Time evolution of an infinite projected entangled pair state: a neighborhood tensor update

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The simple update (SU) and full update (FU) are the two paradigmatic time evolution algorithms for a tensor network known as the infinite projected entangled pair state (iPEPS). They differ by an error measure that is either, respectively, local or takes into account full infinite tensor environment. In this paper we test an intermediate neighborhood tensor update (NTU) accounting for the nearest neighborhood environment. This small environment can be contracted exactly in a parallelizable way. It provides an error measure that is Hermitian and non-negative down to machine precision. In the 2D quantum Ising model NTU is shown to yield stable unitary time evolution following a sudden quench. It also yields accurate thermal states despite correlation lengths that reach up to 20 lattice sites. The latter simulations were performed with a manifestly Hermitian purification of a thermal state. Both were performed with reduced tensors that do not include physical (and ancilla) indices. This modification naturally leads to two other schemes: a local SVD update (SVDU) and a full tensor update (FTU) being a variant of FU.

I. INTRODUCTION

Weakly entangled states are just a small subset in an exponentially large Hilbert space but they are ubiquitous as stationary ground or thermal states in condensed matter physics. They can be efficiently represented by tensor networks, including the one-dimensional (1D) matrix product state (MPS)3, its two-dimensional (2D) generalization known as a projected entangled pair state (PEPS)4,5, or a multi-scale entanglement renormalization ansatz6–9. The MPS ansatz provides a compact representation of ground states of 1D gapped local Hamiltonians10–11 and purifications of their thermal states12. It is also the ansatz underlying the density matrix renormalization group (DMRG)13–16. Analogously, the 2D PEPS is expected to represent ground states of 2D gapped local Hamiltonians1,2 and their thermal states17,18, though representability of area-law states, in general, was shown to have its limitations19. As a variational ansatz tensor networks do not suffer from the notorious sign problem plaguing the quantum Monte Carlo methods. Consequently, they can deal with fermionic systems20–24, as was shown both for finite25 and infinite PEPS (iPEPS)26,27.

The PEPS was originally proposed as an ansatz for ground states of finite systems28,29, generalizing earlier attempts to construct trial wave-functions for specific models3. The subsequent development of efficient numerical methods for infinite PEPS (iPEPS)30–33, shown in Fig. 1(a), promoted it as one of the methods of choice for strongly correlated systems in 2D. Its power was demonstrated, e.g., by a solution of the long-standing magnetization plateaus problem in the highly frustrated compound SrCu2(BO3)234,35, establishing the striped nature of the ground state of the doped 2D Hubbard model36, and new evidence supporting gapless spin liquid in the kagome Heisenberg antiferromagnet37. Recent developments in iPEPS optimization38–40, contraction41,42, energy extrapolations43, and universality-class estimation44–46, pave the way towards even more complicated problems, including simulation of thermal states47–62, mixed states of open systems63,64, excited states65,66, or real-time evolution55,66–70. In parallel with iPEPS, there is continuous progress in simulating systems on cylinders of finite width using DMRG. This numerically highly stable method that is now routinely used to investigate 2D ground states66,71 was applied also to thermal states on a cylinder72–76. However, the exponential growth of the bond dimension limits the cylinder’s width to a few lattice sites. Among alternative approaches are direct contraction and renormalization of a 3D tensor network representing a 2D thermal density matrix77–84.

This article readdresses the problem of real/imaginary time evolution with iPEPS55. There are two most popular simulation schemes: the simple update (SU) and full update (FU). In both the time evolution proceeds by small time steps, each of them subject to the Suzuki–Trotter decomposition. In both after a Trotter gate is applied to a pair of nearest neighbor (NN) sites a bond dimension of the index between the sites is increased by a factor equal to the rank of the gate. In order to prevent its exponential growth with time the dimension is truncated to a predefined value, D, in a way that minimizes error incurred by the truncation. The two schemes differ by a measure of the error: FU takes into account full infinite tensor environment while SU only the bonds adjacent to the NN sites. The former is expected to perform better in case of long range correlations while the latter is, at least formally, more efficient thanks to its locality. In this paper an intermediate scheme is considered — a neighborhood tensor update (NTU) — where the error measure is induced by the sites that are NN to the Trotter gate. It is shown to compromise the SU accuracy only a little for a price of small numerical overhead over SU, hence it may turn out to be a reasonable trade off for many applications.
The neighborhood tensor update is a special case of a cluster update\textsuperscript{85} where the size of the environment is a variable parameter interpolating between a local update and the infinite FU. In NTU only the neighboring sites are taken into account because they allow the error measure to be calculated exactly with little numerical overhead over SU as it involves only tensor contractions that are fully parallelizable. Its exactness warrants the error measure to be a manifestly Hermitian and non-negative quadratic form. This property is essential for stability of NTU and makes it distinct from FU where an approximate corner transfer matrix renormalization\textsuperscript{2,33} often breaks the Hermiticity and non-negativeness. In case of long range correlations the small environment can, admittedly, make NTU converge with the bond dimension more slowly than FU but this may be compensated by its better numerical efficiency and stability that allow NTU to reach higher bond dimensions.

At a more technical level, unlike in FU but similarly as in Ref. \textsuperscript{86}, we define reduced tensors not before but after application of the Trotter gate. Our reduced tensors do not have any physical (and ancilla) indices. Unlike in Ref. \textsuperscript{86}, we do not introduce any bond tensors in our iPEPS to avoid the necessity of their inversion. This redefinition of the reduced tensors naturally leads to two schemes that are complementary to NTU: a local SVD update (SVDU) and a full tensor update (FTU). The former is more local than SU, as it ignores even the adjacent bonds’ environment, while the latter is a variant of FU with the infinite but approximate environment.

Another technical modification, in case of thermal states represented by their purifications, is to make the purification manifestly Hermitian between physical and ancilla degrees of freedom. The Hermitian purification is an iPEPS in a space of Hermitian operators. An important symmetry is protected thus enhancing stability and in general also numerical efficiency.

This paper is organized as follows. In section II we provide a detailed introduction to SVDU, NTU, and FTU that includes the definition of reduced tensors. In section III the algorithms are applied to unitary real time evolution after a sudden quench of the 2D quantum Ising Hamiltonian. In section IV we describe the manifestly Hermitian thermal state purifications and in section V thermal states of the 2D quantum Ising model are simulated by imaginary time evolution of their purifications. We summarize in section VI.

II. ALGORITHMS

The algorithms considered in this paper are summarized in figures 1, 2, 3, 4, and 5. Figures 1(b,c) show the most basic singular value decomposition update (SVDU) in a schematic form. After a two-site Trotter gate is applied to a pair of nearest neighbor iPEPS tensors, $A$ and $B$, the resulting network in Fig. 1(b) is SV-decomposed into a pair of new tensors $A'$ and $B'$. The dimension of their common bond index is truncated to the original $D$ by keeping only the $D$ largest singular values. Numerical cost of this scheme is $\propto D^6$. Its equivalent but more efficient version is shown in Fig. 2. The cost is cut down to $\propto D^5$ by reduction to smaller matrices $R_{A,B}$ before the SVD truncation. The truncation yields new reduced matrices $M_{A,B}$ that are fused with fixed isometries $Q_{A,B}$ into updated iPEPS tensors $A'$ and $B'$.

The SVDU minimizes the Frobenius norm of the difference between diagrams in Figs. 2(b) and (d). For this norm all directions in the $(Dr)^2$-dimensional space are equally important. Thus, though formally cheap, the SVDU does not make optimal use of the available bond dimension $D$ which is wasted to preserve accuracy in all directions including those that are not important from the perspective of the infinite tensor environment of the two sites. Even zero modes, that are not important at all, instead of being truncated are preserved as accurately as the dominant directions. On the positive side, the SVDU is inverse free.
FIG. 2. Efficient SVDU and beyond. In (a) the Suzuki-Trotter gate $G$ is applied to physical indices of NN tensors $A$ and $B$ as in Fig. 1(b). Here the 2-site gate is replaced by two tensors, $G_A$ and $G_B$, contracted by an index with dimension $r$. In (b) the tensor contraction $A \cdot G_A$ is QR-decomposed into $Q_AR_A$. Similarly $B \cdot G_B = Q_BR_B$. Isometries $Q_{A,B}$ will remain fixed. In (c) after SVD, $R_AR_A^T = U_ASU_T^B$, $S$ is truncated to $D$ leading singular values. In (d) matrices $M_A = U_AS^{1/2}$ and $M_B = S^{1/2}U_B^T$ are made by absorbing square root of truncated $S$ symmetrically. In (e) in SVDU new iPEPS tensors are obtained as $A' = Q_AG_A$ and $B' = Q_BG_B$ ending the story. A step beyond SVDU, whose cost is still $\propto D^5$, is the simple update (SU). In this scheme the iPEPS ansatz in Fig. 1(a) is generalized by inserting its bonds with diagonal bond tensors $\lambda_i$, where $i$ is numbering four inequivalent bonds on the checkerboard lattice. The Frobenius norm is replaced by a metric

$$g_{SU} = 1_d \otimes 1_d \otimes \prod_j \lambda_j,$$

where $j$ runs over the six bonds stemming out from the considered pair of NN sites. These bonds are the nearest tensor environment providing the nontrivial metric tensor that assigns different weights to different directions. SU can afford the same bond dimension as SVDU but, in principle, can make better use of it. A potential caveat is inversion of the bond tensors: $\lambda_i \rightarrow \lambda_i^{-1}$ that has to be done after every gate.

In this paper we advocate a step beyond the SU where a cluster of nearest neighbor (NN) tensors, shown in Fig. 4(b), is the environment providing the metric. This NN cluster can be contracted exactly, as outlined in Fig. 4, to yield metric $g$ that is Hermitian and non-negative within machine precision. The cost of optimal contraction is $\propto D^8$ but, as it involves only matrix multiplication, can be fully parallelized. The key advantage of the metric in Fig. 4(e) over the local SVDU/SU are the two NN bonds, parallel to the considered one, that connect the left and right side of the environment. They are essential to prevent virtual loop entanglement from being build into the iPEPS and parasite its bond dimension. We call the scheme a neighborhood tensor update (NTU) to distinguish it from a full tensor update (FTU), where the infinite environment in Fig. 4(a) provides the metric tensor.

This infinite environment is the same as in the popular full update (FU) scheme. FU and FTU differ in the way the iPEPS tensors are decomposed into isometries $Q_{A,B}$ and reduced tensors/matrices $R_{A,B}$. In this paper both schemes serve mainly as a benchmark. Their infinite environment takes into account long range correlations but calculation of the metric tensor $g$ requires an expensive corner transfer matrix renormalization group (CTMRG) whose approximate character makes it difficult to keep

FIG. 3. Full/neighborhood tensor update. In FTU the truncated diagram in Fig. 2(d) is inserted in place of the two missing tensors in the middle of the infinite PEPS in (a). In NTU the same truncated diagram is inserted into a finite fragment of the iPEPS in (b). In FTU/NTU the tensor network obtained after the truncated insertion is compared with a similar network (a)/(b) but inserted with the exact diagram in Fig. 2(b). In both schemes truncated matrices $M_A$ and $M_B$ are optimized to minimize norm of the difference between the two networks: the one with the truncated insertion and the other with the exact one.
FIG. 4. **NTU.** Norm squared of the matrix product, $||M_A M_B^T||^2$, is shown in (e). Here $g$ is a metric tensor obtained in (d). The upper/lower free indices in diagram (d) correspond to the upper/lower indices of $g$ in (e). Diagram (d) is obtained by inserting the two empty central sites in Fig. 3(b) with isometries $Q_A$ and $Q_B$ and then contracting the inserted (ket) network with its complex conjugate (bra) through pairs of their corresponding indices, except for the bond indices stemming from the two isometries along the considered bond. This is done in steps (a,b,c,d). In (a) double iPEPS tensors are defined. Edge double tensors are obtained by contracting pairs of corresponding external bra and ket indices, as exemplified in (b). In (c) double isometries are defined. The double isometries and edge tensors are assembled in (d). Cost of their contractions can be optimized to scale like $D^8$.

the metric tensor Hermitian and non-negative. In NTU

the CTMRG is used only for calculation of expectation values which can be done less frequently and may require less precision than the Trotter gates.

With metric tensor $g$ matrices $M_A$ and $M_B$ are optimized in order to minimize the norm squared of the difference between the two diagrams in Fig. 5(a), where $R_A R_B^T$ is the exact (untruncated) product in Fig. 2(b).
Sudden quench. Unitary evolution of the transverse magnetization $\langle \sigma^x \rangle$ after a sudden quench from a fully polarized state. We show three bunches of curves corresponding to evolution with (from top to bottom) $h_x = 2h_c, h_c, h_c/10$. Each curve is terminated when the energy per site deviates by 0.01 from the initial value. The squares are data from FU simulations. They extend up to the time where they appear converged in $D$ for $D = 8$ (for $h_x = 2h_c, h_c$) or up to $t = \pi/2$ where they were terminated (for $h_x = h_c/10$). Here we use the same time step, $dt = 0.01$, as for the FU, the same second order Suzuki-Trotter scheme and environmental bond dimension: $\chi = 4D$.

The error is measured with respect to the metric in Fig. 4(d,e):

$$\varepsilon = [M_AM_B^T - R_AR_B^T]^T g [M_AM_B^T - R_AR_B^T].$$

For a fixed $M_B$ it becomes a quadratic form in $M_A$:

$$\varepsilon = M_A^T g_A M_A - M_A^T J_A M_A + \varepsilon_A,$$

where $g_A$, $J_A$, and $\varepsilon_A$ depend on the fixed $M_B$, see Fig. 5(b) and (c). The matrix is optimized as

$$M_A = \text{pinv} (g_A) J_A,$$

where tolerance of the pseudo-inverse can be dynamically adjusted to minimize $\varepsilon$. Thanks to the exactness of $g$ in NTU, the optimal tolerance is usually close to machine precision. This optimization of $M_A$ is followed by a similar optimization of $M_B$. The optimizations are repeated in a loop,

$$\rightarrow M_A \rightarrow M_B \rightarrow,$$

until convergence of $\varepsilon$. Except for SVD of small matrices, $R_AR_B^T$ and $M_AM_B^T$, NTU is fully parallelizable.

III. UNITARY EVOLUTION AFTER A SUDDEN QUENCH

To begin with we consider a sudden quench in the transverse field quantum Ising model on an infinite square lattice:

$$H_{QI} = - \sum_{\langle j,j' \rangle} \sigma^z_j \sigma^z_{j'} - \sum_j h_x \sigma^x_j.$$  (6)

At zero temperature the model has a ferromagnetic phase with non-zero spontaneous magnetization $\langle \sigma^z \rangle$ for magnitude of the transverse field, $|h_x|$, below a quantum critical point located at $h_c = 3.04438(2)$.

Here we simulate unitary evolution after a sudden quench at time $t = 0$ from infinite transverse field down to a finite $h_x$. After $t = 0$ the fully polarized ground state of the initial Hamiltonian is evolved by the final Hamiltonian with $h_x = 2h_c, h_c, h_c/10$. The same quenches were simulated with FU and neural quantum states. Our present results obtained with SVDU, NTU, and FTU are shown in Fig. 6. As a benchmark we also show the FU results with $D = 8$ up to times where they appear converged with this bond dimension.

The evolution with the weakest $h_x = h_c/10$ remains weakly entangled for a long time and can be extended to long simulation times by any iPEPS method. This is not surprising given that for $h_x = 0$, when the Hamiltonian is classical, exact evolution can be represented with mere $D = 2$. All the considered simulation schemes reproduce the exact $D = 2$ evolution for $h_x = 0$. The quenches to $h_x = 2h_c, h_c$ are more challenging as they create a lot of entanglement.

We show SVDU, NTU, and FTU results with, respectively, $D = 12, 12, 8$. These bond dimensions require similar simulation time as FU with $D = 8$. All simulations,
IV. SIMULATION OF THERMAL STATES

In a series of tautologies a thermal state, \( \rho(\beta) \equiv e^{-\beta H} \), can be written as \( \rho(\beta) = \rho(\beta/2) \rho(\beta/2) \), where

\[
\rho(\beta/2) = e^{-\beta H/4} \rho(0/2) \left( e^{-\beta H/4} \right)^\dagger. \tag{7}
\]

We represent this \( \rho(\beta/2) \) as an iPEPO and the evolution operator is a product of small time steps,

\[
e^{-\beta H/4} = \prod_{i=1}^{N} e^{-d \beta H/4}. \tag{8}
\]

A small time step for the iPEPO is

\[
\rho((\beta + d \beta)/2) = e^{-d \beta H/4} \rho(\beta/2) \left( e^{-d \beta H/4} \right)^\dagger \tag{9},
\]

where \( e^{-d \beta H/4} \) is approximated by a Suzuki-Trotter decomposition into a product of Trotter gates. \( \rho((\beta + d \beta)/2) \) would be manifestly Hermitian if it were not necessary to truncate the bond dimension after each Trotter gate.

In order to preserve the Hermitian symmetry in Fig. 8 we introduce a manifestly Hermitian parametrization of the iPEPO. In effect, the iPEPO \( \rho \) is represented by an iPEPS \( \tilde{\rho} \) made of real tensors. In addition to manifestly preserving the symmetry, that may improve numerical stability, this real parametrization should speed up floating number computations by a factor of 4.

In the next section we test the algorithm in the 2D quantum Ising model, where the non-trivial nearest-neighbor 2-site Trotter gate is

\[
e^{d \beta \sigma^z \sigma^z/4} \equiv 1_j 1_{j'} + \tanh(d \beta/4) \sigma^z_j \sigma^z_{j'} \equiv G. \tag{10}
\]

Under its action the basis operators \( O^a_j O^b_{j'} \), defined in Fig. 8, transform as

\[
G O^a_j O^b_{j'} G^\dagger = \sum_{a'b'} G_{a'b'}^{ab} O^{a'}_{j} O^{b'}_{j'}. \tag{11}
\]

Therefore, the action of the gate \( G \) on the iPEPO, \( G \rho G^\dagger \), is equivalent to contracting the iPEPS \( \tilde{\rho} \) with the tensor \( G_{a'b'}^{ab} \). The upper indices of the latter, \( a \) and \( b \), are contracted with the physical indices of the iPEPS on sites \( j \) and \( j' \), respectively, as shown in Fig. 1(b). The SVDU, NTU, and FTU algorithms follow as in section II.

V. 2D QUANTUM ISING MODEL AT FINITE TEMPERATURE

The Hamiltonian of the quantum Ising model with a longitudinal bias on an infinite square lattice is

\[
H = H_{QI} - \sum_j h_z \sigma^z. \tag{12}
\]

Here \( H_{QI} \) is the transverse field quantum Ising model (6) and \( h_z \) is a longitudinal field providing a tiny symmetry-breaking bias that allows for smooth evolution across a
finite-temperature phase transition by converting it into a smooth crossover. For zero longitudinal field and \( h_x < h_c \) the model has a second order phase transition at a finite temperature, \( T_c(h_x) \), belonging to the 2D classical Ising universality class. For \( h_x = 0 \) it becomes the 2D classical Ising model with \( T_c(0) = 2/\ln(1 + \sqrt{2}) \approx 2.27 \).

In all simulations in this section we use \( d\beta = 0.0025 \) and the second order Suzuki-Trotter decomposition. The data are converged in the environmental bond dimension which is set at \( \chi = 40 \). Finally, in all FTU simulations we begin with a short SVDU evolution stage up to \( \beta = 0.1 \). This avoids dealing with zero modes which arise when the bond dimension is too big\(^{52}\).

First we consider \( h_x = 2.9 \) — which is very close to \( h_c = 3.04438(2) \)\(^{87}\) — where the critical temperature is estimated as \( T_c(2.9) \approx 0.6085(8) \)\(^{90}\). Due to strong quantum fluctuations this is almost four times less than the Onsager’s \( T_c(0) \). We generate thermal states across this transition with a bias field \( h_z = 5 \cdot 10^{-4} \) which is one of the weakest biases considered in Ref. \(^{55}\) where the same states were obtained with SU and FU schemes. The SU data\(^{55}\) in Fig. 9 show that under these extreme conditions SU is not able to converge to the converged FU results (with \( D = 5.6 \)) even for the largest considered bond dimension \( D = 14 \). Pushing the simulations beyond \( D = 14 \) becomes more costly than the more accurate FU and thus becomes impractical\(^{55}\).

Figure 10(a) shows new FTU results which are converged for \( D = 5 \) similarly as the old FU. Quite remarkably, as the bond dimension in SVDU is increased from \( D = 3 \) up to a mere \( D = 6 \), which is still very cheap for this local update, the results get closer to the converged FTU results than the SU ones with \( D = 14 \). For \( D = 6 \) a maximal correlation length \( \xi \approx 15 \) is achieved at \( \beta = 1.44 \ldots 1.48 \) which is more than might have been expected from a local update. However, this record is a warning sign that anticipates the following decline in accuracy as the bond dimension is increased further beyond \( D = 6 \). The decline is most visible for \( \beta = 1.44 \ldots 1.48 \) where the record long correlations make
the local update method the most problematic. The same Fig. 10(a) shows results from NTU as they slowly converge for $D = 7, \ldots, 9$. The converged NTU curve slightly differs from the FTU one but much less than the SVU results.

In order to see how SVDU and NTU perform under less severe conditions, in Fig. 10(b) we show results for the same $h_z = 2.9$ but with a stronger bias $h_x = 5 \cdot 10^{-4}$. Again, $D = 5$ is enough to converge FTU. With $D$ growing from 3 to 6 the SVDU gets much closer to the converged FTU benchmark than for the weaker bias. Beyond $D = 6$ some decline in accuracy is observed but it is much less significant than for the weaker bias. The better convergence can be explained by a much shorter correlation length which peaks at $\xi \approx 4$ near $\beta = 1$. The same correlation length explains why the NTU magnetization curves with $D \geq 6$ coincide with the FTU one.

In order to see if the correlation length is the sole factor determining quality of the SVDU/NTU convergence, we move away from the quantum critical point down to $h_x = 2.5$ and consider again the weaker bias $h_z = 5 \cdot 10^{-4}$. The critical temperature is $T_c(2.5) = 1.2737(6)^{90}$ which is a little more than half of $T_c(0)$ indicating that quantum fluctuations are much less influential than for $h_x = 2.9$ but still significant. The results are shown in Fig. 11. Again, FTU is converged for $D = 5$ and SVDU is the closest to the FTU benchmark for $D = 6$ and slightly drifts up for $D = 7, 8$ but this time the difference between SVDU and FTU is negligible: SVDU with $D = 5, 6, 7, 8$ are practically converged to the benchmark though they have some scatter. The correlation length calculated at

\[ \beta = 0.76 \] is $\xi \approx 22$, i.e., the longest of the three examples. In spite of this it does not prevent convergence of either SVDU or NTU: NTU is converged already for $D = 5$. Therefore, it is not the correlation length alone that matters but the quantum nature of the correlations.

The convergence of the NTU results encourages us to attempt estimation of critical temperature $T_c(h_x)$ from magnetization curves — $\langle \sigma^z \rangle$ in function of $\beta$ — obtained for different $h_z$, see Ref.\textsuperscript{55} for more details of the procedure. For each $h_z$ we find a pseudo-critical temperature, $T^*(h_z)$, where the slope of the magnetization in function of $\beta$ is the steepest. Then we make a fit:

\[ T^*(h_z) = T_c + A h_z^{1/\tilde{\beta} \delta}, \] (13)

where $\tilde{\beta}, \delta$ are critical exponents. Treating $T_c, A$ and $1/\tilde{\beta} \delta$ as fitting parameters we obtain estimates of critical temperatures $T_c$ for $h_x = 2.9$ and $h_x = 2.5$ that are listed in tables I and II, respectively. The best fits (13) are shown in Fig. 12. For both values of transverse field NTU yields estimates of $T_c$ that are consistent with those from FU\textsuperscript{55} and quantum Monte Carlo\textsuperscript{90} although their convergence requires higher $D$ than FU. The error bars

\[ \begin{array}{|c|c|c|}
\hline
\text{method} & D & T_c \pm 1/\tilde{\beta} \delta \\
\hline
\text{SU}\textsuperscript{55} & 12 & 0.704(11) \pm 0.85(11) \\
\text{NTU} & 5 & 0.5858(28) \pm 0.586(7) \\
\text{NTU} & 6 & 0.5995(38) \pm 0.606(11) \\
\text{NTU} & 7 & 0.6021(21) \pm 0.611(6) \\
\text{NTU} & 8 & 0.6084(42) \pm 0.611(13) \\
\text{NTU} & 9 & 0.6080(40) \pm 0.618(14) \\
\text{FU}\textsuperscript{55} & 5 & 0.6100(7) \pm 0.571(3) \\
\text{QMC}\textsuperscript{90} & - & 0.6085(8) \pm - \\
\text{exact} & - & 8/15 \approx 0.533 \\
\hline
\end{array} \]

TABLE I. Comparison of $T_c$ and $1/\tilde{\beta} \delta$ obtained with NTU for $h_x = 2.9$ and the bias in the range: $0.0005 \leq h_x \leq 0.01$. For comparison we also list the SU and FU results\textsuperscript{55}. The quantum Monte Carlo estimate\textsuperscript{90} is shown as a benchmark. In brackets we show 95% confidence intervals.

\[ \begin{array}{|c|c|c|}
\hline
\text{method} & D & T_c \pm 1/\tilde{\beta} \delta \\
\hline
\text{NTU} & 2 & 1.2820(10) \pm 0.576(13) \\
\text{NTU} & 3 & 1.2430(20) \pm 0.570(9) \\
\text{NTU} & 4 & 1.2450(20) \pm 0.573(11) \\
\text{NTU} & 5 & 1.2740(20) \pm 0.578(14) \\
\text{NTU} & 6 & 1.2740(15) \pm 0.579(13) \\
\text{FU}\textsuperscript{55} & 5 & 1.2745(7) \pm 0.549(4) \\
\text{QMC}\textsuperscript{90} & - & 1.2737(6) \pm - \\
\text{exact} & - & 8/15 \approx 0.533 \\
\hline
\end{array} \]

TABLE II. Comparison of $T_c$ and $1/\tilde{\beta} \delta$ obtained with NTU for $h_x = 2.5$ and the bias in the range: $0.0005 \leq h_x \leq 0.0056$. For comparison we also list the FU result\textsuperscript{55}. The quantum Monte Carlo estimate\textsuperscript{90} is shown as a benchmark. In brackets we show 95% confidence intervals.
VI. CONCLUSION

We considered three evolution algorithms that can be ordered according to their increasing size of tensor environment that is taken into account when optimizing tensors: SVDU, NTU, and FTU. In general, the increasing size translates to faster convergence with bond dimension $D$. On this scale the traditional SU sits between SVDU and NTU while FTU is a variant of FU:

$$\text{SVDU} < \text{SU} < \text{NTU} < \text{FTU} \approx \text{FU}. $$

The increasing environment correlates with increasing numerical cost. However, in the latter respect NTU is in practice not much more expensive than SU. Although formally its cost of calculating the neighborhood environment scales like $D^8$, as compared to the leading cost of $D^5$ for SU, the $D^8$ is a fully parallelizable tensor contraction while the $D^5$ is a non-parallelizable SVD. When compared with FTU/FU, on the other side, NTU convergence with $D$ is in general slower but, thanks to the numerically exact environment, it offers more stability/efficiency for higher $D$ that allow to compensate for the limitations of the small environment. Therefore, for many applications NTU may be an attractive alternative for SU and FU alike.

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