Finite-temperature dynamics with the density-matrix renormalization group method

J. Kokalj[1] and P. Prelovšek[1,2]

[1]*J. Stefan Institute, SI-1000 Ljubljana, Slovenia*
[2]*Faculty of Mathematics and Physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia*

We present a numerical method for the evaluation of dynamical response functions at finite temperatures in one-dimensional strongly correlated systems. The approach is based on the density-matrix renormalization group method, combined with the finite-temperature Lanczos diagonalization. The feasibility of the method is tested on the example of dynamical spin correlations in the anisotropic Heisenberg chain, in particular, it yields nontrivial results for the critical behavior in the isotropic case.

I. INTRODUCTION

Strongly correlated systems present one of the major theoretical challenges in last decades and are stimulating the intensive search for adequate numerical methods to evaluate their properties. Within the low-dimensional systems, in particular one-dimensional (1D) systems the breakthrough has been achieved with the introduction of the density-matrix renormalization group (DMRG) method[1] allowing accurate calculation of the ground-state wave function and its static properties on large systems far beyond those available with the exact-diagonalization methods. Among various DMRG extensions[2] we concentrate here on the goal to study the dynamical response of such systems at finite temperatures $T > 0$. It should be observed that in spite of the satisfactory description and an understanding of static properties of generic 1D systems at $T > 0$ the corresponding dynamics, in particular, the low-frequency one as manifested in the transport quantities, NMR relaxation, is far less understood and approachable via numerical methods.

For dynamical response within the ground state the targeting within the DMRG has been extended to contain also excited states.[3,4] Transfer-matrix DMRG (Refs. 5–7) is very efficient to evaluate thermodynamic properties of models with short-range interactions as well as some dynamical correlations of very limited range. Time dependent DMRG (Refs. 8 and 9) developed recently enables studies of short-time evolution of general many-body systems hence also of $T > 0$ behavior but is rather limited in reaching the low-ω response. Recently, a DMRG method extended with the polynomial expansion has been proposed to treat low-T dynamics.[10] On the other hand, methods emerging from the exact-diagonalization approach as the finite-temperature Lanczos method (FTLM) (Ref. 11) and the low-T version[12] have high-ω resolution and provide the information on the nontrivial dynamics of correlated models but are still restricted to small systems reachable with exact diagonalization.

The paper is organized as follows. In Sec. II we first present our method, with which we calculate some static and dynamical properties of the model described in Sec. III. In Sec. III we also show our results, first the test of our method on the *XY* model and then our main results for the isotropic Heisenberg model. In Sec. IV we present our conclusions.

II. METHOD

In this paper we propose a method for the calculation of the $T > 0$ dynamics which is a combination of the FTLM and the DMRG, namely, the finite-temperature dynamical DMRG (FTD-DMRG) method. It is constructed to calculate dynamical response functions in 1D systems at $T > 0$ with the emphasis on the low-ω regime. As a test we consider highly nontrivial spin correlations within the anisotropic Heisenberg model on a chain.

In the standard $T = 0$ DMRG the ground state is used to construct the basis. In our case we use the full $T > 0$ density matrix, which can in general be expressed with eigenstates $|n\rangle$ and corresponding eigenvalues E_n

$$\hat{\rho} = \frac{1}{Z} e^{-\beta \hat{H}} = \frac{1}{Z} \sum_{n=1}^{N_{st}} |n\rangle e^{-\beta E_n} \langle n|, \qquad (1)$$

where $\beta = 1/T$ and Z is the (grand) canonical sum. We proceed by extending the density matrix, Eq. (1), with the sampling over the random vectors $|r\rangle = \Sigma_n \beta_{rn} |n\rangle$ where β_{rn} denote random amplitudes

$$\hat{\rho} \sim \frac{N_{st}}{ZR} \sum_{r=1}^{R} e^{-\beta \hat{H}/2} |r\rangle \langle r| e^{-\beta \hat{H}/2}. \qquad (2)$$

It is easy to show that Eq. (2) reduces to Eq. (1) expressed in diagonal basis $|n\rangle\langle n|$ since offdiagonal terms vanish assuming normalized and random $|r\rangle$.[11] In Eq. (2) we evaluate the operator $e^{-\beta \hat{H}/2}$ on $|r\rangle$ by starting the Lanczos procedure from $|r\rangle$. After diagonalization of the Lanczos tridiagonal $\hat{H}$, we obtain the first series of Lanczos eigenvectors $|\psi_i^r\rangle$ with corresponding eigenenergies ϵ_i^r

$$|\tilde{\psi}_r\rangle = \sum_{i=1}^{M} e^{-\beta \epsilon_i^r/2} |\psi_i^r\rangle \langle \psi_i^r | r\rangle,$$

$$\hat{\rho} \sim \frac{N_{st}}{ZR} \sum_{r=1}^{R} |\tilde{\psi}_r\rangle \langle \tilde{\psi}_r|. \qquad (3)$$

It is evident that for M approaching N_{st} Eq. (3) reproduces fully Eq. (1) while for $M \ll N_{st}$ as used in practice represents an efficient way of evaluation of density matrix. The sum Z

may be evaluated in the same manner as within the FTLM (Ref. 11)

$$Z \sim \frac{N_{st}}{R} \sum_{r=1}^{R} \sum_{i=1}^{M} e^{-\beta \epsilon_i^r} |\langle \psi_i^r | r \rangle|^2. \tag{4}$$

In the original $T=0$ DMRG procedure one targets the ground state.[1,2] Instead, at $T>0$ we target states $|\tilde{\psi}_r\rangle$ and construct the density matrix according to Eq. (3).

Since our aim is to calculate dynamical response functions, expressed as autocorrelation functions, we also require a good representation of the operator density matrix

$$\hat{\rho}_A = \frac{1}{Z} \sum_{n=1}^{N_{st}} |\hat{A}n\rangle e^{-\beta E_n} \langle \hat{A}n|. \tag{5}$$

It replaces the operator on the ground state in original $T=0$ DMRG (Refs. 2 and 3) and is evaluated by extending Eq. (3)

$$|\tilde{\psi}_r^A\rangle = \sum_{i=1}^{M} e^{-\beta \epsilon_i^r/2} \hat{A} |\psi_i^r\rangle \langle \psi_i^r | r \rangle = \hat{A} |\tilde{\psi}_r\rangle,$$

$$\hat{\rho}_A \sim \frac{N_{st}}{R} \sum_{r=1}^{R} |\tilde{\psi}_r^A\rangle \langle \tilde{\psi}_r^A|. \tag{6}$$

In the proposed targeting we sum up above contributions with weighting factors

$$\hat{\rho}_{tot} = p_1 \frac{\hat{\rho}}{\text{Tr } \hat{\rho}} + p_2 \frac{\hat{\rho}_A}{\text{Tr } \hat{\rho}_A} \tag{7}$$

with the restriction $p_1 + p_2 = 1$. From $\hat{\rho}_{tot}$ we prepare the reduced density matrix by integrating out the environment, which is then used to construct the basis within the infinite and finite algorithms of the DMRG.[2] Our way of targeting is in fact very similar to the one in Ref. 10 with an additional random sampling suppressing the nondiagonal terms of $\hat{\rho}$. In such a way we prepare the basis for any $T>0$ whereby limitations are emerging from the truncation of the basis being more under control for low T. It should also be mentioned that for dynamical response at particular ω there is an improvement to target also excited states corresponding to so-called correction vectors.[4,10] Still, the latter does not affect quality of the most interesting and challenging regime $\omega \sim 0$ as well as it increases the computational demand hence we do not employ it here.

Physical quantities are calculated in the measurement part of the FTD-DMRG procedure in the same manner as within the FTLM.[11] A dynamical autocorrelation function

$$A(\omega) = \frac{1}{Z} \sum_n e^{-\beta E_n} \langle n | \hat{A}^\dagger \frac{1}{\omega - (\hat{H} - E_n) + i\eta} \hat{A} | n \rangle \tag{8}$$

is evaluated with the use of two Lanczos series of eigenstates and eigenenergies

$$A(\omega) \approx \frac{N_{st}}{ZR} \sum_{r=1}^{R} \sum_{i,j=1}^{M} e^{-\beta \epsilon_i^r} \frac{1}{\omega - (\epsilon_j^{Ar} - \epsilon_i^r) + i\eta}$$

$$\times \langle r | \psi_i^r \rangle \langle \psi_i^r | \hat{A}^\dagger | \psi_j^{Ar} \rangle \langle \psi_j^{Ar} | \hat{A} | r \rangle. \tag{9}$$

The second Lanczos series of eigenstates $|\psi_j^{Ar}\rangle$ and eigenenergies ϵ_j^{Ar} is obtained from second Lanczos procedure starting from the initial vector $\hat{A}|r\rangle$.

III. MODEL AND RESULTS

As a nontrivial test of the method we analyze the dynamics of the 1D anisotropic Heisenberg model

$$\hat{H} = J \sum_{i=1}^{L} \left[\frac{1}{2} (S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+) + \Delta S_i^z S_{i+1}^z \right], \tag{10}$$

where $S_i^\pm, S_i^z$ are local spin $S=1/2$ operators, L is the chain length, J is the exchange coupling (in the following we use $J=1$), and Δ is the anisotropy parameter. In our calculations we focus on systems in the absence of the magnetic field hence on the subspace $S_{tot}^z = 0$. As the quantity of interest we choose the dynamical spin structure factor $S(q,\omega)$ and the corresponding susceptibility $\chi(q,\omega)$

$$S(q,\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dt e^{i\omega t} \langle S^z(q,t) S^z(q,0) \rangle,$$

$$\chi''(q,\omega) = \pi (1 - e^{-\beta \omega}) S(q,\omega). \tag{11}$$

As usual within the DMRG technique more accurate results are obtained with open-boundary conditions[2] hence one defines $S^z(q) = \sqrt{2/(L+1)} \Sigma \sin(qi) S_i^z$ whereby $q = \pi j/(L+1)$ with $j=1,\ldots,L$. In our calculations we concentrate on most challenging $q = Q = \pi$, i.e., $j=L$.

The relaxation function $\Phi(q,\omega) = \chi''(q,\omega)/\omega$ should be an even function of ω. This represents another nontrivial test for the FTD-DMRG method. In addition to considering complete spectra $\chi''(q,\omega)$ better defined criteria are frequency moments

$$M^{(n)}(q) = \frac{1}{\pi} \int \Phi(q,\omega) \omega^n d\omega. \tag{12}$$

Due to symmetry only even $M^n(q)$ are finite while the static susceptibility corresponds to $\chi^0(q) = M^0(q)$. In the following we employ the FTD-DMRG method to evaluate $\Phi(Q,\omega)$ for $\Delta = 0, 1$ and various T. In the actual implementation we use the infinite and finite-size DMRG basis preparation and the calculation of $S(Q,\omega)$ via Eq. (9) [$A = S_z(Q)$] performed on the system divided into two subblocks of size $(L-2)/2$ and two coupling sites in between.[2] In the preparatory sweeping typically 1 or 2 sweeps are sufficient for the convergence of the basis. Important parameters for the final quality of results are the (subblock) DMRG truncation number m and the number of Lanczos steps M. We are typically restricted to $m \sim 1000$ and $M \sim 100$. We have two kinds of sampling. One in the determination of the density matrix Eq. (2), $R = R_1$ for the basis preparation, and the other in the evaluation of the
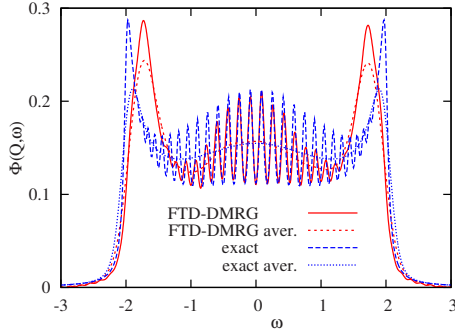
FIG. 1. (Color online) Relaxation function $\Phi(Q,\omega)$ within the XY model for $T=0.25$ and a system of $L=36$ sites. For comparison the exact grandcanonical result for spinless fermions is shown and the corresponding smoothed curve relevant for $L \to \infty$.

final Eq. (9), $R=R_2$. While only modest $R_1 \sim 50$ is adequate, $R_2 \gg 1$ is needed, in particular, at low T (Ref. 11) to get accurate matrix elements. At higher T R_2 can be reduced effectively to $R_2 \sim 1$.[11] Further on we mainly consider $T < 0.5$ with $R_2 \sim 100$. When evaluating the feasibility of various methods we should keep in mind that the full exact-diagonalization evaluation of $S(q,\omega)$ at $T>0$ for the model at hand can be performed up to $L=14-16$ with the FTLM technique up to $L=24$ while in the following we present the FTD-DMRG results up to $L=40$.

A. *XY* model

The $\Delta=0$ case maps onto noninteracting spinless fermions via the Jordan-Wigner transformation and $S(Q,\omega)$ can be expressed for any $T>0$ in a Lindhard form. For finite L the only caveat is that the FTD-DMRG is performed within a canonical systems with fixed $S^z_{tot}=0$, i.e., with fixed number of fermions $N_e=L/2$ while the usual (easier) evaluation is within the grandcanonical ensemble. In Fig. 1 we present the FTD-DMRG result for (unsymmetrized) relaxation function $\Phi(Q,\omega)$ at low $T=0.25$. Results are for $L=36$ where the basis is heavily reduced, i.e., only 5×10^{-4} of all states are retained within the final evaluation. For comparison we show the exact (grandcanonical) fermionic result for the same system with open boundary condition and for all presented spectra we use the damping $\eta=0.05$. Oscillations are a clear sign of finite-size system and slowly disappear with increasing T and L. The finite-size effect can be avoided by smoothing with a Gaussian filter with the width adapted to the frequency $\propto 1/L$. From Fig. 1 it is evident that at low $|\omega| < 1$ the agreement between the FTD-DMRG and the exact result is very satisfactory. At high $\omega \sim 2$ the FTD-DMRG does not fully reproduce the sharp spectral edge which could be improved by the introduction of the correction vector targeting for $\omega \neq 0$ within the method.[2,4,10]

Figure 2 shows the corresponding results for the frequency moments $M_n(Q)$ displayed vs $1/L$ obtained with the full basis for $L \leq 22$ and with the FTD-DMRG method for $L \leq 40$. For comparison also corresponding exact results are shown within the canonical calculation at $N_e=L/2$. It is evident that $T=0.25$ is already high enough so that moments are essentially size independent. Also up to $L=40$ FTD-DMRG
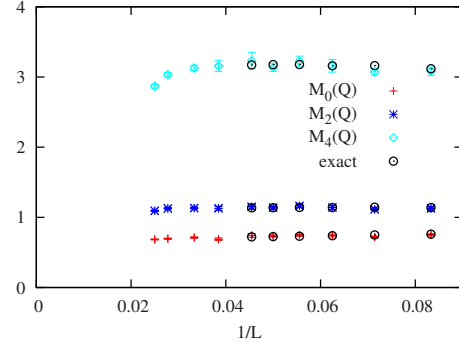

FIG. 2. (Color online) Lowest frequency moments $M_n(Q)$ vs $1/L$ for $T=0.25$. For comparison exact moments are shown up to $L=22$.

results are well stable, at least for lowest M_0, M_2, while for M_4 some deviations originate from high-ω regime and are also visible in Fig. 1. At the same time, $M_1, M_3 \approx 0$ is well reproduced as required by the symmetry of $\Phi(Q,\omega)$.

B. Isotropic Heisenberg model

The isotropic $\Delta=1$ case (at $S^z_{tot}=0$) representing marginally gapless system is by far more challenging. For $T>0$ there are no exact results for dynamical quantities. The bosonization approach provides a form for $S(q,\omega)$ within the low $\omega-T$ regime.[13,14] Relative to the $\Delta=0$ case the divergence for $\Delta=1$ is stronger and nontrivial. The isotropic model has been an obvious target for numerical methods. Static quantities, as the structure factor $S(q)$ and $\chi^0(q)$ have been evaluated using the quantum Monte Carlo (QMC) method and the high-T expansion,[15,16] recently also with the time-dependent DMRG[17] but only for $q \neq Q$ so far. An obvious deficiency is in results for dynamic quantities at $\omega \sim 0$ since the QMC approach (due to the maximum entropy procedure) seems to have considerable uncertainty in this regime.[16] On the other hand, the latter regime is frequently just the most interesting, e.g., in connection with the NMR relaxation rate $1/T_1 \propto \Sigma_q A_q S(q,\omega \to 0)$, with transport quantities, etc.

In Fig. 3 we present results for $\Phi(Q,\omega)$ obtained for $L=40$ sites and different T. Since spectra are peaked at $\omega=0$ (in contrast to Fig. 1) finite-size oscillations are more pro-
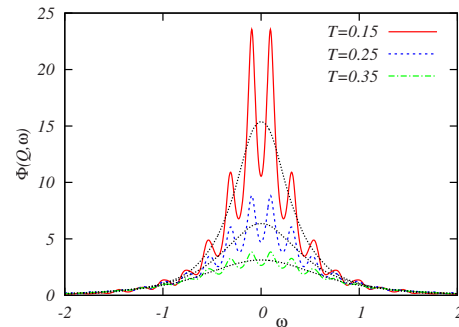

FIG. 3. (Color online) Symmetrized $\Phi(Q,\omega)$ for the isotropic Heisenberg model shown for $L=40$ and $T=0.15, 0.25, 0.35$. Presented are also finite-size smoothed spectra (dotted line).
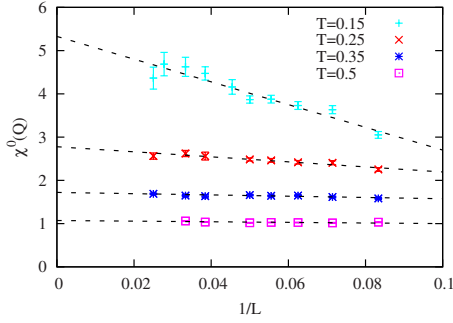
FIG. 4. (Color online) $\chi^0(Q)$ for the isotropic model vs $1/L$ for different T as calculated via the FTD-DMRG method for $L = 22-40$ and via FTLM for $L = 12-20$.
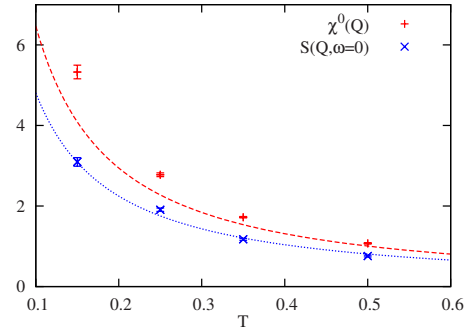

FIG. 5. (Color online) Scaled values for $\chi^0(Q)$ and $S(Q, \omega=0)$ vs T for the isotropic model. The dashed curve represents $\chi^0(Q)$ using the analytical form as extracted from the QMC results (Ref. 15). Dotted $S(Q, \omega=0)$ curve is the fit as deduced from the analytical approximation (Ref. 14).

nounced. Hence, also smoothed curves [Gaussian width $\sigma = 4 \cos[\pi L/2(L+1)]/\sqrt{2}$] are presented as relevant for $L \to \infty$. We note that such spectra are nearly L independent ($L = 16-40$) for $\omega > 0.5$ whereas for $\omega \sim 0$ still scale as $a + b/L$.

On the other hand, static $\chi^0(Q)$ can be extracted directly without invoking any smoothing and FTD-DMRG results combined with the FTLM results for $L = 12-20$ are shown in Fig. 4 scaled vs $1/L$. Deviations from the linear scaling mostly emerge from the random sampling in the basis preparation and the dynamical quantity evaluation and for the latter are indicated with error bars. Final scaled FTD-DMRG results for $\chi^0(Q)$ vs T are shown in Fig. 5 together with the result of the QMC analysis[15] of the analytical expression

$$\chi^0(Q) = \frac{a}{T}[\ln(b/T)]^{1/2}. \tag{13}$$

Our FTD-DMRG result is quite consistent with QMC results at higher $T > 0.3$. Still it is indicative that we get higher values (beyond error bars) for $T < 0.3$.

Finally, we present in the same Fig. 5 also scaled values of $S(Q, \omega=0)$ vs T. Bosonization theory gives[14]

$$S(Q, 0) = \frac{A}{T}[\ln(\Lambda/T)]^{1/2} \tag{14}$$

also fitted to our results with $\Lambda = 24.27$ taken from Ref. 18 and adjusted $A \sim 0.205$. The agreement with the analytical fit is very good although there seems to be substantial difference in the prefactor A.[14] On the other hand, it should be reminded that for this quantity there are no reliable larger-system alternative results since the QMC analysis[15,16] appears to have some difficulties in the regime $\omega \sim 0$.

IV. CONCLUSIONS

In conclusion, we have introduced the FTD-DMRG method, which is the extension of the density-matrix-based optimization of target states and the FTLM method for the evaluation of dynamical quantities at $T > 0$. It is so far well founded and tested for relatively low T and not too large systems, e.g., $L < 40$ while the feasibility or possible breakdown at larger T should still be understood. Presented results are obtained for systems with $\tilde{Z} < 200$ [normalized so that $\tilde{Z}(T=0) = 1$] although the method is not, in principle, limited to low T since it is not essential that all relevant many-body states are well represented, in analogy to the FTLM.[11] The emphasis so far is on the most challenging $\omega \sim 0$ dynamical response while higher ω could be improved by extending the density matrix by optimizing the correction vector at particular ω.[4,10] As the test we use the $\Delta = 0$ case which is nontrivial for the FTD-DMRG method while exact results are available via the spinless-fermion representation. On the other hand, results for the isotropic $\Delta = 1$ case where we concentrate on the low $\omega - T$ regime of dynamical spin correlations $S(Q, \omega)$ show that the presented method goes beyond the capabilities of up-to-date numerical methods, e.g., in the case of $S(Q, \omega=0)$. Clearly, more effort is needed to examine in more detail the feasibility of the new method.

ACKNOWLEDGMENTS

[1] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).

[2] U. Schollwöck, Rev. Mod. Phys. **77**, 259 (2005).

[3] K. A. Hallberg, Phys. Rev. B **52**, R9827 (1995).

[4] T. D. Kühner and S. R. White, Phys. Rev. B **60**, 335 (1999).

[5] T. Nishino and K. Okunishi, J. Phys. Soc. Jpn. **64**, 4084 (1995).

[6] R. J. Bursill, T. Xiang, and G. A. Gehring, J. Phys.: Condens.

Matter **8**, L583 (1996).

[7] F. Naef, X. Wang, X. Zotos, and W. von der Linden, Phys. Rev. B **60**, 359 (1999).

[8] M. A. Cazalilla and J. B. Marston, Phys. Rev. Lett. **88**, 256403 (2002).

[9] M. Zwolak and G. Vidal, Phys. Rev. Lett. **93**, 207205 (2004).

[10] S. Sota and T. Tohyama, Phys. Rev. B **78**, 113101 (2008).

[11] J. Jaklič and P. Prelovšek, Phys. Rev. B **49**, 5065 (1994); Adv. Phys. **49**, 1 (2000).

[12] M. Aichhorn, M. Daghofer, H. G. Evertz, and W. von der Linden, Phys. Rev. B **67**, 161103(R) (2003).

[13] T. Giamarchi and H. J. Schulz, Phys. Rev. B **39**, 4620 (1989).

[14] M. Bocquet, F. H. L. Essler, A. M. Tsvelik, and A. O. Gogolin, Phys. Rev. B **64**, 094425 (2001).

[15] O. A. Starykh, A. W. Sandvik, and R. R. P. Singh, Phys. Rev. B **55**, 14953 (1997).

[16] S. Grossjohann and W. Brenig, Phys. Rev. B **79**, 094409 (2009).

[17] T. Barthel, U. Schollwöck, and S. R. White, Phys. Rev. B **79**, 245101 (2009).

[18] V. Barzykin, Phys. Rev. B **63**, 140412(R) (2001).