Dynamic structure factor from real time evolution and exact correction vectors with matrix product states

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We propose two complimentary numerical methods for rigorous computation of dynamic structure factor at zero temperature. One solution is to solve Schrodinger equation using time dependent variational principle (TDVP) with matrix product states (MPSs) proposed by Haegeman et al. [Physical Review B 94, 165116], and Fourier transform correlation functions in time to frequency domain. Another way is to directly compute the transition rate between ground state and several low lying momentum eigenstates that are accessed using MPSs method amended with momentum filtering process. We benchmark both methods on a spin-1/2 Antiferromagnetic (AF) Heisenberg chain with periodic boundary condition. With finite size scaling analysis, the asymptotic line shape as a function of $\omega$ can be reproduced at various momentum $k$ with both methods.

I. INTRODUCTION

Dynamic structure factor is an important physical quantity observed directly in inelastic neutron scattering and resonating inelastic X-ray spectroscopy \[2\]. Numerical exact computation of them is extremely important for experimental data analysis and theoretical predictions. The definition of dynamic structure factor involves either real time evolution operators $e^{\pm iHt}$, which leads to a sign problem, or a set of exact eigenstates that is often inaccessible for non-integrable systems. Recent numerical advances proposed several remedies to the above problem. For a sign free Hamiltonian, analytical continuation with constraint can generate reliable spectral functions with certain known physical input \[3\]. On the other hand, for frustrated systems, approximated methods have to be used. Variational methods, such as Variational Monte Carlo (VMC) method \[4,4\], matrix product states (MPSs) method \[7,11\], and projected entangled pair states (PEPSs) method \[12\], have made translational invariant variational ansatz for single or two particle excited states, from which the transition rate between ground state and excited states can be calculated. These methods are strongly restricted by their number of variational parameters, yet they are efficient in getting all momentum eigenstates and eigen energies within a single run. Apart from variational approaches, exact diagonalization within certain quantum sectors \[13\] is still a simple and practical choice to get important physical insight, but it can not handle relatively large system sizes. Follow the streamline of working in a Krylov space, Gagliano et al. proposed continued fraction method \[14\]. With the success of Density Matrix Renormalization Group (DMRG) method, it was naturally adapted within a DMRG approach \[15,16\], where the exponential wall effect can be significant. Subsequently, correction vectors were introduced as a remedy, however with the expenses that each $\omega$ has to be targeted separately \[16,18\]. To circumvent this issue, Chebyshev MPSs (ChMPS) approach was proposed \[19,21\] to compute the full spectral functions. However the intrinsic limitation of ChMPS method is at the size of the subspace expand by a set of orthogonal finite bond dimensional MPSs \[22\].

Another approach within the MPSs/DMRG framework is to compute the real time evolution of an initial state using so called time dependent DMRG (tDMRG) method \[23,28\]. The accuracy of this method depends on evolution time step $\tau$, the order of Trotter-Suzuki expansion, and the number of Schmidt states $m$ kept. Usually with $\tau$ ranges from 0.01 to 0.1 and the expansion order from second to fifth, a maximum evolution time of 20 to 40 (in unit of coupling strength) can be reached up-to $m = 1200$ \[26\]. One obstacle of tDMRG method is the balancing between the order of expansion to operator $e^{-i\tau H}$ expressed by a Matrix Product Operator (MPO) and the efficiency (bond dimension) of it \[26,28\].

A recent development in the MPSs context for real time evolution \[1\] overcomes the above problem and brings additional benefits. It deals with real time evolution by numerically computing exponential of Hamiltonian (without Trotter-Suzuki expansion), whose procedure is similar to the ground state search DMRG algorithm, therefore the computational cost is also comparable to that of the standard algorithm. The second advantage is that energy conservation for unitary transformation is preserved, in contrary to the tDMRG method. Most importantly, the optimization at each step $\tau$ explores the entire MPSs manifold, which can be dynamically expanded when needed. This can be thought of as the wavefunction $\ket{\psi(t)}$ is fully optimized in a subspace spanned by all possible orthogonal states of MPSs with bond dimension $m$. The detail of this method is re-visited in Sec. II.

We propose using this method for computing correlation functions in time, then Fourier transform into frequency domain to get the spectral functions.

Come back to correction vectors in DMRG algorithm for spectral functions. If a correction vector is an eigenstate, thus calculated spectral function is exact. We
here propose a new generic MPSs/DMRG algorithm to numerically exactly compute physically important correction vectors. This benefits from the MPSs formalism, which can deal with non-local operations, such as global projection operator or translation operator, and can efficiently express them as local matrix product operators (MPO). These non-local operations if included as a constraint in the wavefunction, or added as extra terms in the Hamiltonian, can lead to energy level reshuffle [30] or reshaping. Inspired by the excited state MPSs/DMRG algorithm proposed by Wang and Sandvik [30], a MPSs/DMRG algorithm amended with momentum filtering process is proposed to explicitly compute several energy eigenstates with a wave momentum \( \mathbf{k} \). This leads to direct computation of the spectral weight (transition rate) of low-lying excitations, for example the des Cloizeaux-Pearson (dCP) states [31] in the spin-1/2 Antiferromagnetic Heisenberg chain. The rest of the paper is organized as following: after revisit the TDVP in Sec. II we discuss the transformation needed to obtain spectral functions in Sec. III where an alternative way to compute the spectral weight, is also discussed. Sec. IV is devoted for a benchmark demonstration of both methods. Conclusions and remarks are given in Sec. V.

II. TIME DEPENDENT VARIATIONAL PRINCIPLE APPLIED TO MATRIX PRODUCT STATES MANIFOLD

Time dependent variational principle was formulated recently to solve the Schrodinger equation approximately in a variational manifold \( \mathcal{M} \) of MPSs [1]. Consider Schrodinger equation, taking \( \hbar = 1 \),

\[
\frac{d\psi(t)}{dt} = -iH\psi(t).
\]

(1)

When restricted to a variation manifold \( \mathcal{M} \), it becomes

\[
\frac{du(t)}{dt} = -i\mathcal{P}_uH\psi(t),
\]

(2)

where \( u(t) \) is an approximate solution to \( \psi(t) \) within the manifold \( \mathcal{M} \), and \( \mathcal{P}_u \) denotes a tangent space at \( u(t) \). Projection to the tangent space \( \mathcal{P}_u \) guarantees that, under unitary evolution, the norm of wavefunction doesn’t change. Ref. [1] has shown how to Trotter decompose a tangent space projector rather than the Hamiltonian terms. Here we briefly outline this idea following Ref. [1].

The wavefunction at time \( t \) can be written as

\[
|\psi(A)| = \sum_{\{s\}=1}^{d} \text{Tr}[A_1^s A_2^s \cdots A_N^s]|s_1 s_2 \cdots s_N\rangle, \quad (3)
\]

which depends on a set of site-dependent matrices \( A_i^s \). It is convenient to rewrite Eq. (3) in a mixed canonical form

\[
|\psi(A)| = \sum_{\alpha\beta s_n s_{n+1}} \left[ A^C_n A^C_{n+1}\right]_{\alpha\beta}^{s_n s_{n+1}} \times
\]

\[
|\Phi_{La}\rangle\langle\Phi_{Ra}|_{n+1}\rangle\langle n|_{n+2:N} \rangle,
\]

(4)

where \( |\Phi_{La}\rangle \langle \Phi_{Ra}|_{n+2:N} \rangle \) is a set of orthonormal basis for the left (right) block of the lattice respect to the center two sites \( n \) and \( n+1 \), \( A^C_n \) and \( A^C_{n+1} \) are the center matrices of the two-site mixed canonical form. The tangent space of above wavefunction is defined as

\[
|\Theta[B]| = \sum_{n=1}^{N-2} \sum_{\alpha\beta s_n s_{n+1}} \left[ B_n B_{n+1}\right]_{\alpha\beta}^{s_n s_{n+1}} \times
\]

\[
|\Phi_{La}\rangle\langle\Phi_{Ra}|_{n+1}\rangle\langle n|_{n+2:N} \rangle.
\]

(5)

Under the "left gauge fixing condition"

\[
\sum_{s_n\beta} \left[ A_L \right]_{\beta\alpha}^s (n) B^s_{\alpha\beta} (n) = 0, \quad \forall n = 1, \ldots, N - 1, (6)
\]

where \( A_L(n) \) denotes the left canonical form of \( A_n \), one can check that \( \langle\psi[A]|\Theta[B]\rangle = 0 \). To minimize the distance of an arbitrary vector \( |\varepsilon\rangle \) with tangent vector \( |\Theta[B]\rangle \) under constraint Eq. (6) the projector is derived as

\[
\mathcal{P}_u = \sum_{n=1}^{N-1} P_L^{[1:n-1]} \otimes I_n \otimes I_{n+1} \otimes P_R^{[n+2:N]} - \sum_{n=1}^{N-2} P_L^{[1:n]} \otimes I_{n+1} \otimes P_R^{[n+2:N]},
\]

(7)

where \( P_L^{[1:n-1]} \) and \( P_R^{[n+2:N]} \) are defined as in Fig. 1. Once Trotter decompose the tangent space projector into parts, one can then integrate one by one following naturally the sweeping order of the standard DMRG algorithm.

The two-site algorithm can be organized as following: (1) prepare initial state in a right canonical form. (2) For any \( n = 1, \cdots, N - 2 \) integrate the Schrodinger equation in a subspace centered around \( n \) and \( n + 1 \)

\[
\frac{dA_C(n,t)}{dt} = -iH_{\text{eff}}A_C(n,t), \quad (8)
\]

where \( A_C(n,t) = \sum_{\alpha\beta s_n s_{n+1}} \left[ A^C_n (t) A^C_{n+1}(t)\right]_{\alpha\beta}^{s_n s_{n+1}} \). The solution is

\[
A_C(n,t + \tau) = e^{-iH_{\text{eff}}\tau} A_C(n,t).
\]

(9)

(3) Reformulate the wavefunction as a one-site \( (A^C_{n+1}) \) centered mixed canonical form to integrate the Schrodinger equation backward in time

\[
\frac{dA_C^{n+1}(t + \tau)}{dt} = -iH_{\text{eff}}A_C^{n+1}(t + \tau), \quad (10)
\]
Note that step (2) and (3) together complete evolving where the solution is

\[ A_{n+1}(t) = e^{-iH_{\text{ext}}(-\tau)}A_{n+1}(t + \tau). \]  

(11)

where \( A_{n+1}(t) \) is a coordinate index runs over all sites in the system. The space Fourier transformed operator \( S_{n+1}(t) = \sum_{r=1}^{N} e^{-i\mathbf{r}\cdot(\mathbf{r}-1)} \int_{-\infty}^{\infty} dt e^{i\mathbf{r}\cdot(\mathbf{r}-1)} \langle 0 | S_{n+1}(t) S_{1}^{0}(0) | 0 \rangle, \)

(12)

where \( | 0 \rangle \) denotes the ground state, \( \alpha, \beta = x, y \) or \( z \), and \( \mathbf{r} \) is a coordinate index runs over all sites in the system. The space Fourier transformed operator \( S_{n+1}(t) \) can be conveniently expressed as a matrix product operator (MPO) of bond dimension 2, where the left and right boundary MPO can be written as \( \left( 1, e^{i\mathbf{r}\cdot\mathbf{r}} S_{n}^{0} \right)^{T} \) respectively, and the bulk MPO is written as

\[ \left( \begin{array}{cc} 1 & 0 \\ e^{i\mathbf{r}\cdot\mathbf{r}} S_{n}^{0} & 1 \end{array} \right). \]

(13)

The dynamic structure can be re-expressed as

\[ S_{n}^{0}(\mathbf{k}, \omega) = \int_{-\infty}^{\infty} dt e^{i\mathbf{k}\cdot\mathbf{r}+i\omega t} \langle 0 | S_{n+1}(t) S_{1}^{0}(0) | 0 \rangle \]

(14)

Insert a complete set of basis \( \sum_{i=0}^{\infty} | i \rangle \langle i | \) into Eq. 14, the dynamic structure factor can be written as following

\[ S_{n}^{0}(\mathbf{k}, \omega) = 2\pi \sum_{i} \langle 0 | S_{-1}^{0}(\mathbf{k}) | i \rangle \langle i | S_{0}^{0}(0) \rangle \delta(\omega - \omega_{i}), \]

(15)

where \( \omega_{i} = E_{i} - E_{0}, E_{0} = \langle i | H | i \rangle \) and \( E_{0} = \langle 0 | H | 0 \rangle \). The dynamic structure factor reduces to a set of poles (delta function) with transition rate \( M_{i}^{0}(\mathbf{k}, \omega) = \langle 0 | S_{-1}^{0}(\mathbf{k}) \langle i | S_{0}^{0}(0) \rangle \), which is nonzero only when eigenstate \( | i \rangle \) has momentum \( \mathbf{k} \).

In the MPSS formalism, momentum eigenstates can be selected by adding an extra cost \( H_{\Lambda} \) in the Hamiltonian

\[ H_{\Lambda} = \lambda \left[ \left( T_{\alpha} + T_{\alpha}^{-1} - \cos k_{\alpha} \right)^{2} + \left( T_{\alpha} - T_{\alpha}^{-1} - \sin k_{\alpha} \right)^{2} \right] \]

(16)

where \( T_{\alpha} \) is a translation operator in \( \alpha = x \) or \( y \) direction, \( \lambda \) is a large number to favor energy eigenstate with wave momentum \( k_{\alpha} \). The translation operator can be written efficiently as a MPO of bond dimension \( d^{2} \), as illustrated in Fig. 2 with \( \mathcal{T} = 1_{s1r1} \otimes 1_{s2r2}, \mathcal{R} = 1_{s1l1} \otimes 1_{s2l1}, \mathcal{T} = 1_{s1r1} \otimes 1_{s2l2} \otimes 1_{s2l2} \) and \( T^{-1} = 1_{s1r1} \otimes 1_{s2l2} \otimes 1_{s1l1}, \)

\[ \mathcal{T} = 1_{s1r1} \otimes 1_{s2r2}, \mathcal{R} = 1_{s1l1} \otimes 1_{s2l1}, \mathcal{T} = 1_{s1r1} \otimes 1_{s2l2} \otimes 1_{s2l2} \] and \( T^{-1} = 1_{s1r1} \otimes 1_{s2l2} \otimes 1_{s1l1}, \)

where \( 1 \) is a \( d \times d \) identity matrix.

In the selected momentum \( k_{\alpha} \) sector, the ground state as well as several low lying excited states can be computed successively using Hamiltonian

\[ H_{j} = H + H_{\Lambda} - \sum_{i=0}^{j-1} E_{j} | i \rangle \langle i | \] (17)

where \( | i \rangle \) (for any \( i < j \), \( E_{i} < E_{j} \)) are energy eigenstates with wave momentum \( k_{\alpha} \) that are pre-computed before targeting the next state \( | j \rangle \). The transition rate \( M_{i}^{0}(\mathbf{k}, \omega) = \langle 0 | S_{-1}^{0}(\mathbf{k}) \langle i | S_{0}^{0}(0) \rangle \) therefore can be computed directly using eigenstates \( | 0 \rangle \) and \( | i \rangle \).

III. DYNAMIC STRUCTURE FACTOR AND TRANSITION RATE MATRIX

Dynamic structure factor can be expressed as Fourier transformation of space and time separated correlation function

\[ S_{n}^{0}(\mathbf{k}, \omega) = \sum_{r=1}^{N} e^{-ik\cdot(\mathbf{r}-1)} \int_{-\infty}^{\infty} dt e^{i\mathbf{k}\cdot(\mathbf{r}-1)} \langle 0 | S_{n+1}(t) S_{1}^{0}(0) | 0 \rangle, \]

(12)

The dynamic structure can be re-expressed as

\[ S_{n}^{0}(\mathbf{k}, \omega) = \int_{-\infty}^{\infty} dt e^{i\omega t} \langle 0 | S_{n+1}(t) S_{1}^{0}(0) | 0 \rangle \]

(14)

Insert a complete set of basis \( \sum_{i} | i \rangle \langle i | \) into Eq. 14, the dynamic structure factor can be written as following

\[ S_{n}^{0}(\mathbf{k}, \omega) = 2\pi \sum_{i} \langle 0 | S_{-1}^{0}(\mathbf{k}) | i \rangle \langle i | S_{0}^{0}(0) \rangle \delta(\omega - \omega_{i}), \]

(15)

The dynamic structure factor of this model has been well studied with Bethe Ansatz \([31, 32]\), symmetries and quantum groups analysis \([33, 35]\), and various numerical methods, such as time dependent DMRG method \([25]\), the Krylov-space approach with correction vectors \([13]\), the MPS-based Chebyshev expansion method \([24]\). We study this model by computing the spin correlation function in real time, i.e. the integrand \( \langle 0 | S_{n+1}(t) S_{1}^{0}(0) \rangle \) of Eq. 14 then Fourier transform into frequency domain to obtain the dynamic structure factor \( S(\mathbf{k}, \omega) \). Since the Hamiltonian is one dimensional, we here and after replace the wave momentum \( \mathbf{k} \) by a scalar \( k \) for

![ FIG. 2. Demonstration of translation operators \( T_{x} \) and \( T_{x}^{-1} \) in a form of matrix product operator.](image-url)
The integrand is calculated by separately evolving \( |S_k^\beta(t/2)\rangle = e^{-i\beta H t/2} S_k^\beta |0\rangle \) and \( |S_k^{\alpha\beta}(t/2)\rangle = e^{i\beta H t/2} S_k^{\alpha\beta} |0\rangle \) in time, and taking the inner product of them to get the time dependent correlation function

\[
\langle S^{\alpha\beta}(k, t) \rangle = \langle 0 | S_{-k}^\alpha(t) S_k^\beta | 0 \rangle = e^{iE_0 t} \langle S_k^{\alpha\beta}(t/2) | S_k^\beta(t/2) \rangle. \tag{19}
\]

The correlation functions \( \langle S^{zz}(k, t) \rangle \) for a size \( N = 64 \) chain at momentum \( k = \pi \), \( \frac{3\pi}{4} \), and \( \frac{\pi}{2} \) are shown in Fig. 3. Here we take \( \tau = 0.02 \) and iterate 1400 times to reach \( T_{\text{max}} = 112 \). The bond dimension is dynamically adjusted such that the error throw away in a single SVD \( \epsilon < 10^{-7} \). For \( N = 64 \), maximum bond dimension can reach \( m = 2000 \).

When Fourier transform time dependent correlation functions into frequency domain, we multiply the integrand by a contour \( 1 + \cos(\frac{\pi x}{T_{\text{max}}}) \), therefore, each delta function peak becomes a Gaussian with a broadening \( \approx \frac{1}{T_{\text{max}}} \). Fig. 4 illustrates the dynamic structure factors of \( N = 64 \) chain at momentum \( \pi \), \( \frac{3\pi}{4} \), and \( \frac{\pi}{2} \) obtained from the Fourier transform of spin correlation functions in Fig. 3. We fit each peak in the spectral function with a Gaussian \( a_i e^{-\frac{(\omega_\text{fit} - \omega_i)^2}{2b_i^2}} \) (shown in black solid lines in Fig. 4), where \( b_i \approx 0.02 \) for all fits.

**B. Comparison to two-spinon analytical transition rates**

For the AF Heisenberg chain, its lowest excited states are the famous des Cloizeaux-Pearson (dCP) triplets \( \frac{\pi}{2} \)

\[
\omega_L(k) = \frac{\pi}{2} |\sin k|. \tag{20}
\]

Bethe Ansatz approach revealed an extended two-spinon continuum whose lower boundary is the dCP expression and upper boundary is given by \( \frac{\pi}{2} |\sin k/2| \).

\[
\omega_U(k) = \frac{\pi}{2} |\sin k/2|. \tag{21}
\]

By approaches based on concept of infinite dimensional symmetries developed in the context of quantum groups, exact two-spinon dynamic structure factor has been derived \( \frac{\pi}{2} \), the asymptotic behavior at \( k = \pi \) and \( \omega \to 0 \) is

\[
S^{\alpha\beta}(\pi, \omega) \propto \frac{1}{\omega} \sqrt{\ln \frac{1}{\omega}}, \tag{22}
\]

whereas for all other \( k \) at \( \omega \to \omega_L \) is

\[
S^{\alpha\beta}(k, \omega) \propto \frac{1}{\sqrt{\omega - \omega_L(k)}} \sqrt{\ln \frac{1}{\omega - \omega_L(k)}}, \tag{23}
\]
To verify the above asymptotic behaviors using finite size
dynamic structure factor from real time evolution in solid symbols, and size scaled transition rate from exact eigenstates in open symbols. Asymptotic behavior $\frac{1}{c} (\ln \frac{1}{d})^d$ is fitted to above results, with $c, d$ the fitting parameters, red solid lines show fitting results from solid symbols, and black solid lines show fitting results from open symbols.

FIG. 5. Size scaled and normalized dynamic structure factor from real time evolution in solid symbols, and size scaled transition rate from exact eigenstates in open symbols. Asymptotic behavior $\frac{1}{c} (\ln \frac{1}{d})^d$ is fitted to above results, with $c, d$ the fitting parameters, red solid lines show fitting results from solid symbols, and black solid lines show fitting results from open symbols.

and normalized dynamic structure factor $NS^{zz}(k,\omega,N)$ for the first pole $\omega_1$ as a function of $\omega$ for sizes $N = 64, 56, 48, 40, 32, 24, 16$ at momentum $k = \pi, \frac{3}{2}\pi, \frac{1}{2}\pi$ in solid red squares. Fig. (a) also plots $NS^{zz}(k,\omega,N)$ for the second pole $\omega_2$ at $k = \pi$ in solid green dots. Whereas the open symbols in Fig. 5 are the scaled transition rate $NM^{zz}(k,\omega,N) = N|\langle i|S_x^z|0\rangle|^2$ directly computed from the lowest momentum eigenstates $|i\rangle$ for sizes $N = 160, 144, 128, 112, 96, 80, 64, 56, 48, 40, 32, 24, 16$ at $k = \pi, \frac{3}{2}\pi, \frac{1}{2}\pi$ (in red open squares) and the second lowest momentum eigenstates for sizes $N = 64, 56, 48, 40, 32, 24, 16$ at $k = \pi$ (in green open circles) via the momentum filtering method mentioned in Sec. III. Fig. (a) indicates that the two complementary methods produce exactly the same spectral functions, with solid and open symbols lie on top of each other. Fitting with the asymptotic behavior $\frac{1}{c} (\ln \frac{1}{d})^d$, where $\omega_L(\pi) = 0$, we found $c = 1.00(3), d = 0.28(8)$, which is very consistent with Bethe Ansatz analytical results $c = 1, d = 0.5$. Fig. (b-c) show that the weight of the first peak is a bit over-counted in the Fourier transformation of correlation functions in time for large system sizes. It means that longer evolution time and larger bond dimension is needed to resolve small and close-by spectral peaks in higher energy excitations. With the same analytical function we found in Fig. 5(b) for $k = 3\pi/4$, $c = 0.59(4), d = 0.11(11)$ for open symbols, $c = 0.42(4), d = 0.54(8)$ for solid symbols; while in Fig. 5(c) for $k = \pi/2$, $c = 0.43(2), d = 0.69(5)$ for open symbols, and $c = 0.40(7), d = 0.83(17)$ for solid symbols.

V. REMARKS AND DISCUSSIONS

We proposed two different methods to compute dynamic structure factor, both methods are formulated within the framework of matrix product states (MPSS). One involves real time evolution using a recently proposal, where time dependent variational principle (TDVP) is applied to MPSS \[1\]. Another method directly target exact eigenstates in the middle of the spectra by modifying Hamiltonian to favor eigenstates with wave momentum \( k \). We applied both method to the spin-1/2 Antiferromagnetic Heisenberg chain. From real time evolution, $T_{\text{max}} = 112$ can be reached at a maximum bond dimension $m = 2000$. Linear prediction for real time correlation, which is believed to be unreliable for complicated spectral functions, is not used here. Still the Fourier transformation with a cut $T_{\text{max}}$ in time can rigorously reproduce the exact spectral function for size $N = 64$. Larger system sizes can be studied with a slightly relaxed condition $\epsilon < 10^{-6}$ for one singular value decomposition (SVD). The computational cost of evolving a wavefunction $2\tau$ forward in time is comparable to one full sweep in the standard density matrix renormalization group (DMRG) algorithm. Given a relatively small bond dimension $m = 2000$, a much longer time $T_{\text{max}}$ can be reached compared to tDMRG algorithm.
formulated with matrix product operator (MPO). Even though there is no explicit estimation of Trotter error in orders of $\tau$ for Trotter expansion of the tangent space projector, the forward plus backward evolution scheme make error in $\tau$ cancel thus generate very accurate solution to the Schrodinger equation. On the other hand, direct computation of energy eigenstates in the middle of the spectrum proposed in this paper is way more powerful than previous correction vector method in DMRG, in a way that it can reshuffle and reshape the energy eigenvalues such that around the target state, the density of states are much smaller. With additional techniques, such as fixing total spin quantum number with SU(2) symmetric MPS/DMRG program, the convergence of eigenstates can be even faster. The time evolution method, although powerful, can not evolve too long with restricted bond dimension $m$. However it will predict a qualitatively correct position $\omega$ of the important physics. Applying shift-and-invert method using the proposed Hamiltonian in the main text can precisely compute the corresponding eigenvector, and allows direct analysis of other observable. The two methods combined together provide a numerical powerful tool to explore excitations in quantum many-body systems.

Upon completing this manuscript, we saw manuscript [37], which shares similar idea with one of the two proposals within our manuscript.

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