Dynamical Spectral Function From Numerical Renormalization Group: A Full Excitation Approach

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For a given quantum impurity model, Wilson’s numerical renormalization group (NRG) naturally defines a NRG Hamiltonian whose exact eigenstates and eigenenergies are obtainable. We give exact expressions for the free energy, static, as well as dynamical quantities of the NRG Hamiltonian. The dynamical spectral function from this approach contains full excitations including intra- and inter-shell excitations. For the spin-boson model, we compare the spectral function obtained from the present method and the full density matrix (FDM) method, showing that while both guarantee rigorous sum rule, the full excitation approach avoids the causality problem of FDM method.

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I. INTRODUCTION

Wilson’s numerical renormalization group (NRG) method\textsuperscript{1,2} is powerful for studying quantum impurity models. Since its invention, NRG has witnessed a series of development, including z-averaging to mitigate the discretization error\textsuperscript{9–11} and merging with matrix product state\textsuperscript{7} networks, etc. Today, both the sophistication and applicability of NRG have been advanced significantly compared to Wilson’s original work.

The calculation of spectral function of an quantum impurity model from the NRG-produced eigenstates and eigenenergies is an important problem. The patching method\textsuperscript{12} combines the spectral functions from successively lower energy shells to produce a full spectral function which does not guarantee the exact sum rule. Using the reduced density matrix of the full system to combine the spectral functions of different energy shells, Hofstetter\textsuperscript{13} developed the density-matrix NRG that can take into account the influence of the low energy states to the high frequency spectral function. In the full density matrix (FDM) NRG method,\textsuperscript{5} the Lehmann representation of the spectral function is treated with a complete basis proposed by Anschel et al.\textsuperscript{6} The set of exact eigenstates of $\hat{H}$, dubbed NRG Hamiltonian. The complete basis proposed by Anderson et al.\textsuperscript{8} is the set of exact eigenstates of $\hat{H}$, with their eigenenergies being generated by NRG calculation. Then, we propose an algorithm to calculate the exact free energy, static, as well as dynamical quantities of $\hat{H}$, which constitute well-controlled approximations to those of the original impurity model. The obtained spectral function contains both the intra- and inter-shell excitations. It satisfies the rigorous sum rule and positivity. Hereafter this new algorithm is called full excitation (FE) NRG method.

II. FE FORMALISM

In this section, we derive the formalism of FE method for general quantum impurity models. The Hamiltonian of a generic quantum impurity model reads $H = H_{imp} + H_{bath} + H_{c}$. A small quantum system described by $H_{imp}$ is coupled through $H_{c}$ to a continuous non-interacting reservoir described by $H_{bath} = \sum_{i} \epsilon_{i} c_{i}^{\dagger} c_{i}$. Here, $c_{i}^{\dagger}$ creates a particle (fermion or boson) with energy $\epsilon_{i}$. The indices such as spin and orbital are included in $i$. The impurity is coupled directly to the local bath degrees of freedom $f_{0} = 1/L \sum_{i} V_{i} c_{i}$, with $L$ the normalization constant.

The NRG algorithm consists of three steps:\textsuperscript{14} (i) The continuous bath degrees of freedom are discretized into bath sites with exponentially descending energies $\omega_{n} \sim \Lambda^{-n}$. $\Lambda \geq 1.0$ is the logarithmic discretization parameter. This step introduces the logarithmic discretization error which diminishes as $\Lambda$ decreases to unity. (ii) The discretized Hamiltonian is canonically transformed into a semi-infinite chain of the form (truncated to length $N$
and neglecting possible indices of spin, orbital, etc.)

\[ H_N = H_{imp} + c_0 \left( f_0^A + A \hat{f}_0 \right) + \sum_{n=0}^{N} \epsilon_n f_{n}^A f_n 
+ \sum_{n=0}^{N-1} t_n \left( f_{n}^A f_{n+1} + f_{n+1}^A f_n \right). \]  

Here, \( A \) is an impurity operator. \( H_N(\Lambda) \) is a function of \( \Lambda \). Both \( \epsilon_n \) and \( t_n \) decay as \( \Lambda^{-n/2} \) for fermionic bath (\( \Lambda^{-n} \) for bosonic bath). (iii) The chain Hamiltonian is diagonalized iteratively. Starting from the longest chain \( H_{n_0} \) whose all eigenstates can be kept, we add one bath site and diagonalize the enlarged system. This is done iteratively until all the chain sites are added and diagonalized. To handle the divergence of the Hilbert space in this process, after diagonalizing \( H_n \), only the \( M \) eigenstates with lowest eigenenergies are kept. The matrix of \( H_{n+1} \) is built in the product space of these kept states and the bare states of the newly added site. The truncation error introduced in this step diminishes in the limit \( M = \infty \).

NRG calculation generates many eigenstates \( |s \rangle_n \) and the degeneracies of \( \Lambda \). Both the theoretical equations where the truncation is not taken into account explicitly.

Let us analyse the structure of the eigen spectrum generated by NRG. Suppose \( H_{n+1} = H_n + \Delta H_n \). \( \Delta H_n \) contains the on-site energy of the newly added bath site \( n + 1 \) and the hopping between sites \( n + 1 \) and \( n \). If \( \Delta H_n \) is not considered, adding bath site \( n + 1 \) will increase the degeneracy of each eigenstate of \( H_n \) by a factor of \( d \). If \( \Delta H_n \) is fully added, all these degeneracies will be lifted. In NRG calculation, \( \Delta H_n \) is added only partly. That is, the matrix of \( \Delta H_n \) is constructed in the space of kept states of \( H_n \) multiplying the bare states of bath site \( n + 1 \). Therefore, the degeneracies in the extended spectrum of \( H_n \) are partly lifted. The resulting Hamiltonian matrix corresponds to the Hamiltonian

\[ \tilde{H}_{n+1} = \tilde{H}_n + P_n \Delta H_n P_n \]  

instead of to the theoretical \( H_{n+1} = H_n + \Delta H_n \). Here \( P_n \) is the projecting operator of the kept space of \( H_n \). The full spectrum of \( H_{n+1} \) (rectangular boxes in Fig.1 for \( n = 1 \) and 2) is composed of those low energy eigenstates obtained from lifting the degeneracies of \( \tilde{H}_n \) by \( P_n \Delta H_n P_n \) (red horizontal levels in Fig.1), and those high energy eigenstates generated by multiplying new bath states to previous eigenstates while maintaining degeneracies (green and blue horizontal levels in Fig.1). A schematic picture is shown in Fig.1 for illustration of the above process, using the number of kept states \( M = 4 \), Hilbert space dimension of bath site \( d = 4 \), and chain length \( N = 3 \). Detailed explanation is in figure caption.

Grouping all the discarded states (extended to include the degeneracies) generated in the calculation for \( H_N \) (e.g., the rectangular box of \( H_B \) in Fig.1), we obtain not only a complete basis set for \( H_N \) but also the exact eigenstates of the following NRG Hamiltonian \( \tilde{H}_N \)

\[ \tilde{H}_N = H_{n_0} + \sum_{n=n_0+1}^{N} \epsilon_n f_{n}^A f_n 
+ \sum_{n=n_0}^{N-1} t_n \left[ (P_n f_{n}^A P_n) f_{n+1} + f_{n+1}^A (P_n f_{n} P_n) \right], \]  

which is obtained by iterating Eq.(2) and setting \( \tilde{H}_{n_0} = H_{n_0}, \tilde{H}_N = \tilde{H}_N(\Lambda, M) \) depends on the NRG parameter \( \Lambda \) and \( M \). It is a many-body Hamiltonian defined in the original Hilbert space of \( H_{n_0} \), with eigenstates \( |se \rangle_{n}^{D} \) and eigenenergies \( E_{n_0s}^{D} (n \in [n_0 + 1, N]) \),

\[ H_N |se \rangle_{n}^{D} = E_{n_0s}^{D} |se \rangle_{n}^{D}. \]  

Here, \( |se \rangle_{n}^{D} = |s_n\rangle \otimes |s_n \rangle \otimes |s_{n-1} \rangle \otimes \cdots \otimes |s_0 \rangle \otimes |s_{n+1} \rangle \) are matrix product states with degeneracy \( d^{N-n} \). \( |s_n \rangle \)'s \( \sigma_n \in [1, d] \) are the bare basis states of site \( n \). The eigenstates fulfill the standard orthonormal and complete relations. We have \( H = H_{N=\infty}(\Lambda = 1.0) \) and \( H_N(\Lambda) = \tilde{H}_N(\Lambda, M = \infty) \). Therefore, \( \tilde{H}_N \) approximates
$H_N$ of Eq.(1) with the control parameter $M$ and $H_N$ approximates $\hat{H}$ with the control parameter $\Lambda$. Thanks to the exponential separation of energy scales due to the logarithmic discretization and the truncation scheme of NRG, $\hat{H}_N$ has very accurate low energy states. Note that the extended kept states $|se\rangle_K^N$ ($n = 0, 1, ..., N - 1$) are not exact eigenstates of $\hat{H}_N$.

We now consider to produce the exact physical quantities of $\hat{H}_N$ from the obtained $\{|s\rangle_n\}$ and eigenenergies $\{E_{ns}\}$. The partition function $Z$ at temperature $T$ reads

$$Z = \sum_{n=n_0+1}^{N} \sum_{s} \exp{-\beta E_{ns}},$$

The exact free energy of $\hat{H}_N$ is $F = -(1/\beta) \ln Z$. The statistical average of an impurity operator $\hat{O}$ reads

$$\langle \hat{O} \rangle = \frac{1}{Z} \sum_{n=n_0+1}^{N} \sum_{s} \exp{-\beta E_{ns}} \langle s \hat{O} s \rangle_n.$$  \hspace{1cm} (6)

The above expressions were already employed in the FDM method which treats the density matrix exactly. FE and FDM differ in their formalisms for dynamical quantities. Consider, for example, the time correlation function $\langle A(t)B \rangle = \text{Tr}[\rho A(t)B]$ of two impurity operators $A$ and $B$. The density operator reads $\rho = e^{-\beta \hat{H}}/Z$. Inserting $1 = \sum_{n,s} |se\rangle_n \langle se|$ twice, we obtain

$$\langle A(t)B \rangle = \sum_{n,s} \sum_{s'} \text{Tr}[\rho |se\rangle_n \langle se| e^{i\hat{H}t} A e^{-i\hat{H}t} |s'e\rangle_n \langle s'e| B].$$  \hspace{1cm} (7)

Once the exact expression Eq.(4) is used to evaluate the matrix elements of $A(t)$, excitations of the form $E_{ns}^D = E_{n's'}^D$ will be generated, which include both inter-($n \neq n'$) and intra-shell ($n = n'$) excitations. Before we present the FE formalism, we first make a brief analysis for the FDM method. To obtain the formalism of FDM, we first reduce Eq.(7) into the single-shell form with the help of the exact relation $1_{d,D,N,n_0} = \sum_{s} |se\rangle_K^n \langle se|$ + $\sum_{n=n_0+1}^{N} \sum_{s} |se\rangle_n \langle se|$ ($m \in [n_0, N]$). We obtain

$$\langle A(t)B \rangle = \sum_{n=n_0+1}^{N} \sum_{s} \text{Tr}[\rho |se\rangle_n \langle se| e^{i\hat{H}t} A e^{-i\hat{H}t} |s'e\rangle_n \langle s'e| B] + \sum_{n} \sum_{s} \text{Tr}[\rho |se\rangle_n \langle se| e^{i\hat{H}t} A e^{-i\hat{H}t} |s'e\rangle_n \langle s'e| B] + \sum_{n} \sum_{s} \text{Tr}[\rho |se\rangle_n \langle se| e^{i\hat{H}t} A e^{-i\hat{H}t} |s'e\rangle_n \langle s'e| B].$$  \hspace{1cm} (8)

The exact relation $\rho |se\rangle_n \langle se| = e^{-\beta E_{ns}^D}/Z$ is used for the density operator $\rho$. To calculate the matrix elements of $e^{i\hat{H}t} A e^{-i\hat{H}t}$ in the second and third terms, the NRG approximation $H_N|se\rangle_K^N \approx E_{ns}^K |se\rangle_K^N$ is used on one side of $A$ and the exact Eq.(4) is used on the other side. The $e^{\pm i\hat{H}t}$ factors on two sides of $A$ are hence not treated on equal footing. The obtained expression reads

$$\langle A(t)B \rangle = \sum_{n,s,s'} \sum_{D} \left[ B^{(n)}_{DD} |s's\rangle_D \langle s| A^{(n)}_{DD} |s's\rangle_D e^{i(E_{ns}^D - E_{n's}^D)t} d_n - n \right] + \sum_{n,s,s'} \sum_{D} \left[ B^{(n)}_{KD} |s's\rangle_D \langle s| A^{(n)}_{KD} |s's\rangle_D e^{i(E_{ns}^D - E_{n's}^D)t} d_n - n \right]$$  \hspace{1cm} (9)

Here, the matrix elements are defined as $\left[ O^{(n)}_{XX'} \right]_{ss'} = \langle X| O |se\rangle_{n}^N |X' \rangle$, for $O = A, B$, and $\rho$. Eq.(9) contains only intra-shell excitations among which the kept-discarded excitations are approximate for $\hat{H}_N$. For the case $B = A^\dagger$, the first two terms have positive weights since the matrix $\rho^{-1}_{DD}$ is diagonal and positive. In the third term, the matrix $\rho^{-1}_{KK}$ is not diagonal. For fixed $n, s$, and $s'$, the prefactor of exp $i \left( E_{ns}^D - E_{n's}^D \right) t$ is not guaranteed to be positive unless the same NRG approximation is used for $\rho^{-1}_{KK}$. In summary, in the FDM formalism, the density operator $\rho$ is evaluated exactly but the matrix elements of $A(t)$ are treated with the NRG approximation. The inter-shell excitations are approximately replaced by the kept-discarded intra-shell excitations. As a result, albeit the spectral function fulfills the rigorous sum rule, the positiveness of the diagonal spectral function is lost.

In contrast, in deriving the FE formalism, we start from Eq.(7) and use Eq.(4) only. The obtained expression for the spectral function is exact for $\hat{H}_N$. Naturally, it has no causality problem. Below, we focus on the retarded Green’s function (GF) of the impurity operators $A$ and $B$, $G_{f_A B}^{f_b} (\omega) \equiv -i \int_0^\infty \langle A(t)B(t') \rangle_\pm e^{i(\omega + i\eta)(t-t')} dt - t'$. $G^f (G^b)$ denotes Fermi- (Bose-) type GF which is defined with anti-commutator (commutator). Starting from the exact Lehmann representation of $G_{A,B}^{f,b}$, inserting the complete relation of the complete basis, and using Eq.(4) to compute the matrix elements of both $\rho$ and $e^{\pm i\hat{H}t}$, we obtain the FE formula for GF. Details of the derivation are summarized in Appendix. We obtain

$$G_{A,B}^{f,b} (\omega) = \sum_{m=n_0+1}^{N} \sum_{s} w_{ms'} G_{A,B}^{f,b} (\omega),$$  \hspace{1cm} (10)
with the weight \( w_{ms'} = (1/Z)d^{N-m}e^{-\beta E_{ms'}} \) and
\[
G_{A,B}^{(ms')}(\omega) = \\
\sum_s \left[ 1 + e^{-\beta(E_{ms}^{A} - E_{ms'}^{A})} \right] \left[ \frac{AB_{\omega}^{(nm)}}{D_{\omega}^{(m)\omega} + i\eta + E_{ms}^{D} - E_{ms'}^{D}} \right] + \sum_{n=n_0+1}^{m-1} \sum_s \left[ 1 + e^{-\beta(E_{ms}^{A} - E_{ms'}^{A})} \right] \left[ \frac{BA_{\omega}^{(nm)}}{D_{\omega}^{(m)\omega} + i\eta + E_{ms}^{D} - E_{ms'}^{D}} \right]
\]
(11)

In the equation, \( D_{\omega}^{(m)\omega} = \sum_s |O_{\omega}^{(m)}| s s' D_{m}s' \), \( (O = A, B) \).

\( [XY]^{(nm)}_{s s'} \) \((XY = AB \text{ or } BA)\) is given by \((n_0 + 1 \leq n \leq m - 1)\)
\[
[XY]^{(nm)}_{s s'} = \sum_{n_1, s_2} \left[ X^{(n_1)}_{DK} \right]_{s_1 s_2} V^{(n,m)}_{s_1 s', s_2} \left[ Y^{(n)}_{DK} \right]_{s s_2} .
\]
(12)

The transition matrix \( V \) is calculated recursively through
\[
V^{(n-1,m)}_{s_1 s', s_2} = \sum_{\sigma_m, s_3, s_4} \left[ U^{(\sigma_m)}_{KK} \right]_{s_1 s_3} V^{(n,m)}_{s_3 s', s_4} \left[ U^{(\sigma_m)}_{KK} \right]_{s_4 s_2} ,
\]
(13)

with the initial value
\[
V^{(m-1,m)}_{s_1 s', s_2} = \sum_{\sigma_m} \left[ U^{(\sigma_m)}_{KK} \right]_{s_1 s'} \left[ U^{(\sigma_m)}_{KK} \right]_{s_2 s_2} .
\]
(14)

Here, the matrices \( U^{(\sigma_m)}_{KK} \) and \( U^{(\sigma_m)}_{KD} \) are respectively the kept-kept and kept-discarded blocks of the unitary transformation matrices produced by the diagonalization of \( H_m \) in NRG. Eqs.(10)-(14) are the main results of this paper. This FE formalism contains both intra- and inter-shell excitations. The unitarity of quantum evolution in \( A(t) \) is maintained at the expense of introducing inter-shell excitations of \( \tilde{H}_N \). For \( B = A^\dagger \), Eq.(11) has a hermitian symmetry and naturally guarantees the positiveness of the spectral function \(-1/\pi\text{Im}G^{f/b}_{A,A^\dagger}(\omega)\) in \( \omega > 0 \).

III. RESULTS AND COMPARISON

Below, we use the spin-boson model (SBM) to demonstrate FE algorithm and to make comparison with the patching method and FDM method. SBM describes a two-level quantum system coupled to a dissipative bosonic bath. It has been widely studied in many contexts ranging from superconducting qubits to photosynthetic biosystems. NRG has played an important role in the understanding of this model. The Hamiltonian reads
\[
H_{SB} = -\frac{\Delta}{2} \sigma_x + \frac{\epsilon}{2} \sigma_z + \sum_i \omega_i a_i^\dagger a_i + \frac{\sigma_+}{2} \sum_i \lambda_i (a_i^\dagger + a_i) .
\]
(15)

The two-level system is described by Pauli matrices and the influence of bath is encoded into the spectral function \( J(\omega) = \frac{1}{\pi} \sum \lambda_i^2 \delta(\omega - \omega_i) \), for which we use \( J(\omega) = 2\pi m \omega^\epsilon \omega_{c}^{1-\epsilon} \) \((0 < \omega < \omega_c, \omega_c = 1.0)\) with coupling strength \( \alpha \) and exponent \( s \). As usual, we truncate the Hilbert space of each boson site to \( N_b \) states in the occupation basis. Now, the NRG Hamiltonian becomes \( H_N(\Lambda, M, N_b) \) and FE method produces the exact quantities for it. In this paper, we study the Fourier transform of the anti-symmetric dynamical correlation function,
\[
C(\omega) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{1}{1/2} \langle [\sigma_z(t), \sigma_z(0)] \rangle e^{i\omega t} dt = -\frac{1}{2\pi} \text{Im}G^{f}_{\sigma_z \sigma_z}(\omega) .
\]
(16)

In Fig.2(a), we plot the regular part of \( C(\omega) \) obtained from the patching method, FDM method, and FE for a sub-Ohmic bath \( s = 0.3 < \alpha > \alpha_c \), \( \epsilon > 0 \), and a low temperature. In this paper, we use the standard log-Gaussian broadening for the spectral function at all frequencies, being different from the fermion case where a Lorentzian broadening is used instead for \( \omega < T \). The broadening is controlled by the width \( B \) of the log-Gaussian function. The curve from FDM method agrees well with that of FE in the frequency regime \( \omega / \Delta \gtrsim 10^{-3} \) but becomes negative in lower frequencies. Both curves fulfill the sum rule \( \int_{-\infty}^{\infty} C(\omega) d\omega = 1.0 \) to machine precision. The curve from the patching method is higher in the intermediate regime and matches the FE result in the low frequency regime. It violates the sum rule since the spectral function is obtained by approximately patching up the spectral function of each energy shell.

The Lehmann representation of FDM-produced \( C(\omega) \) can be written as \( C(\omega) = \sum_k w_k \delta(\omega - \epsilon_k) \). We separate the positive and negative components as
\[
C(\omega) = C^{(+)}(\omega) + C^{(-)}(\omega) \\
C^{(+)}(\omega) = \sum_k \left( w_k \delta(\omega - \epsilon_k) \right) \\
C^{(-)}(\omega) = \sum_k \left( w_k \delta(\omega - \epsilon_k) \right).
\]
(17)

Here, \( w_k \) and \( \epsilon_k \) are the weight and energy of the \( k \)-th pole in \( C(\omega) \), respectively. In Fig.2(b), we compare \( C^{(+)}(\omega) \), \( |C^{(-)}(\omega)| \), and \( C(\omega) \). In a wide frequency range including where FDM agrees well with FE, \( C^{(+)}(\omega) \) and \( |C^{(-)}(\omega)| \) are larger than \( C(\omega) \), showing that a cancellation of errors occurs in the FDM-produced \( C(\omega) \). In contrast, FE produces \( C^{(-)}(\omega) = 0 \) at machine precision for all parameters.
The converged part agrees well with the FE curve. However, at different parameters of NRG, the frequency regime with negative weight problem in C(ω) is not remedied by increasing M and N_b. The only curve of C(ω) > 0 is obtained at s = 0.8, using Λ = 4.0 and a relatively larger broadening parameter B = 1.2. In agreement with Fig.3, this shows that the positive C(ω) is obtained through a more effective cancellation of errors between C(-)(ω) and C(+)(ω) at larger Λ and B. Our data for s = 0.3 (not shown) gives the same conclusion.

FDMD method should produce the exact C(ω) of H_N(Λ, M = ∞, N_b) at M = ∞. We expect that the negative weight problem in C(ω) will disappear at sufficiently large M. Fig.4(b) shows how the FDMD-produced C(ω) evolves with increasing M. The high frequency regime of C(ω) (ω/Δ > 10^{-4}) converges already for M = 60. With increasing M, the frequency regime with converged C(ω) extends slowly towards lower frequency. The converged part agrees well with the FE curve. However, we find that the integrated negative weight |W(-)| does not decrease with increasing M. To understand this observation, using a smaller N_b = 4, we show in the inset |W(-)| as functions of chain length N for different M. For a fixed M, |W(-)| is zero for the short chain whose states
So far, the spectral function of SBM has not been studied in detail in this parameter regime. We plot both FDM and FE results. From the FE curves (solid lines), one can find a narrow frequency window around $\omega \gtrsim T$ where $C(\omega) \sim \omega^s$ occurs (dot-dashed straight eye-guiding lines). Below an $\alpha$-dependent low frequency $\omega_r$, $C(\omega)$ increases sharply. In the range $\omega_r \lesssim \omega \lesssim T$, a pseudo-gap forms. As $T$ decreases (not shown here), the lower boundary of this pseudo-gap range shifts towards lower frequency, forming an extended range with $C(\omega) \sim \omega^s$ behavior. In the limit $T = 0$, the expected Shiba relation for the symmetry broken phase will be recovered. In contrast, FDM method produces negative or irregular curve (dashed lines) in the $C(\omega) \sim \omega^s$ range and the pseudo-gap range, failing to give the complete scenario.

Finally, we investigate the computing time of the FDM
and FE methods. Fig.7 and Fig.8 show the scaling of the computation time of FE (Fig.7) and FDM (Fig.8) with respect to NRG parameters $N$, $M$, and $N_b$. They show that FE is more computationally demanding, with computing time proportional to $M^2N_b^2N^1/2$, while FDM method is much faster, with the scaling to $M^2N_b^2N^1/2$. This is expected because the FE formalism of GF includes inter-shell excitations while the FDM one includes only intra-shell excitations. It is an open question how to modify the FE method to accelerate the computation while keeping its advantages of positiveness. Both FE and FDM algorithms can be implemented with efficient parallel computing.

IV. DISCUSSION AND SUMMARY

The time-dependent NRG employs the same NRG approximation as FDM does and the unitary quantum evolution is not treated accurately. Similar to the equilibrium situation, the exact result for $H_N$ will provide well-behaved time evolution of $\langle O(t) \rangle$. Therefore, the present FE for equilibrium state can be extended to time-dependent NRG for studying quantum quench problems. A comparison study will shed light on to what extent the FE method can improve the result for non-equilibrium time evolution of interested quantities.

The concept of exactly solvable effective projected Hamiltonian, such as the $H_N$ in the present work, can also be extended to other algorithms. The energy-based truncating criterion used in ordinary NRG algorithm does not produce the optimal matrix product eigenstates. By replacing the energy-based truncating criterion of NRG with the density matrix-based criterion, or using the variational scheme of matrix product states NRG algorithm can be improved and a bridge between NRG and density matrix renormalization group (DMRG) has been established. The idea of FE could also be applied to these new NRG algorithms for better precision. For the one-dimensional quantum many-body systems with short-range entanglement, it is an interesting open question whether the exactly solvable effective projected Hamiltonian like $H_N$ can be constructed and an accurate full spectrum algorithm for the dynamical quantities can be developed.

In summary, we propose the FE algorithm for calculating the dynamical quantities of quantum impurity models in the equilibrium state. This algorithm is based on the exact solution of the projected NRG Hamiltonian and hence it circumvents the negative spectral function problem of FDM NRG. We demonstrate the effect of FE and its advantage over FDM method by a comparison study of $C(\omega)$ for SBM.

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Appendix A: Derivation of FE Formalism for $G_{A,B}(\omega)$

In this appendix, we derive the FE formalism for the retarded GF $G_{A,B}(\omega)$ defined in the main text. We use the notations as Ref. 24. For completeness, we also summarize the basic formulas about the complete basis developed there.

We denote the recursive relation of NRG Hamiltonian as $H_n = H_{n-1} + \Delta H_{n-1}$. $H_n$ is the Hamiltonian of the full chain with length $N$. $H_{n0}$ is Hamiltonian of the longest chain whose eigenstates are all kept. In the NRG iteration, after diagonalizing $H_n$, we obtain its eigenstates and eigenenergies, which are denoted as $|s\rangle_n^X$ and $E_{n,s}^X$ (Ref.13), respectively. Here $X = D$ for the discarded states and $X = K$ for the kept states. According to the NRG algorithm, there is the following recursive relation between $|s\rangle_n^X$ and $|s\rangle_{n-1}^X$,

$$|s_{n+1}\rangle^X_n = \sum_{\sigma_n,s} |\sigma_n\rangle \otimes |s_{n-1}\rangle^K_n \left[U^{(\sigma_n)}_{K\times X} \right]_{ss'}.$$  \hspace{1cm} (A1)

Here, $\{|\sigma_n\rangle\}$ ($n = 1, 2, ..., d$) are the local states of the $n$-th chain site and $d$ is the dimension of the local Hilbert space of bath site $n$. $U^{(\sigma_n)}_{K\times X}$ is the $K$-$X$ block of the unitary transformation matrix used to diagonalize $H_n$. 

FIG. 8: Scaling of computing time of the FDM method with respect to parameters (a) $N$; (b) $M$; and (c) $N_b$. The dashed lines are fitting lines of the form $y = cx^{1/2}$ in (a), and $y = cx^2$ in (b) and (c). Data are obtained on a single core of Intel Xeon E5-2670 with 2.6GHz frequency.
which has been written in the matrix product state representation. The orthonormal relation for a single shell, \( \langle s'| X^\sigma_{n,m} X \rangle = \delta_{X,X'} \delta_{s,s'} \), gives

\[
\sum_{\sigma_m} \left[ U_{n,K}^{(\sigma_m)} \right] \left[ U_{K,X}^{(\sigma_m)} \right] = \delta_{X,X'} \quad (A2)
\]

According to Ref[8], a complete orthonormal basis for the full NRG chain Hamiltonian \( H_N \) can be constructed by the discarded states \( |s\rangle^D_n \) and the environment states \( \{|e\rangle^D_n \} \),

\[
|s\rangle^D_n = |e_n\rangle \otimes |s\rangle^D_n = |\sigma_N \sigma_{N-1} ... \sigma_{n+1}\rangle \otimes |s\rangle^D_n \quad (A3)
\]

For the last chain site \( n = N \), all the eigenstates of \( H_N \) are regarded as discarded. Similarly, one can construct the kept states \( \{|se\rangle^K_n \} \) but they do not form complete orthonormal basis. These states have the following properties:

(i) Orthonormal relation. For the same shell \( n = m \),

\[
\langle X'(s' e'|s e') \rangle^{X,K}_n = \delta_{X,X'} \delta_{s,s'} \delta_{e,e'} \quad (X, X' \in \{K, D\}) \quad (A4)
\]

For different shell \( n < m \),

\[
\langle s'| e' \rangle^{X,K}_n = 0 \quad (X = K, D) \quad (A5)
\]

(ii) Inner product. For \( n < m \),

\[
\langle s'| e' \rangle^{X,K}_n = \delta_{e>e_m} \delta_{e'>e_m} \left[ U_{n,K}^{(\sigma_{m+1})} U_{n,K}^{(\sigma_{m+2})} ... U_{K,K}^{(\sigma_m)} \right]^{X}_{ss'} \quad (A6)
\]

Here, \( \delta_{e>e_m} \delta_{e'>e_m} \) equals to unity if \( \sigma_1 ... \sigma_{m+1} \) of environment \( e \) equals to \( \sigma_1' ... \sigma_{m+1}' \) of environment \( e' \). It equals to zero otherwise.

(iii) Complete relation.

\[
\sum_{n=0}^{N} \sum_{s,e} |s\rangle^{D,D}_n \langle s| = \mathbb{1}_{d^N} \quad (A7)
\]

\[
\sum_{s,e} |s\rangle^{K,K}_n \langle s| = \mathbb{1}_{d^N-n_0} \quad (A8)
\]

\[
\sum_{n=n_0+1}^{m} \sum_{s,e} |s\rangle^{D,D}_n \langle s| + \sum_{s,e} |s\rangle^{K,K}_m \langle s| = \mathbb{1}_{d^N-n_0} \quad (A9)
\]

Here \( d_0 \) is the number of eigenstates of \( H_{n_0} \).

In this work, we suggest the following exact relation,

(iv) Eigenstates of \( H_N \).

\[
H_N |s\rangle^D_n = E_n^D |s\rangle^D_n \quad (A10)
\]

The NRG Hamiltonian \( H_N \) here is defined in Eq. (3) of the main text. This equation, together with \( H_N |s\rangle^K_n \approx E_n^K |s\rangle^K_n \), was called NRG approximation in Ref[8]. In fact, Eq. (A10) is an exact equation while the corresponding equation for the kept states is an approximation. In the derivation of FDM formalism, both equations were used. In this work, we only use the exact equation Eq. (A10) for FE.

We start from Lehmann representation of the Fourier transformation of \( \langle A(t)B \rangle \)

\[
\frac{1}{i} \int_0^\infty \text{Tr} [\rho A(t)B] e^{i(\omega + \nu)t} dt = \frac{1}{Z} \sum_{m,n} e^{-\beta E_n} \langle n|A|m\rangle \langle m|B|n\rangle \quad (A11)
\]

Here \( Z = Tr(e^{-\beta H}) \) is the partition function and \( \rho = e^{-\beta H}/Z \) is the density operator. Replacing \( H \) with \( \tilde{H}_N \) and \( \{|n\rangle \} \) with \( \{|se\rangle^K_n\} \) in the above equation, and using Eq. (A10), we obtain

\[
\frac{1}{i} \int_0^\infty \text{Tr} [\rho A(t)B] e^{i(\omega + \nu)t} dt = \frac{1}{Z} \sum_{m,n=0}^{N} \sum_{s,e} e^{-\beta E_n} \langle s|A|s\rangle^K_n \langle m|B|n\rangle \langle s|e\rangle^K_N \langle m|e\rangle^K_N \quad (A12)
\]

For the matrix element \( D_n^D |s\rangle^K_n \langle e| D_m^K \) with \( m > n \), inserting Eq. (A9) into the right-hand side of \( A \) and using Eq. (A5), we obtain

\[
D_n^D |s\rangle^K_n \langle e| D_m^K = \sum_{\tilde{s}} D_n^D |s\rangle^K_n \langle \tilde{s}| \langle \tilde{s}| \langle e| D_m^K \quad (m > n).
\]

Using Eq. (A6) and

\[
D_n^D |s\rangle^K_n \langle \tilde{s}| \approx D_n^D |s\rangle^K_n \delta_{s,\tilde{s}} \quad (A13)
\]

we further obtain for \( n > m \)

\[
D_n^D |s\rangle^K_n \langle e| D_m^K = \sum_{\tilde{s}} \left[ U_{n,K}^{(\sigma_{m+1})} U_{n,K}^{(\sigma_{m+2})} ... U_{K,K}^{(\sigma_{m})} \right]^{D,K}_{\tilde{s} e_m} D_m^D |s\rangle^K_m \delta_{e,e_m} \quad (A14)
\]

Here, we have assumed that \( A \) is a local operator defined in the impurity Hilbert space. \( D_n^D |s\rangle^K_n \langle e| D_m^K \) can be obtained similarly. We then obtain the nominator of Eq. (A12) for \( m > n \) as

\[
\sum_{s,e} D_n^D |s\rangle^K_n \langle e| D_m^K |s\rangle^K_m \langle e| B |s\rangle^K_m \quad (A15)
\]

In the above equation, \( T_{K,N}^{(nm)} = U_{n,K}^{(\sigma_{m+1})} U_{n,K}^{(\sigma_{m+2})} ... U_{K,K}^{(\sigma_{m})} \). The sum over environmental indices \( \sigma_i \) (\( i = n+1, n+2, ..., m \)) contains exponentially large number of terms. We carry out this summation efficiently using the recursive formula Eqs. (12)-(14) of the main text.

The expression for \( m < n \) can be obtained from Eq. (A15) by using the exchange \( m \leftrightarrow n, s \leftrightarrow s', e \leftrightarrow e' \).
\( A \leftrightarrow A^\dagger, \ B \leftrightarrow B^\dagger \) and taking complex conjugate. We split the summation \( \sum_{m,n} \) in Eq.(A12) into those for \( m = n, \ m > n, \) and \( m < n. \) Inserting the respective expressions and after some simplification, we obtain

\[
\frac{1}{i} \int_0^\infty Tr [\rho A(t) B] e^{i(\omega + i\eta)t} dt = \frac{1}{Z} \sum_{n=n_0+1}^{N} \sum_{ss'} d^{N-n} e^{-\beta E_{n,s}} \left[ B_{DD}^{(m)} \right]_{ss'} \left[ A_{DD}^{(m)} \right]_{ss'} + \frac{1}{Z} \sum_{n=n_0+1}^{N} \sum_{m=n+1}^{N} \sum_{ss'} d^{N-m} e^{-\beta E_{n,s}} [AB]_{ss'}^{(nm)} + \frac{1}{Z} \sum_{n=n_0+1}^{N} \sum_{m=n+1}^{N} \sum_{ss'} d^{N-m} e^{-\beta E_{m,s'}} [BA]_{ss'}^{(nm)}.
\]

(A16)

Here, \( [A_{DD}^{(n)}]_{ss'}, \) and \( [B_{DD}^{(n)}]_{ss'} \) are defined below Eq.(9) of the main text. \( [AB]_{ss'}^{(nm)} \) and \( [BA]_{ss'}^{(nm)} \) are given by Eqs.(12)-(14) of the main text. Eq.(A16) gives the particle part of the retarded GF. The hole part \((1/i) \int_0^\infty Tr [\rho B A(t)] e^{i(\omega + i\eta)t} dt\) can be obtained similarly. From them, one obtains the full expression for \( G^{R/b}_AB(\omega), \) i.e., Eqs.(10)-(14) of the main text. One can estimate that the FE computation time for GF scales as \( N^2 M^4. \) Parallel computation can be easily implemented for this formalism.

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