

# Variational Numerical Renormalization Group: Bridging the Gap between NRG and Density Matrix Renormalization Group

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The numerical renormalization group (NRG) is rephrased as a variational method with the cost function given by the sum of all the energies of the effective low-energy Hamiltonian. This allows us to systematically improve the spectrum obtained by NRG through sweeping. The ensuing algorithm has a lot of similarities to the density matrix renormalization group (DMRG) when targeting many states, and this synergy of NRG and DMRG combines the best of both worlds and extends their applicability. We illustrate this approach with simulations of a quantum spin chain and a single impurity Anderson model where the accuracy of the effective eigenstates is greatly enhanced as compared to the NRG, especially in the transition to the continuum limit.

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The density matrix renormalization group [1] (DMRG), devised to improve on the Wilson's numerical renormalization group (NRG) [2], has become the method of choice to simulate one-dimensional quantum many-body systems at zero temperature and has found a large number of applications in the fields of the condensed matter physics, quantum chemistry and quantum information theory where it turned out that DMRG is essentially equivalent to simulating quantum systems in terms of matrix product states (MPS) [3]. In all these methods, a quantum many-body state is represented by associating matrices to local configurations at sites, and the coefficients in the expansion over the configuration states are given as products of the corresponding matrices. The DMRG can be used to calculate not only the ground state but also the excited states through the concept of *targeting* where these matrices are chosen such that they well represent many states at the same time. In the NRG, on the other hand, the low-energy states of a system are expressed in terms of the low-energy states of a smaller system which is a suitable description of impurity systems with energy scale separation. In this context, the NRG gives remarkably good results and has retained the position as a widely used impurity solver [4], whereas the DMRG is rarely used to calculate the excited states [5] except for the spectral gap. One of the reasons is that the NRG is less costly as it provides  $D$  excited states at the cost of  $O(D^3)$  as compared to DMRG with targeting with the cost  $O(D^4)$ . Presently, the DMRG is mostly used in its time dependent form (see, e.g., [6]) which is also true for impurity systems [7–11] where other density-matrix related concepts are used also [12–14]. Still, DMRG's remarkable ability to calculate and optimize many excited states has not been used in this context.

Even as an impurity solver, the NRG has certain limitations: the hopping terms should fall off sufficiently fast which means lower resolution of the spectral densities at higher energies, e.g., Hubbard bands. Otherwise it

becomes inaccurate for longer chains which is seen as a violation of the Friedel sum rule [15]. It also becomes highly expensive for many-band impurity problems, whereas an additional self-consistency constraint in the context of dynamical mean-field theory, see, e.g., [16], calls for more accurate impurity solvers. What makes the NRG really different from the DMRG is that it does not provide any feedback mechanism to optimize the matrices by sweeping along the chain and a method along this line has already been used with quantum fields [17]. In this Letter, we identify the cost function in the NRG algorithm and introduce a feedback mechanism by which the states can be optimized in a variational way under the original NRG cost function. We relate the NRG and the DMRG by identifying the common cost function in both approaches, showing that the proposed scheme improves the results of both methods while it retains the lower, NRG-like, scaling of computational costs.

*Numerical renormalization group.*—In the context of the NRG, the lowest energy eigenstates of a quantum many-body system on  $n$  sites,  $\hat{H}|\psi_\alpha\rangle = E_\alpha|\psi_\alpha\rangle$ , are approximated by orthonormal states  $\mathcal{S}^{[n]} \equiv \{\psi_1^{[n]}, \dots, \psi_{D_n}^{[n]}\}$  defining an effective low-energy Hamiltonian

$$\hat{H}_{\text{eff}}^{[n]} = \sum_{\alpha=1}^{D_n} E_\alpha^{[n]} |\psi_\alpha^{[n]}\rangle \langle \psi_\alpha^{[n]}|, \quad (1)$$

with effective energies  $E_\alpha^{[n]} = \langle \psi_\alpha^{[n]} | \hat{H} | \psi_\alpha^{[n]} \rangle$ . The set of effective states  $\mathcal{S}^{[n]}$  is obtained recursively from  $\mathcal{S}^{[n-1]}$ , the effective description of a system on  $n-1$  sites, extended by an extra site of a local dimension  $d_n$ , resulting in an extended Hamiltonian  $\mathbf{H}_{\text{ext}}^{[n]} \in \mathbb{C}^{(D_{n-1}d_n) \times (D_{n-1}d_n)}$  that, in order to prevent exponential growth, has to be projected to a subspace of a smaller dimension  $D_n$ . In the NRG, this subspace is spanned by the lowest energy eigenvectors as  $\mathbf{H}_{\text{eff}}^{[n]} = \mathbf{U}^H \mathbf{H}_{\text{ext}}^{[n]} \mathbf{U}$  where  $\mathbf{H}_{\text{eff}}^{[n]} \in \mathbb{C}^{D_n \times D_n}$  is a new effective

Hamiltonian and  $\mathbf{U} \in \mathbb{C}^{(D_{n-1}d_n) \times D_n}$  is an isometry matrix  $\mathbf{U}^H \mathbf{U} = \mathbf{1}$ . The set of effective states  $\{\psi_\alpha^{[n]}\}$  is given as a MPS with an external  $\alpha$  index [8]

$$|\psi_\alpha^{[n]}\rangle = \sum_{\{s_j\}} \mathbf{e}_0 \cdot \mathbf{A}^{[1]s_1} \mathbf{A}^{[2]s_2} \dots \mathbf{A}^{[n]s_n} \mathbf{e}_\alpha |s_1, \dots, s_n\rangle, \quad (2)$$

with the right boundary vector  $\mathbf{e}_\alpha$  enumerating basis states. The set  $\mathcal{S}^{[n]}$  is orthonormal due to the isometry constraint for matrices  $\mathbf{A}^{[j]}$  defined as  $[\mathbf{A}^{[j]}]_{(ls)r} \equiv A_{lr}^{[j]s}$ .

The NRG projection is equivalent to requiring that the sum of the new effective energies  $E_\alpha^{[n]}$  is minimal which, according to (1), corresponds to the trace of  $H_{\text{eff}}^{[n]}$  and leads to a cost function

$$f(\mathbf{A}) = \text{tr}(\mathbf{A}^H \mathbf{H}_{\text{ext}}^{[n]} \mathbf{A}) \quad \text{where} \quad \mathbf{A}^H \mathbf{A} = \mathbf{1}, \quad (3)$$

which is minimized exactly by the NRG isometry  $\mathbf{U}$ . This cost function is different from other DMRG-based approaches (e.g., [8,12]) where the cost is determined from the ground state alone.

*Variational optimization.*—The identification of the NRG cost function allows us to optimize not only the tensor associated with the last site in the NRG-MPS (2), but an arbitrary tensor in the chain. The cost  $f(\mathbf{A}^{[j]}) = \sum_\alpha \langle \psi_\alpha^{[n]} | \hat{H} | \psi_\alpha^{[n]} \rangle$  can easily be understood as a tensor network depicted on Fig. 1 where the  $\alpha$  index enumerating states  $|\psi_\alpha^{[n]}\rangle$  is contracted with the  $\alpha$  index in the conjugate MPS  $\langle \psi_\alpha^{[n]} |$ . The cost can thus be minimized by varying an arbitrary isometry  $A^{[j]}$  in the NRG-MPS (2) which we will illustrate by expressing the Hamiltonian as a matrix product operator (any 1D operator can be written as a matrix product operator)  $\hat{H} = \sum_{\{s_j\}} \mathbf{e}_0 \cdot \mathbf{H}^{[1]s_1} \dots \mathbf{H}^{[n]s_n} \mathbf{e}_0 |s'_1, \dots, s'_n\rangle \langle s_1, \dots, s_n|$  where tensors  $\mathbf{H}^{[j]}$  are represented by squares on Fig. 1. An arbitrary isometry  $\mathbf{A}^{[j]}$  is extracted out of the cost function (3) which now takes a form

$$f(\mathbf{A}) = \sum_\gamma \text{tr}(\mathbf{L}_\gamma^{[j]} \mathbf{A} \mathbf{R}_\gamma^{[j]T} \mathbf{A}^H) \quad \text{for} \quad \mathbf{A}^H \mathbf{A} = \mathbf{1}, \quad (4)$$

where  $\mathbf{L}^{[j]}$  and  $\mathbf{R}^{[j]}$  correspond to the contractions of the tensor networks on the left and right side of the chosen site  $j$ , respectively, (Fig. 1), explicitly defined as

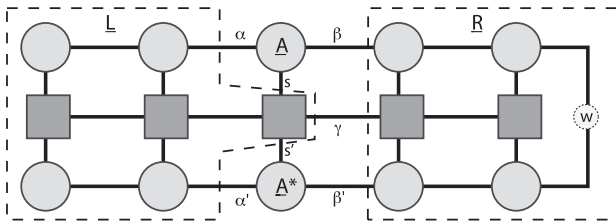


FIG. 1. Tensor network representation of the (weighted) cost function (4) in the optimization of a tensor  $\mathbf{A}^{[j]}$  (circles) under the Hamiltonian matrix product operator (squares).

$[\mathbf{L}_\gamma^{[j]}]_{(\alpha's')(\alpha s)} = L_{\alpha s \gamma s' \alpha'}$  and  $[\mathbf{R}_\gamma^{[j]}]_{\beta' \beta} = R_{\beta \gamma \beta'}$ . Furthermore, a modified weighted cost function may be considered where the effective states are weighted according to their importance, e.g., by a Boltzmann factor  $w_\alpha = e^{-\beta E_\alpha^{[n]}}$  (see Fig. 1). The cost (4) is minimized using the conjugate gradient method with a unitary constraint [18] in a variational way (i.e., the sum of energies can only decrease) and the computational costs scale as  $O(D^3)$ , the same as in the original NRG. The number of optimization steps depends on the quality of the initial state and the desired accuracy.

*Density matrix renormalization group.*—A special property of the NRG-MPS states is the twofold nature of the external  $\alpha$  index which acts both as an enumerating index as well as a virtual bond in extending the system for a site. For a fixed system size, the external index can be associated with any site in the chain and moved along the chain by means of the singular value decomposition (SVD). Interestingly, the concept of a moveable external index is intrinsic to the finite size DMRG algorithm *with targeting* [1]. The basic concept of the finite size DMRG is as follows: split the system as  $\{1, \dots, j-1\}, \{j\}, \{j+1\}, \{j+2, \dots, n\}$ , find the optimal tensor at site  $j$ , and move to the next site  $j+1$ . The way one finds the optimal tensor at site  $j$  is by considering the reduced density-matrix (DM) for  $\{1, \dots, j\}$ , obtained by tracing the DM of the complete system (“universe”) over the environment  $\{j+1, \dots, n\}$  whereas the universe can be either in a pure state (ground state) or in a mixed state of lowest energy states as is the case with the targeting. Formally, the eigenstates of the universe can be written as  $|\Psi_\alpha\rangle = \sum G_{(l, s_j, s_{j+1}, r), \alpha} |\varphi_l^{1, \dots, j-1}\rangle |s_j\rangle |s_{j+1}\rangle |\varphi_r^{j+2, \dots, n}\rangle$ , where the index  $\alpha$  enumerates the states and the optimal tensor  $\mathbf{A}^{[j]}$  is obtained by the SVD as  $G_{(l, s_j, s_{j+1}, r), \alpha} = \sum_c A_{lc}^{[j]s_j} \sigma_c V_{cs_{j+1} \alpha r}$ . Identifying  $A_{l, r}^{[j+1]s_{j+1} \alpha} \equiv \sigma_l V_{ls_{j+1} \alpha r}$ , we recover a NRG-MPS with the index  $\alpha$  associated with the site  $j+1$  (instead of site  $n$ ). However, this part is ignored in the DMRG since the tensor at site  $j+1$  is obtained in the subsequent step. Therefore, the index  $\alpha$  is intrinsic to but hidden in the DMRG and is carried back and forth along the chain. In the DMRG, only the central sites are optimized (the boundary parts are treated exactly). We can however sweep to the very end of the chain and end up exactly with the NRG-MPS (2) where the last tensor  $\mathbf{A}^{[n]}$  carries the  $\alpha$  index which now allows us to enlarge the chain for an extra site by a NRG step. Looking back, we realize that the optimal tensor  $G_{(l, s_j, s_{j+1}, r), \alpha}$  is an isometry matrix minimizing the same cost function (3) as in the NRG context, just that it represents an arbitrary pair of neighboring sites instead of the last site only. Hence, the DMRG minimizes the same cost function as the NRG.

We also realize that the truncation in the SVD decreases the accuracy of states and it is not guaranteed that the optimization at the next site will recover the same accuracy (in fact the highest accuracy is reached in the center of the

chain). Therefore, the set of excited states obtained by the DMRG can be further optimized by means of the variational principles proposed earlier.

**Results.**—The variational optimization algorithm for a NRG-MPS set of states is put to the test on two qualitatively distinct models. First, we consider a quantum Ising chain in a tilted magnetic field

$$H = \sum_{j=1}^{n-1} \sigma_j^x \sigma_{j+1}^x + \sum_{j=1}^n (h_x \sigma_j^x + h_z \sigma_j^z), \quad (5)$$

which is a simple example of nonintegrable quantum spin chains. The accuracy of the approximate eigenstates of (5) is quantified by a measure  $\langle H^2 \rangle - \langle H \rangle^2$  which puts a lower bound to the fidelity (see Supplemental Material [19]). We consider a chain of 200 sites, obtain the excited states by means of the DMRG and optimize them using the variational approach. The DMRG provides highly accurate results as seen from Fig. 2, leaving little space for improvements. However, the results are not optimal and can be improved by the variational NRG. Higher improvement is observed for smaller bond dimensions  $D$  which suggests a possibility of improving the excited states in the regime where sufficiently large  $D$  are not reachable due to higher entanglement, such as in two-dimensional or critical (see Supplemental Material [19]) systems. It is also worth noting that the computational costs of one DMRG sweep targeting  $M$  states scale as  $O(nd^3MD^3)$ , compared to  $O(MD^3 + nd^3D^3)$  or  $O(nd^3D^3)$  for the variational optimization where the  $\alpha$  index is associated with an internal boundary site, respectively. The prefactors to  $O(MD^3)$  are similar (related to the number of Lanczos steps).

As the second example we consider the single impurity Anderson model (SIAM) which, after a logarithmic discretization [4] of the conduction band, is described by a semi-infinite linear chain of sites nearest-neighbor coupled to a chain of  $N$  sites.

With the same parameters as in the previous section, we obtain the excited states of the SIAM Hamiltonian with  $U = 1$  and  $\Lambda = 1.7$ . We obtain a fixed bond dimension of  $D = 100$  for the eigenstates obtained by the DMRG. The variational optimization (vNRG) is seen to provide results better than the NRG results. Our results are obtained for the absolute ground state (see Supplemental Material [19]).

We now consider the interacting case, with  $U = -2\epsilon_f = 0.1$  on 40 sites. In the interacting case, we employ the same parameters as in the previous section.

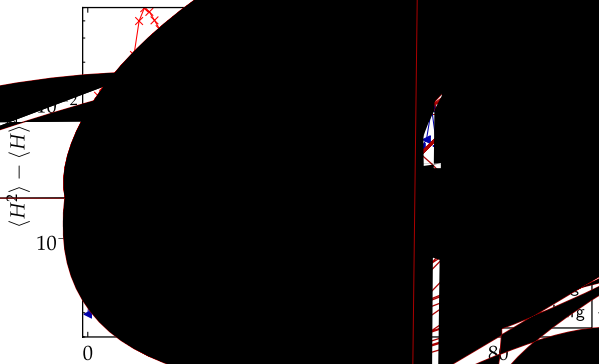


FIG. 2 (color online) Variance of the Hamiltonian  $\langle H^2 \rangle - \langle H \rangle^2$  for the excited states obtained by the DMRG (blue circles) and optimized by the variational NRG (red crosses) for various bond dimensions  $D$ .

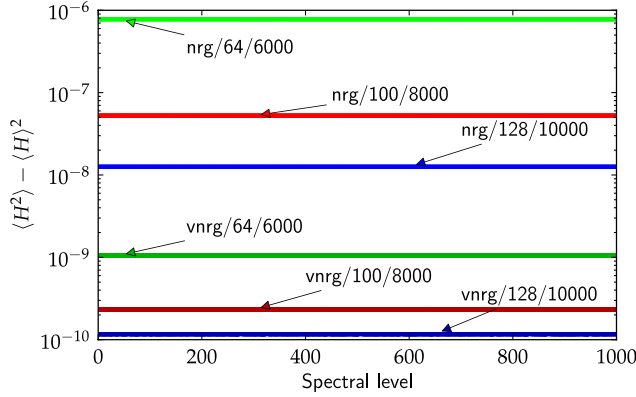


FIG. 4 (color online). Accuracy of the lowest 1000 states for the interacting SIAM chain (6) on 40 sites ( $N = 38$ ), for NRG and the variational NRG *with symmetries*. Subsector bond dimensions are taken  $D \in \{64, 100, 128\}$ , truncated to  $\{6000, 8000, 10\,000\}$  states of lowest energy. We have set  $\Lambda = 2$ ,  $\xi_0 = 0.01$ ,  $\epsilon_f = -0.05$ , and  $U = 0.1$ .

due to scale separation ( $\Lambda = 2$ ). Because of the symmetries, the bond dimension  $D \in \{64, 100, 128\}$  (which determines the computational complexity) now refers to the maximal number of states in individual subsectors whereas the total number of kept states is denoted by  $M \in \{6000, 8000, 10\,000\}$ . As shown in Fig. 4, the accuracy of eigenstates is greatly enhanced by the optimization. While the cost of an optimization step is comparable to the cost of a NRG step, a smaller bond dimension is needed to represent states using the vNRG as compared to the NRG. This effect is more pronounced for small values of  $\Lambda$  while for larger values of  $\Lambda$  the NRG already gives highly accurate results, only requiring little improvement. The results are consistent also for the fidelity of excited states and the absolute errors of energies (see Supplemental Material [19]). We stress that the logarithmic discretization is not needed for the variational scheme proposed in this Letter.

**Conclusion.**—We have proposed a variational method to simulate or optimize the effective low-energy description of one-dimensional quantum systems, introducing a feedback mechanism to the NRG and identifying the cost function. Furthermore, we have expressed the DMRG method with targeting as a NRG method with a moveable external index enumerating states and shown that the DMRG results can be further improved by the variational optimization. We have tested the methods on the quantum Ising chain in a tilted magnetic field and the single impurity Anderson model where we observed significant improvement of the approximate low-energy eigenstates. The

proposed technique can be directly applied to optimize existing NRG results [20] and could be a beneficial improvement of impurity solvers in the context of dynamical mean-field theory, see, e.g., [16].

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