Editors' Suggestion

Time-Dependent Variational Principle with Controlled Bond Expansion for Matrix Product States

Jheng-Wei Li,[1,2] Andreas Gleis,[1] and Jan von Delft[1]
[1]Arnold Sommerfeld Center for Theoretical Physics, Center for NanoScience, and Munich Center for Quantum Science and Technology, Ludwig-Maximilians-Universität München, 80333 Munich, Germany
[2]Université Grenoble Alpes, CEA, Grenoble INP, IRIG, Pheliqs, F-38000 Grenoble, France

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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 and accuracy of CBE-TDVP with several numerical examples on finite quantum lattices, including new results on bipolaron formation in the Peierls-Hubbard model and spin pumping via adiabatic flux insertion in a chiral spin liquid.

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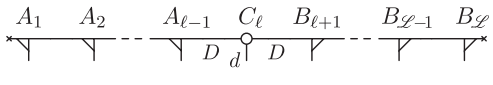
Introduction.—The time-dependent variational principle (TDVP) [1–4] is a standard tool for time-evolving the Schrödinger equation on a constrained manifold parametrizing the wave function. Tensor networks (TN) offer efficient parametrizations based on low-rank approximations [5–12]. Their combination, 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 [15,45], 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).

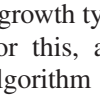
To remedy this drawback, we introduce a rank-adaptive integrator for 1TDVP that is more efficient than previous ones [49–52]. It ensures properties (i)–(iv) at the same numerical costs as 1TDVP, with marginal overhead. Our key idea is to control the TDVP projection error [22,49,53] by adjusting MPS ranks 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 and energy reduction 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. [54,55]. For an $\mathcal{L}$-site system an open boundary MPS wave function Ψ having dimensions d for physical sites and D for virtual bonds can always be written in site-canonical form,

$$\Psi =$$ 

$$. \quad (1)$$

The tensors C_ℓ ( ), A_ℓ ( ) and B_ℓ ( ) are variational parameters. A_ℓ and B_ℓ are left- and right-sided isometries, respectively, projecting Dd-dimensional *parent* (P) spaces to D-dimensional *kept* (K) images spaces; they obey

$$A_\ell^\dagger A_\ell =$$ 

$$= \mathbb{1}_\ell^{\mathrm{K}}, \qquad B_\ell B_\ell^\dagger =$$ 

$$= \mathbb{1}_{\ell-1}^{\mathrm{K}}. \quad (2)$$

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_ℓ from one site to another.

The Hamiltonian can likewise be expressed as a matrix product operator (MPO) with virtual bond dimension w,

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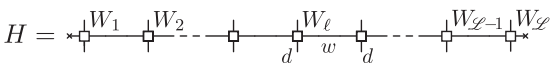
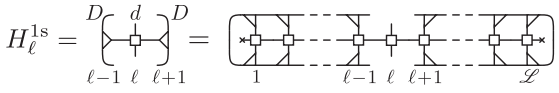
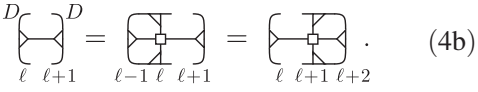
$H =$  . (3)

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

$H_\ell^{1s} =$  , (4a)

$H_\ell^{b} =$  . (4b)

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

Let $\overline{A}_\ell$ () and $\overline{B}_\ell$ () be isometries that are orthogonal complements of A_ℓ and B_ℓ, with *discarded* (D) image spaces of dimension $\bar{D} = D(d-1)$, obeying orthonormality and completeness relations complementing Eq. (2) [54]:

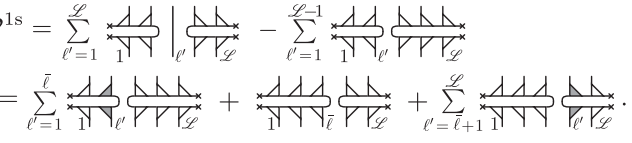
 (5a)

 (5b)

Tangent space projector.—Next, we recapitulate the TDVP strategy. It aims to solve the Schrödinger equation, $i\dot{\Psi} = H\Psi$, 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 Ψ and hence does not lie in $\mathcal{M}$, the TDVP aims to minimize $\|i\dot{\Psi} - H\Psi\|$ within $\mathcal{M}$. This leads to

$$i\dot{\Psi}(t) = \mathcal{P}^{1s}(t) H \Psi(t), \tag{6}$$

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

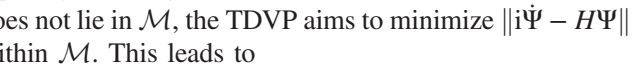
 (7)

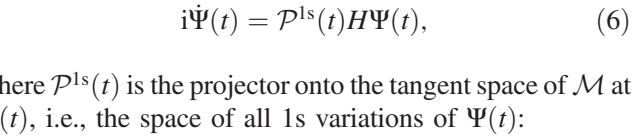
The form in the first line was found by Lubich, Oseledets, and Vandereycken [21] (Theorem 3.1) and transcribed into MPS notation in Ref. [22]. For further explanations of its form, see Refs. [55,56]. The second line, valid for any $\overline{\ell} = 1, \ldots, \mathcal{L}-1$, follows via Eq. (5b); Eq.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

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

1TDVP has two leading errors. One is the Lie-Trotter decomposition error. It can be reduced by higher-order integration schemes [45,60]; we use a third-order integrator with error $\mathcal{O}(\delta^3)$ [61]. The second error is the projection error from projecting the Schrödinger equation into the tangent space of $\mathcal{M}$ at $\Psi(t)$, quantified by $\Delta_P = \|(\mathbb{1} - \mathcal{P}^{1s}) H\Psi(t)\|^2$. 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], which enriches the basis representing $\Psi(t)$ by adding a few *global* Krylov vectors, $\{H\Psi(t), \ldots, H^k\Psi(t)\}$. 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 Δ_P, given by $\Delta_P^{2\perp} = \|\mathcal{P}^{2\perp} H\Psi\|^2$, where $\mathcal{P}^{2\perp} = \mathcal{P}^{2s}(1 - \mathcal{P}^{1s})$. Here, $\mathcal{P}^{2s}$ is the projector onto 2s variations of Ψ, and $\mathcal{P}^{2\perp}$ its component orthogonal to the tangent space projector (see also [55]):

 (8a)

 (8b)

Now note that $\Delta_P^{2\perp}$ is equal to $\Delta_E^{2\perp} = \|\mathcal{P}^{2\perp}(H - E)\Psi\|^2$, the 2s contribution to the energy variance [53–55]. In Ref. [54], discussing ground state searches via CBE-DMRG, we showed how to minimize $\Delta_E^{2\perp}$ at 1s costs: each bond ℓ can be expanded in such a manner that the added subspace carries significant weight from $\mathcal{P}^{2\perp} H\Psi$. This expansion removes that subspace from the image of $\mathcal{P}^{2\perp}$, thus reducing $\Delta_E^{2\perp}$ significantly. Consider, e.g., a

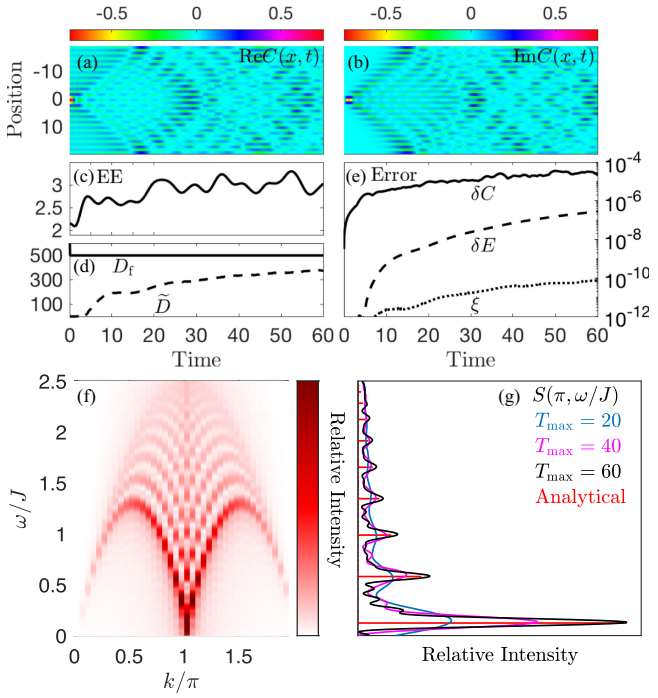


FIG. 1. 40-site SU(2) Haldane-Shastry model: Time evolution of a spin excitation, computed with $\delta = 0.05$ and SU(2) spin symmetry. (a),(b) Real and imaginary parts of $C(x,t)$, (b) entanglement entropy $\mathrm{EE}(t)$, and (c) bond dimensions $D_\mathrm{f}^*(t)$ and $\tilde{D}_\mathrm{f}^*(t)$. (e) Error analysis for $D_\mathrm{max} = 500$: $\delta C(t)$, the maximum of $\delta C(x,t)$ over x, energy drift $\delta E(t)$ (should remain zero for unitary time evolution), and discarded weight $\xi(t)$. (f) Normalized spectral function $S(k,\omega)/S(\pi,0)$, obtained using $t_\mathrm{max} = 60$. (g) $S(\pi,\omega)/S(\pi,0)$, obtained using $t_\mathrm{max} = 20$, 40, 60; red lines indicate exact peak heights.

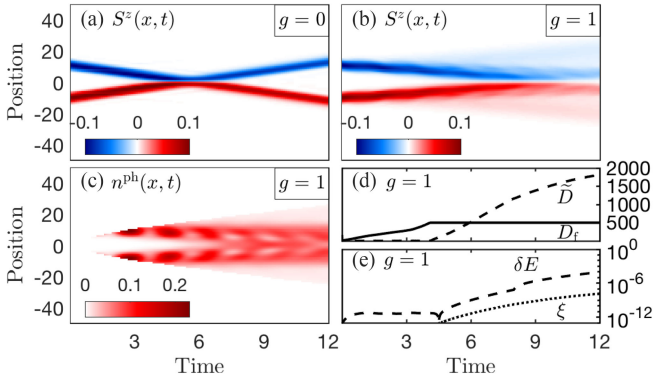
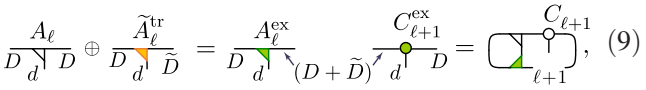
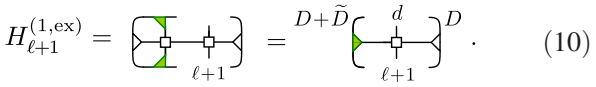


FIG. 2. Peierls-Hubbard model: Real-space scattering of two electron wave packets, computed for $U = 10$, $\omega_\mathrm{ph} = 3$, $\delta = 0.05$, $n^\mathrm{ph}_\mathrm{max} = 8$ and U(1) spin symmetry. (a),(b) Spin magnetic moment $S^z(x,t)$ for $g = 0$, $g = 1$. (c) Phonon density $n^\mathrm{ph}(x,t)$, (d) bond dimensions, and (e) error analysis: energy $\delta E(t)$ and discarded weight $\xi(t)$, all computed for $g = 1$, $D_\mathrm{max} = 500$.

right-to-left sweep and let $\widetilde{A}^\mathrm{tr}_\ell$ ( ) be a truncation of $\overline{A}_\ell$ ( ) having an image spanning such a subspace, of dimension $\tilde{D}$, say. To expand bond ℓ from D to $D + \tilde{D}$, we replace A_ℓ( ) by A^ex_ℓ( ), $C_{\ell+1}$( ) by $C^\mathrm{ex}_{\ell+1}$( ) and $H^\mathrm{1s}_{\ell+1}$ by $H^\mathrm{1s,ex}_{\ell+1}$, with expanded tensors defined as



(9)



(10)

Note that Ψ remains unchanged, $A^\mathrm{ex}_\ell C^\mathrm{ex}_{\ell+1} = A_\ell C_{\ell+1}$.

Similarly, the projection error $\Delta^{2\perp}_P$ can be minimized through a suitable choice of the truncated complement $\widetilde{A}^\mathrm{tr}_\ell$( ) [54]. We find $\tilde{A}^\mathrm{tr}_\ell$ using the so-called *shrewd selection* strategy of Ref. [54] (Figs. 1 and 2 there); it avoids computation of , and has 1s costs regarding CPU and memory, thus becoming increasingly advantageous for large D and d. Shrewd selection involves two truncations ($D \to D'$ and $\hat{D} \to \tilde{D}$ in Ref. [54]). Here, we choose these to respect singular value thresholds of $\epsilon' = 10^{-4}$ and $\tilde{\epsilon} = 10^{-6}$, respectively; empirically, we found these to yield good results for various benchmark studies [56].

CBE-TDVP.—It is straightforward to incorporate CBE into the 1TDVP algorithm: simply expand each bond ℓ from $D \to D + \tilde{D}$ before time evolving it. Concretely, when sweeping right-to-left, we add step (0): expand $A_\ell, C_{\ell+1}, H^\mathrm{1s}_{\ell+1} \to A^\mathrm{ex}_\ell, C^\mathrm{ex}_{\ell+1}, H^\mathrm{1s,ex}_{\ell+1}$ following Eq. (9) (and by implication also $\Lambda_\ell, H^\mathrm{b}_\ell \to \Lambda^\mathrm{ex}_\ell, H^\mathrm{b,ex}_\ell$). 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 $D + \tilde{D}$ to a final value D_f, as needed in two situations [49,51,62]: 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 $D + \tilde{D}$ exceeds D_max, we trim it back down to D_max, aiming to limit computational costs. The trimming error is characterized by its discarded weight, $\xi(t)$, which we monitor throughout. The TDVP properties of (ii) unitary evolution and (iii) energy conservation [51] hold to within order $\xi(t)$.

Results.—The Supplemental Material [56] benchmarks the performance of CBE-TDVP for two exactly solvable models. Here, we illustrate its power with three numerically challenging applications containing interesting physics: spin dynamics in the Haldane-Shastry model, scattering dynamics in the Peierls-Hubbard model, and spin pumping via flux insertion for a chiral spin liquid on a cylinder.

Haldane-Shastry model: Spin dynamics.—The SU(2) Haldane-Shastry model on a $\mathcal{L}$-site ring is defined by

$$H_{\mathrm{HS}} = \sum_{0\le\ell<\ell'\le\mathcal{L}-1} \frac{\pi^2 \mathbf{S}_\ell \cdot \mathbf{S}_{\ell'}}{\mathcal{L}^2 \sin^2 \frac{\pi}{\mathcal{L}}(\ell-\ell')}. \tag{11}$$

Its ground state correlator, $C(\ell,t) = \langle\Psi_0|\mathbf{S}_\ell(t)\mathbf{S}_0(0)|\Psi_0\rangle$, is related by discrete Fourier transform to its spectral function [63,64], $S(k,\omega)$, given by $(0<\ell'<\ell\le\mathcal{L}/2)$

$$S\left(2(\ell+\ell')\frac{\pi}{\mathcal{L}}, \frac{\pi^2}{\mathcal{L}^2}[(\ell+\ell')\mathcal{L} - 2(\ell^2+\ell'^2) + \ell - \ell']\right) = \frac{2\ell-2\ell'-1}{(2\ell-1)(\mathcal{L}-2\ell'-1)} \prod_{\bar{\ell}=\ell'+1}^{\ell-1} \frac{2\bar{\ell}(\mathcal{L}-2\bar{\ell})}{(2\bar{\ell}-1)(\mathcal{L}-2\bar{\ell}-1)}. \tag{12}$$

Figures 1(a) and 1(b) show the real and the imaginary parts of $C(x,t)$, computed using CBE-TDVP. For early times ($t\le 20$), the local excitation introduced at $\ell=0$, $t=0$ spreads ballistically, as reported previously [28,65,66]. Once the counterpropagating wavefronts meet on the ring, an interference pattern emerges. Figures 1(c)–1(e) show that our numerical results remain accurate throughout: the entanglement entropy $\mathrm{EE}(t)$ and bond expansion per time step $\tilde{D}_{\mathrm{f}}^*(t)$ do not grow rapidly, and error measures remain small. Figure 1(f) shows the corresponding spectral function $S(k,\omega)$, obtained by discrete Fourier transform of $C(x,t)$ using a maximum simulation time of $t_{\max}=60$. Figure 1(g) shows a cut along $k=\pi$: peaks can be well resolved by increasing $t_{\max}$, with relative heights in excellent agreement with the exact Eq. (12).

Peierls-Hubbard model: Scattering dynamics.—Next, we consider the scattering dynamics of interacting electrons coupled to phonons. This interaction leads to nontrivial 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 one-dimensional Peierls-Hubbard model,

$$H_{\mathrm{PH}} = \sum_\ell U n_{\ell\uparrow} n_{\ell\downarrow} + \sum_\ell \omega_{\mathrm{ph}} b_\ell^\dagger b_\ell + \sum_{\ell\sigma} (c_{\ell\sigma}^\dagger c_{\ell+1\sigma} + \mathrm{H.c.}) \times \left(-t + g(b_\ell^\dagger + b_\ell - b_{\ell+1}^\dagger - b_{\ell+1})\right). \tag{13}$$

Spinful electrons with onsite interaction strength U and hopping amplitude $t=1$, and local phonons with frequency ω_{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 $W=4$ [85,86], initialized as $|\Psi_\pm\rangle = \sum_\ell A e^{-[(x_\ell \mp x_0)/W]^2} e^{\mp i k x_\ell} c_{\ell\pm}^\dagger |0\rangle$, where $|0\rangle$ describes an empty lattice. Without electron-phonon coupling [$g=0$, Fig. 2(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. 2(b)–2(e)], phonons are excited by the electron motion [Fig. 2(c)]. 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. 2(b)]; they thus seem to form a bipolaron, stabilized by a significant phonon density in the central region [Fig. 2(c)].

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

Chiral spin liquid: Spin pumping via flux insertion.—A hallmark of topologically ordered systems is the quantized charge or spin transport. Laughlin famously argued that adiabatically threading an axial magnetic flux through a quantum Hall cylinder pumps quantized charge from one side to the other. This thought experiment, requiring high control of the time evolution, has recently been realized in the lab using a cold-atom integer quantum Hall system [87], but not yet for fractional quantum Hall systems. Here, we numerically demonstrate quantized spin transport for a $S=\frac{1}{2}$ chiral spin liquid (CSL) model with same topological order as the $\nu=\frac{1}{2}$ fractional quantum Hall state [88]. The spin Hamiltonian is

$$H_{\mathrm{CSL}} = \sum_{\langle ij\rangle} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\Delta_{ijk}} (\mathbf{S}_i \times \mathbf{S}_j)\cdot \mathbf{S}_k \tag{14}$$

on a square lattice, $\langle ij\rangle$ enumerates nearest neighbors, and Δ_{ijk} the four clockwise three-site terms of each plaquette [89,90]. We study a $\mathcal{L}_x\times\mathcal{L}_y = 20\times 4$ cylinder threaded by an axial flux θ, implemented via a twisted boundary condition, $S_{x,1+\mathcal{L}_y}^\pm \to e^{\pm i\theta} S_{x,1}^\pm$ [91–93]. Starting from the ground state, we adiabatically ramp up the flux as $\theta(t) = 2\pi t/T$ over a total time $T=20$. According to Laughlin, this transports one spinon from the left to the right edge of the cylinder [94,95]. The challenge is to demonstrate this numerically. To this end, we performed a single, uninterrupted CBE-TDVP evolution run [96].

Figure 3(a) shows the time evolution of the local spin moment per column, $M_x(t) = \sum_{y=1}^{\mathcal{L}_y} S_{x,y}^z(t)$: it decreases (increases) near the left (right) edge at $x=1$ ($\mathcal{L}_x$) while remaining close to zero in between. Importantly, the transferred spin, i.e., the left deficit (right surplus), $\Delta M(t) = -\sum_{x=1}^{\mathcal{L}_x/2} M_x(t) = \sum_{x=(\mathcal{L}_x+1)/2}^{\mathcal{L}_x} M_x(t)$, increases linearly and reaches 0.5 [Fig. 3(a), inset]. Thus, the final

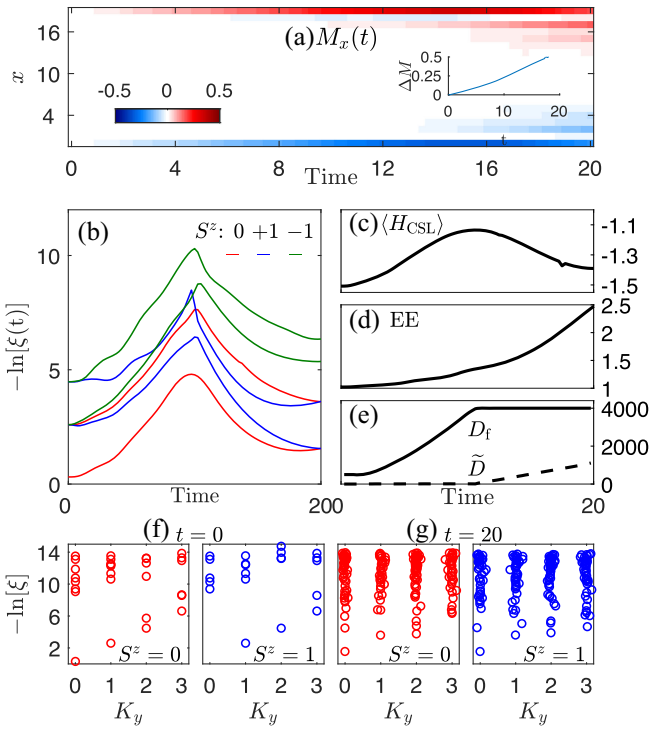


FIG. 3. Adiabatic flux insertion for a chiral spin liquid ($\nu = 1/2$ Laughlin state) on a cylinder, computed with $\delta = 0.05$, $D_{\mathrm{max}} = 4000$, and U(1) spin symmetry. (a) Time evolution of $M_x(t)$, the local spin moment of column x. Inset: $\Delta M(t)$, the spin transferred between the left and right cylinder edges. (b) Spectral flow of the six lowest entanglement eigenvalues for $S^z = 0, \pm 1$. (c) Energy $\langle H_{\mathrm{CSL}}(t)\rangle$; the initial and final values differ due to finite-size effects. (d) Entanglement entropy EE(t). (e) Bond dimensions $D_{\mathrm{f}}^*(t)$, $\tilde{D}_{\mathrm{f}}^*(t)$. (f),(g) Momentum-resolved entanglement spectra of the initial and final states.

state has a fractional Chern number, $C = \frac{1}{2}$, in accord with the fundamental bulk-edge correspondence [98].

Figure 3(b) shows the time evolution of the six lowest-lying levels of the many-body entanglement spectrum (ES) [97,99]. For an integer Chern insulator ($C = n$), a 2π flux insertion is known to shift the ES by n units. Here, by contrast, the degeneracy structure changes: the lowest four levels at $t = 0$ form a singlet and triplet, those at $t = T$ form two doublets. This suggest, again, that a spin-$\frac{1}{2}$ entity has indeed been pumped from left to right.

As a consequence, the initial and final states lie in different topological sectors. Figures 3(f) and 3(g) confirm this by displaying their momentum-resolved entanglement spectra [95,100]. According to conformal field theory, the ES levels in each sector can be labeled by the quantum numbers (S^z, K_y) with integer transverse momentum K_y, and exhibit the multiplicities $\{1, 1, 2, 3, \ldots\}$ [101]. The initial state [Fig. 3(f)] shows a linear K_y dispersion (up to minor finite-size effects) with degeneracies that indeed match this pattern, lying higher for $J^z = 1$ than $J^z = 0$. For the final state [Fig. 3(g)], by contrast, the lowest-lying levels (which again have nearly integer K_y), are almost degenerate for $S^z = 0$ and $S^z = 1$.

Summary 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, $\mathcal{O}(d^2 w D^3)$, and is able to simulate dynamics reliably [44]. CBE-TDVP achieves the same accuracy as 2TDVP, but at 1s costs, $\mathcal{O}(dwD^3)$ (see Ref. [56]). Our benchmark tests of CBE-TDVP demonstrate its reliability. Our results on the Peierls-Hubbard model suggest that bipolarons form during electron scattering—an effect not previously explored numerically. We further simulated adiabatic flux insertion in a CSL and demonstrated the pumping of a spinon through the system. This illustrates the potential of CBE-TDVP for tracking complex dynamics over long times in computationally very challenging models.

For applications involving the time evolution of MPSs defined on "doubled" local state spaces, with effective local bond dimensions $d_{\mathrm{eff}} = d^2$, the cost reduction of CBE–TDVP vs 2TDVP, $\mathcal{O}(d^2 w D^3)$ vs $\mathcal{O}(d^4 w D^3)$, will be particularly dramatic. Examples are finite temperature properties, treated by purification of the density matrix [102], dissipation-assisted operator evolution [103], or tangent tensor renormalization [104]; and the dynamics of open quantum systems [105], described by Liouville evolution of the density matrix [106–108] or by an influence matrix approach [109].

1TDVP-equivalent integrators are also used in computational chemistry for the computation of molecular quantum dynamics [110], where d, the size of the basis sets describing molecular orbitals, easily exceeds 100. There, suboptimal subspace expansion schemes can lead to dramatic problems—CBE offers a solution, and its d^2 to d cost reduction relative to 2TDVP would be huge.

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