Density matrix algorithm for the calculation of dynamical properties of low dimensional systems

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I extend the scope of the density matrix renormalization group technique developed by White to the calculation of dynamical correlation functions. As an application and performance evaluation I calculate the spin dynamics of the 1D Heisenberg chain.

The density matrix renormalization group method (DMRG) as developed recently by S. White is a powerful algorithm for calculating ground state energies and static properties of low dimensional systems. This technique leads to highly accurate results for much larger systems than those which can be solved by straightforward exact diagonalization. The method has been applied successfully to several problems such as the Haldane gap of spin-1 chains, the one-dimensional Kondo insulator and the two-chain Hubbard model.

An effective way of extending the basic ideas of this method to the calculation of dynamical quantities was lacking, mainly due to the fact that it is performed in real space and it is not possible to fix the momentum as a quantum number. It also involves a strong truncation of the Hilbert space and therefore much information of the excited states is lost.

In this paper I present a way to calculate the dynamical properties using the DMRG method. As an application I calculate the spin dynamics of the 1D isotropic Heisenberg model. The dynamics of this model has been studied extensively and therefore presents a good test of the method.

The DMRG allows for a systematic truncation of the Hilbert space by keeping the most probable states in de-
\[
G_A(z) = \frac{\langle \psi_0 | A^\dagger A | \psi_0 \rangle}{z - a_0 - \frac{b_0^2}{z - a_1 - \frac{b_1^2}{z - a_2 - \ldots}}} \tag{6}
\]

The coefficients \(a_n\) and \(b_n\) can be obtained using the following recursion equations [13,14]:

\[
|f_{n+1}\rangle = H|f_n\rangle - a_n|f_n\rangle - b_n^2|f_{n-1}\rangle \tag{7}
\]

where

\[
|f_0\rangle = A|\psi_0\rangle
\]

\[
a_n = \frac{\langle f_n | H | f_n \rangle}{\langle f_n | f_n \rangle},
\]

\[
b_n = \frac{\langle f_n | f_{n-1} \rangle}{\langle f_{n-1} | f_{n-1} \rangle}; \quad b_0 = 0 \tag{8}
\]

An alternative way for calculating the spectra is by means of the Liouvillian representation of the recursion method presented above [15,16]. This method leads to quasi size-independent coefficients. In the example given below, it has been seen that the results are the same as with the Hamiltonian representation using Eqs. (7) and (8) [16].

For finite systems the Green’s function \(G_A(z)\) has a finite number of poles so only a certain number of coefficients \(a_n\) and \(b_n\) have to be calculated. The DMRG technique presents a good framework to calculate such quantities. With it, the ground state, Hamiltonian and the operator \(A\) required for the evaluation of \(C_A(\omega)\) are obtained. An important feature is that the reduced Hilbert space should also describe with great precision the relevant excited states \(|\psi_n\rangle\). This is achieved by choosing the appropriate target states. For most systems it is enough to consider as target states the ground state \(|\psi_0\rangle\) and the first few \(|f_n\rangle\) with \(n = 0, 1, \ldots\) and \(|f_0\rangle = A|\psi_0\rangle\) as described above. In doing so, states in the reduced Hilbert space relevant to the excited states connected to the ground state via the operator of interest \(A\) are included. The fact that \(|f_0\rangle\) is an excellent trial state, in particular, for the lowest triplet excitations of the two-dimensional antiferromagnet was shown in Ref. [17].

Another straightforward election of target states is to take the excited eigenstates and the ground state. But this is possible only when the quantum number of the above mentioned states can be fixed. Otherwise, when diagonalizing the Hamiltonian, the lowest lying excitations of the whole space are obtained and not those of the appropriate symmetry sector. With the DMRG technique we can fix the total \(S^z_\|\) and parity but not, for example, the momentum \(q\) of the system. In the example given below, I attempted to obtain the first excited states for a given \(q\) by using \(|f_0\rangle = S_{\|}^z|\psi_0\rangle\) (where \(S_{\|}^z = \sum_j e^{iqR_j} S_j^z\)) as a trial state for the diagonalization procedure in step (i) above. Due to the fact that there is a small but non-zero overlap between \(|f_0\rangle\) and \(|\psi_0\rangle\), the algorithm does not remain in the symmetry sector with a given \(q\). Because of this, I found it convenient to use \(|\psi_0\rangle\) and \(|f_n\rangle\) with \(n = 0, 1, \ldots\) as target states.

Of course, if the number \(m\) of states kept per block is fixed, the more target states considered, the less precisely each one of them are described. An optimal number of target states and \(m\) has to be found for each case. Due to this reduction, the algorithm can be applied up to certain lengths, depending on the states involved. For longer chains, the higher energy excitations will become inaccurate. Proper sum rules have to be calculated to determine the errors in each case.

As an application of the method I calculate

\[
S^{zz}(q, \omega) = \sum_n \langle \langle \psi_n | S_n^z | \psi_0 \rangle \rangle^2 \delta(\omega - (E_n - E_0)), \tag{9}
\]

for the 1D isotropic Heisenberg model.

As I already mentioned, the spin dynamics of this model has been extensively studied. The lowest excited states in the thermodynamic limit are the famous des Cloiseaux-Pearson (dCP) triplets [11], having total spin \(S^z = 1\). The dispersion of this spin-wave branch is:

\[
\omega_q^\perp = \frac{J\pi}{2} |\sin(q)| \tag{10}
\]

Above this lower boundary there exists a two-parameter continuum of excited triplet states that have been calculated using the Bethe ansatz approach [18] with an upper boundary given by

\[
\omega_q^\parallel = J\pi |\sin(q/2)| \tag{11}
\]

It has been shown [18], however, that there are excitations above this upper boundary due to higher order scattering processes, with a weight that is at least one order of magnitude lower than the spin-wave continuum. Based on selection rules, Bethe ansatz calculations and numerical diagonalization of small clusters, Müller et al. [19] proposed the following approximate expression for the out-of-plane dynamical structure factor:

\[
S^{zz}(q, \omega) = \frac{A}{\sqrt{\omega^2 - \omega_q^\perp}} \Theta(\omega - \omega_q^\perp) \Theta(\omega_q^\parallel - \omega) \tag{12}
\]

where \(A\) is a constant and \(\Theta(x)\) a cutoff step function that was considered so that the sum-rules are satisfied. A similar expression for an exactly solvable model (the Haldane-Shastry model) has been obtained [17]. The low energy properties of this model and those of the nearest neighbour Heisenberg model we are considering belong to the same universality class.

In the following I will present the numerical results. The values for \(N = 20\) sites (without reduction of the Hilbert space) and exact calculations using the Lanczos technique and exploiting all the symmetries coincide exactly. For larger systems I used \(m = 200\) states per block and periodic boundary conditions.

In Fig. 1 I show the spectrum for various systems lengths and \(q = \pi\) and \(q = \pi/2\). The delta peaks of
Eq. (11) are broadened by a Lorentzian for visualizing purposes. For this case it was enough to take 3 target states, i.e. |ψ₀⟩, |f₀⟩ = S₂π/2|ψ₀⟩ and |f₁⟩. I also plot the analytical expression (12). There is good agreement up to N ≈ 40 with the envelope of our data. For larger values the peaks at ω/J ≈ 2 acquire high weight, which grows with N. The second peak seems to be somewhat shifted, also having a higher weight. Due to the truncation of the Hilbert space the spectrum of ω/J is also reduced. I notice that if we consider only the first (≈ 10) coefficients aₙ and bₙ, the spectrum at low energies remains essentially unchanged. Minor differences arise at ω/J ≈ 3. This is another indication that only the first |fₙ⟩ are relevant for the low energy dynamical properties for finite systems.

In the inset of Fig. 1 the spectrum for q = π/2 and N = 28 is shown. For this case I considered 5 target states i.e. |ψ₀⟩, |f₀⟩ = S₂π/2|ψ₀⟩, |fₙ⟩ n = 1, 3 and m = 200. Here, and for all the cases considered, I have verified that the results are very weakly dependent on the weights pⱼ of the target states, as long as the appropriate target states are chosen. For lenthgs where this value of q is not defined I took the nearest value. I found that with these parameters the spectrum starts developing spurious peaks for larger systems. The coefficients also present a larger dispersion with N than for the q = π case. To be able to go further, one should consider larger m values.

The q = π/2 case is the most unfavourable one because it involves high energy excitations. Although I have included some of these states as target states, the reduced Hilbert space related to |ψ₀⟩ and S₂π/2|ψ₀⟩ have very small overlap and many states are needed to describe correctly both target states. For q = π, instead, the overlap of Hilbert spaces is very high and the target states and low energy excitations are better described. The difference between the q = π/2 and q = π cases can be seen by comparing the ground state energy, it being more precise in the latter case by a factor of 3 in the relative error for m = 200 and N = 28 (the relative error of the ground state for the q = π case is 10⁻⁶).

Even though I am including states with a given momentum as target states, due to the particular real-space construction of the reduced Hilbert space, this translational symmetry is not fulfilled and the momentum is not fixed. To check how the reduction on the Hilbert space influences the momentum q of the target state |f₀⟩ = S₂|ψ₀⟩, I calculated the expectation values

\[ \langle ψ₀|S_{-q}^z S_q^z|ψ₀⟩ \] (13)

for all q’. If the momenta of the states were well defined, this value is proportional to δ₁−q if q ≠ 0. For q = 0, \( \sum S_{q=0}^z = 0 \). In Fig. 2a) I show the expectation values (13) for q = π/2 (using S₂π/2|ψ₀⟩ as one of the target states) and different lengths. I see that, as the system becomes larger (higher reduction of the Hilbert space), the q value becomes less defined, presenting a wider distribution. The figure shows a marked oscillation in the expectation value. This is due to the fact that the system is built from two identical blocks and that |ψ₀⟩|S₂π|ψ₀⟩| is small but non-zero (≈ 10⁻³ for the largest system). These should disappear when using the finite-size method (11). The momentum distribution for q = π is shown in Fig. 2b) in a semilogarithmic scale. In this figure I have shifted the values by .003 so as to have well-defined logarithms. I have also neglected the points where Eq. (13) is zero, mentioned above (i.e. between any two successive values in the figure there is a q’ that leads to a zero expectation value). I can see here that the momentum is better defined, even for much larger systems, but, as expected, more weight on other q’ values arise for larger N. I also calculated Eq. (13) for N = 28 and q = π/2 but using S₂π|ψ₀⟩ as a target state. I find a very poorly defined momentum centered at q’ = π/2. This is expected since the reduced Hilbert space targeted q = π states (in addition to the ground state).

In Fig. 3, I show the dispersion curve for 28 sites as compared to the exact dCP dispersion (Eq. (11)). The difference in the values at higher values of q is due to finite-size effects. These results are in very good agreement with those of Ref. [19]. The inset shows the first excitation energy ω¹ for q = π as a function of 1/N. In the thermodynamic limit this value must go to zero. The upwards curvature for the largest systems is due to the approximation of the method.

I find excellent agreement in excitation energies and weights for all values of q with exact results for N = 24 sites [14].

As a check of the approximation I calculated the sum rule

\[ \frac{1}{4π} ∫_0^∞ dω ∫_0^{2π} S_{zz}(q, ω) ≡ \langle ψ₀|S_{z=0}^zz|ψ₀⟩ = \frac{1}{4} \] (14)

for N = 28, 5 target states and m = 200. I obtain a relative error of 0.86%. I have also found that the expression for the static structure factor S_{z'z}(q) given in Ref. [13] i.e. S_{z'z}(q) = −1/4 ln(1−q/π), fits very accurately our data for N = 28 (details will be given elsewhere).

To conclude, I have developed a method to calculate dynamical correlation functions precisely using the DMRG technique to evaluate the coefficients of the continuous fraction representation of the Green’s function. I show that even by considering a 0.1% of the total Hilbert space (for N = 28 only ~ 40000 states are kept) a reasonable description of the low energy excitations is obtained. I also show that it is possible to obtain states with well defined momenta if the appropriate target states are used. The numerical computation has been performed on a workstation. A better performance (more accurately described excitations, larger systems) can surely be obtained by supercomputers, where, due to a larger memory space, a larger reduced Hilbert space can be considered.
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FIG. 1. Spectral densities for \( q = \pi \) and \( N = 28 \) (continuous line), \( N = 40 \) (dotted line) and \( N = 60 \) (dashed line). The analytical expression (12) is shown with a dashed-dotted line. Inset: Spectral density for \( q = \pi/2 \) for \( N = 28 \) (\( \eta = 0.05 \)).

FIG. 2. Momentum weights (Eq. (13)) of a target state with a) \( q = \pi/2 \) and \( N = 24 \) (circles), \( N = 28 \) (squares) and \( N = 36 \) (diamonds); b) \( q = \pi \) for \( N = 28 \) (circles), \( N = 44 \) (squares), \( N = 60 \) (diamonds) and \( N = 72 \) (triangles). The dotted lines are a guide for the eye.

FIG. 3. Dispersion relation of the lowest energy excitation. The full line is the spin wave curve \( \omega^\perp_q \) (Eq. (14)). The dots are our data for \( N = 28 \) and \( m = 200 \). Inset: First excitation energy as a function of \( 1/N \) for \( N = 14, 20, 28, 32, 36, 40, 44, 52, 60 \) and 72. The dotted line is a guide to the eye.
Fig. 2a
Fig. 2b
Fig. 3

A graph showing a relationship between $\omega / J$ and $1/N$. The inset graph illustrates $q = \pi$. The main graph varies $q$ from 0 to 3 on the horizontal axis and $\omega / J$ from 0 to 3 on the vertical axis.