When do conservation laws improve the efficiency of the Density Matrix Renormalization Group?

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We explore matrix product state approximations to wavefunctions which have spontaneously broken symmetries, or are critical. We are motivated by the fact that symmetries, and their associated conservation laws, lead to block-sparse matrix product states, which often can be used to speed-up numerical calculations. For the symmetry broken and critical phases studied here, we find that block-sparse matrix product states are less efficient than dense states that explicitly break the underlying symmetry.

I. INTRODUCTION

Our most powerful numerical techniques for studying one dimensional quantum systems, such as the Density Matrix Renormalization Group (DMRG) or its time-dependent generalizations [1, 2], are based upon a systematic truncation of the entanglement between neighboring regions of space. Within these approaches, the quantum mechanical wavefunction has the structure of a matrix product state (MPS): The amplitude of any quantum mechanical wavefunction has the structure of a larger matrices to achieve the same accuracy. Finding an MPS which respects the symmetry requires a larger matrices to achieve the same accuracy.

According to Noether’s theorem, symmetries are closely related to conservation laws [3, 4]. As a relevant example, consider a Hamiltonian that is invariant under the transformation

\[ \hat{H} \rightarrow \hat{U} \hat{H} \hat{U}^\dagger, \]

where \( \hat{U}(\theta) = e^{i\theta \hat{N}} \) and \( \hat{N} \) is the total particle number operator. Equation (1) defines a continuous U(1) symmetry, parameterized by \( \theta \). This can only be true if \( [\hat{H}, \hat{N}] = 0 \), which is the formal quantum-mechanical statement that \( \hat{N} \) is conserved. Consequently, we can find simultaneous eigenstates of \( \hat{H} \) and \( \hat{N} \).

One of the most profound features of many-body physics is that, in the thermodynamic limit, the symmetry may be spontaneously broken [5]: An infinitesimal symmetry breaking field leads to a ground state which is neither invariant under the symmetry operation, nor is it an eigenstate of the conserved charge. A relevant example is a Bose-Einstein condensate, which chooses a particular phase and contains an indefinite number of particles. Spontaneous symmetry breaking is always associated with a ground degeneracy, and one can restore the symmetry by taking an appropriate quantum superposition of the degenerate ground states. In the case of a discrete symmetry, such symmetry-restored states are “Schrodinger cats.”

In Sec. III A we study the transverse-field Ising model, which possesses a discrete \( \mathbb{Z}_2 \) symmetry. It has two zero-temperature phases: a paramagnetic phase, in which the ground state respects the symmetry; and a ferromagnetic phase, which breaks it. In both phases one can use a symmetry-preserving MPS to describe the ground state. In the ferromagnetic phase, however, the resulting MPS corresponds to the aforementioned Schrodinger cat, which is a superposition of the two symmetry-broken solutions. These symmetry-broken constituents are less entangled than the symmetry-preserving Schrodinger cat, and hence are more efficient to express as a MPS. Aspects of this behavior are known by the community, but rarely discussed in the literature.

The situation is far more complicated for continuous symmetries. One-dimensional systems with short-ranged interactions cannot break a continuous symmetry [6, 7]. Instead, strong quantum fluctuations lead to correlation functions which fall off as a power-law [8]. It is far from obvious if they are better described by an MPS that respects the symmetry, or one that explicitly breaks it. We consider two examples: The Bose-Hubbard model and the Fermi-Hubbard model. In both cases we find that for fixed bond dimension (i.e. the linear size of the MPS matrices) a symmetry-broken MPS is a better variational wavefunction than one which obeys the symmetry. For the Fermi-Hubbard case the improvement is fairly modest, while for the Bose-Hubbard case it is quite substantial. We show that the key difference is the scaling of density fluctuations, which is characterized by the Lut-
tunger parameter $K$. We quantify this relationship.

In Section II we review how Abelian symmetries lead to block-sparse MPS tensors. In Sec. III we present our results for the transverse-field Ising model (Sec. III A), the Bose-Hubbard model (Sec. III B), and the Fermi-Hubbard model (Sec. III C). In Sec. IV we present a more general interpretation of the results in Secs. III B and III C in terms of the Luttinger parameter. We conclude in Sec. V.

II. CONSERVATION LAWS IN MPS

An MPS incorporates conservation laws by placing restrictions on which matrix elements can be non-zero. This sparse structure can be exploited to dramatically speed up tensor contractions. For the purpose of this paper, we will only consider Abelian symmetries generated by a global operator $Q = \sum_i Q_i$ that commutes with the Hamiltonian: $[\hat{H}, Q] = 0$. Here $Q_i$ are a set of mutually-commuting single-site operators, where $i$ indexes the sites of the MPS in real space — for concreteness, one can envision $Q = N$, as in Eq. (1), and take $Q_i = N_i$ to be the number of particles on site $i$.

We consider a matrix product state wavefunction on $L$ sites. The MPS ansatz can be schematically written as $|\psi\rangle = \prod_s A^s_1 A^s_2 \cdots A^s_L |\sigma_1 \sigma_2 \cdots \sigma_L\rangle$, where $A^s_i$ corresponds to a matrix with elements $\langle A_i | \sigma_i \rangle \sigma_j |s_i\rangle$. The sum is taken over all $\sigma_1, \sigma_2, \cdots \sigma_L$, where $\sigma_i$ corresponds to the allowed states on site $i$, and over shared indices $s_i$ between adjacent matrices. Here $s_i - 1$ and $s_i$ are the left and right MPS bond indices. The bond dimension $\chi$ is the number of different possible values of $s$. In order to make use of the conservation law we write the local Hilbert space in the eigenbasis of the local operator $Q$, and define a function $q(\sigma_i)$ which associates a charge with each possible value of the bond indices. The conservation law is imposed by requiring that the only non-zero elements of $A_i$ obey

$$q(s_{i-1}) + q(\sigma_i) - q(s_i) = 0.$$  \hspace{1cm} (2)

In the case of number conservation, one can interpret $q(s_{i-1})$ as the number of particles to the left of site $i$, and $q(s_i)$ as the number of particles to the left of site $i + 1$. In finite chains, it is convenient to define $q(\sigma_i)$ as the deviation of the quantum number from its average so that the charges of the bond indices are more readily truncated.

As should be clear, the block-sparse condition in Eq. (2) greatly reduces the number of matrix elements which need to be stored, and speeds up all matrix operations. Its limitations, however, are illustrated by considering a simple Gutzwiller mean-field wavefunction: $|\Psi\rangle = \prod_{i=1}^L \otimes (a|0\rangle_i + b|1\rangle_i)$, which represents a Bose-Einstein condensate in which each site contains the superposition of 0 and 1 particle. This is a MPS with bond dimension $\chi = 1$, but it does not obey Eq. (2). One can rewrite it using the conservation laws, but that comes at the cost of greatly increasing $\chi$. For a chain of length $L$, for example, one needs $\chi = L$, and the MPS matrices can take the form

$$A_i = \begin{pmatrix} a|0\rangle_i & b|1\rangle_i \\ a|0\rangle_i & b|1\rangle_i \\ \vdots & \vdots \end{pmatrix}.$$  \hspace{1cm} (3)

The rows correspond to configurations where there are 0, 1, 2, $\cdots$ particles to the left of this site. The bond index increments whenever a site is occupied.

III. RESULTS

We characterize the distinction between a quantum-number-conserving (sparse) MPS and a non-conserving (dense) MPS by running iDMRG simulations on a few well-known models. We begin by discussing the transverse-field Ising model in Sec. III A, which exhibits discrete spontaneous symmetry breaking. In this particular model, we show how one can explicitly construct the dense MPS out of the sparse MPS (and vice versa). We then move to examples of Luttinger liquids, namely the Bose-Hubbard (Sec. III B) and Fermi-Hubbard (Sec. III C) models. These are more complicated systems that do not explicitly break any symmetries, so they necessitate more detailed numerical comparisons. We make use of the ITensor library for an efficient implementation of quantum number conservation [9]. Further details of the numerical simulations are discussed in Appendix A.

A. Transverse-field Ising model

The one-dimensional transverse-field Ising model is an exactly-solvable model of $s = 1/2$ spins on a lattice with nearest-neighbor interactions. The Hamiltonian is given by

$$\hat{H}_{\text{TFI}} = -J \sum_j (\sigma^x_j \sigma^x_{j+1} + \alpha \sigma^z_j)$$  \hspace{1cm} (4)

where $\sigma^\beta_j$ is the Pauli spin matrix ($\beta = x, y, z$) acting on the spin on site $j$. The ratio of the transverse field strength to the nearest-neighbor interaction strength, $\alpha$, is the only non-trivial parameter in the ground state phase diagram (here we consider the ferromagnetic model: $J, \alpha > 0$). While $\hat{H}_{\text{TFI}}$ does not conserve total magnetization, it has a global $Z_2$ symmetry, $[\hat{H}_{\text{TFI}}, \hat{P}] = 0$, where the parity operator, $\hat{P} = \prod_j \sigma^z_j = \exp(i\pi \sum_j (\sigma^z_j - 1)/2)$, rotates all spins about the $\hat{z}$ axis by $\pi$. This parity symmetry implies that the magnetization along the $\hat{z}$ direction is conserved modulo 2.
The transverse-field Ising model has two zero-temperature phases. When $\alpha > 1$, the $\sigma^z$ term dominates and spins tend to align with the transverse field. This phase is even under parity transformations: $P|\psi_{\alpha>1}\rangle = |\psi_{\alpha>1}\rangle$. When $\alpha < 1$, the exchange term dominates and spins will tend to align with one another in the $\pm \hat x$ direction. In the thermodynamic limit, an infinitesimal field in the $\hat x$ direction will result in a ground state $|+\rangle$ with a finite magnetization in the $\hat x$ direction. This is an example of spontaneous symmetry breaking: The state $|-\rangle = P|+\rangle$ is orthogonal to $|+\rangle$ and has a magnetization in the $-\hat x$ direction. Two parity-conserving ground states can be formed by taking $|+\rangle \pm |-\rangle$. In the limit $\alpha \to 0$, parity-conserving ground states are given by GHZ states $|1\rangle$,

$$\frac{1}{\sqrt{2}} (|\rightarrow\rightarrow\rightarrow\ldots\rangle \pm |\leftarrow\leftarrow\leftarrow\ldots\rangle),$$

where $|\rightarrow\rangle_j$ denotes a spin on site $j$ oriented in the $\hat x$ direction.

We use the infinite DMRG algorithm (iDMRG) to find the ground state of Eq. (4) as a function of $\alpha$. We separately run the algorithm with and without enforcing parity conservation, using appropriate initial conditions. In Fig. 1(a) we plot the resulting entanglement entropy across a bipartition of the infinite chain. Filled red dots denote the behavior of the parity-conserving MPS, while open blue circles show the non-parity-conserving results. For $\alpha > 1$ the ansatze converge to the same state, which has zero entanglement entropy as $\alpha \to \infty$. This parent state is simply a product state with all spins oriented in the $\hat z$ direction. The entanglement entropy diverges at the critical point, $\alpha = 1$. For $\alpha < 1$, the two simulations converge to distinct, degenerate ground states. As shown by the arrows, the parity-conserving ansatz has exactly ln(2) more entanglement entropy at every point with $\alpha < 1$. This relationship is expected when the parity-conserved state is a simple superposition of the two symmetry-broken ground states.

We investigate this correspondence more closely in Figs. 1(b) and (c), where we plot the spectrum of singular values, $\lambda_i$, at representative points in both phases: $\lambda_i^2$ are the eigenvalues of the reduced density matrix when one traces over half the chain. Figure 1(b) shows the spectrum at a representative point in the symmetry broken phase. The spectrum is effectively doubled by conserving parity – each blue singular value matches up with exactly two red singular values in each degenerate plateau. This is precisely what one would expect by taking a superposition of symmetry-broken states. Note that the slight offset between corresponding blue and red plateaus is due to the normalization condition, $\sum_i \lambda_i^2 = 1$, and the fact that the parity-conserving ansatz has twice as many singular values. By contrast, Fig. 1(c) shows that the singular values of both states match up perfectly when $\alpha > 1$.

A consequence of this spectral doubling is that the symmetry-preserving MPS in the symmetry-broken phase needs twice the bond dimension to yield the same accuracy as the wavefunction which explicitly breaks the symmetry. The MPS tensors therefore contain four times as many matrix elements – only half of which are eliminated by the block-sparseness condition in Eq. (2). Thus, instead of making the calculation more efficient, enforcing parity conservation requires storing twice as many matrix elements. On the paramagnetic side of the transition, the situation reverses, and the parity-conserving ansatz requires half as many elements.

The transverse field Ising model is simple, and the algorithmic costs/benefits here are small. Nonetheless, it provides a clear illustration of how spontaneous symmetry breaking interacts with conservation laws in DMRG.
B. Bose-Hubbard model

The Bose-Hubbard model is a paradigmatic strongly-interacting model of lattice bosons. In one dimension (1D) the Hamiltonian is

\[ \mathcal{H}_{\text{BH}} = -t \sum_j (a_j^\dagger a_{j+1} + h.c.) + U \sum_j n_j n_j \]  

where \( a_j^{(1)} \) is a bosonic annihilation (creation) operator on site \( j \) of a lattice, and \( n_j = a_j^\dagger a_j \) is the number operator. We focus on the superfluid phase, which in 1D is a critical phase described by Tomonaga-Luttinger liquid theory [8, 11–13]. Unlike a Bose-Einstein condensate, it does not spontaneously break U(1) gauge invariance. There is, however, quasi-long range order corresponding to a power law decay of the single particle density matrix. In contrast to the phases in Sec. III A, it is not \textit{a priori} obvious whether this superfluid phase would be better described by a variational wavefunction that breaks or conserves particle-number conservation.

The most interesting part of the phase diagram is near the BKT transition at the tip of the Mott lobe. Thus we focus on the point \( U/t = 3 \) with an average of \( \bar{n} = 1 \) particles per site. We use the standard iDMRG algorithm. For our particle-number-conserving simulations, fixing the average density is trivial, while in our unrestricted simulations we add an extra step in each iteration which corrects the chemical potential, \( \mu \). This procedure is described in Appendix A 2. As described in Ref. [13], this gapless, critical phase is best analyzed using “finite entanglement scaling,” meaning that one understands the properties of the state by considering a sequence of bond dimensions, \( \chi \).

Our results are summarized in Fig. 2. In the main panel we plot the density matrix \( \langle a_i^\dagger a_j \rangle \) as a function of spatial separation \( |i - j| \). For the number-conserving ansatz, the correlation function falls off exponentially at sufficiently long distances. For the dense ansatz, the correlation function instead approaches a constant. This constant corresponds to a Bose-Einstein condensate, indicating that the finite-bond dimension approximation spontaneously breaks the symmetry even though exact ground state is critical. One typically refers to this phenomenon as “quasicondensation,” which we discuss at greater length in Sec. IV. The dashed black line shows the asymptotic power-law scaling of the density matrix,

\[ \langle a_i^\dagger a_j \rangle \propto |i - j|^{-\kappa/2}, \tag{7} \]

where we used a scaling analysis to find the Luttinger parameter \( \kappa \) (see Appendix B). The dense MPS better captures the correlations: while both curves eventually bend away from the dashed line, the dense MPS curves show approximate power-law decay out to distances almost an order of magnitude larger than those of the sparse MPS.

The inset of Fig. 2 shows the variational energy of the dense and sparse ansatze as a function of bond dimension on a log-log scale. The dense MPS has a substantially lower energy at each bond dimension, while both curves exhibit power-law scaling of the form

\[ E(\chi) = E_0 + A/\chi^{2\kappa} + \ldots \quad A > 0, \tag{8} \]

As argued in Ref. [14], one expects that \( \kappa = 6/(c + \sqrt{12c}) \) for an MPS approximation of a conformal critical point with central charge \( c \). The low-energy description of the Bose-Hubbard model takes the form of a single-component Luttinger liquid, which is a conformal field theory with \( c = 1 \). This theoretical prediction is given by the shaded gray line in the inset, clearly showing that the data is in close agreement with Eq. (8). The dense ansatz is roughly an order of magnitude more accurate for the same bond dimension.

In contrast to the energy, the correlation length behaves counterintuitively. We define

\[ \xi^2 = \frac{\sum_j j^2 \left( \langle a_j^a \rangle - \langle a_j^b \rangle \right)^2}{\sum_j \langle a_j^a \rangle^2} \]

which is the characteristic length-scale of the fluctua-
tions. Despite the fact that the number non-conserving ansatz yields a density matrix which is closer to the exact result (which has an infinite correlation length), its correlation length is shorter. This unexpected result is a consequence of subtracting off the constant term in Eq. (9).

In addition to the U(1) symmetry described here, at the BKT point the Bose-Hubbard model exhibits an emergent $\mathbb{Z}_2$ particle-hole symmetry. As the number-conserving ansatz encodes particle and hole fluctuations with different singular values, this implies that near the BKT point many of its singular values will have nearly-degenerate partners. Similar degeneracies have been used to detect forms of order $[15–17]$. They also indicate that the ansatz contains redundant information. These degeneracies do not show up in the singular values for the non-conserving ansatz.

C. Fermi-Hubbard model

The 1D Fermi-Hubbard model describes spin-1/2 lattice fermions with on-site interactions and Hamiltonian

$$\mathcal{H}_{\text{FH}} = -t \sum_{j,\sigma} (c_{j,\sigma}^\dagger c_{j+1,\sigma} + h.c.) + U \sum_j n_{j,\uparrow} n_{j,\downarrow}. \quad (10)$$

Here $c_{j,\sigma}^{(1)}$ is a fermionic annihilation (creation) operator for a particle with spin $\sigma$ on site $j$ and $n_{j,\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma}$ is the number operator. Like the 1D Bose-Hubbard model, the ground state of the 1D Fermi-Hubbard model is either a Mott insulator or a Luttinger liquid. We will again focus on the latter phase. This model is exactly solvable via the Bethe ansatz $[18, 19]$.

At half filling (one particle per site) this model is in the Mott insulator phase for any $U/t > 0$. Thus we work at quarter filling and zero net magnetization, $\bar{n}_\uparrow = \bar{n}_\downarrow = 1/4$. Our block-sparse simulations conserve both the total particle number and the total magnetization. Number-conserving simulations at a fractional filling $p/q$, where $p$ and $q$ are integers, requires a unit cell of length $qm$ sites where $m \in \mathbb{Z}^+$ $[20]$. The dense MPS simulations have no restriction on the allowed unit cell size. For the purpose of providing a reliable comparison between methods, we perform both the number-conserving and non-number-conserving simulations with a unit cell of 4 sites. A good discussion of multi-site iDMRG can be found in Ref. $[21]$.

Figure 3(a) shows the momentum distribution function for up spins, $\langle n_{k,\uparrow} \rangle$, in the vicinity of $k_F = \pi/4$. Both data sets show a step at $k_F$ that grows increasingly sharp with bond dimension. Note that on this scale the distribution never goes to 0 or 1. The step height is somewhat analogous to the Fermi liquid quasiparticle weight $Z$. As $\chi \to \infty$ the distribution function near $k = k_F$ should approach $[8]$

$$\langle n_{k,\sigma} \rangle \approx \frac{1}{2} - \text{sign}(k - k_F)|k - k_F|^\alpha. \quad (11)$$

where the exponent in the power-law singularity depends on the Luttinger parameter for charge degrees of freedom, $K_p$:

$$\alpha = (K_p + 1/K_p - 2)/4. \quad (12)$$

For $U/t = 4$ and $\bar{n}_\uparrow = \bar{n}_\downarrow = 1/4$ the Bethe ansatz solution gives $K_p \approx 1.4$ $[19]$.

At $k = k_F$, the derivative $\frac{\partial \langle n_{k,\uparrow} \rangle}{\partial k}$ in Eq. (11) diverges. At finite $\chi$, this singularity is cut off and one instead expects $\frac{\partial \langle n_{k,\uparrow} \rangle}{\partial k} \sim \chi^{\kappa(1-\alpha)}$ where $\kappa = 3/(1 + \sqrt{6})$ is the conformal scaling exponent corresponding to a central charge $c = 2$ $[14]$. The width of the deviation from Eq. (11) scales as $\delta q \propto \chi^{-\kappa}$. Figure 3(b) demonstrates the resulting scaling collapse: For a given ansatz, all of the curves from panel (a) lie on top of one-another. We use the theoretical values of $\kappa$ and $K_p$, without any
free parameters.

Strikingly, in Fig. 3(b), the dense and sparse MPS exhibit two distinct scaling collapses, the former notably sharper than the latter. Thus, while both data sets exhibit the expected conformal scaling, the dense MPS yields wavefunctions with a sharper singularity at \( k_F \). These two scaling collapses can be made to line up with one another by rescaling the bond dimension by a factor of 1.8.

In Fig. 3(c) we plot the variational energy as a function of the bond dimension on a log-log scale. We again find that the energy obtained by the dense MPS is lower than that of the sparse MPS. Fixing the bond dimension, the ratio of the errors in the energy for the two ansatze is roughly 1.5. The shaded gray line denotes the scaling behavior in Eq. (8), which is clearly consistent with both data sets.

\[ \text{EQ. (8)} \]

\[ \Gamma = \frac{A_{\text{QN}}}{A_{\text{dense}}} \]

\[ \text{versus the Luttinger parameter. Blue, orange and green data correspond to the Bose-Hubbard model at particle densities } \bar{n} = 1, 1/2, \text{ and } 1/4, \text{ respectively. Strikingly, these data lie on a single scaling function, independent of the microscopic parameters. The function exhibits a power-law divergence as } K \to 0, \text{ where the ground state is proximate to a Bose-Einstein condensate, while it should approach 1 as } K \to \infty. \]

This therefore corresponds to a topological order in the fermionic system, which is revealed via a string correlation function. There is no obvious way to experimentally measure this topological quasi-order.

Comparing the inset of Fig. 2 with Fig. 3(c), it is clear that the advantage gained from breaking the symmetry is larger for the bosons than for the fermions. As noted in Eq. (8), the leading deviation of the variational energy is \( \delta E = A_{\chi} \chi^{-2\kappa} \). Here \( A \) is smaller for the dense ansatz, and the improvement in accuracy from using the dense ansatz is quantified by the dimensionless ratio \( \Gamma = A_{\text{QN}}/A_{\text{dense}} \). To achieve a fixed error in the energy, the number-conserving ansatz requires a bond dimension which is \( \Gamma^{1/2\kappa} \) times larger than the dense ansatz. In our bosonic example (Sec. III B), \( \Gamma = 6.7 \), while in the fermionic one (Sec. III C), \( \Gamma = 1.5 \).

The reason for this difference is that the fermionic system has much smaller density fluctuations. In the number conserving ansatz, there is a configurational entropy associated with number fluctuations between two halves of the system, requiring a larger bond dimension. The scale of these number fluctuations is set by the Luttinger parameter [23]: A region of size \( L \) will have fluctuations \( \langle (\bar{\hat{N}} - \langle \hat{N} \rangle)^2 \rangle \sim (2\pi^2 K)^{-1} \ln L \). In a MPS of fixed bond dimension, the correlation length \( \xi \) plays the role of \( L \). In our examples \( K_{\text{Fermi}}^{\text{Bose}} = 0.42 \) is much smaller than \( K_{\text{Fermi}}^{\text{Fermi}} = 1.4 \).

In Figure 4 we show how \( \Gamma \) depends on Luttinger parameter for the Bose-Hubbard model at three different fillings: \( \bar{n} = 1, 1/2, \text{ and } 1/4 \). We find that these data
collapse onto a single universal curve which diverges as a power law, \( \Gamma \propto K^{-1.27(2)} \), for small \( K \). The maximum value of \( K \) in the superfluid phase of the Bose-Hubbard model is \( K = 1 \), beyond which the system undergoes a Mott transition. If one were to continue the scaling function out to \( K > 1 \), e.g. with the inclusion of long-range interactions, one would expect the power-law behavior to break down so that \( A_{\text{dense}}/A_{\text{QN}} \to 1 \) as \( K \to \infty \).

The metallic phase of the 1D Fermi-Hubbard model with \( U > 0 \) has distinct Luttinger parameters for spin \((K_s)\) and charge \((K_p)\) degrees of freedom. The spin Luttinger parameter is fixed at \( K_s = 1 \), while the charge Luttinger parameter \( K_p > 1 \). Both spin and density fluctuations are relevant here, so the fermionic results do not collapse onto the bosonic data in Fig. 4.

V. CONCLUSIONS

Conservation laws allow one to write matrix product states in a block-sparse manner (Eq. (2)). It is not, however, always favorable to take advantage of this block-sparse structure. In particular, if the ground state spontaneously breaks the symmetry then the resulting MPS contains redundant information whose only purpose is to impose the constraint.

Critical Luttinger liquid phases act similarly to the symmetry-broken states: they are modeled more efficiently by ignoring the conservation laws. The degree of savings depends on the Luttinger parameter. We emphasize that these Luttinger liquid results are also relevant to quasi-2D calculations, where one performs DMRG in a cylindrical geometry.

Our considerations apply to all tensor network approaches [24, 25]. Efficient numerical calculations require an awareness of the interplay between spontaneous symmetry breaking and conservation laws.

VI. ACKNOWLEDGEMENTS

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Appendix A: iDMRG Details

In our calculations we start with a product state, then implement the iDMRG algorithm with two-site updates to find MPS approximations of the ground state in the thermodynamic limit. Simulations are carried out using the iTensor library [9]. Here we describe several technical details.

1. Truncation Error

For calculations of the transverse-field Ising model in Sec. III A, we increase the bond dimension as necessary until the properties of the state have all converged. We find that it is sufficient to reduce the truncation error \( e_{\text{trc}} \leq 10^{-12} \) to achieve convergence. One can interpret the data in Fig. 1 as numerically exact results.

As for the Bose-Hubbard (Sec. III B) and Fermi-Hubbard (Sec. III C) simulations, “convergence” is no longer a meaningful criterion. The ground states are gapless critical states and the long distance properties of the correlation functions cannot be modeled by matrix product states with fixed bond dimension. As has been argued elsewhere [13, 14], however, features of the asymptotic ground state can be inferred by studying the behavior of variational wavefunctions as a function of the bond dimension. This is known as finite-entanglement scaling. For the data shown in Figs. 2 and 3, we increase the bond dimension from \( \chi = 40 \) to 120 in steps of \( \Delta \chi = 10 \). We find that the truncation error scales as a power law of the bond dimension, \( e_{\text{trc}} \propto \chi^{-2\kappa} \), consistent with the Luttinger liquid scaling observed in other observables [14].

2. Fixing the chemical potential

Throughout this paper, we calculate properties at fixed density. This constraint is simple to incorporate into the sparse number conserving MPS ansatz. For the dense ansatz, one instead has to specify a suitable chemical potential, \( \mu_i \), to fix the density at the desired value.

To achieve our target density, \( \bar{n}^* \), we vary the chemical potential in the early iterations of the dense DMRG algorithm. The update procedure involves approximating the inverse compressibility based on measurements made in subsequent iterations:

\[
\frac{\partial \mu_i}{\partial \bar{n}_i} \approx \frac{\bar{n}_i - \bar{n}_{i-1}}{\bar{n}_i - \bar{n}_{i-1}}
\]

We then define the chemical potential for iteration \( i + 1 \) based on the compressibility computed in iteration \( i \):

\[
\mu_{i+1} = \mu_i + \alpha_i (\bar{n}^* - \bar{n}_i) \frac{\partial \mu_i}{\partial \bar{n}_i}
\]

Here the convergence factor, \( \alpha_i \), controls how large of an update we allow from iteration to iteration. Smaller \( \alpha \) results in a more stable algorithm, but slower convergence. In all our calculations we take \( \alpha_i = 0.1 \).

Appendix B: Scaling Analysis

Here we describe how we use a scaling analysis of the single particle density matrix to extract the Luttinger parameter for the Bose-Hubbard model. We use this analysis in Sec. III B and Sec. IV.
As argued in the main text, the correlation length of the MPS is expected to scale as $\chi^{\kappa}$ where $\kappa = 6/(1 + \sqrt{12})$ [14]. For distances that are smaller than this correlation length, we expect $\langle a_i^\dagger a_j \rangle \propto |i - j|^{-K/2}$. Given a guess for the optimal Luttinger parameter, $K_0$, we rescale:

$$|i - j| \rightarrow |i - j|^{\chi^{-\kappa}},$$

$$\langle a_i^\dagger a_j \rangle \rightarrow \langle a_i^\dagger a_j \rangle^{\chi^{\kappa K_0/2}}.$$

Following a procedure similar to Ref. [13], we then define an objective function which measures the deviation between the scaled density matrices with different values of $\chi$. These should all collapse when $K_0 = K$. We adjust $K_0$ to minimize our objective function.

For the case in Sec. III B, where $\bar{n} = 1$ and $U/t = 3$, we find $K = 0.423(2)$. Note that the value of the Luttinger parameter at the Mott lobe tip is 0.5, so this result is consistent with being on the superfluid side of the Mott-superfluid transition.

This same bond dimension scaling procedure is used to generate the data in Fig. 4.

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