Comparative Study of State-of-the-Art Matrix-Product-State Methods for Lattice Models with Large Local Hilbert Spaces without $U(1)$ symmetry

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Abstract

Lattice models consisting of high-dimensional local degrees of freedom without global particle-number conservation constitute an important problem class in the field of strongly correlated quantum many-body systems. For instance, they are realized in electron-phonon models, cavities, atom-molecule resonance models, or superconductors. In general, these systems elude a complete analytical treatment and need to be studied using numerical methods where matrix-product states (MPS) provide a flexible and generic ansatz class. Typically, MPS algorithms scale at least quadratic in the dimension of the local Hilbert spaces. Hence, tailored methods, which truncate this dimension, are required to allow for efficient simulations. Here, we describe and compare three state-of-the-art MPS methods each of which exploits a different approach to tackle the computational complexity. We analyze the properties of these methods for the example of the Holstein model, performing high-precision calculations as well as a finite-size-scaling analysis of relevant ground-state observables. The calculations are performed at different points in the phase diagram yielding a comprehensive picture of the different approaches.

1. Introduction

In the past two decades, tensor-network state (TNS) based methods have become very successful tools to study strongly correlated, low-dimensional quantum systems in and out of equilibrium [1–7]. In principle, these methods can reach a very high accuracy that is controlled by a successive scaling in the bond dimensions. The prerequisites are a sufficiently small amount of entanglement encoded in the wave function and an efficient means of computing energies and expectation values [6]. Re-expressing the early algorithms of the density-matrix renormalization group (DMRG) [1, 2] using matrix-product state (MPS) [3, 8] representations paved the way for the formulation of new efficient and flexible variational algorithms to study correlated quantum systems with excellent precision in one dimension [5, 6, 9, 10]. Exploring the tensor-product structure of the many-body Hilbert space to decompose the coefficients of a quantum state into local tensors yields a powerful formulation of DMRG and allows the exploitation of ideas from quantum-information theory [5, 11, 12]. Thereby, numerical optimization schemes that work on the local tensors can be formulated, which is at the heart of their high efficiency.

Unfortunately, such a decomposition becomes numerically very costly if the local quantum systems have a large number of internal degrees of freedom that do not obey conservation laws. Indeed, these situations are not too exotic as may be illustrated by the simple example of lattice fermions locally coupled to Einstein
phonons, the Holstein model \[13\]. Describing such a system by means of MPS requires, in principle, an infinite number of local degrees of freedom, while in practice, one needs to introduce a cutoff in the local Hilbert space dimension \[14, 15\]. As is well known, these systems can feature rich physics. Modeling the influence of phonons on interacting fermions on a numerically unbiased footing \[16–22\] is an important problem with many intensively studied questions, such as the formation, stability, and dynamics of (bi-)polarons in the (Hubbard-)Holstein model \[23–30\]. Various numerical approaches have been employed to study these systems ranging from exact diagonalization \[31, 32\] over quantum Monte-Carlo methods \[33, 34\] to dynamical mean-field theory (DMFT) \[35–37\].

Ultracold atoms provide another relevant platform in which large local Hilbert spaces play an important role for the theoretical description. For instance, models involving Feshbach-resonances feature a molecular and an atomic channel as well as a term that converts two atoms into one molecule. As a consequence, the particle numbers of molecules and atoms are not conserved individually. These models are called Bose-Fermi or Bose-Bose resonance models \[38–41\]. Models of single atoms coupled to optical cavities \[42–44\] have to account for the bosonic nature of the light field and are important systems to understand the interplay between light and matter on the atomic scale. Finally, in heterostructures of proximity-coupled s-wave superconductors, the condensate can be described separately, yielding an effective bosonic bath with pairwise creation and annihilation of particles. Recently, these systems have been suggested as promising candidates for an experimental realization of Majorana quasi particles, potential building blocks of topological qubits \[45–48\].

Here, we discuss three state-of-the-art MPS methods that can be utilized to efficiently deal with such a large number of required local degrees of freedom: The pseudosite DMRG (PS-DMRG) method \[23\], DMRG with local basis optimization (DMRG-LBO) \[26, 49–52\], and the projected purified two-site DMRG (PP-2DMRG) \[53\]. The first method was introduced by Jeckelmann and White to extend the applicability of DMRG to describe electrons coupled to phonons \[23\]. Local basis optimization (LBO) proposed by Zhang \textit{et al.} \[49\] is based on a rotation into the eigenbasis of the single-site reduced density-matrix (1RDM). It allows for a faithful truncation yielding an optimal approximation of the 1RDM. The PP-2DMRG developed recently by some of the authors consists of a mapping of the initial problem into a purified Hilbert space with a subsequent projection into an invariant subspace to generate an artificial $U(1)$ symmetry that collapses the local dimensions of the bosonic degrees of freedom and allows to exploit canonical MPS truncation schemes \[53\].

We compare the methods by applying them to the Holstein model at half filling. This system undergoes a phase transition from a gapless Luttinger-liquid (LL) phase to a gapped charge-density wave (CDW) phase upon changing the electron-phonon-coupling strength \[18, 54–56\]. To this end, we conduct high-precision calculations at an intermediate system size of $L = 51$ (where $L$ is the number of sites) and perform a finite-size extrapolation of the ground-state energy and the CDW order parameter from data at $L = 51, 101, 151, 201$ with relaxed precision demands. According to our analysis, all three methods agree within their anticipated error margins. We further find that the PS-DMRG and the PP-2DMRG require a larger bond dimension in order to reach a comparable precision as DMRG-LBO. However, the efficient representation of states using the DMRG-LBO method comes at the cost of additional numerical control parameters in which the calculations have to be converged. Here, the PS-DMRG and PP-2DMRG benefit from being conceptually simpler approaches. PS-DMRG can be converged with respect to a scaling analysis in the bond dimension and comparative calculations using different local Hilbert-space dimensions. Finally, using PP-2DMRG, it suffices to converge the calculations in the discarded weight, only. On the one hand, this comes at the cost of the largest growth in bond dimension compared to the other methods, but, on the other hand, this can be compensated by exploiting the restored global $U(1)$ symmetries.

The paper is organized as follows: In section 1.1, we briefly review the Holstein model and its phase diagram at half filling. In section 2, we introduce the different numerical methods. After recapitulating some basic facts about MPSs in section 2.1, we introduce the PS-DMRG in section 2.2, the strictly single-site DMRG with LBO (DMRG3S+LBO) in section 2.3, and the PP-2DMRG in section 2.4. Section 3 is devoted to the comparison between the methods, where section 3.1 and section 3.2 contain the high-precision calculations, while section 3.3 contains the finite-size extrapolations. Finally, in section 5, we give a conclusion of our work.
1.1. Holstein Model

In order to demonstrate the applicability of the different methods, we conduct numerical ground-state calculations of the half-filled 1D Holstein model with spinless fermions [13]. The model is defined by a set of spinless fermions with creation/annihilation operators $\hat{c}^\dagger_j$ on a lattice, where every lattice site possesses an associated harmonic oscillator with bosonic creation/annihilation operators $\hat{b}^\dagger_j$. The oscillators are decoupled from each other and play the role of a single Einstein-phonon branch. The density of the fermions $\hat{n}^f_j = \hat{c}^\dagger_j \hat{c}_j$ at a specific site $j$ couples to the displacement ($\hat{b}^\dagger_j + \hat{b}_j$) of the associated harmonic oscillator:

$$\hat{H} = \hat{H}_f + \hat{H}_{ph} + \hat{H}_{f-ph}$$

$$\hat{H}_f = -t_0 \sum_j \left( \hat{c}^\dagger_j \hat{c}_{j+1} + \text{h.c.} \right)$$

$$\hat{H}_{ph} = \omega_0 \sum_j \hat{b}^\dagger_j \hat{b}_j$$

$$\hat{H}_{f-ph} = \gamma \sum_j \hat{n}^f_j \left( \hat{b}^\dagger_j + \hat{b}_j \right).$$

An important exact relation between the different particle species and for eigenstates is given by [54, 57]

$$\langle \hat{b}^\dagger_j + \hat{b}_j \rangle = 2 \frac{\gamma}{\omega_0} \langle \hat{n}^f_j \rangle.$$  

At half filling, the ground-state phase diagram of this model exhibits a transition from a metallic LL phase into a CDW insulating phase when increasing the ratio $\gamma/t_0$ for fixed $t_0/\omega_0 \neq 0$ [18, 54–56] (see figure 1).

We investigate the Holstein model with open boundary conditions at different points in its parameter space.
The singular-value decomposition (SVD) is one way of obtaining these canonical tensors (see figure 2). Encoding the information of the wave function locally in rank 3 site tensors \( M \) the tensor product of coefficients \( \psi \) 2.1. Matrix-Product States the number of phonons is not conserved, which is one major reason for the numerically challenging situation. decomposing the local degrees of freedom into 1D representations [58, 60]. However, in the Holstein model, a canonical gauge [6]. Site tensors \( \{ \} \) essential, particularly in the intermediate coupling regime. A loophole is to exploit global \( U \) two-site algorithm [6, 65]. Therefore, a generic representation allowing to numerically treat large 1D systems, \( S \) scales only with the surface area of the partitioned subsystems [61]. For instance, for gapped one-dimensional (1D) systems, \( S \) is bounded by a constant. Here, \( \rho_{A/B} \) is the reduced density matrix of a bipartition of the many-particle Hilbert space \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \). There has been great effort to characterize the entanglement properties of generic models and it has been shown that for a wide range of gapped systems with local couplings, the ground states obey the area law and thus can be represented efficiently using MPS [62–64]. For pure fermion or small-spin systems, the dominating numerical costs are caused by contracting the site tensors along the auxiliary index between two lattice sites. However, in typical algorithms such as a ground-state search, the local dimension \( d \) enters the numerical complexity as \( d^2 \) or \( d^4 \) in case of a single- or two-site algorithm [6, 65]. Therefore, a generic representation allowing to numerically treat large \( d \) values is essential, particularly in the intermediate coupling regime. A loophole is to exploit global \( U(1) \) symmetries, decomposing the local degrees of freedom into 1D representations [58, 60]. However, in the Holstein model, the number of phonons is not conserved, which is one major reason for the numerically challenging situation. 2. Methods The applicability of the MPS ansatz is rooted in the fact that in one dimension, an efficient parameterization of so-called area-law states is possible by means of mixed-canonical representations, exploiting the inherent gauge freedom of MPS [6, 9, 10]. In area-law states, the entanglement entropy of so-called area-law states is possible by means of mixed-canonical representations, exploiting the inherent gauge freedom of MPS [6, 9, 10]. In area-law states, the entanglement entropy scales only with the surface area of the partitioned subsystems [61]. For instance, for gapped one-dimensional (1D) systems, \( S \) is bounded by a constant. Here, \( \rho_{A/B} \) is the reduced density matrix of a bipartition of the many-particle Hilbert space \( \mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B \). There has been great effort to characterize the entanglement properties of generic models and it has been shown that for a wide range of gapped systems with local couplings, the ground states obey the area law and thus can be represented efficiently using MPS [62–64]. For pure fermion or small-spin systems, the dominating numerical costs are caused by contracting the site tensors along the auxiliary index between two lattice sites. However, in typical algorithms such as a ground-state search, the local dimension \( d \) enters the numerical complexity as \( d^2 \) or \( d^4 \) in case of a single- or two-site algorithm [6, 65]. Therefore, a generic representation allowing to numerically treat large \( d \) values is essential, particularly in the intermediate coupling regime. A loophole is to exploit global \( U(1) \) symmetries, decomposing the local degrees of freedom into 1D representations [58, 60]. However, in the Holstein model, the number of phonons is not conserved, which is one major reason for the numerically challenging situation. 2.1. Matrix-Product States MPSs supply both a flexible and numerically efficient ansatz class for quantum many-body states. The coefficients \( \psi_{\sigma_1, \ldots, \sigma_L} \in \mathbb{C} \) of a wave function representing a state \( |\psi\rangle \in \mathcal{H} \) in a Hilbert space \( \mathcal{H} \) composed of the tensor product of \( L \in \mathbb{N} \) \( d \)-dimensional local degrees of freedom are expanded in terms of \( d \cdot L \) matrices \( M^\sigma \in \mathbb{C}^{m_j \times m_j} \) [6]

\[
|\psi\rangle = \sum_{\sigma_1, \ldots, \sigma_L} \psi_{\sigma_1, \ldots, \sigma_L} |\sigma_1, \ldots, \sigma_L\rangle \equiv \sum_{\sigma_1, \ldots, \sigma_L} M^{\sigma_1} \cdots M^{\sigma_L} |\sigma_1, \ldots, \sigma_L\rangle .
\] 7

Encoding the information of the wave function locally in rank 3 site tensors \( M_j \) (i.e., the set of matrices \( \{ M^\sigma \} \) per site) provides direct access to the Schmidt coefficients if the site tensors are expressed in the canonical gauge [6]. Site tensors \( A_j \) are called left canonical if they fulfill \( \sum_{\sigma_j, m_{j-1}} \left( A^\sigma_{m_{j-1}, m_j} \right)^\dagger A^\sigma_{m_{j-1}, m_j} = 1_{m_j' \cdot m_j} \) and site tensors \( B_j \) are called right canonical if they fulfill \( \sum_{\sigma_j, m_j} B^{\sigma}_{m_{j-1}, m_j} \left( B^{\sigma}_{m_{j-1}, m_j} \right)^\dagger = 1_{m_{j-1} \cdot m_j} \).

The singular-value decomposition (SVD) is one way of obtaining these canonical tensors (see figure 2).
Expanding the site tensors of a canonically gauged state by means of a SVD

\[ M^\sigma_j = M(\sigma_j, m_{j-1}), m_j = \sum_{s_j} U(\sigma_j, m_{j-1}), s_j \Sigma s_j V_{s_j, m_j} \]  

allows for an optimal approximation with respect to the reduced density matrix \( \hat{\rho} = \text{Tr}_{k \leq j} |\psi\rangle \langle \psi| \) by truncating the series of Schmidt values \( \Sigma s_j \) below a certain threshold \( \delta_0 \), leading to a cutoff bond dimension \( m_{\text{max}} \). The squared and summed discarded parts of the Schmidt spectrum are commonly referred to as discarded weight \( \delta(m_{\text{max}}) \)

\[ \delta = \sum_{s_j > m_{\text{max}}} \Sigma^2 s_j. \]

Rapidly decaying Schmidt values \( \Sigma s_j \) are thus a necessary condition for a compact approximation of a state by means of a MPS and small truncation error controlled by \( \delta \).

Further numerical benefits can be achieved if \( |\psi\rangle \) transforms under a global symmetry group \( G \). In this situation, the Wigner-Eckhardt theorem ensures a decomposition of the site tensors in terms of irreducible representations \( \Gamma(g) \) of the elements in the symmetry group \( g \in G \) [58–60]. The dimensions of the tensor indices decompose under the action of \( G \):

\[ m_j = \sum g_j m_{g_j} \]  

so that by working on each block separately, the computational costs typically are reduced by an order of magnitude in the case of a global \( U(1) \) symmetry.

### 2.2. Pseudosite Method

In this section, we summarize the PS-DMRG method for large local dimensions \( d \). Details can be found in [23, 31]. The pseudosite approach is based on the original two-site DMRG method [1, 2]. Without special techniques for large sites, the complexity of the two-site DMRG method scales as \( SLD^3m_{\text{max}}^3 \), where \( L \) is the number of sites in the lattice and \( m_{\text{max}} \) is the maximum bond dimension. In the spinless Holstein model, \( d = 2(n_{\text{ph}} + 1) \), where \( n_{\text{ph}} \) is the maximum number of phonons per site. \( S \) represents the number of iterations required to achieve convergence and combines both the iterative diagonalization of the superblock Hamiltonian at each DMRG step and the repeated DMRG sweeps through the lattice.

The key idea of the PS-DMRG method is to substitute \( n_{\text{pseudo}} = \log_2(n_{\text{ph}} + 1) \) pseudosites of dimension 2 for the phonon site of dimension \( n_{\text{ph}} + 1 \). As the computational cost increases linearly with the number of sites but with the cube of the site dimension, PS-DMRG can handle this representation more efficiently. The exact mapping between the truncated phonon Hilbert space and the Hilbert space spanned by the \( n_{\text{pseudo}} \)
Figure 4: Relative deviation of the ground-state energy obtained with PS-DMRG from reference values as a function of the maximum bond dimension \(m_{\text{max}}\) and varying phonon cutoff \(n_{\text{ph}}\). The reference values are obtained by taking the best approximations to the ground state from high-precision calculations using the DMRG3S+LBO and PP-2DMRG methods, as discussed in section 3.1.

Pseudosites can be implemented using the binary number representation of the boson number \(n\) (0 ≤ \(n\) ≤ \(n_{\text{ph}}\)) on a site. An occupied pseudosite corresponds to the binary digit 1 while an empty pseudosite corresponds to the binary digit 0 (cf., figure 3). Boson operators have to be represented in terms of pseudosite operators to perform PS-DMRG calculations.

2.2.1. Number of Pseudosites

For the Holstein model, the pseudosite Hamiltonian contains \(\sim n_{\text{ph}}\) many-particle terms acting over a range of up to \(n_{\text{pseudo}}\) pseudosites. Thus, the computational cost of the PS-DMRG method scales as \(SL(n_{\text{ph}} + 1) \log_2(n_{\text{ph}} + 1)n_{\text{max}}^3\), which is significantly more efficient than the usual DMRG method applied to large phonon sites. Due to the longer interaction range in the pseudosite representation, however, the PS-DMRG method requires a larger bond dimension \(m_{\text{max}}\) and a larger number of iterations \(S\) to reach a given accuracy. The difference becomes more pronounced for larger site dimensions. Thus, the precision increases first with increasing the number of pseudosites, but may deteriorate for too large \(n_{\text{pseudo}}\) if the number of sweeps and the bond dimension are kept constant, as observed in figure 4(b). Nonetheless, the PS-DMRG method allows much larger numbers of bosons than the usual DMRG method [66–68]. It was successfully used to study the metal-insulator transition in various Holstein-type models [14, 57, 69–71].

2.2.2. Benchmark Setup

For the high-precision calculations presented in section 3.1, we use \(n_{\text{pseudo}}\) from 3 to 6 (7 ≤ \(n_{\text{ph}}\) ≤ 63). The PS-DMRG calculation always starts with a small bond dimension \(m\), which is increased progressively up to \(m_{\text{max}}\). Three to six DMRG sweeps (back and forth) through the full lattice are carried out for each bond dimension for a total of up to 30 sweeps. The bond dimensions are so large that the discarded weight \(\delta\) vanishes within double precision (10⁻¹⁵). Thus \(\delta\) is not a helpful quantity to decide whether a calculation has converged and extrapolations of observables to vanishing discarded weights are not used [31]. The accuracy of the calculated energies is limited by the slow convergence with the number of iterations rather than by the DMRG truncation error or the phonon Hilbert-space truncation.

For the study of the finite-size scaling of the order parameter in section 3.3, we use several bond dimensions \(m\) up to \(m_{\text{max}} = 200\) or 400 with 3 to 6 sweeps for each value of \(m\). From the scaling with varying bond dimension \(m\), we estimate the relative errors of the finite-system energies to be smaller than 10⁻⁶, while the absolute errors of the finite-system order parameters are smaller than 10⁻⁵.
2.3. DMRG with local basis optimization

Here, we recapitulate the DMRG3S+LBO introduced in [30] (see also [72]). The method is based on the LBO introduced by Zhang et al. [49]. At the core, the DMRG3S+LBO is a combination of the variational matrix-product state (VMPS) method originally formulated for spin-boson models and introduced by Guo et al. [73] (see also [74–76]) with the single-site DMRG method with subspace expansion introduced by Hubig et al. [65].

2.3.1. LBO

The LBO tackles the problem of large local Hilbert spaces by dynamically finding an optimized local basis for the problem at hand. The optimized basis at site \( j \) can by found by computing the 1RDM:

\[
\hat{\rho}_j = \text{Tr}_{k \neq j} |\psi\rangle \langle \psi| ,
\]

where the trace is over all degrees of freedom \( \sigma_k \) that are not on site \( j \). Upon diagonalization of \( \hat{\rho}_j \), a local basis transformation matrix \( U_l \) as well as the spectrum of \( \hat{\rho}_j \) is found. Along the lines of the DMRG strategy, the local basis can be truncated according to the spectrum of \( \hat{\rho}_j \) and the state can be transformed into the new local basis. If only a few of the eigenvalues of \( \hat{\rho}_j \) have considerable magnitude, the truncation will retain most of the information in the state. In case of the Holstein model, this strategy can be motivated by the insight that the ground state of the Holstein model in the atomic limit (\( t_0 = 0 \)) needs just a single state at every site [54]. In the ground state of the Holstein-polaron model, an exponential decay of the spectrum was found numerically for several sets of parameters [49, 77]. A similar behavior in the spectrum of \( \hat{\rho}_j \) was also found in the Bose-Bose resonance model [41].

A MPS with LBO takes the form:

\[
|\psi\rangle \approx \sum_{\sigma_1, \ldots, \sigma_L} M_{\tilde{\sigma}_1, \sigma_1} \cdots M_{\tilde{\sigma}_L, \sigma_L} |\sigma_1, \ldots, \sigma_L\rangle ,
\]

where truncated local basis transformations \( R_j \) (with entries \( R_{\tilde{\sigma}_j, \sigma_j} \)) are attached to every local tensor \( M_j \) (i.e., the set of matrices \( \{ M_{\tilde{\sigma}_j, \sigma_j} \} \) (cf., figure 5 left). The matrices \( R_j \) have dimension \( d_o \times d \), where \( d_o \) is the number of optimal modes, i.e., the number of local basis states that are kept after the truncation.

2.3.2. DMRG3S+LBO

The DMRG3S+LBO method consists of two stages, an optimization of the local basis matrix \( R_j \) and an optimization of the local site tensor \( M_j \). Both of these are performed by a DMRG-like optimization step. The tensor manipulations necessary are sketched in figure 5. Consider a MPS with LBO in mixed-canonical form where all site tensors left of site \( j \) are left canonical and all tensors to the right are right canonical. In the first step, a SVD of the site tensor is performed such that [cf., figure 5(1)]:

\[
M_{(m_{j-1}, m_j), \tilde{\sigma}_j} = \sum_{s_j} U_{(m_{j-1}, m_j), s_j} \Sigma_{s_j} V_{s_j, \tilde{\sigma}_j} .
\]

Subsequently, \( \Sigma \) and \( V \) are contracted with \( R_j \) and a DMRG optimization of the resulting matrix is performed [cf., figure 5(2)]. The original form of the MPS is then restored by a SVD of the optimized matrix [cf., figure 5(3)]. In this step, a truncation of the optimal basis may be done. However, note that the optimized basis dimension cannot grow throughout the optimization step. A truncation is therefore only necessary if the left dimension of the matrix \( R_j \) is larger than the desired \( d_o \) before the optimization. In practice, it is more common that the dimension has to be enlarged artificially (e.g., in the first sweep if the initial state has a simple structure) so that future optimization steps can explore the full \( d_o \) local states. Note further that we utilize particle-number conservation of the fermions in the Holstein model so that the local-basis-transformation matrices consist of two symmetry blocks. The maximal number of optimal modes \( d_o \) refers to the maximal number per block. In the truncation step, the singular values from both blocks are combined.
in one list and the blocks are filled according to the size of the singular values until one of the blocks reaches the maximal size \( d_0 \). The smaller block is then filled with zeros so that both blocks have the same size.

The second step is a DMRG optimization of the local site tensor \( M_j \) [cf., figure 5(4)]. These two steps of optimizing the local basis and then the site tensor can be done in a loop until no further improvements are detected [73]. However, in the implementation of the DMRG3S+LBO algorithm used for this work, every optimization is done for a fixed number of two times.

After the optimization of both, the local basis and the site tensor is finished, the center of the mixed-canonical MPS is moved to the next site. To prevent the algorithm from getting stuck in local minima of the energy landscape, an enrichment step on the bonds has to be implemented. For this purpose, the subspace expansion described in [65] is used.

### 2.3.3. Convergence of the DMRG3S+LBO method

In a single-site DMRG method, the bond dimension does not grow on its own during the algorithm. Therefore, it is crucial to implement a procedure that enhances the bond dimension artificially. This procedure has the second purpose of preventing the algorithm from getting stuck in local energy minima. In the DMRG3S+LBO, we choose the subspace expansion developed by Hubig et al. in [65] (see also [58, 78] for earlier work on single-site DMRG algorithms). The crucial steps of the method are recapitulated here. In a left-to-right sweep, after the DMRG optimization of the local tensor \( M_j \), the tensor is enlarged by \( P_j \) with entries:

\[
P^{\hat{\sigma}_j}_{k_{j-1},l_j,m_j} = \alpha \sum_{l_{j-1},m_{j-1},\hat{\sigma}_j} L_{k_{j-1},l_{j-1},m_{j-1},M_{m_{j-1},m_j}} H_{l_{j-1},l_j} \tilde{\sigma}_j, \tilde{\sigma}'_j
\]

(13)

where \( H_j \) (with entries \( H^{\hat{\sigma}_j,\hat{\sigma}'_j}_{l_{j-1},l_j} \)) is the local matrix-product operator (MPO) site tensor of the Hamiltonian transformed into the optimal basis:

\[
H_{l_{j-1},l_j}^{\hat{\sigma}_j,\hat{\sigma}'_j} = \sum_{\sigma_j,\sigma'_j} R^{\hat{\sigma}_j,\sigma_j}_j H^{\hat{\sigma}_j,\sigma'_j}_{l_{j-1},l_j} (R^\dagger)^{\sigma'_j,\hat{\sigma}'_j}_j
\]

(14)
and the tensor \( L_{j-1} \) is recursively defined as having entries:

\[
L_{k_j-1,l_j-1,m_j-1} = \sum_{k_{j-2},l_{j-2},m_{j-2},\tilde{\sigma}_{j-1},\tilde{\sigma}'_{j-1}} L_{k_{j-2},l_{j-2},m_{j-2},\tilde{\sigma}_{j-1},\tilde{\sigma}'_{j-1}} A^\dagger_{m_{j-2},m_j-1} H^{\dagger}_{l_{j-2},l_j-1} (A^\dagger)_{k_{j-2},k_j-1},
\]

where the \( A_j \) are the left-canonical site tensors of the MPS and \( L_0 = 1 \). The parameter \( \alpha \) is a mixing factor that has to be chosen appropriately. The tensor on site \( j \) is enlarged by \( P_j \) and the MPS tensor on the following site \( j+1 \) is enlarged by zeros in such a way that the tensors fit together:

\[
\tilde{M}_j = [M_j P_j], \quad \tilde{B}_{j+1} = \begin{bmatrix} B_{j+1} & 0 \\
0 & 0 \end{bmatrix}.
\]

This enrichment step can be interpreted as an expansion of the local site tensor into a two-dimensional Krylov space, as \( P_j \) provides the left-contraction of the current state multiplied by the system's Hamiltonian. If the MPS is already close to the global ground state, the site tensors are essentially eigenstates of the effective single-site Hamiltonian \( H_j \), contracted with the proper left- and right-contractions \( L_{j-1} \) and \( R_{j+1} \), respectively. In this case, the mixing factor should be chosen as \( \alpha = 0 \).

The previous step of enlarging the tensor \( M_j \) by \( P_j \) does not change the state at all, since the expansion tensor \( P_j \) is multiplied by zeros on the next site. However, the bond dimension between site \( j \) and \( j+1 \) is increased by \( w \cdot \chi \), where \( w \) is the bond dimension of the MPO and \( \chi \) is the bond dimension of the MPS. In most cases, it is therefore necessary to truncate the bond dimension to the maximal bond dimension \( m_{max} \) immediately after the enrichment step. After the truncation, the change done to the state becomes manifest and in most cases, the subspace enlargement and subsequent truncation increases the energy.

To monitor the effect of the subspace expansion on the state, one compares the energy after the truncation on the last bond \( E_{\text{last}} \) with the energy after the DMRG optimization on the current site \( E_{\text{opt}} \) and the energy after the truncation on the current bond \( E_{\text{trunc}} \). This provides the energy differences \( \Delta_{\text{opt}} = E_{\text{last}} - E_{\text{opt}} \) and \( \Delta_{\text{trunc}} = E_{\text{trunc}} - E_{\text{opt}} \). On the one hand, it is, of course, important to keep \( \Delta_{\text{opt}} > \Delta_{\text{trunc}} \), as otherwise the energy actually grows and one does not approach the ground state. On the other hand, one has to apply a strong enough mixing so that the global energy minimum can be found. Comparing both energy differences provides a measure for the competing effects of the subspace expansion. An optimal expansion strategy maximizes the energy gain when optimizing the current site tensor (measured by \( \Delta_{\text{opt}} \)), while at the same time it minimizes the perturbation of the optimized site tensor when expanding the next bond (measured by \( \Delta_{\text{trunc}} \)). It also needs to account for the previously described situation, in which the site tensors are eigenstates of the effective Hamiltonian in which no expansion should occur, or, the mixing factor should be decreased, at least.

As suggested in [65], we update the mixing factor with a multiplicative adaption factor \( \eta \) such that \( \alpha' = \eta \alpha \). This allows for a gradual change of the expansion rates that mimics the increase or decrease of correlations throughout the system. The overall strategy is to increase the mixing factor if the ratio \( \Delta_{\text{trunc}}/\Delta_{\text{opt}} \) is very small (or even negative) but to decrease it if the ratio exceeds 0.3. The exact procedure to choose the adaption factor \( \eta \) is given in algorithm 1. Further, the adaption factor is restricted to \( 0.99 < \eta < 1.01 \) and the mixing factor to \( 10^{-8} \leq \alpha \leq 100 \). If the mixing factor falls below \( 10^{-8} \) this is interpreted as a signal for the site tensor being an eigenstate of the effective single-site Hamiltonian and the subspace expansion is suspended entirely.

To achieve convergence of our DMRG3S+LBO method, it turns out to be beneficial to postpone the adaptation of the mixing factor \( \alpha \) in the first few sweeps to keep it at a relatively high value. Furthermore, we noticed that the algorithm is still prone to getting stuck despite the use of the subspace expansion. This behavior is especially common in the CDW phase of the Holstein model when polaron becomes heavy and hard to move around in the lattice. It is therefore beneficial to use initial states that are already close to the targeted ground state and possess key features of it. We therefore pursue the strategy of first calculating the ground state at \( \gamma = 0 \) for a relatively small maximal bond dimension, in an initialization run. In the following, we increase the coupling \( \gamma \) from run to run while keeping the maximal bond dimension fixed, until the desired coupling strength is reached. Then, the bond dimension is increased from run to run until the desired precision is reached.
We illustrate potential pitfalls of our method in figure 6. In this example, three runs with \( L = 51 \), \( \omega_{\nu}/t_o = 1 \), and \( \gamma/t_o = 2 \), which corresponds to the CDW phase, are compared. The maximal bond dimension is set to \( n_{\text{max}} = 20 \), the maximum phonon number per site to \( n_{\text{ph}} = 31 \), and \( d_o = 5 \) optimal modes per symmetry block are considered. In the first run \( R_1 \), the initial state is the ground state at \( \omega_{\nu}/t_o = 1 \), \( \gamma/t_o = 1.5 \), \( n_{\text{max}} = 20 \), \( n_{\text{ph}} = 31 \), and \( d_o = 5 \) \( (|\Psi_{\text{in},1}\rangle) \). Furthermore, the mixing factor \( \alpha \) is fixed to 1 in the first 30 sweeps \( (s_{\alpha=1} = 30) \). In the second run \( R_2 \), the initial state is the same as in the first run \( (|\Psi_{\text{in},1}\rangle) \), but the fixation of \( \alpha \) is only done in the first sweep \( (s_{\alpha=1} = 1) \). For the third run \( R_3 \), the initial state is chosen to be the ground state at \( \gamma = 0 \) and \( n_{\text{max}} = 15 \) \( (|\Psi_{\text{in},2}\rangle) \), while \( \alpha \) is again fixed for the first 30 sweeps \( (s_{\alpha=1} = 30) \).

The inset of figure 6(a) shows the electron density on the sites in the different initial states. As expected, the density profile is flatter in the ground state at \( \gamma = 0 \) \( (|\Psi_{\text{in},2}\rangle) \) and has more structure in the ground state at \( \gamma/t_o = 1.5 \) \( (|\Psi_{\text{in},1}\rangle) \). In the main panel of figure 6(a), the mixing factor \( \alpha \) is plotted against the sweeps. After the first 30 sweeps where \( \alpha \) is fixed, the mixing factor falls off quickly to \( \approx 10^{-7} \) in \( R_1 \). In \( R_2 \), the mixing factor falls off immediately with a small peak at around the 40th sweep before \( \alpha \) also settles at \( \approx 10^{-7} \). In \( R_3 \), the decay of \( \alpha \) is more gradual but after the 160th sweep, it also has a value of \( \approx 10^{-7} \) with small fluctuations.

In figure 6(b), the relative energy difference between the lowest energy found during the run and the current energy estimate in the middle of a specific sweep is presented:

\[
\delta_{\text{self}} E = \frac{E_{\text{sweep}} - E_{\text{min,run}}}{|E_{\text{min}}|}. \tag{17}
\]

The evolution of \( \delta_{\text{self}} E \) can be extracted from a single run. In contrast, figure 6(c) displays the energy difference between the current energy estimate in the middle of a sweep and the lowest energy between all three runs:

\[
\delta E = \frac{E_{\text{sweep}} - E_{\text{min}}}{|E_{\text{min}}|}. \tag{18}
\]

It can, of course, only be extracted from a comparison between different runs.

The runs \( R_1 \) and \( R_2 \) show a plateau in \( \delta_{\text{self}} E \) in figure 6(b) until approximately the 40th sweep. Then, the energy quickly drops over the course of about 20 sweeps and \( \delta_{\text{self}} E \) stays below \( 10^{-10} \) after the 60th sweep. In contrast, the energy drops slower in \( R_3 \), but after the 300th sweep, \( \delta_{\text{self}} E \) also stays below \( 10^{-10} \).

While figure 6(b) suggests that all three runs are converged, the data for \( \delta E \) in figure 6(c) gives evidence that this is not the case. The data for \( R_1 \) is the same in figure 6(b) and figure 6(c) since in \( R_1 \) the lowest

---

**Algorithm 1** Procedure to choose the adaption factor \( \eta \) for the update of the mixing factor \( \alpha \) from the energy differences \( \Delta_{\text{opt}} \) and \( \Delta_{\text{trunc}} \).

\[
\begin{align*}
\delta_{\text{opt}} &= \frac{\Delta_{\text{opt}}}{|E_{\text{opt}}|} \\
\delta_{\text{trunc}} &= \frac{\Delta_{\text{trunc}}}{|E_{\text{trunc}}|} \\
\text{if} \ (|\delta_{\text{opt}}| < 10^{-14} \text{ or } |\delta_{\text{trunc}}| < 10^{-14}) \text{ then} & \quad \eta = 1 \\
\text{else if } \delta_{\text{trunc}} < 0 \text{ then} & \quad \eta = 2(1 + \frac{|\delta_{\text{trunc}}|}{|\delta_{\text{opt}}|}) \\
\text{else if } \frac{|\delta_{\text{trunc}}|}{|\delta_{\text{opt}}|} < 0.05 \text{ then} & \quad \eta = 1.2 - \frac{|\delta_{\text{trunc}}|}{|\delta_{\text{opt}}|} \\
\text{else if } \frac{|\delta_{\text{trunc}}|}{|\delta_{\text{opt}}|} > 0.3 \text{ then} & \quad \eta = \frac{1}{\eta_{\text{min}}} \\
\text{else} & \quad \eta = 1 \\
\end{align*}
\]
energy was found. $\mathcal{R}_2$ finds an energy that is about $\delta E \approx 10^{-6}$ above the one found by $\mathcal{R}_1$. The energy found in $\mathcal{R}_3$ is $\delta E \approx 10^{-2}$ above the one of $\mathcal{R}_1$.

The inset of figure 6(b) shows the real-space electron-density profile in the final states of the runs. The final states of $\mathcal{R}_1$ and $\mathcal{R}_2$ have the expected profile of a charge-density wave. The final state of $\mathcal{R}_3$ does not have such a structure in the electron density at all.

This example illustrates the impact of initial states and the choice of the mixing factor on the convergence of the DMRG3S+LBO. Choosing an initial state that already possesses structural features of the ground state one is trying to find can prevent the algorithm from getting stuck in local minima. This can be achieved by gradually changing the parameters in the Hamiltonian (here $\gamma$) by performing several runs of complete ground-state searches. In this procedure, the initial state of the subsequent run is chosen to be the optimized ground state of the previous parameter set. Finally, the mixing factor should be fixed at a large value for the first few runs to explore a large enough portion of the Hilbert space before it can be lowered to achieve
Further increasing the DMRG3S+LBO method can be reached, which turns out to be a relative energy difference of about $10^{-12}$.

As a function of $m_{\text{max}}$, the maximal bond dimension, the energy decreases as expected. For a certain choice of $n_{\text{ph}}$ and $d_o$, the energy can, however, only reach a certain precision that does not substantially improve as the bond dimension is increased further. With $n_{\text{ph}} = 31$ and $d_o = 10$, the maximal precision of our implementation of the DMRG3S+LBO method can be reached, which turns out to be a relative energy difference of about $10^{-12}$. Further increasing $n_{\text{ph}}$ does not improve the energies.

Figure 7(b) shows the variance of the energy versus the maximal bond dimension $m_{\text{max}}$. The variance can be taken as a measure of proximity of a certain state to an eigenstate of the Hamiltonian. As expected, a small choice of $d_o$ limits the reachable precision in the variance. However, limiting $n_{\text{ph}}$ does not limit the precision in such a way. As mentioned earlier, changing $n_{\text{ph}}$ alters the Hilbert space and the system altogether and, therefore, one can be close to the ground state in the case of a small $n_{\text{ph}}$, but the state is still substantially different from the ground state in the limit $n_{\text{ph}} = \infty$. This difference, however, does not manifest itself in the variance.

The ultimate goal is to get results that do not change upon further increase of $n_{\text{ph}}$, $n_{\text{ph}}$ changes the dimension of the Hilbert space and, in principle, the nature of the whole system. However, limiting $n_{\text{ph}}$ alters the Hilbert space and the system altogether and, therefore, one can be close to the ground state to an eigenstate of the Hamiltonian. As expected, a small choice of $d_o$ limits the reachable precision in the variance. However, limiting $n_{\text{ph}}$ does not limit the precision in such a way. As mentioned earlier, changing $n_{\text{ph}}$ alters the Hilbert space and the system altogether and, therefore, one can be close to the ground state in the case of a small $n_{\text{ph}}$, but the state is still substantially different from the ground state in the limit $n_{\text{ph}} = \infty$. This difference, however, does not manifest itself in the variance.
2.4. Projected Purification

![Diagram](image)

Figure 8: (a) A schematic representation of the local Hilbert space doubling via the introduction of a bath site for each local degree of freedom as used in PP-2DMRG is shown. (b) The decomposition and projection of a general MPS tensor (top) into the subspace \( \mathcal{P} \) enforcing the local gauge conditions is depicted. The decomposition of the introduced auxiliary index into irreducible representations of the local conservation law generated by \( \hat{n}_{P,j} + \hat{n}_{B,j} \) as described in [53] is sketched by the double bond \((n_{P,j}, \alpha_{j-1})\).

In the following, we describe the projected-purification ansatz [53], which is based on a doubling of the Hilbert space and a subsequent projection into an invariant subspace. This scheme allows us to formulate operators and states that transform under a restored global \( U(1) \) symmetry and to efficiently represent and truncate the local phononic degrees of freedom. A simple pictorial representation of the ansatz is sketched in figure 8(a). Every physical site with electron and phonon degrees of freedom is accompanied by a phonon bath site that acts as a reservoir. Creating or annihilating a phonon on the physical site means that it hops from or to the bath site. This way, an artificial \( U(1) \) symmetry is generated, namely the combined number of phonons on the physical and bath site is conserved.

2.4.1. Projected Purified Operators

Consider a Hilbert space \( \mathcal{H} = \mathcal{H}_d^\otimes L \) with basis states labeled by the eigenvalues of the local density operators \( \hat{n}_j = \text{diag}(0, 1, \ldots, d - 1) \). We define a doubling \( \mathcal{H}_{PB} = \mathcal{H}_P \otimes \mathcal{H}_B \), introducing two copies \( \mathcal{H}_{P/B} \) of the original Hilbert space \( \mathcal{H} \) as shown in figure 8(a) and refer to \( \mathcal{H}_P \) and \( \mathcal{H}_B \) as the physical and bath Hilbert space, respectively. Operators acting on (local) Hilbert spaces \( \mathcal{H}_{P/B} \) will be equipped with an additional label, for instance, \( \hat{n}_{P/B,j} \) denotes the density operators acting on the local physical or bath degrees of freedom at site \( j \). A projected purified operator \( \hat{O}_{PP} : \mathcal{P} \rightarrow \mathcal{P} \) acts on a subspace \( \mathcal{P} \subset \mathcal{H}_{PB} \) of the purified Hilbert space and satisfies the constraints

\[
\left[ \hat{O}_{PP}, \hat{n}_{P,j} + \hat{n}_{B,j} \right] = 0
\]

for every \( j \). Defining global operators \( \hat{N}_{P/B} = \sum_j \hat{n}_{P/B,j} \), any projected purified operator manifestly conserves the global \( U(1) \) symmetry generated by \( \hat{N}_P + \hat{N}_B \):

\[
\left[ \hat{O}_{PP}, \hat{N}_P + \hat{N}_B \right] = 0.
\]
An explicit construction scheme for the subspace $\mathcal{P}$ can be found by fixing gauge constraints between the physical and bath site to

$$\hat{n}_{P,j} + \hat{n}_{B,j} \equiv (d - 1).$$  \hspace{1cm} (23)

In [53], we showed that this choice implies $\dim \mathcal{P} = \dim \mathcal{H}$ and that there is a one-to-one mapping between states and operators in these Hilbert spaces. It follows that for any operator $\hat{O}$ acting on the original Hilbert space, an analogous projected purified operator can be constructed. This is achieved by introducing balancing operators $\hat{\beta}_{B,j}^{\dagger}$

$$\hat{\beta}_{B,j} = \sum_{n_{B,j} = 1}^{d-1} |n_{B,j} - 1 \rangle \langle n_{B,j}|, \quad |n_{B,j}\rangle \in \mathcal{H}_{B,d}.$$ \hspace{1cm} (24)

Writing $\hat{O}$ in terms of ladder operators $\hat{b}_{j}^{\dagger}$, the mapping to the corresponding projected purified operator $\hat{O}_{PP}$ is achieved by pairing up ladder operators with conjugated balancing operators:

$$\hat{b}_{j}^{\dagger} \rightarrow \hat{b}_{P,j}^{\dagger} \hat{\beta}_{B,j}, \quad \hat{b}_{j} \rightarrow \hat{b}_{P,j} \hat{\beta}_{B,j}^{\dagger}.$$ \hspace{1cm} (25)

The phononic part of the Holstein model breaking the global $U(1)$ symmetry in $\mathcal{H}$ is then represented by a projected purified operator $\hat{H}_{PP,f-ph}$ acting only on $\mathcal{P}$

$$\hat{H}_{PP,f-ph} = \gamma \sum_{j} \hat{n}_{P,j}^{f} \left( \hat{b}_{P,j}^{\dagger} \hat{\beta}_{B,j} + \hat{b}_{P,j} \hat{\beta}_{B,j}^{\dagger} \right).$$ \hspace{1cm} (26)

Note that $\hat{H}_{PP,f}$ and $\hat{H}_{PP,ph}$ remain unaltered except for a formal replacement of local operators acting on $\mathcal{H}_{d}$ with their counterparts acting on $\mathcal{P}$:

$$\hat{c}_{j}^{\dagger} \rightarrow \hat{c}_{P,j}^{\dagger} \hat{1}_{B,j}, \quad \hat{n}_{j}^{f} \rightarrow \hat{n}_{P,j}^{f} \hat{1}_{B,j} \quad \text{and} \quad \hat{b}_{j}^{\dagger} \rightarrow \hat{b}_{P,j}^{\dagger} \hat{b}_{P,j} \hat{1}_{B,j}.$$ \hspace{1cm} (27)

2.4.2. Projected Purified MPS

The gauge-fixing condition (23) allows us to construct a projector to $\mathcal{P}$. Using the action of this projector on MPSs in the enlarged Hilbert space, we derived a condition on the combined physical and bath system’s site tensors [53]. In a practical ground-state-search calculation, it suffices to create an initial state whose physical indices reflect the gauge fixing. For instance, let $T_{j ; \alpha_{j} \gamma_{j}}^{n_{P,j}}$ and $T_{j ; \gamma_{j} \alpha_{j}}^{n_{B,j}}$ be $U(1)$-invariant MPS site tensors with physical and bath local degrees of freedom labeled by $n_{P,j}$ and $n_{B,j}$, respectively. The condition for the MPS to represent a projected purified state $|\psi\rangle_{PP} \in \mathcal{P}$ is then given by

$$\sum_{\gamma_{j}} T_{j ; \alpha_{j} \gamma_{j}}^{n_{P,j}} T_{j ; \gamma_{j} \alpha_{j}}^{n_{B,j}} \neq 0 \Leftrightarrow n_{P,j} + n_{B,j} \equiv (d - 1),$$ \hspace{1cm} (28)

and shown graphically in figure 8(b). Since $\mathcal{P}$ is a subspace of the enlarged Hilbert space $\mathcal{H}_{PB}$, projected purified operators acting on such states conserve this condition. This is an important point as it minimizes the implementational effort. In fact, by doubling the Hilbert space and using projected purified operator representations only, DMRG codes that are able to initialize states $|\psi\rangle_{PP}$ obeying (28) can readily work in $\mathcal{P}$ and thereby exploit restored global $U(1)$ symmetries. For the dimensions of the indices representing the local degrees of freedom, this implies $\dim n_{P/B,j} \equiv 1$.

2.4.3. Truncation and Connection to 1RDM

Projected purified states $|\psi\rangle_{PP} \in \mathcal{P}$ exhibit an intimate relation to the 1RDM $\hat{\rho}_{j} = \text{Tr}_{k \neq j} |\psi\rangle \langle \psi|$ of the corresponding state in the original Hilbert space $\mathcal{H}$, which is displayed graphically in figure 9. The crucial
upon truncation. An important conclusion is that having restored the global contractions scaling as

\[ \text{degrees of freedom} \]

allows us to employ a local solver based on two-site tensors, which is less prone of getting

\[ \text{advantages in MPS calculations when the local dimension } d \text{ of the problem is large and the system does not} \]

conserve global symmetries, initially. When re-establishing a global \( U(1) \)-symmetry in the subspace \( \mathcal{P} \), local degrees of freedom \( \hat{n}_{\mathcal{P}/B,j} \) decompose into one-dimensional representations. As a consequence, contractions scaling as \( d^l \) for some exponent \( l \in \mathbb{N} \) can be parallelized over the local degrees of freedom.

Additionally, the connection to the IRDM reveals that if for some \( n_0 \in \{0, \ldots, d-1\} \) the diagonal elements \( \rho_{n_0,n_0,n_0,n_0} \) are decaying fast enough, the number of relevant tensor blocks can be reduced drastically upon truncation. An important conclusion is that having restored the global \( U(1) \) symmetry w.r.t. phononic degrees of freedom allows us to employ a local solver based on two-site tensors, which is less prone of getting
Figure 10: Weight $w_0$ of optimal modes $d_0$ as a function of the maximal bond dimension at the auxiliary bonds $\gamma_{25}$ (a) and (b) using the projected purification. Data is extracted from the single-site reduced density matrix $\rho_{n_{25}/n_{25}}$ at the center site ($j = 25/24$) in the calculated ground state of the Holstein model with $L = 51$ sites and $N = 25$ fermions, $\omega/t_0 = 1.0, \gamma/t_0 = 1.5$. The inset shows the diagonal elements $\rho_{n_{25},n_{25}}$ indicating the immediate effect of truncations. For comparison, the phonon excitation probabilities obtained for $t_0 = 0$ at occupied sites (left) are overlayed, indicated by yellow crosses.

stuck in local minima (PP-2DMRG). Furthermore, the truncation argument implies that the dimension of the auxiliary bond $\gamma_j$ between physical and bath site tensors controls the quality of the approximation of $\rho_{n_j,n'_j}$.

As a consequence, the same scaling analysis in terms of auxiliary bond dimensions, which is usually employed in DMRG algorithms to extrapolate observables towards their exact value, can be used for the projected purification. This is demonstrated in figure 10(a), where we show the weight $w_0$ of the optimal modes $d_0$ of the single-site reduced density-matrix as a function of the auxiliary bond dimension $\gamma_j$ used to approximate the ground state of the Holstein model near the phase boundary (P.2). Upon increasing the bond dimension we find a well-converging behavior for the weights $w_0(d_0)$. Note that in these calculations, we allowed for a maximum number of $n_{ph} = 63$ phonons per lattice site. However, as shown in the inset, the maximum occupation number for the phonons kept after truncation is $n_{ph} \leq 20$, i.e., a significant amount of tensor blocks is discarded due to the vanishing contribution of high-occupation phonon modes. Therein, we also indicate the diagonal elements calculated for the atomic limit $t_0 = 0$ using the Lang-Firsov transformation of the Holstein Hamiltonian [79]. It can be seen that the phonon excitation probability (i.e., $\rho_{n,n'}$), obtained from projected purification, is already very close to the limit of decoupled fermions, which is the asymptotic distribution when sending $t_0 \to 0$.

2.4.4. Effects of Truncation

Performing ground-state searches using PP-2DMRG allows to monitor the actual discarded weight $\delta_j$ on a bond $j = (j,j+1)$ after each, local-optimization step as a function of the maximally allowed bond dimension $m_{\text{max}}$. As a consequence, an estimate for the quality of the obtained ground-state energy can be
constructed from the maximally found discarded weight per bond

\[ \Delta = 2L \max_{j} \delta_j \equiv 2L \delta_{\text{max}} . \]  

(34)

This provides an alternative convergence test for the approximation of the ground state as we expect the difference of the approximated energy $E$ to the exact ground-state energy $E_{\text{ex}}$ to scale as $E - E_{\text{ex}} \sim \Delta$. For PP-2DMRG, this is important, since the phonon correlations are encoded into the auxiliary bond between the physical- and bath-site tensors. If the number of phonons is large and their excitation probability is broadly distributed, this implies the requirement of significantly larger auxiliary bond dimensions to keep the discarded weight below a certain threshold [53].

The necessity to monitor the discarded weight can be illustrated by studying the system near the phase boundary where strong fluctuations in both the fermionic and phononic subsystem are present, which have to be captured by the auxiliary bonds. The bond dimensions between the original lattice sites are multiplied by the additional number of states required to capture the phononic degrees of freedom on the auxiliary bonds $\gamma_j$. Thus, near the phase boundary, where we have strong fluctuations on large length scales also in the fermionic systems, the value of $m_{\text{max}}$ on the auxiliary bonds between physical and bath sites has to be chosen comparably large in order to achieve a certain quality $\Delta$ of the approximated ground states. We demonstrate this observation in figure 11(a) (blue curve) where the chosen cutoff $m_{\text{max}} = 2000$ is not sufficient to reach the desired discarded weight per bond $\delta_j = 10^{-14}$. However, it should be pointed out that using the restored global $U(1)$ symmetries, $m_{\text{max}} = 2000$ is not fixed because of numerical limitations, but only to allow consistent comparisons.

2.4.5. Benchmark Setup

For the benchmark simulations, the maximum allowed bond dimensions are varied from $m_{\text{max}} = 100$ up to $m_{\text{max}} = 2000$ and the number of phonons is bound by $n_{\text{ph}} = 63$. The initial state for the ground-state searches are constructed as a Fermi sea of non-interacting, spinless fermions and no phonons in the physical system ($n_{P,j} \equiv 0$). In order to achieve convergence, the maximally allowed number of sweeps for a single ground-state calculation was set to 200 (which is never reached) and the calculations were terminated once

Figure 11: Truncation effects in the PP-2DMRG method at three different points in parameter space, i.e., in the LL phase (P.3) (green), near the phase boundary (P.2) (blue), and in the CDW phase (P.3) (yellow). In (a), the maximal discarded weight $\delta_{\text{max}}$ as a function of the maximally allowed bond dimension $m_{\text{max}}$ is shown demonstrating the impact of strong fluctuations near the phase boundary on the required bond dimensions to achieve a particular accuracy. (b) shows the scaling of the relative distance $\Delta E$ to the minimally found ground-state energies with the maximal discarded weight revealing that near the phase boundary, the maximally allowed number of states $m_{\text{max}} = 2000$ is not sufficient to achieve the same numerical precision as in the LL and CDW phase.
the relative fluctuations in the approximated ground-state energy as a function of the number of sweeps fell below a certain threshold. For the high-precision calculations, this threshold was set to $10^{-14}$ while in case of the finite-size extrapolation the condition to terminate the ground-state search was relaxed to a threshold of $10^{-8}$.

3. Comparing the Methods

The Holstein model provides an excellent testing platform to compare the numerical behavior of the presented DMRG methods with respect to two important problem settings: numerical high-precision calculations at intermediate system sizes and finite-size extrapolations, thereby relaxing conditions on the numerical precision as a tradeoff for reaching larger system sizes. For the high-precision calculations, we fix the system size to $L = 51$ lattice sites at nearly half filling with $N = 25$ fermions. The finite-size extrapolation is performed for systems with $L = 51, 101, 151, 201$ lattice sites where the fermion number is set to $N = \frac{L - 1}{2}$. Note that we always use an odd number of lattice sites. One reason for this is the observation that in the CDW phase, the sublattice symmetry between even and odd sites is broken and the unit cell is enlarged to consist of two lattice sites. In a system with an even $L$, this yields two different possibilities of arranging the unit cells. These two choices will hybridize to form the ground state. For DMRG, this is a delicate situation as the site tensors are optimized in a way to minimize entanglement entropy while sweeping through the system. In such situations, an often encountered consequence is that algorithms get stuck in low-lying excited states, which minimize the entanglement entropy but not the global energy. To circumvent this problem, we use odd system sizes, thereby fixing the arrangement of the unit cells in the CDW phase. This has the pleasant side effect that the CDW order parameter actually acquires a finite value in the CDW phase, which is not the case in finite systems with an even number of sites.

3.1. Convergence Analysis of Ground-State Energies

In order to compare the methods’ capabilities of approximating the ground state, we perform a scaling analysis in the maximum bond dimension $m_{\text{max}}$. We calculate the relative distance of the approximated ground-state energies $E_0(m_{\text{max}}) = \langle \psi(m_{\text{max}}) | \hat{H} | \psi(m_{\text{max}}) \rangle$ to the lowest energy found from all methods, $E_{\text{min}}$.

$$\Delta E(m_{\text{max}}) = \frac{E_{\text{min}} - E_0(m_{\text{max}})}{E_{\text{min}}}.$$  \hspace{1cm} (35)

For the DMRG3S+LBO and PP-2DMRG methods, we also systematically evaluated the variance for the found ground-state approximations $|\psi(m_{\text{max}})\rangle$:

$$\text{Var}[\hat{H}] = \langle \psi(m_{\text{max}}) | (\hat{H} - E_0(m_{\text{max}}))^2 | \psi(m_{\text{max}}) \rangle.$$  \hspace{1cm} (36)

In practice, a systematic dependency of the variance on the ground-state energy allows us to extrapolate toward the limit of infinite bond dimension $E_0(m_{\text{max}} \to \infty)$ [80].

During the numerical calculations, the maximally allowed discarded weight per bond is set to $\delta = 10^{-14}$ for the DMRG3S+LBO and PP-2DMRG methods. The PS-DMRG calculations were not limited with respect to $\delta$. Here, for the given parameter sets, the discarded weight is not a helpful quantity to decide whether a calculation converges or not and therefore, for PS-DMRG, we focus on the bond dimension as the sole control parameter.

Having discussed each method’s peculiarities in sections 2.2 to 2.4, in the following, we only show one dataset per method and parameter set. For the comparison, we pick those datasets yielding the lowest ground-state energies for the largest bond dimension.
Figure 12: Relative deviations from the minimal ground-state energy found (a) and their scaling w.r.t. the relative variance (b) using PS-DMRG ($\Delta E$ only), PP-2DMRG and DMRG3S+LBO for the parameter set (P.1). We vary the maximal bond dimensions and for the case of PS-DMRG and DMRG3S+LBO, we only show data points belonging to those datasets that yield the lowest ground-state energies. The maximal bond dimensions $m_{\text{max}}$ in (a) are rescaled by a factor of 3 in the case of the PS-DMRG and PP-2DMRG calculations.

**LL phase.** Figure 12 displays the results of the scaling analysis in the LL phase (P.1). The maximum bond dimension $m_{\text{max}}$ used during the PS-DMRG and PP-2DMRG calculations are rescaled by a factor of 3. For the latter, this yields a dependency of the ground-state energies on $m_{\text{max}}$ comparable to the data obtained using DMRG3S+LBO, as shown in figure 12(a). The smallest ground-state energy reached is $E_{\text{min}}/t_0 = -36.15999956298296$ obtained by PP-2DMRG with a relative precision $\sim 10^{-13}$, which is consistent with the chosen discarded weight $\delta = 10^{-14}$.

The relative variance $\frac{\text{Var}[\hat{H}]}{E_0^2(m_{\text{max}})}$ as a function of the relative distance $\Delta E$ is shown in figure 12(b). For both the DMRG3S+LBO and PP-2DMRG methods, we find a similar systematic dependence up to a very high precision. Note that the saturation of $\frac{\text{Var}[\hat{H}]}{E_0^2(m_{\text{max}})}$ at $\Delta E(m_{\text{max}}) < 10^{-12}$ is numerically consistent with the overall truncation error $\propto L \cdot \delta$ introduced by the chosen discarded weight per bond $\delta = 10^{-14}$.

**Phase boundary.** Figure 13 shows the results near the phase boundary between the LL and CDW phase. The scaling of $\Delta E(m_{\text{max}})$ displayed in figure 13(a) reveals that the appearance of heavy polarons and strong fluctuations in the fermion system require a much larger bond dimension to approximate the ground state with a high precision. This is reflected by a rescaling of $m_{\text{max}}$ with a factor of 1.5 for the PS-DMRG method and a factor of 5 for PP-2DMRG in order to achieve a convergence behavior similar to the one observed in DMRG3S+LBO. Here, the ground-state approximations obtained using DMRG3S+LBO yield the smallest energy, which is given by $E_{\text{min}}/t_0 = -70.862628874727$ with a relative precision of $\lesssim 10^{-11}$ as can be seen by the variance displayed in figure 13(b).

**CDW phase.** In figure 14, the scaling analysis is shown for the parameter set (P.3) for which the system is in the CDW phase. All tested methods are capable of faithfully representing the ground state with a very high precision and comparably small bond dimensions with the lowest energy given by $E_{\text{min}}/t_0 = -107.32209423031215$ with a relative precision of $10^{-14}$ using PP-2DMRG. For the PS-DMRG method, we rescaled the maximally allowed bond dimension by a factor of 4 while a factor of 7.5 was required for the PP-2DMRG method in order to achieve a similar scaling behavior of $\Delta E$ for the three methods. This large rescaling factor is based on the broadly distributed excitation probabilities of the phonons requiring a larger local Hilbert-space dimension. Here, for all three methods tested, we use $N_{\text{ph}} = 63$ to achieve the best results.

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3.2. Local Observables - Oscillator Displacement

Having studied the convergence of the ground-state approximation for the different methods, we turn to physical observables next. In the Holstein model, the CDW phase is characterized by the formation of lattice distortions with a period of twice the lattice constant, i.e., the translation symmetry of the lattice is broken into two translational invariant sublattices $\mathcal{A}/\mathcal{B}$ with even/odd lattice sites. We evaluate the oscillator displacement of the $j$th lattice site for different maximum bond dimensions $m_{\text{max}}$ near the phase transitions.
Figure 15: Oscillator displacement \( x_{ph}(j) = \langle \hat{b}_j^\dagger + \hat{b}_j \rangle \) in the ground state near the phase boundary. The data shown here is taken from the calculations with the largest bond dimension for each method. For convenience, even-(a) and odd-site (b) expectation values are plotted separately. Insets display differences of the calculated oscillator displacements between the different methods.

boundary (P.2)

\[ x_{ph}(j) = \langle \hat{b}_j^\dagger + \hat{b}_j \rangle, \quad (37) \]

breaking translational symmetry. In figure 15, the results are shown for \( \omega_0/t_0 = 1.0 \) and \( \gamma/t_0 = 1.5 \). We separately plot even-(figure 15(a)) and odd-site (figure 15(b)) expectation values to illustrate the behavior of \( x_{ph}(j) \) in the two sublattices. All methods yield the same behavior, i.e., we find developing CDW modulations in the two sublattices caused by finite displacements with larger values \( x_{ph}(j) \) for \( j \in B \) compared to those \( x_{ph}(j) \) for \( j \in A \). In order to visualize the numerical deviations, in the insets, we plot the difference \( \Delta x_{ph}(j) \) between the displacements obtained from the datasets with the largest \( m_{max} \) for each method, as they exhibit the highest precision (\( m_{max} = 2000 \) for PP-2DMRG, \( m_{max} = 440 \) for DMRG3S+LBO and \( m_{max} = 200 \) for PS-DMRG). In the analyzed data, the deviations \( \Delta x_{ph}(j) \) rapidly decrease and, for the largest bond dimensions, are located around \( 10^{-6} \) as shown in figure 15.

3.3. Finite-Size Extrapolation

Practically, one is often interested in a finite-size extrapolation of intensive quantities such as the energy density \( \frac{E_0}{L} \) or the order parameter

\[ \mathcal{O}_{\text{disp}}(L) = \frac{1}{L} \sum_j (-1)^j x_{ph}(j), \quad (38) \]

where the extrapolation towards \( L \rightarrow \infty \) allows us to approach the thermodynamic limit. Here, we perform a scaling analysis of the ground-state energy density \( \epsilon(L) = \frac{E_0}{L} \) in units of \( t_0 \equiv 1 \) and \( \mathcal{O}_{\text{disp}}(L) \). The extrapolations are done using fitting functions

\[ \epsilon(L) = \frac{A_\epsilon}{L} + \epsilon_\infty \quad (39) \]

\[ \mathcal{O}_{\text{disp}}(L) = \frac{A_O}{L} + \frac{B_O}{L^2} + \mathcal{O}_{\text{disp},\infty} \quad (40) \]

For the order parameter, we add a contribution \( \propto \frac{1}{L^2} \) to account for boundary effects, which are important for the parameter sets (P.1) and (P.2).
Table 1: Energy densities $\epsilon_\infty = \lim_{L \to \infty} \epsilon(L)$ in units of $t_0$ obtained from finite-size scaling of ground-state energies.

| Method   | Energy Density   |
|----------|------------------|
| (P.1)    | $-0.71862 \pm (2 \cdot 10^{-5})$ |
| (P.2)    | $-1.41606 \pm (1 \cdot 10^{-5})$ |
| (P.3)    | $-2.1462830 \pm (1 \cdot 10^{-7})$ |

Energy density. The extrapolated energy density in the thermodynamic limit is shown in table 1. All methods agree within their confidence intervals for the investigated parameter sets (P.1) and (P.2). For illustrational purposes, in figure 16(a), the finite-size extrapolation is displayed for the parameter set (P.2). In the CDW phase (P.3), the finite-size extrapolations seem to underestimate the fitting error. We attribute this to the fact that in the CDW phase, and at weakened conditions on the precision, the formation of heavy polarons effectively suppresses the energy gains due to fermion delocalization. As a consequence, domain walls in the fermionic system are harder to resolve and the calculations can get stuck in a local minimum. In our calculations, it appears that all three methods are affected by this problem, though in a different way owing to their different approximations, and practically, convergence has to be checked very carefully.

Order parameter. The extrapolated values for the CDW order-parameter in the thermodynamic limit are shown in table 2; and the explicitly calculated system-size dependencies are plotted in figure 16(b) for the
PS-DMRG

DMRG3S+LBO

PP-2DMRG

System enlargement

$\times \log_2(n_{ph} + 1)$

$\times 1$

$\times 2$

Local Hilbert space truncation

none

w.r.t. eigenvalues of 1RDM $\hat{\rho}_j$

w.r.t. diagonal elements of 1RDM $\hat{\rho}_j$

Convergence parameter

$n_{ph}, \delta(m_{\text{max}})$

$n_{ph}, \delta(m_{\text{max}}), d_o$

$n_{ph}, \delta(m_{\text{max}})$

Phonon symmetries

none

none

$U(1)$

Additional code requirements

pseudo-site operators

1RDM computation, diagonalization & DMRG optimization of 1RDM trafo, MPS and MPO transformation

balancing operators

Table 3: Comparison of method specific properties when applied to the Holstein model. Local Hilbert space truncation refers to the possibility of reducing the local Hilbert space dimension of the phononic degrees of freedom. Listed, additional code requirements assume that the given implementation is capable of dealing with long-ranged couplings. It is also assumed that the implementation is capable to truncate site tensors w.r.t. control parameters such as the maximal bond dimension $m_{\text{max}}$ or the discarded weight $\delta$ per bond.

parameter set (P.2). In the LL phase (P.1), we expect $\mathcal{O}_{\text{disp,\infty}} \equiv 0$. With a relative precision $\sim \mathcal{O}(10^{-5})$, this is found for the PS-DMRG method, whereas the PP-2DMRG and DMRG3S+LBO calculations are about an order of magnitude smaller $\sim \mathcal{O}(10^{-6})$. Near the phase boundary (P.2), all methods yield a small but finite value coinciding with a relative precision of $\sim \mathcal{O}(10^{-2})$, which is comparably small and most probably a signature of the strong fluctuations. Note that it is not too surprising that near the phase boundary, the methods may produce different outcomes for the order parameter. In the CDW phase, the three methods coincide up to 4 significant digits yielding a finite value of the order parameter, as expected. In particular, the DMRG3S+LBO and PP-2DMRG methods coincide up to a relative precision of $10^{-5}$. However, at (P.3) all methods do not agree with respect to their error bounds obtained from the finite-size scaling, which was also found in the ground-state energy extrapolation.

A more careful convergence analysis is essential to achieve consistent extrapolations, which, however, is not the goal of this comparison. Instead, we want to point out that for the case of heavy polarons, ensuring the convergence with respect to all numerical control parameters is of particular importance.

4. Discussion

The technical properties of the discussed methods are summarized and compared in table 3. It should be noted that both PS-DMRG and PP-2DMRG require fewer modifications to an existing code compared to an implementation of DMRG3S+LBO. In particular, PS-DMRG can be readily used if the implementation supports combined fermionic and hardcore-bosonic lattice degrees of freedom. In order to use PP-2DMRG, the most relevant required modification is the implementation of the balancing operators which, however, are only local operators, i.e., they can be realized in a straightforward manner. In contrast, the implementation of DMRG3S+LBO is more involved and requires the evaluation, optimization and truncation of the 1RDM during each site update as well as a transformation of the local Hilbert space representation for both, the MPS and MPO site tensors. The technical prerequisites in table 3 are put in the context of the numerical behavior of the different approaches, described in section 3.

**PS-DMRG.** The extension of the system size by introducing pseudo sites controls the numerical behavior. There are long-ranged couplings between the fermionic sites and the pseudo sites, as well as long-ranged hoppings between the fermionic sites with a maximum range spanning $\log_2(n_{ph} + 1) + 2$ lattice sites. The situation can be analyzed by considering a bipartition of the system right in the middle of the chain of pseudo sites. In such a bipartition, the cut bond has to account for both, fermionic correlations between the physical lattice sites and off-diagonal phonon correlations on the current, physical lattice site. For
the latter, strong phonon fluctuations contribute to the entanglement entropy with a scaling that can be estimated as $S_{\text{PS}} \sim N_{\text{PS}}/2$ where $N_{\text{PS}} = \log_2(n_{\text{ph}} + 1)$ is the number of pseudo sites. This contribution to the entanglement entropy superimposes the fermionic correlations. The convergence behavior of the PS-DMRG high-precision calculations in the LL phase (c.f. figure 12) and near the phase boundary (c.f. figure 13) can be related to this picture. In both regions, the fermionic degrees of freedom exhibit critical behavior that translates to very long-ranged correlations when introducing pseudo sites. A local DMRG-optimization step in the middle of the chain of pseudo sites, subject to a finite bond dimension, then preferably optimizes with respect to the local correlations. If the maximally allowed bond dimension $n_{\text{max}}$ is not sufficient, this results in a situation in which the optimization is mainly constrained to the phonon system. Upon increasing $n_{\text{max}}$, at some point the bond dimension is large enough to reproduce the long-ranged fermionic correlations with high fidelity. A similar reasoning can be employed to interpret the behavior of the PS-DMRG when increasing the number of pseudo sites (c.f. figure 4). Here, larger values of $S_{\text{PS}}$ in the middle of the chain of pseudo sites yield a slower convergence with respect to the bond dimension. Note that this behavior can also serve as a convergence criterion, i.e., if the maximum phonon number $n_{\text{ph}}$ is large enough so that $S_{\text{PS}}$ saturates, the convergence of the ground-state energy when scaling the bond dimension becomes independent of $n_{\text{ph}}$. Finally, once the system is in the CDW phase, the fermions localize, allowing for a very fast convergence of the PS-DMRG as seen in figure 14.

**DMRG3S+LBO.** In comparison to the other methods, the DMRG3S+LBO method achieves excellent convergence of the ground-state energy with the smallest required bond dimensions. This is achieved by representing on-site phonon-correlations in terms of the truncated transformation matrices $R_j$ acting on the physical legs. A careful optimization of the $R_j$’s in order to find the optimal modes representing the phononic 1RDM is thus a necessary condition for a well-behaved simulation. For that reason, a convergence analysis with respect to the number of optimal modes $d_o$ is crucial and requires various ground-state searches, since $d_o$ cannot be increased in the current implementation of the groundstate search (an adaptive increase of $d_o$ is possible, though, see [26, 30, 81]). During a DMRG sweep one has to perform various optimizations per lattice site. A single site optimization updates both, the site tensor and the transformation matrix. In the current setup, two subsequent optimizations are sufficient to achieve converged results, but dynamic and more involved convergence criteria may become necessary for more complicated systems.

Using a single-site DMRG-solver [65], the convergence behavior during DMRG-sweeps does not only depend on the maximally allowed bond dimension and the chosen optimal modes but also the initial state, as well as the subspace expansion mixing factor. A reasonable choice of the initial state is of particular importance (c.f. figure 6). Here, the separation of the optimization of the transformation matrix, updating the 1RDM approximation of the phononic degrees of freedom, from the local site-tensor optimization, appears to be an important contribution to the tendency of the ground-state search to get stuck. In the scope of our investigations, a Fermi sea with power-law correlations has proven to be a reliable initial guess state in the three investigated regions of the phase diagram.

**PP-2DMRG.** The projected purification combines the ideas of the other methods and, thus, inherits some of their properties. The convergence behavior is dominated by the off-diagonal correlations that build up in the phononic system, which control the growth of the bond dimension between physical and bath sites. Since these bonds carry both, fermionic and phononic correlations, the number of sites required to approximate the ground-state to a given precision is in general larger than in the case of the DMRG3S+LBO method. As already discussed for the case of the PS-DMRG method, this may translate to convergence problems, if the available maximal number of states $m_{\text{max}}$ between physical and bath sites is not sufficient so that mainly the phononic degrees of freedom are optimized. However, since the coupling range between the fermions is only increased from nearest-neighbor to next-to-nearest-neighbor, convergence issues typically are not drastic and can be overcome by warm-up sweeps in which the fermion-phonon coupling is increased gradually. Notably, in our implementations the PP-2DMRG is the only method that allows for a faithful extrapolation in terms of the discarded weight $\delta$. On the one hand, this is based on the fact that by restoring the global $U(1)$-symmetry, the 1RDM can be truncated according to its diagonal elements and thereby the approximation quality of the phonon system is only controlled by $\delta$. On the other hand, a small bond
dimension yields local optimizations to be biased towards the phononic degrees of freedom as observed in the PS-DMRG method. However, in our calculations we found these effects to be less prominent, since the coupling range between the fermions is increased only moderately. Since the approximation quality of the phononic 1RDM crucially depends on the discarded weight, a scaling analysis with respect to this control parameter is nevertheless of particular importance.

5. Conclusion

We discussed three state-of-the-art matrix-product-state methods to simulate numerically challenging systems with large local Hilbert spaces and broken $U(1)$-symmetries that appear in various physical problem settings [13, 38–48]. The presented methods exploit different representations and optimization schemes to reduce the computational costs. The pseudosite method (PS-DMRG) unfolds the large local Hilbert space into additional sites using a compact binary encoding of the local degrees of freedom. Efficiently representing large local Hilbert spaces by means of the local basis optimization (DMRG3S+LBO) directly operates on the physical degrees of freedom. These are rotated into an optimal basis in which the 1RDM is diagonal and can be truncated faithfully. The recently developed projected purification (PP-2DMRG) interpolates between both approaches in the sense that the system is extended by pairing up each lattice site with a bath site, and truncated according to the diagonal elements of the 1RDM. Being conceptually very different, it is not immediately clear which method is best suited for a given problem setting. For that reason, we applied these methods to the Holstein model at half filling, which is a prototypical system featuring Einstein phonons with large local Hilbert spaces and broken $U(1)$-symmetries. We performed two different common numerical analyses: a high-precision scaling analysis of the model’s ground-state energy as a function of the maximally allowed bond dimension at an intermediate system size ($L = 51$ sites) as well as finite-size extrapolations for intensive quantities such as the CDW order parameter in the ground state up to systems with $L = 201$ sites. Our comparisons demonstrate that, in general, all methods characterize the different phases with high numerical precision and allow for an extrapolation of observables towards the thermodynamic limit.

Analyzing the different methods in more detail, we also identify situations in which it can be beneficial to use a particular method. For instance, in the case of broadly distributed phonon-excitation probabilities, the DMRG3S+LBO and PP-2DMRG methods benefit from their capability of truncations on the phononic degrees of freedom. Here, in particular, the DMRG3S+LBO method achieves very compact representations with the smallest bond dimensions found in our calculations (figures 12 to 14). This comes at the cost of a larger amount of numerical control parameters such as the number of phonons per lattice site in combination with the amount of optimal modes kept, or the mixing factor used in the ground-state search. As discussed in section 2.3.3, using improper configurations can produce a strong dependency on the initial state, which becomes particularly important in the CDW phase, where heavy polarons slow down the overall convergence of the ground-state search. In these situations, the 2-site solvers used in the PS-DMRG and PP-2DMRG methods together with the fact that the only relevant control parameter is the maximum bond dimension seem to be easier to control. Finally, it should be pointed out that PP-2DMRG is capable of exploiting restored global $U(1)$ symmetries, which reduces computational costs associated with the local degrees of freedom. Therefore, even though larger maximal bond dimensions are required to achieve the same numerical precision as the PS-DMRG and DMRG3S+LBO methods, this is compensated by the more efficient representation of matrix-product states and operators as can be seen in figures 12 and 14 where the most accurate ground-state approximations are found by PP-2DMRG. However, since the maximally allowed bond dimension is limited to $m_{\text{max}} \leq 2000$ in our calculations, close to the phase boundary, the more compact representation of DMRG3S+LBO yields the best approximation (see figure 13).

Another important aspect is the question of the applicability of the described methods to study out-of-equilibrium setups. The DMRG-LBO already proved its capability to simulate the dynamics of systems with small fermion densities coupled to lattice phonons [26, 82], global quenches [27, 30] and also finite-temperature simulations [81] by using a Trotter decomposition of the time-evolution operator. A very natural, further development would be to employ time-evolution schemes such as the time-dependent variational principle (TDVP) [83, 84] or the $W^{1}$-representation [85] for time-evolution allowing the efficient
treatment of long-ranged interactions and larger time-steps (TDVP). From our previous discussion, we expect the DMRG-LBO as well as the projected purification to be well-suited for an adoption of TDVP as the time-evolution scheme (see [86] for developments to combine LBO with TDVP), while due to the continuously required basis transformations of the Hamiltonian, the W method seems to be more suitable for the projected purification.

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