Time-dependent variational principle with controlled bond expansion for matrix product states

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We present a controlled bond expansion (CBE) approach to simulate quantum dynamics based on the time-dependent variational principle (TDVP) for matrix product states. Our method alleviates the numerical difficulties of the standard, fixed-rank one-site TDVP integrator by increasing bond dimensions on the fly to reduce the projection error. This is achieved in an economical, local fashion, requiring only minor modifications of standard one-site TDVP implementations. We illustrate the performance of CBE–TDVP with several numerical examples on finite quantum lattices.

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Introduction.— The time-dependent variational principle (TDVP) [1–4] is a standard tool for time-evolving the Schrödinger equation on a constrained manifold parametrizing the wave function. Tensor networks (TN) offer efficient parametrizations based on low-rank approximations [5–12]. Their combination, TN–TDVP, holds much potential for studying the dynamics of quantum lattice models [13–32], quantum field theories [33, 34], and quantum chemistry problems [35–40].

Here, we focus on matrix product states (MPSs), an elementary class of TN states. Their time evolution, pioneered in Refs. 41–43, can be treated using a variety of methods, reviewed in Refs. 8, 44. Among these, MPS–TDVP [15, 18–22], which uses Lie-Trotter decomposition to integrate a train of tensors sequentially, arguably gives the best results regarding both physical accuracy and performance [44]: it (i) is applicable for long-ranged Hamiltonians, and its one-site (1s) version (1TDVP) ensures (ii) unitary time evolution, (iii) energy conservation and performance [45] and (iv) numerical stability [18, 21, 23].

A drawback of 1TDVP, emphasized in Refs. 46–48, is use of a fixed-rank integration scheme. This offers no way of dynamically adjusting the MPS rank (or bond dimension), as needed to track the entanglement growth typically incurred during MPS time evolution. For this, a rank-adaptive two-site (2s) TDVP (2TDVP) algorithm can be used [22], but it has much higher computational costs and in practice does not ensure properties (ii–iii).

To remedy this drawback, we introduce a rank-adaptive integrator for 1TDVP that is more efficient than previous ones [49–52]. It ensures properties (i–iv) at the same numerical costs as 1TDVP, with marginal overhead. Our key idea is to control the TDVP projection error [22, 49, 53] by adjusting MPS ranks on the fly via the controlled bond expansion (CBE) scheme of Ref. [54]. CBE finds and adds subspaces missed by 1s schemes but containing significant weight from $H\Psi$. When used for DMRG ground state searches, CBE yields 2s accuracy with faster convergence per sweep, at 1s costs [54]. CBE–TDVP likewise comes at essentially 1s costs.

MPS basics.— Let us recall some MPS basics, adopting the notation of Refs. 54 and 55. For an $L$-site system an open boundary MPS wave function $\Psi$ having dimensions $d$ for physical sites and $D$ for virtual bonds can always be written in site-canonical form,

$$\Psi = A_1 A_2 A_{\ell-1} C_{\ell} B_{\ell+1} B_{\ell+2} \cdots B_k.$$  \hspace{1cm} (1)

The tensors $C_{\ell}(\gamma)$, $A_{\ell}(\gamma)$ and $B_{\ell}(\gamma)$ are variational parameters. $A_{\ell}$ and $B_{\ell}$ are left and right-sided isometries, respectively, projecting $Dd$-dimensional parent (p) spaces to $D$-dimensional kept (k) images spaces; they obey

$$A_{\ell}^\dagger A_{\ell} = \left(\begin{array}{c} 1 \end{array}\right), \quad B_{\ell}^\dagger B_{\ell} = \left(\begin{array}{c} 1 \end{array}\right).$$  \hspace{1cm} (2)

The gauge relations $C_{\ell} = A_{\ell}\Lambda_{\ell} = \Lambda_{\ell-1}B_{\ell}$ ensure that Eq. (1) remains unchanged when moving the orthogonality center $C_{\ell}$ from one site to another. The Hamiltonian can likewise be expressed as a matrix product operator (MPO) with virtual bond dimension $w$,

$$H = W_1 \cdots W_{\ell-1} W_{\ell} \cdots W_L.$$  \hspace{1cm} (3)

Its projection to the effective local state spaces associated with site $\ell$ or bond $\ell$ yields effective one-site or zero-site Hamiltonians, respectively, computable recursively via

$$H_{\ell}^D = D_{\ell-1} D_{\ell+1} D_{\ell} = \begin{array}{c} 1 \end{array}, \quad H_{\ell}^w = D_{\ell-1} D_{\ell+1} D_{\ell} = \begin{array}{c} 1 \end{array}.$$  \hspace{1cm} (4a, 4b)

These act on 1s or bond representations of the wave function, $\psi_{\ell}^1 = C_{\ell}^\dagger(\gamma)$ or $\psi_{\ell}^D = A_{\ell}(\gamma)$, respectively.

Let $A_{\ell}(\gamma)$ and $B_{\ell}(\gamma)$ be isometries that are orthogonal complements of $A_{\ell}$ and $B_{\ell}$, with discarded (b) image spaces of dimension $D = D(d-1)$, obeying orthonormality and completeness relations complementing Eq. (2) [54]:
\( \sum_{\ell} = (I_{\ell}^p, \quad \sum_{\ell} = 0, \quad \sum_{\ell} = I_{\ell}^{p-1}, \quad \sum_{\ell} = 0, \quad (5a) \)

\( \sum_{\ell} + \sum_{\ell} = \sum_{\ell} = I_{\ell}^p, \quad \sum_{\ell} + \sum_{\ell} = \sum_{\ell} = I_{\ell}^{p-1}, \quad (5b) \)

**Tangent space projector.**—Next, we recapitulate the TDVP strategy. It aims to solve the Schrödinger equation, \( i\hbar \dot{\Psi} = H\Psi \), constrained to the manifold \( \mathcal{M} \) of all MPSs of the form (1), with fixed bond dimensions. Since \( H\Psi \) typically has larger bond dimensions than \( \Psi \) and hence does not lie in \( \mathcal{M} \), the TDVP aims to minimize \( ||\Psi - H\Psi|| \) within \( \mathcal{M} \). This leads to

\[
\dot{\Psi}(t) = P^{1s}(t)H\Psi(t),
\]

where \( P^{1s}(t) \) is the projector onto the tangent space of \( \mathcal{M} \) at \( \Psi(t) \), i.e. the space of all 1s variations of \( \Psi(t) \):

\[
P^{1s} = \sum_{\ell=1}^{L-1} \sum_{\ell+1}^{L} \left[ \begin{array}{c} A_{\ell} \hbar \\ B_{\ell} \hbar \end{array} \right] - \sum_{\ell=1}^{L-1} \sum_{\ell+1}^{L} \left[ \begin{array}{c} A_{\ell+1} \hbar \\ B_{\ell+1} \hbar \end{array} \right] + \sum_{\ell=t+1}^{L} \left[ \begin{array}{c} A_{\ell} \hbar \\ B_{\ell} \hbar \end{array} \right] \tag{7}
\]

The form in the first line was derived by Lubich, Oseledets, and Vandereycken [21] (Theorem 3.1), and transcribed into MPS notation in Ref. [22]. For further explanations of its form, see Refs. [55, 56]. The second line, valid for any \( \ell = 1, \ldots, L-1 \), follows via Eq. (5b); Eq. (5a) implies that all its terms conveniently are mutually orthogonal, and that the projector property \( (P^{1s})^2 = P^{1s} \) holds [55].

**One-site TDVP.**—The 1TDVP algorithm [21, 22] represents Eq. (6) by 2\( L-1 \) coupled equations, \( i\dot{C}_\ell = H^{1s}_\ell C_\ell \) and \( i\dot{A}_\ell = -H^{1*}_\ell A_\ell \), stemming, respectively, from the \( L \) single-site and \( L-1 \) bond projectors of \( P^{1s} \) (Eq. (7), first line). Evoking a Lie-Trotter decomposition, they are then decoupled and for each time step solved sequentially, for \( C_\ell \) or \( A_\ell \) (with all other tensors fixed). For a time step from \( t \) to \( t+\delta \), one repeatedly performs four steps, e.g. sweeping right to left: (1) Integrate \( i\dot{C}_{\ell+1} = H^{1s}_{\ell+1} C_{\ell+1} \) from \( t \) to \( t+\delta \); (2) QR factorize \( C_{\ell+1}(t') \); (3) integrate \( i\dot{A}_\ell = -H^{1*}_\ell A_\ell \) from \( t' \) to \( t \); and (4) update \( A_{\ell}(t)C_{\ell+1}(t) \rightarrow C_{\ell}(t)B_{\ell+1}(t') \), with \( C_{\ell}(t) = A_{\ell}(t)L_{\ell}(t) \).

1TDVP has two leading errors. One is the Lie-Trotter decomposition error. It can be reduced by higher-order integration schemes [45, 57]; we use a third-order integrator with error \( \mathcal{O}(\delta^3) \) [58]. The second error is the projection error from projecting the Schrödinger equation into the tangent space of \( \mathcal{M} \) at \( \Psi(t) \), quantified by \( \Delta_P = \| (I - P^{1s}) H\Psi(t) \|^2 \). It can be reduced brute force by increasing the bond dimension, as happens when using 2TDVP [22, 44, 47], or through global subspace expansion [50]. Here, we propose a local approach, similar in spirit to that of Ref. [52], but more efficient, with 1s costs, and without stochastic ingredients, in contrast to [40].

**Controlled bond expansion.**—Our key idea is to use CBE to reduce the 2s contribution in \( \Delta_P \), given by \( \Delta_P^{2s} = \| P^{2s} H\Psi \|^2 \), where \( P^{2s} = P^{2s}(1 - P^{1s}) \). Here, \( P^{2s} \) is the projector onto 2s variations of \( \Psi \), and \( P^{2s} \) its component orthogonal to the tangent space projector (see also [55]):

\[
P^{2s} = \sum_{\ell=1}^{L-1} \sum_{\ell+1}^{L} \left[ \begin{array}{c} A_{\ell} \hbar \\ B_{\ell} \hbar \end{array} \right] - \sum_{\ell=1}^{L-1} \sum_{\ell+1}^{L} \left[ \begin{array}{c} A_{\ell+1} \hbar \\ B_{\ell+1} \hbar \end{array} \right] + \sum_{\ell=t+1}^{L} \left[ \begin{array}{c} A_{\ell} \hbar \\ B_{\ell} \hbar \end{array} \right] \tag{8a}
\]

\[
P^{2s} = \sum_{\ell=1}^{L-1} \sum_{\ell+1}^{L} \left[ \begin{array}{c} A_{\ell} \hbar \\ B_{\ell} \hbar \end{array} \right] + \sum_{\ell=t+1}^{L} \left[ \begin{array}{c} A_{\ell} \hbar \\ B_{\ell} \hbar \end{array} \right] \tag{8b}
\]

Now note that \( \Delta_P^{2s} \) is equal to \( \Delta_P^{2s} = \| P^{2s}(H - \bar{\Psi})\|^2 \), the 2s contribution to the energy variance [53-55]. In Ref. [54], discussing ground state searches via CBE-DMRG, we showed how to minimize \( \Delta_P^{2s} \) at 1s costs; each bond \( \ell \) can be expanded in such a manner that the added subspace carries significant weight from \( P^{2s} H\Psi \). This expansion removes that subspace from the image of \( P^{2s} \), thus reducing \( \Delta_P^{2s} \) significantly. Consider, e.g., a right-to-left sweep and let \( \tilde{A}_{\ell}^t (\tilde{\Psi}) \) be a truncation of \( \bar{\Psi} (\Psi) \) having an image spanning such a subspace, of dimension \( \bar{D} \), say. To expand bond \( \ell \) from \( D \) to \( D + \bar{D} \), we replace \( A_{\ell}(\Psi) \) by \( A_{\ell}^{ex}(\tilde{\Psi}) \) (see also [55]) and \( \bar{D} \) ex varies through a suitable choice of the truncated complement \( \bar{A}_{\ell}^t (\tilde{\Psi}) \) [54]. We find \( \tilde{A}_{\ell}^t \) using the so-called shread selection strategy of Ref. [54] (Figs. 1 and 2 there); it avoids computation of \( \Psi, \bar{\Psi} \) and has 1s costs regarding CPU and memory, thus becoming increasingly advantageous for large \( D \) and \( \bar{D} \). Shread selection involves two truncations \( (D \rightarrow D') \) and \( (D' \rightarrow D) \) in Ref. [54]). Here, we choose these to respect singular value thresholds of \( \epsilon = 10^{-4} \) and \( \epsilon = 10^{-6} \), respectively; empirically, these yield good results in the benchmark studies presented below.

**CBE-TDVP.**—It is straightforward to incorporate CBE into the 1TDVP algorithm: simply expand each bond \( \ell \) from \( D \rightarrow D + \bar{D} \) before time-evolving it. Concretely, when sweeping right-to-left, we add step (0): expand \( A_{\ell}, C_{\ell+1}, H^{1s}_{\ell+1} \rightarrow A^{ex}_{\ell}, C^{ex}_{\ell+1}, H^{1s,ex}_{\ell+1} \) following Eq. (9) (and by implication also \( \Lambda_{\ell}, H^{1*}_{\ell}, A^{ex}_{\ell}, H^{1s,ex}_{\ell} \)). The other steps remain as before, except that in (2) we replace the QR factorization by an SVD. This allows us to reduce (trim) the bond dimension from \( D \rightarrow D + \bar{D} \) to a final value \( D_t \), as needed in two situations [49, 51, 59]: First, while standard 1TDVP requires keeping and even padding small singular values in order to retain a fixed bond dimension [13, 18], that is not necessary here. Instead, for bond trimming, we discard small singular values below an empirically determined threshold \( \epsilon = 10^{-12} \). This keeps the MPS rank as low as possible, without impacting the accuracy [49]. Second, once \( D + \bar{D} \) exceeds
D_{\text{max}}$, we trim it back down to $D_{\text{max}}$ aiming to limit computational costs. The trimming error is characterized by its discarded weight, $\xi(t)$, which we either control or monitor. The TDVP properties of (ii) unitary evolution and (iii) energy conservation [51] hold to within order $\xi(t)$.

Results.— We now benchmark CBE–TDVP for three spin models, then illustrate its performance for large $d$ using the Peierls–Hubbard model with $d = 36$. Our benchmark comparisons track the time evolution of the entanglement entropy $E(t)$ between the left and right halves of a chain, the bond dimensions $D_1(t)$ and $D_2(t)$, the discarded weight $\xi(t)$, the deviations from exact results of spins expectation values, $\delta S^{i}(t)$, and the energy change, $\delta E(t)$, which should vanish for unitary time evolution.

**XX model: domain wall motion.**— We consider a spin chain with Hamiltonian $H_{\text{XX}} = \sum_\ell \left( S^{x}_\ell S^{x}_{\ell+1} + S^{y}_\ell S^{y}_{\ell+1} \right)$. We compute the time evolution of the local magnetization profile $S^{z}_\ell(t) = \langle \Psi(t)|S^{z}_\ell|\Psi(t)\rangle$, initialized with a sharp domain wall, $|\Psi(0)\rangle = \uparrow\uparrow\cdots\uparrow\downarrow\cdots\downarrow$. For comparison, the analytical solution for $\varphi \to \infty$ reads [60] $S^{z}_\ell(t) = -1/2 \sum_{n=\ell-1}^{\ell} J_n(t)^2$, for $\ell \geq 1$ (right half) and $S^{z}_\ell = -S^{z}_{\ell-1}$ otherwise, where $J_n(t)$ is the Bessel function of the first kind. The domain wall spreads with time [Fig. 1(a)], entailing a steady growth of the entanglement entropy (EE) between the left and right halves of the spin chain [Fig. 1(b)]. $D_1(t)$ and $D_2(t)$ [Fig. 1(c)] start from 1 and 0. Initially, $D$ remains remarkably small ($\lesssim 10$), while $D_1$ increases in steps of $D$ until reaching $D_{\text{max}}$. Thereafter $D$ increases noticeably, but remains below $D_{\text{max}}$ for all times shown here. This reflects CBE frugality—bonds are expanded only as much as needed.

![FIG. 1. 100-site XX spin chain: Time evolution of a domain wall, computed with time step $\delta = 0.05$ and $U(1)$ spin symmetry. (a) Local magnetization profile $S^{z}_\ell(t)$. (b) Entanglement entropy $E(t)$ between the left and right halves of the chain. (c) Bond dimension $D_1(t)$ and its pre-trimming expansion $\tilde{D}(t)$ per time step, for $D_{\text{max}} = 120$. (d,e) Error analysis: magnetization $\delta S^{z}(t)$ (solid line), the maximum deviation of $\ell$ of $S^{z}_\ell(t)$ from the exact result, and, energy $\delta E(t)$ (dashed line), and discarded weight $\xi(t)$ (dotted line) for $D_{\text{max}} = 40$ (red), 80 (blue) and 120 (black), computed with (d) CBE–TDVP or (e) 2TDVP. Remarkably, the errors are comparable in size, although CBE–TDVP has much smaller computational costs.](image1)

![FIG. 2. 100-site one-axis twisting model: Time evolution of an initially $x$–polarized spin state, computed using $\delta = 0.01$ and $Z_2$ spin symmetry. (a) Total spin $S^{z}_x(t)$, (b) entanglement entropy, and (c) bond dimensions. (d) Error analysis: error in total spin density $\delta S^{z}_x(t)$ (solid line), energy $\delta E(t)$ (dashed line), and discarded weight $\xi(t)$ (dotted line), for $D_{\text{max}} = 500$.](image2)
Its ground state correlator, \( S \) function, is related by discrete Fourier transform to its spectral evolution of a spin excitation, computed with \( \delta = 0.05 \), \( n_{\text{ph}} = 8 \) and U(1) spin symmetry. (a1,a2) Real and imaginary parts of \( S(\pi,\omega/J) \) for \( g = 0 \) and \( g = 1 \). (c) Phonon density \( n_{\text{ph}}(x,t) \), (d) bond dimensions, and (e) error analysis: energy \( \delta E(t) \) (dashed line) and discarded weight \( \xi(t) \) (dotted line), all computed for \( g = 1 \), with \( D_{\text{max}} = 500 \).

**Peierls–Hubbard model: scattering dynamics.**—Finally, we consider the scattering dynamics of interacting electrons coupled to phonons. This interaction leads to non-trivial low-energy physics involving polarons [67–79]; the numerical study of polaron dynamics is currently attracting increasing attention [69, 80–84]. Here, we consider the 1-dimensional Peierls–Hubbard model,

\[
H_{\text{PH}} = \sum_{\ell} U n_{\ell \uparrow} n_{\ell \downarrow} + \sum_{\ell} \omega_{\text{ph}} b_{\ell}^\dagger b_{\ell} + \sum_{\ell \sigma} (c_{\ell \sigma}^\dagger c_{\ell+1 \sigma} + \text{h.c.}) (-t + b_{\ell}^\dagger b_{\ell} - b_{\ell+1}^\dagger b_{\ell+1}).
\]

Spinful electrons with onsite interaction strength \( U \) and hopping amplitude \( t = 1 \), and local phonons with frequency \( \omega_{\text{ph}} \), are coupled with strength \( g \) through a Peierls term modulating the electron hopping.

We consider two localized wave packets with opposite spins, average momenta \( k = \pm \pi/2 \) and width \( W \) [85, 86], initialized as \( |\Psi_{\pm}\rangle = \sum_{\ell} A e^{-\left(\pi u_{\text{ph}} k \pi x\right)^2} e^{ikx} c_{\ell \uparrow}^\dagger |0\rangle \), where \( |0\rangle \) describes an empty lattice. Without electron-phonon coupling \( g = 0 \), Fig. 4(a), there is little dispersion effect through the time of flight, and the strong interaction causes an elastic collision. By contrast, for a sizable coupling in the nonperturbative regime [77, 79] \( g = 1 \), Figs. 4(b–c), phonons are excited by the electron motion [Fig. 4(e)]. After the two electrons have collided, they show a tendency to remain close to each other (though a finite distance apart, since \( U \) is large) [Fig. 4(b)]; they thus seem to form a bi-polaron, stabilized by a significant phonon density in the central region [Fig. 4(e)].

We limited the phonon occupancy to \( n_{\text{ph}} = 8 \) per site. Then, \( d = 4(n_{\text{ph}} + 1) = 36 \), and \( D = 35D_1 \) is so large that 2TDVP would be utterly unfeasible. By contrast, CBE–
TDVP requires a comparatively small bond expansion of only $D(t) \leq 4D_{\text{max}}$ for the times shown; after that, the discarded weight $\xi(t)$ becomes substantial [Figs. 4(d,e)].

**Conclusions and outlook.**— Among the schemes for MPS time evolution, 1TDVP has various advantages (see introduction), but its projection error is uncontrolled. 2TDVP remedies this, albeit at 2s costs, $O(d^2wD^3)$, and is able to simulate dynamics reliably [44]. CBE–TDVP at 1s costs, $O(dwD^3)$ achieves the same accuracy as 2TDVP. Moreover, CBE–TDVP comes with significantly slower growth of bond dimensions $D$ in time, which speeds up the calculations further (see Ref. [56]).

Our benchmark tests of CBE–TDVP, on three exactly solvable state spaces, with effective local bond dimensions $d_{\text{eff}} = d^2$, the cost reduction of CBE–TDVP vs. 2TDVP, $O(d^2wD^3)$ vs. $O(d^4wD^3)$, will be particularly dramatic. Examples are finite temperature properties, treated by purification of the density matrix [87] or dissipation-assisted operator evolution [88]; and the dynamics of open quantum systems [89], described by Liouville evolution of the density matrix [90–92] or by an influence matrix approach [93].

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See Supplemental Material at [url] for: (S-1) an explanation of the structure of the tangent space projector P^2; (S-2) an analysis of the fidelity of CBE–TDVP: we show that under backward time evolution (implemented by changing the sign of \( L \delta \)), the domain wall retracts to a point; and (S-3) a comparison of the CPU time costs of CBE–TDVP vs. 2TDVP. The Supplemental Material includes Refs. [21, 22, 51].

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A first-order integrator, with error \( O(\delta^2) \), involves a single left-to-right sweep \( L_S \) or right-to-left sweep \( R_S \) through the entire chain. For 1TDVP, \( L_S \) and \( R_S \) are adjoint operators, with \( L_S \delta \circ R_S = 1 \), hence higher-order integrators can be obtained through symmetric compositions [57]. We use one of third order (error \( O(\delta^3) \)): \( L^4_S \circ R^2_S \circ L^4_S \), for one time step, \( R^4_S \circ L^2_S \circ R^4_S \) for the next.

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Supplemental material: Time-dependent variational principle with controlled bond expansion for matrix product states

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S-1. SINGLE SITE (FIXED RANK) TANGENT SPACE PROJECTOR

The structure (7) of the tangent space projector $P^{1s}$ can be motivated by the following short-cut argument (equivalent to invoking gauge invariance [21, 22]). If $\Psi$ is represented as an MPS, then its tangent vectors $\delta \Psi$ under the fixed-rank approximation can be expressed as a sum of MPSs each containing one derivative of a local tensor. This representation is not unique, but its gauge redundancy can be easily removed. To do so, let us first consider the variation of MPS in Eq. (1) on a single bond $\ell$, i.e., $A_{\ell}C_{\ell+1} = A_{\ell}A_{\ell}B_{\ell+1}$, while the other tensors remain fixed (and hence are not depicted below). Its first order variation then gives us $\delta A_{\ell}A_{\ell}B_{\ell+1} + A_{\ell}\delta A_{\ell}B_{\ell+1} + A_{\ell}\delta B_{\ell+1}$. By further rewriting $\delta A_{\ell}A_{\ell}$ as $A_{\ell}A_{\ell} + A_{\ell}A_{\ell} + \Lambda^\ell B_{\ell+1}$ and $\Lambda^\ell B_{\ell+1}$ as $\Lambda^\ell B_{\ell+1} + \Lambda^\ell B_{\ell+1} + \Lambda^\ell B_{\ell+1}$, we obtain the following unique decomposition,

$$
\delta \frac{\partial}{\partial \ell} \frac{\partial}{\partial \ell} = \frac{\partial}{\partial \ell} \frac{\partial}{\partial \ell} \frac{\partial}{\partial \ell} + A_{\ell} \frac{\partial}{\partial \ell} B_{\ell+1} + A_{\ell} \frac{\partial}{\partial \ell} B_{\ell+1},
$$

(S1)

with $\Lambda^\ell = \Lambda^\ell + \delta A_{\ell} + \Lambda^\ell$. The three terms on the right are mutually orthogonal to each other. Each of them belongs to the image space of one of the following three orthogonal projectors:

$$
\frac{\partial}{\partial \ell} \frac{\partial}{\partial \ell}, \frac{\partial}{\partial \ell} \frac{\partial}{\partial \ell}, \frac{\partial}{\partial \ell} \frac{\partial}{\partial \ell};
$$

(S2)

their sum is a tangent space projector for $A_{\ell}A_{\ell}B_{\ell+1}$. Repeating the same argument for all the bonds, while avoiding double counting, i.e., including every term only once, we readily obtain $P^{1s}$ given by the second line of Eq. (7).

Therefore, given an MPS of the form (1), $P^{1s}$ is indeed the orthogonal projector onto its tangent space under the fixed-rank approximation. For real-time evolution, applying the Hamiltonian to $|\Psi\rangle$ leads the state out of its tangent space. In the 1TDVP scheme, $H$ is approximated by $P^{1s}H|\Psi\rangle$, its orthogonal projection onto the tangent space, leading to Eq. (6).

S-2. ANALYSIS OF CBE-TDVP ERROR PROPAGATION

The TDVP time evolution of an MPS under the fixed-rank approximation is unitary, with energy conservation if the Hamiltonian is time-independent. Expanding the tangent space does not spoil these desirable properties, provided that no truncations are performed. However, then the bond dimension would keep growing with time, which is not practical for studies of long-time dynamics.

With our CBE approach, we instead restrict the bond dimension growth by bond trimming using $\epsilon = 10^{-12}$, and also stopping the increase of $D_1$ once it has reached a specified maximal value $D_{\text{max}}$. Due to these truncations, the desirable TDVP properties are no longer satisfied exactly. However, for each time step they do hold within the truncation error, as shown by Ceruti, Kusch, and Lubich [51]. Thus, the time evolution per time step is almost unitary. Nevertheless, errors can accumulate with time, hence it is unclear a priori to what extent the desirable TDVP properties survive over long times.

To investigate this, we revisit our first benchmark example for the domain wall motion of the XX model. We use CBE-TDVP (while exploiting $U(1)$ spin symmetry) to compute the forward-backward fidelity [Fig. 1(a)]

$$
F(t) = |\langle \Psi_-(t) | \Psi_+(t) \rangle|^2, \quad t = t_{\text{max}} - t \in [0, t_{\text{max}}].
$$

(S3)

Here, $|\Psi_+(t)\rangle = e^{-iHt}|\Psi(0)\rangle$ is obtained through forward evolution for time $t$, and $|\Psi_-(t)\rangle = e^{iHt}|\Psi_+(t_{\text{max}})\rangle$ through forward evolution until time $t = t_{\text{max}}$, then back-evolution for $t = t_{\text{max}} - t$ to get back to time $t$. The deviation of the fidelity from unity, $\delta F(t) = 1 - F(t)$, equals zero for unitary evolution; increases with $t$ if time evolution is computed using truncations; and tends to 1 for $t \to t_{\text{max}}$ if truncations are too severe.

Figure 1(b) shows the back-evolution of the domain wall described by $|\Psi_-(t)\rangle$ as $t$ increases from 0 to $t_{\text{max}} = 40$, where both $|\Psi_+(t)\rangle$ and $|\Psi_-(t)\rangle$ were computed using CBE-TDVP with the truncation parameters stated in the main text, namely $\epsilon = 10^{-6}$ and $D_{\text{max}} = 120$. The corresponding $\delta F(t)$ (Fig. 1(d), black dashes) shows initial transient growth, but then saturates at a remarkably small plateau value of $6.7 \times 10^{-5}$. Moreover, the corresponding bond expansion per update, $\bar{D}(t)$ (Fig. 1(c), black dots), increases only fairly slowly. For these truncation settings, the CBE-TDVP errors are thus clearly under good control and do not accumulate rapidly, so that long-time evolution can be computed accurately.

The fidelity becomes worse ($\delta F(t)$ increases) if the singular-value threshold for bond expansion, $\epsilon$, is raised (Fig. 1(d), dashed lines). Nevertheless, even for $\epsilon$ as large as $10^{-2}$ we find long-time plateau behavior for $\delta F(t)$, implying that the errors remain controlled. This illustrates...
Finally, Figs. 1(c) and 1(d) (dash-dotted, purple line) also show 1TDVP results, computed with $D = 120$: the domain wall fails to recontract to a point, and the fidelity reaches zero ($\delta F(\hat{\tau})$ reaches 1). This occurs even though 1TDVP uses no truncations besides the tangent space projection, and hence yields unitary time evolution. This poor performance illustrates a key limitation of 1TDVP when exploiting symmetries (as here): time evolution involves transitions to sectors having quantum numbers not yet present, but 1TDVP cannot include these, due to the fixed-rank nature of its tangent space projection. CBE–TDVP by construction lifts this restriction.

S-3. COMPARISON OF CPU TIME FOR CBE–TDVP AND 2TDVP

In this section, we compare the CPU time for CBE–TDVP and 2TDVP. As a demonstration, we use the one-axis twisting (OAT) model discussed in Results in the main text. All CPU time measurements were done on a single core of an Intel Core i7-9750H processor.

First, we compare the early-time behavior of CBE–TDVP and 2TDVP. From $t = 0$ to 1.5, both methods yield good accuracy as shown in Fig. S-2(a). The CPU time spent to achieve this, however, is quite different. In Fig. S-2(b), we see that while the 2TDVP takes about two days, CBE–TDVP accomplishes the same time span overnight.

The main reason for this difference does not lie in the 1s vs. 2s scaling of CBE–TDVP vs. 2TDVP (discussed below), because $d = 2$ (for $S = 1/2$) is small, and CBE involves some algorithmic overhead for determining the truncated complement $A^3(t)$. Instead, the difference reflects the fact that the growth in MPS bond dimension $D(t)$ with time is much slower for CBE–TDVP than 2TDVP. This implies dramatic cost savings, since both methods have time complexity proportional to $D^3$. Figure S-2(c,d) show the time evolution of bond dimensions for all MPS bonds for CBE–TDVP and 2TDVP respectively. For 2TDVP [Fig. S-2(c)], the bond dimensions grow almost exponentially and quickly saturate to their specified maximal value, here $D_{\text{max}} = 500$. This saturation is reflected by the early onset of linear growth in the CPU time in Fig. S-2(b). By contrast, the bond dimensions of CBE–TDVP show a much slower growth [Fig. S-2(d)], yielding a strong reduction in CPU time compared to 2TDVP.

Second, we demonstrate that when $D$ is fixed, the time complexity of CBE–TDVP vs. 2TDVP scales as $d$ vs. $d^2$, implying 1s vs. 2s scaling. Figure S-3 shows this by displaying the CPU time per sweep for the OAT model for several different values of the spin $S$, with the MPS bond dimension fixed at $D_{\text{max}} = 500$. 
FIG. S-3. CPU time per sweep for the 20-site one-axis twisting model, computed for several values of $S$, at $D_{\text{max}} = 500$. 

$D = D_{\text{max}} = 500$ 

fit: 
- CBE-TDVP 
- $ax + b$ 
- $ax^3 + bx + c$