

Ground-state dynamical correlation functions: An approach using the density-matrix renormalization-group method

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(Received 21 August 1995)

A numerical approach to ground-state dynamical correlation functions from the density-matrix renormalization group (DMRG) is developed. Using sum rules, moments of a dynamic correlation function can be calculated with DMRG, and with the moments the dynamical correlation function can be obtained by the maximum entropy method. We apply this method to a one-dimensional spinless fermion system, which can be converted to the spin-1/2 Heisenberg model in a special case. The dynamical density-density correlation function is obtained.

Dynamical correlation functions of a model are of special interest, because they can provide a comprehensive comparison to experimental measurements. Unfortunately they are very difficult to calculate analytically or numerically for strongly correlated systems. Even for one-dimensional systems, the dynamical correlation functions are hard to obtain. For example, the $S=1/2$ Heisenberg model, although its exact solution from Bethe ansatz has been known for a long time, its ground-state dynamical correlation functions have not yet been obtained. Until now there are only a few general ways to obtain dynamical correlation functions. Analytically, only the asymptotic behavior of correlation functions for one-dimensional models in the quantum critical regime are able to be obtained by bosonization or conformal field theory.¹ Numerically, one way to calculate dynamical correlation functions is the analytic continuation of quantum Monte Carlo simulations with the maximum entropy method.^{2,3} But this method will encounter essential difficulties if we are interested in zero-temperature properties. Another numerical method to calculate the ground-state dynamical properties⁴ is based on the Lanczos method. The method is limited to very small systems.

The density-matrix renormalization-group (DMRG) method proposed by White⁵ is a powerful method to study the ground-state of one-dimensional interacting systems. With this method the ground-state energy, a few excitation energies, and static correlation functions can be calculated for a large system. However, it was not clear if one can obtain dynamical properties from this method.

In this paper, we describe a numerical method for calculating ground-state dynamical correlation functions in a systematic way, which is a combination of DMRG and maximum entropy methods⁶ (MEM). (After we finished this work we noticed the work by Hallberg,⁷ which provides another way to obtain the correlation function based on DMRG.) In general the moments of a dynamical correlation function can be expressed as static correlation functions, which can be calculated by the DMRG method. With these moments we can obtain the dynamic correlation function with MEM. We apply this method to the one-dimensional spinless fermion system with nearest neighbor interaction. This model is equivalent to the spin-1/2 XXZ chain. We have considered two special cases of this model, corresponding to the XY

model and the Heisenberg model. The dynamical density-density correlation [namely the structure function $S(q, \omega)$ in spin chain] is obtained. For the noninteracting case (the XY model) we compare our result with the exact result, and obtain a very good agreement.

The one-dimensional spinless fermion model we consider has the following Hamiltonian:

$$H = -t \sum_i (c_i^\dagger c_{i+1} + \text{H.c.}) + V \sum_i n_i n_{i+1}, \quad (1)$$

where $c_i^{(\dagger)}$ are annihilation (creation) operators for a fermion at site i , and $n_i = c_i^\dagger c_i - 1/2$. The Hamiltonian written in such form ensures the ground state is at half filling. This model may be mapped to the XXZ model by the Jordan-Wigner transformation. Under this transformation $S_i^z = n_i$, $J_x = J_y = 2t$, and $J_z = V$. At $V=0$ this model is equivalent to the XY model, while at $V=2t$ it is equivalent to the Heisenberg model. We only consider these two cases in this work.

The first step of our method is to use sum rules to express the moments of a dynamical correlation function by some static correlation functions. The sum rules for the spin model have been derived.⁸ We use the similar definition of the correlation functions as in Ref. 8:

$$\begin{aligned} \chi_c(q, t) &= \frac{1}{2} \langle \{n(q, t), n(-q, 0)\} \rangle - \langle n(q, t) \rangle \langle n(-q, 0) \rangle, \\ \chi''(q, t) &= \frac{1}{2} \langle [n(q, t), n(-q, 0)] \rangle, \end{aligned} \quad (2)$$

where $n(q) = N^{-1/2} \sum_i n_i e^{iqi}$, the curly bracket indicates an anticommutator, and $\langle n(q) \rangle = \text{Tr}[n(q) e^{-\beta H}]$. The fluctuation-dissipation theorem gives the relation $\chi_c(q, \omega) = \coth(\omega/2k_B T) \chi''(q, \omega)$. The structure function or dynamic form factor $S(q, \omega)$ is defined as $S(q, \omega) = \chi''(q, \omega)/(1 - e^{-\omega/k_B T})$. Due to the parity and time reversal symmetry in our model, $\chi''(q, \omega)$ and $\chi_c(q, \omega)$ have the following properties: $\chi''(q, -\omega) = -\chi''(q, \omega)$ and $\chi_c(q, -\omega) = \chi_c(q, \omega)$. At zero temperature $S(q, \omega) = \chi_c(q, \omega) = \chi''(q, \omega)$ for $\omega > 0$, therefore the sum rules given in Ref. 8 can be written as

$$\begin{aligned}
m_1(q) &= \int_0^\infty \frac{d\omega}{\pi} \frac{\chi''(q, \omega)}{\omega} = \frac{1}{2} \chi(q, \omega=0), \\
m_2(q) &= \int_0^\infty \frac{d\omega}{\pi} \omega \frac{\chi''(q, \omega)}{\omega} = \chi_c(q, t=0), \\
m_3(q) &= \int_0^\infty \frac{d\omega}{\pi} \omega^2 \frac{\chi''(q, \omega)}{\omega} = -\frac{1}{2} \langle [[H, n(q)], n(-q)] \rangle \\
&= 2 \langle c_i^\dagger c_{i+1} \rangle [1 - \cos(q)], \tag{3}
\end{aligned}$$

where $\chi(q, \omega=0)$ is the static susceptibility. These sum rules can be easily generalized to higher moments:

$$\begin{aligned}
m_l(q) &= \int_0^\infty \frac{d\omega}{\pi} \omega^{l-1} \frac{\chi''(q, \omega)}{\omega} \\
&= \begin{cases} -\frac{1}{2} \langle [[H, \dots, [H, n(q)] \dots], n(-q)] \rangle, & l \text{ odd,} \\ \frac{1}{2} \langle \{ [H, \dots, [H, n(q)] \dots], n(-q) \} \rangle, & l \text{ even,} \end{cases}
\end{aligned}$$

where H appears in the commutators $l-2$ times. Apart from the first moment which is given by the static susceptibility, all the other moments can be expressed as equal-time correlation functions. Theoretically if all the moments are known, one can obtain the $\chi''(q, t)$ and thus $\chi''(q, \omega)$. In real calculations, it is tedious to calculate the commutators for higher moments, and there are more and more new equal-time correlation functions that appear in the expression of higher moments. However it is still reasonable to obtain the expression for the first several moments using a symbolic manipulator, such as Mathematica, to calculate the commutators. In this work we have calculated the expressions for the first five moments.

The second step is to obtain the moments by calculating the corresponding static correlation functions with the DMRG. The infinite lattice method (see Ref. 5 for details) is used in our calculations for open ended chains. $t=1$ is chosen, and states kept at each iteration varies from 52 to 64. The equal-time correlations, for example $\langle n_i n_j \rangle$, are usually calculated by putting n_i and n_j on different blocks.^{5,9} In the DMRG calculation, the matrix of a local operator like n_i can be constructed when site i is added into the system, and its elements in the truncated Hilbert space are updated at each iteration. By inserting a complete basis set, the matrix elements of operators like $n_i n_j$ in the truncated Hilbert space can be calculated if we know the matrices of operators n_i and n_j . Since we only have their matrices in the truncated Hilbert space, in general multiplying two matrices does not give the correct matrix for the combined operator. One way to avoid such a problem is to put n_i and n_j on separate blocks. But the precision of a correlation function calculated in this way is much lower than that of a local operator. In contrast to the conventional method, we choose n_i and n_j on the same block and site j at the edge of the block connecting to the other block. Since the site j is one of the two sites which are just added into the system, the Hilbert space at site j is complete for the operator n_j . Therefore we can calculate the matrix

elements of the combined operator $n_i n_j$ by multiplying the matrices of n_i and n_j . We can prove that the precision of $\langle n_i n_j \rangle$ is completely controlled by discarded weight in DMRG calculations, which means the precision can be as high as that for the ground-state energy or any local operators.¹⁰ For a system which has parity and translational symmetries, $\langle n_j n_i \rangle$ only depends on $|i-j|$. Therefore $\langle n_q n_{-q} \rangle = \sum_i \langle n_j n_{j+i} \rangle e^{iqi}$ is independent of j . Since the calculations are done with an open boundary condition, $\langle n_j n_{j+i} \rangle$ depends on the position j . Also due to the open boundary, the correlation $\langle n_j n_{j+i} \rangle$ has an even-odd oscillation in j . We take the mean value of $\langle n_j n_{j+i} \rangle$ at j even and odd, which is closer to the value with period boundary condition for a system having the same size. When the system size goes to infinity, the boundary effect can be neglected. We calculate the moments for system sizes varying from 100 sites to 200 sites, and obtain their values for infinite system by extrapolating the data. Since the first moment is not an equal time correlation but the static susceptibility, it is calculated with the finite lattice method. For a particular momentum q , we apply a small field $h_q \cos(qi)$ which couples with the density in this way: $h_q \sum_i n_i \cos(qi)$, then we calculate the density response $\langle n_q \rangle = 1/N \sum_i \langle n_i \rangle \cos(qi)$ with DMRG. The ratio $\langle n_q \rangle / h_q$ in the $h_q \rightarrow 0$ limit gives the static susceptibility.

The next step is to use the MEM to obtain the dynamical correlation functions. The MEM has become a standard way to extract maximum information from incomplete data.⁶ This method has been applied to the analytic continuation of the quantum Monte Carlo data,¹¹ and in this paper we apply a similar method to extract the dynamic susceptibility $\chi''(q, \omega)$ from the finite number of moments m_l with the corresponding errors σ_l . We define $f(\omega) = \chi''(\omega) / \omega$, which is positive definite, as a distribution function, and the entropy or the information function $S = \sum_\omega f(\omega) - f(\omega) \ln f(\omega)$. By maximizing the entropy under the constraints $m_l - \int_0^\infty (d\omega/\pi) \omega^{l-1} f(\omega) = 0$, $f(\omega)$ has the following form:

$$f(\omega) = \exp\left(-\sum_{l=1}^n (\lambda_l \omega^{l-1})\right), \tag{4}$$

where n is the number of moments and λ_l are the Lagrange multipliers. At this point one may try to find λ_l by requiring the $f(\omega)$ to satisfy the constraints without considering the error bars of the moments. However, in general, the error bars cannot be neglected. The kernel of the transformation is singular, so small errors in moments may produce large errors in $f(\omega)$. By maximizing the posterior probability $e^{\alpha S - L}$ where $L \equiv \sum_l [m_l - \int_0^\infty (d\omega/\pi) \omega^{l-1} f(\omega)]^2 / \sigma_l^2$, one can find the most probable $f(\omega)$, which gives us the moments within the range of error bars.

Let us first discuss the extrapolation and the error bar of our DMRG results. There are two major contributions to the error: that from finite size effects and that from basis set truncation in the DMRG calculations. The error bar of the DMRG calculation for any finite size is obtained by varying the number of states kept at each iteration, whereas the finite size error is obtained by varying the system size. The asymptotic behavior of correlation functions is known for this model,¹ which decay as a power of system size. For a system with a gap, the extrapolation should be done as an exponen-

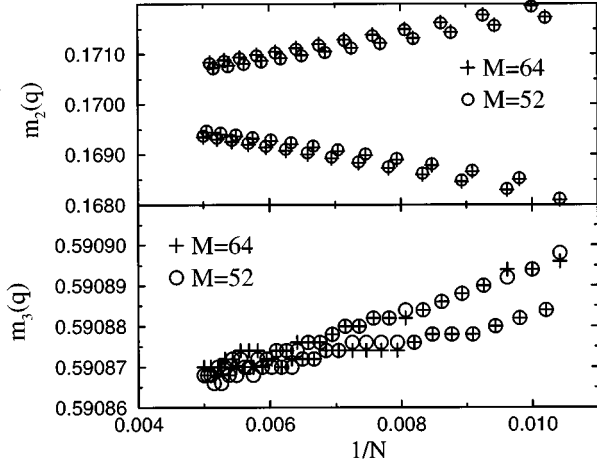


FIG. 1. Moments vs the inverse system size $1/N \rightarrow 0$ for $V=2t$ and $q=\pi/2$, where M is the number of states kept at each iteration in DMRG calculations. The extrapolation is to $1/N \rightarrow 0$, and the error is estimated by the different extrapolations caused by the errors in slope.

tial function of system size. In Fig. 1, we plot the second and third moments at $q=\pi/2$ for $V=2t$ as a function of $1/N$, where N is the number of sites of the system. The error from basis set truncation produces the error in the extrapolated values. We use this resultant error to estimate the error bar of the moments. Extrapolating to $1/N \rightarrow 0$ gives $m_2=0.1700$, and the error bar is estimated as 10^{-4} . For the third moment we have $m_3=0.59085$ and the estimated error bar is 2×10^{-5} . Actually the third moment is known exactly: $m_3 = -(2/3)E[1 - \cos(q)]$ with the ground state energy per site $E = -2(\ln 2 - 1/4)$. The exact value at $\pi/2$ is 0.590863.

We test our method for the noninteracting case. In this case, $\chi''(q, \omega)$ is known exactly:¹²

$$\chi''(q, \omega) = \frac{\theta[\omega - 2t|\sin(q)]\theta[4t|\sin(q/2)| - \omega]}{[16t^2\sin^2(q/2) - \omega^2]^{1/2}}, \quad (5)$$

where $\theta(x)$ is the step function. The moments can also be calculated analytically. In Table I, we compare the moments calculated by the DMRG with the exact results. The error bars obtained by the DMRG provide a very good estimate. Apart from the five moments, there are two more pieces of information in this case: the energy boundaries $2t|\sin(q)| < \omega < 4t|\sin(q/2)|$ for $\chi''(q, \omega)$. The energy bound-

TABLE I. The comparison of the moments obtained by DMRG with the exact results for $V=0$ and $q=2\pi/3$. In the DMRG calculations 64 states are kept at each iteration, and the error bars are estimated by changing the number of states kept and finite size scaling.

	Exact	DMRG	Error
$m_1(2\pi/3)$	0.121013	0.1211	1×10^{-3}
$m_2(2\pi/3)$	0.333333	0.33337	5×10^{-5}
$m_3(2\pi/3)$	0.954930	0.954928	5×10^{-6}
$m_4(2\pi/3)$	2.826993	2.8273	5×10^{-4}
$m_5(2\pi/3)$	8.594367	8.59434	5×10^{-5}

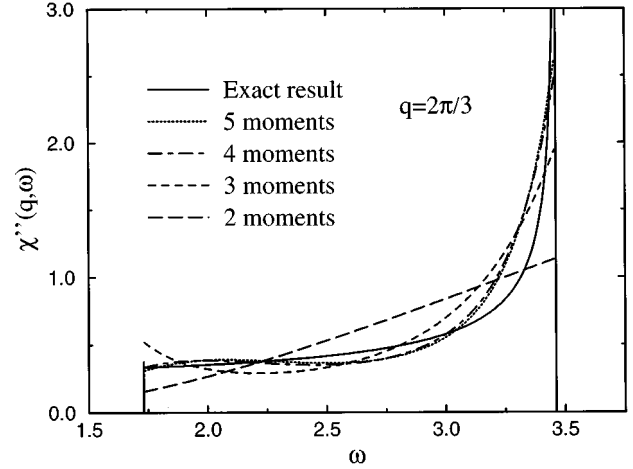


FIG. 2. The dynamical structure function $\chi''(q, \omega)$ for $V=0$ (the XY model) and $q=2\pi/3$. The results obtained by the MEM with a different number of moments are plotted. Two solid vertical lines are the energy boundaries.

aries mean that $\chi''(q, \omega)$ is zero when ω is beyond the boundaries, and we use it as a requirement on $\chi''(q, \omega)$ when we apply the MEM to get $\chi''(q, \omega)$. Using the MEM, we obtain $\chi''(q, \omega)$ for $q=2\pi/3$. In Fig. 2, we plot $\chi''(q, \omega)$ obtained by the MEM with a different number of moments and the exact one from Eq. (5). It shows that the $\chi''(q, \omega)$ obtained by the MEM converges toward the exact one when the number of moments is increased, and $\chi''(q, \omega)$ calculated with five moments is a good approximation for the exact result. We have also calculated $\chi''(q, \omega)$ for other q , they have similar behavior.

For the interacting case with $V=2t$, which corresponds to the Heisenberg model, the elementary excitations are known as $S=1/2$ objects¹³ (spinons). The dispersion relation is $\epsilon(q) = \pi t|\sin(q)|$,¹⁴ which provides the lower bound of excitation energies for each momentum q . The spectral weight is dominated by the continuum of the two-spinon excited states,¹⁵ and the energy range for the continuum is $t\pi|\sin(q)| < \omega < 2t\pi|\sin(q/2)|$. Based on this fact an analytic ansatz for $\chi''(q, \omega)$ was proposed as¹⁵

$$\chi''(q, \omega) = A \frac{\theta[\omega - \pi t|\sin(q)]\theta[2\pi t|\sin(q/2)| - \omega]}{[\omega^2 - \pi^2 t^2 \sin^2(q)]^{1/2}}, \quad (6)$$

where $\theta(x)$ is the step function. This is an approximate solution, because it cannot satisfy the sum rules with a fixed parameter A . Since the contributions from the excited states of more than two spinons are finite, we only have the low energy bound. We use it as a requirement on $\chi''(q, \omega)$ in our MEM calculations. In Fig. 3, the $\chi''(q, \omega)$ obtained by the MEM with different number of moments are plotted for $q=2\pi/3$. The analytic ansatz which satisfies the third sum rule is also plotted in Fig. 3 for comparison. One can see the tendency of the curves as the number of moments increase. $\chi''(q, \omega)$ tends to diverge at the lower bound. We also mark the position of the upper bound for two-spinon excited states.

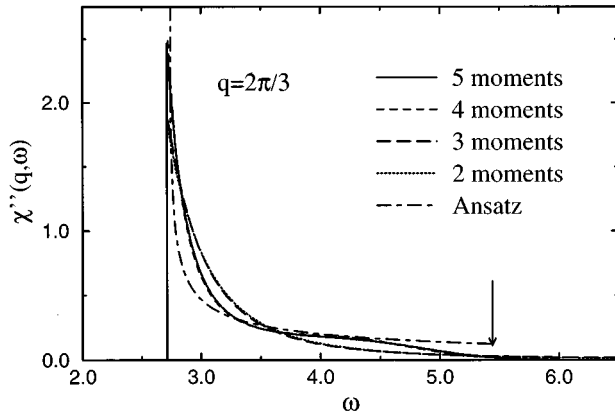


FIG. 3. The dynamical structure function $\chi''(q, \omega)$ for $V=2t$ (the Heisenberg model) and $q=2\pi/3$. The results obtained by the MEM with different number of moments are plotted. The analytic ansatz which satisfies the third sum rule is also plotted for comparison. The solid vertical line is the lower boundary. The arrow marks the position of the upper boundary for the two-spinon excited states.

It is obvious that the contributions from the two-spinon continuum is dominate. In Fig. 4, $\chi''(q, \omega)$ is plotted for other momentums.

In conclusion, we have developed a numerical method for calculating the ground-state dynamical correlation functions in one-dimensional quantum systems based on the density matrix renormalization-group method and the maximum entropy method. We demonstrate this method on the dynamical density-density correlation function $\chi''(q, \omega)$ of the spinless fermion system with nearest neighbor interaction. For the noninteracting case, it corresponds to the XY model, the dynamical density-density correlation function obtained by our method shows very good agreement with the exact result. For the interacting case with $V=2t$, it corresponds to the Heisenberg model, we obtain the $\chi''(q, \omega)$, which was not

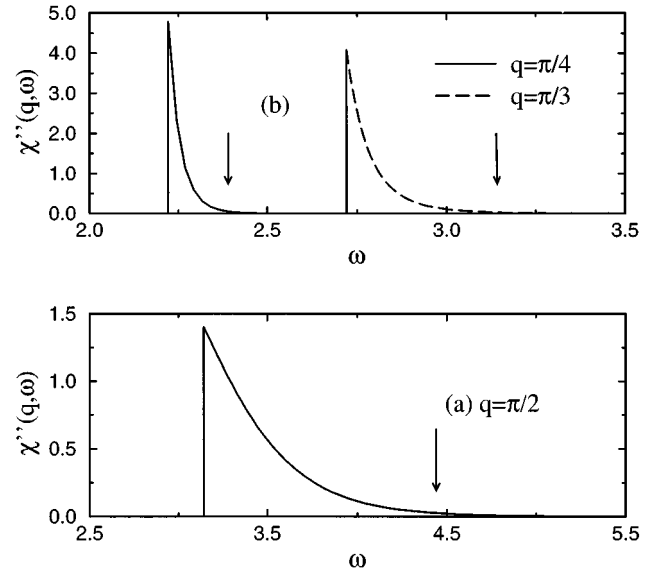


FIG. 4. The dynamical structure function $\chi''(q, \omega)$ for $V=2t$ (the Heisenberg model) at (a) $q=\pi/2$, and (b) $\pi/3$ and $\pi/4$. $\chi''(q, \omega)$ are obtained by the MEM with five moments. The solid vertical lines are the lower boundaries for each momentum. The arrow marks the position of the upper boundary of the two-spinon excited states.

known before. This method is a very general one, which can be applied to any one-dimensional system with short range interaction like, e.g., the Hubbard model, the $S=1$ Heisenberg model, the interacting fermion (or boson) system with randomness.

We would like to acknowledge useful discussions with J. E. Gubernatis, Shoudan Liang, and R. N. Silver. This work was supported by the National Science Foundation grant No. DMR-9107563. In addition M.J. would like to acknowledge the support of the NSF NYI program.

- ¹A. Luther and I. Peschel, Phys. Rev. B **12**, 3908 (1975); I. Affleck in *Fields, Strings and Critical Phenomena*, edited by E. Brezin and J. Zinn-Justin (North-Holland, Amsterdam, 1990).
- ²J. Deisz, M. Jarrell, and D. L. Cox, Phys. Rev. B **42**, 4869 (1990).
- ³R. Preuss, A. Muramatsu, W. von der Linden, P. Dieterich, F. F. Assaad, and W. Hanke, Phys. Rev. Lett. **73**, 732 (1994).
- ⁴E. R. Gagliano and C. A. Balseiro, Phys. Rev. Lett. **59**, 2999 (1987).
- ⁵S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); Phys. Rev. B **48**, 10 345 (1993).
- ⁶T. Brandt, *Statistical and Computational Methods in Data Analysis* (North-Holland, Amsterdam, 1983), Chap. 13; S.F. Gull and J. Skilling, IEE Proc. **131**, 646 (1984); R. K. Bryan, Eur. Bio-

phys. J. **18**, 165 (1990).

⁷K. Hallberg, Phys. Rev. B **52**, 9827 (1995).

⁸P. C. Hohenberg and W. F. Brinkman, Phys. Rev. B **10**, 128 (1974).

⁹E. S. Sørensen and I. Affleck, Phys. Rev. B **49**, 15 771 (1994).

¹⁰Hanbin Pang, H. Akhlaghpour, and M. Jarrell (unpublished).

¹¹R. N. Silver, D. S. Sivia, J. E. Gubernatis, and M. Jarrell, Phys. Rev. Lett. **65**, 496 (1990); J. E. Gubernatis, M. Jarrell, R. N. Silver, and D. S. Sivia, Phys. Rev. B **44**, 6011 (1991).

¹²S. Katsura, T. Horiguchi, and M. Suzuki, Physica **46**, 67 (1970).

¹³L. D. Faddeev and L. A. Taktajan, Phys. Lett. **85A**, 375 (1981).

¹⁴J. des Cloizeaux and J. J. Pearson, Phys. Rev. **128**, 2131 (1962).

¹⁵G. Müller, H. Beck, and J. Bonner, Phys. Rev. Lett. **43**, 75 (1979).