sup>9</sup> at every step of the DMRG sweep. One DMRG sweep through the system thus suffices to calculate the Lanczos vector  $|f_i\rangle$  and the parameters  $a_i$  and  $b_i$ . As one needs to target only three Lanczos vectors simultaneously, the number  $m$  of basis states necessary to obtain an accurate representation is generally substantially smaller than in the original algorithm.<sup>2</sup> We will come back to this point later. Here we emphasize only that we avoid calculating the ground state at each DMRG step, speeding up the calculation dramatically; the most time-consuming part left in the Lanczos iteration is now the diagonalization of the reduced density matrix needed to initialize the next DMRG step. After iterating the recursion relation often enough, one obtains a sequence  $\{(a_i, b_i)\}$  from which one can calculate the Green's function, Eq. (2).

We test the method on a model of spinless fermions on a chain with Hamiltonian

$$\hat{H} = - \sum_i \left( c_{i+1}^\dagger c_i + c_i^\dagger c_{i+1} \right) + U \sum_i n_i n_{i+1},$$

where  $c_i^{(\dagger)}$  denotes the usual creation (annihilation) operators for an electron at site  $i$ , and  $n_i$  denotes the occupation number operator. Here we take  $A = \hat{c}_i$  and calculate the spectral function  $\rho(x = i, \omega)$  at the center of the chain for a system at half filling. In Fig. 1, we compare the original (OLM) and the ALM implementation of the CFE with the exact solution on a chain of length  $L = 40$  in the free-fermion limit,  $U = 0$ . Both implementations do not give a clear hint as to when to stop the Lanczos iteration. We have evaluated the broadened spectral functions after 200 Lanczos iterations, see below. Following Kühner and White,<sup>3</sup> we do not target all Lanczos vectors in the OLM but only a small fraction of them. We then calculate the remaining vectors by straightforward application of the recursion. To achieve good convergence of the DMRG, we assign a weight of 0.5 to the ground state and equal weights to the other Lanczos vectors (one could also give them weights according to their spectral weights). This large freedom, especially in choosing the number of targeted Lanczos states, is in our view a disadvantage of the OLM, as the optimal parameters are not obvious, and the results depend on their choice. Employing the truncation error as measure of the quality of the spectral function is also not possible, as it depends only on the number of targeted states and their weights.

In Fig. 1 we have used  $m = 1500$ , 25 sweeps, and eleven target states, yielding a maximum truncation error of  $10^{-6}$ . There is no way to determine the quality of the

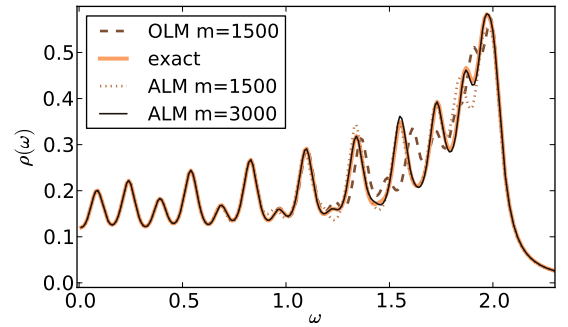


FIG. 1. (Color online) Broadened spectral function for spinless fermions ( $L = 40, U = 0, \eta = 0.05$ , 200 Lanczos vectors) calculated with the new adaptive implementation (ALM), the original implementation (OLM) and compared to the exact solution. The DMRG truncation number is given by  $m$ .

representation of the following Lanczos states (one can only check their orthogonality), but if we would have tried to target all Lanczos states, the truncated weight would have been much higher than  $10^{-6}$ . In addition, the convergence is unstable, as small changes in the first Lanczos vectors will lead to bigger changes in subsequent Lanczos vectors.

In the ALM, we can increase the number of states during the Lanczos iteration, as we do not need to calculate the ground state at each step. We notice that the number of states needed for a good representation of Lanczos vectors increases with the number of iterations desired. For  $m = 1500$ , the maximum truncation error per sweep for the ALM increases from  $10^{-15}$  (ground state and first two Lanczos vectors) to  $10^{-4}$  for the last three Lanczos vectors. As already noted for the OLM,<sup>3</sup> the low-energy portion ( $\omega \lesssim 1$ ) is well-reproduced by both methods. Deviations occur in the high-energy part of the spectrum, notably in both position and weight distribution for the OLM. Here the ALM already shows much better agreement with the exact solution for  $m = 1500$ . Increasing to  $m = 3000$  for the Lanczos iterations in the ALM, one almost perfectly reproduces the exact solution. Note that  $m = 1500$  is the maximum number of states accessible in the OLM with our computational resources; the simultaneous optimization of the ground state and all other Lanczos states prevents calculations with larger  $m$ .

Another advantage of the ALM is its shorter run-time. For  $m = 1500$  our calculations used  $\approx 30h$  on a standard workstation for the ALM and  $\approx 90h$  for the OLM. We emphasize, however, that the run-time is determined by several parameters and thus should be interpreted with some care. For example, the ALM scales linearly with the number of Lanczos iterations, whereas the original implementation is roughly independent of the iteration number. The run-time of the latter, however, strongly depends on the number of Lanczos states targeted, because more target states increase the number of DMRG sweeps needed to achieve convergence.

Since the CFE gives an analytical expression for the

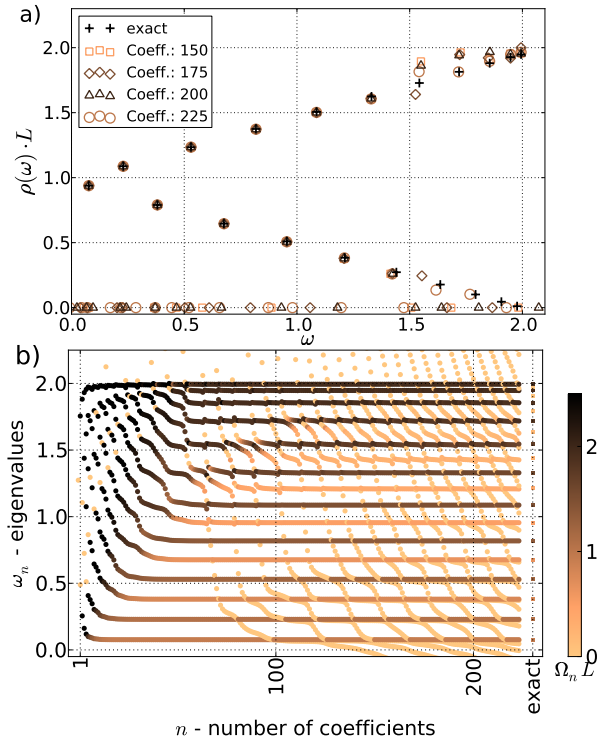


FIG. 2. (Color online) Spectral weights evaluated for different numbers of coefficients (a) and flow of the eigenvalues as a function of the number of Lanczos steps  $i$  (b) for spinless fermions ( $L = 40$ ,  $U = 0$ ,  $m = 3000$ ).

spectral function, we can take the limit  $\eta \rightarrow 0$  so that the spectral function  $\rho_{\hat{A}\hat{A}^\dagger}(\omega) = \sum_n \Omega_n^- \delta(\omega - \omega_n) - s \sum_n \Omega_n^+ \delta(\omega + \omega_n)$  is a series of  $\delta$ -functions, where  $\omega_n = E_n - E_0$ ,  $\Omega_n^{-(+)} = \left| \langle \psi_0 | \hat{A}^{(\dagger)} | n \rangle \right|^2$  and  $|n\rangle$  are the eigenstates of  $\hat{H}$  with eigenenergies  $E_n$ . Evidently, all of the information on the spectral function is contained in the weights  $\Omega_n^\pm$  and poles  $\omega_n = \pm \Delta E_n$ . Furthermore, one will always obtain a discrete and finite set of poles for any finite system. Since the DMRG treats finite systems, the spectral weights and pole positions can be calculated directly. Such a calculation has two important advantages: (i) One can study the size-dependence of spectral properties in a very controlled manner. (ii) It is possible to obtain precise values for the energies of the low-lying excitations;<sup>10</sup> they are given by the pole positions  $\omega_n$ , which can be directly obtained as the eigenvalues of the tridiagonal matrix  $T_{ij} = a_{i-1} \delta_{ij} + b_i (\delta_{j,i+1} + \delta_{i+1,j})$ .<sup>3</sup> The poles of the Green's function are located on the real axis and they are discrete. Therefore, one can integrate along a closed path  $\mathcal{C}$  in the complex plane chosen to enclose one single singularity, say at  $\omega_n$ . According to the residue theorem, the weight  $\Omega_n$  of this pole is then

$$2\pi i \Omega_n = \int_{-\infty}^{\infty} [G(\omega_n - \epsilon + i\gamma) - G(\omega_n + \epsilon + i\gamma)] d\gamma.$$

The parameter  $\epsilon$  must be chosen to be smaller than the distance to the next eigenvalue,  $\epsilon < |\omega_n - \omega_{n\pm 1}|$ . Using

this procedure with the position of the poles known, the spectral weights can be calculated to high precision using numerical integration.

In Fig. 2(a) we compare the weights and positions of the poles calculated with the DMRG and the ALM to the exact values on a chain of length  $L = 40$ , which are given by  $\Omega_n = \frac{2}{L+1} |\sin((k_f + k_n)x)|^2$ ,  $\omega_n = 2 \cos(k_n)$ , where  $k_n = \frac{\pi n}{L+1}$ ,  $n \in \{1, \dots, L\}$ , and  $k_f$  is the Fermi wave vector. For small energies, the agreement is nearly perfect, while deviations occur for large energies. The quality of the agreement depends on the number of coefficients  $a_i, b_i$  taken into account. One finds that after an initial improvement, no improvement occurs when one further increases the number of coefficients.

The origin of this behavior can be understood from Fig. 2(b), which depicts the flow of the eigenvalues of the matrix  $T_{ij}$  as a function of the number of Lanczos coefficients. The convergence of the first few eigenvalues is evidently rapid. The flow of the eigenvalues therefore gives a nice criterion for stopping the iterations (also for the OLM). However, after approximately 50 iterations, an eigenvalue with nearly vanishing weight appears and subsequently moves rapidly to zero energy. More such eigenvalues follow, at rapidly increasing frequency. This appearance of so-called “ghost” eigenvalues is well-known in the Lanczos method. These ghost eigenvalues are caused by the loss of orthogonality of the Lanczos vectors due to numerical error.<sup>11,12</sup> Their appearance here is therefore not surprising, in particular because the calculated Lanczos vectors also include an error from the approximate DMRG representation. We find that this effect is enhanced as one reduces the number of states within the DMRG. Thus, the study of the flow of the eigenvalues makes it possible to control the quality of the spectral function. Note that such ghost eigenvalues also occur within the OLM. As far as we know, this problem was never addressed in detail for this method. While the ghost eigenvalues seem, at first glance, to be a serious problem, we emphasize that, for the spectral function in particular, they do not appear to cause real harm because they possess only very small weight. This is evident from the scaling in Fig. 2(b) and also from the fact that all the ghost eigenvalues are located on the abscissa in Fig. 2(a). This observation is just an empirical one at present. However, as long as this remains true, the method will be insensitive with respect to the occurrence of ghost eigenvalues, except for regions with very small spectral weight. Here it is difficult to distinguish ghosts from small but real spectral weights. One possibility is to examine their convergence.<sup>11,12</sup> Another problem with ghosts is that they lead to a violation of sum rules due to double-counting. If one adds up just the real spectral values there will be a missing weight that is given by the sum of all ghost values. As long as the weight of the ghost values is small, this will not lead to severe violations of sum rules and can be used as a measure for the ghost problem.<sup>13</sup> Another, in our opinion, much more severe problem is the poor convergence at large energies. This

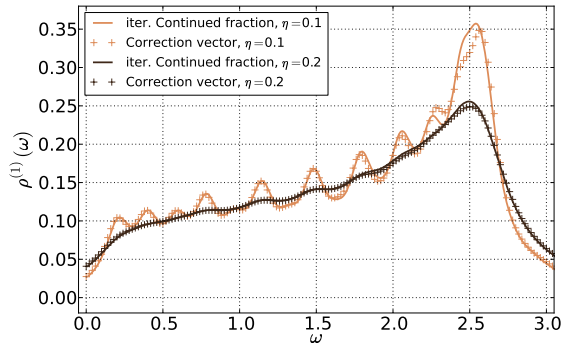


FIG. 3. (Color online) Comparison of the spectral weight calculated using the adaptive Lanczos-vector method with that calculated using the correction vector method for different broadenings  $\eta$  ( $U = 1.0, m_{CV} = 300, m_{ALM} = 3000, 250$  Lanczos vectors).

could be addressed by spectral transformations, which are a standard method for improving convergence of excited states within the Lanczos method.<sup>12</sup>

We now consider finite interaction,  $U = 1$ , and compare our method to the correction vector method.<sup>3,4</sup> The correction vector can be efficiently calculated by minimizing a functional at every step of the DMRG,<sup>14</sup> but one must include a finite broadening in this process. Each broadening requires a separate DMRG run, in contrast to the ALM, which can evaluate the Green's function readily for any set of frequencies and arbitrary broadening once the Lanczos coefficients have been calculated. In Fig. 3, we compare results from the two methods for two different values of the broadening,  $\eta = 0.1$  and  $0.2$ . We find very good agreement overall, especially for small energies. As expected, there are deviations at high energies, which become more pronounced with decreasing broadening.

We have shown that the ALM is capable of calculating the spectral weights and poles accurately within the

DMRG. In contrast to the OLM, we obtain the correct weights and poles of a Green's function up to energies of the order of half the bandwidth with only moderate resources, and, as long as the spectral weight is not too small, a reasonable reproduction of the spectrum even at larger energies. A clear advantage of the CFE in general is that it is based on an analytical expression for the Green's function, making it possible to evaluate it at an arbitrary set of frequencies with any possible broadening without having to repeat the DMRG calculation. In addition, one can extract irreducible quantities such as self-energies directly as continued fractions. The inaccuracies that appear at higher energies can be traced to a loss of orthogonality of the Lanczos vectors due to systematic and numerical errors. In order to improve the accuracy of spectral functions at higher energies, the truncation number  $m$  must be increased. This increase in  $m$  can become quite resource-intensive in standard DMRG implementations. However, an improvement in efficiency could be achieved by using the Matrix-Product-State (MPS) formulation of the DMRG.<sup>15</sup> Within the MPS formulation, one can variationally optimize the three Lanczos vectors in the recursion formula separately, potentially leading to much better performance. Another advantage is that, within the MPS formulation, the Hamiltonian can be represented exactly (see Ref. 16 for an introduction), thereby further reducing systematic errors. Finally, we point out that this recursive approach to calculate a special basis for the evaluation of spectral functions is not limited to the Lanczos basis. For example, expansion in Chebyshev polynomials leads to a similar recursion formula.<sup>17</sup>

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*Note added:* After completion of this work, we learned that Holzner *et al.*<sup>18</sup> have shown that an adaptive method using Chebyshev polynomials in combination with MPS is highly efficient and gives accurate spectral functions.

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<sup>13</sup> Another promising way to deal with this problem would be to carry out a partial or complete reorthogonalization of the calculated Lanczos vectors. This can be done by transforming each of the previous Lanczos vectors to the new DMRG basis (without adding them to the density matrix). This should reduce the ghost problem, but will increase computing time and memory requirements.

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