Integrable Trotterization: Local Conservation Laws and Boundary Driving

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We discuss a general procedure to construct an integrable real-time Trotterization of interacting lattice models. As an illustrative example, we consider a spin-1/2 chain, with continuous time dynamics described by the isotropic (XXX) Heisenberg Hamiltonian. For periodic boundary conditions, local conservation laws are derived from an inhomogeneous transfer matrix, and a boost operator is constructed. In the continuous time limit, these local charges reduce to the known integrals of motion of the Heisenberg chain. In a simple Kraus representation, we also examine the nonequilibrium setting, where our integrable cellular automaton is driven by stochastic processes at the boundaries. We show explicitly how an exact nonequilibrium steady-state density matrix can be written in terms of a staggered matrix product ansatz, and we propose quasilocal conservation laws for the model with periodic boundary conditions. This simple Trotterization scheme, in particular in the open system framework, could prove to be a useful tool for experimental simulations of the lattice models in terms of trapped ion and atom optics setups.

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Introduction.—Quantum integrable systems out of equilibrium are a topic of intense current research, both theoretically and experimentally [1]. Universal relaxation properties of integrable systems based on the hypothesis of local equilibrium, given by the generalized Gibbs ensemble (GGE) [2], depend crucially on the knowledge of local and quasilocal charges of the system. Furthermore, the study of the nonequilibrium quantum transport problem in integrable systems has been fruitful in the context of the boundary driven Lindblad equation [3], where the properties of the nonequilibrium steady state can be connected to a rigorous existence of ballistic transport at high temperatures. However, all these concepts have, so far, been developed for autonomous, time-independent systems, while much recent interest also goes in the direction of periodically-driven (Floquet) many-body systems, in particular in the connection to topological phases [4] and Floquet time crystals [5,6].

A periodically time-dependent system can be naturally viewed as a Trotter approximation of a one-dimensional interacting, continuous time model, on which state-of-the-art matrix product simulation methods are based [7]. This Trotterized evolution is itself a discrete time dynamical system—in fact, a reversible quantum cellular automaton [8]. The quantum transfer matrix approach, proposed by Klümper *et al.*, [9–11], presents a way of generating Bethe-ansatz integrable systems of this form and of improving the efficiency of transfer-matrix renormalization group calculations [12]. Independently, this kind of integrable quantum evolution has been used in lattice discretizations of continuous field theories, such as the famous sine-Gordon model [13–15].

In this Letter, we discuss an integrable unitary circuit that may be viewed as a Trotter formulation of some integrable continuous Hamiltonian, or an integrable Floquet (periodically driven) quantum chain. We take the simplest and perhaps physically most relevant example of the isotropic Heisenberg spin-1/2 model, i.e., the XXX model. First we define the dynamical system from the inhomogeneous (staggered) transfer matrix. We then proceed to show how two independent families of local conservation laws can be constructed along with a boost operator. Next, we present an integrable steady-state density matrix of a boundary driven dissipative protocol, which is formulated in terms of Krauss maps acting on the boundary spins. This is the first time that an explicit solution of an interacting discrete time quantum Markov chain has been presented. Finally, we propose novel quasilocal conservation laws of the model that could be used to describe generalized thermalization.

Integrable Trotterization.—Consider a chain of N spins-1/2. Instead of a continuous time evolution of the density matrix given by the Liouville–von Neumann equation

$$i\frac{d\rho_t}{dt} = [H, \rho_t], \tag{1}$$

and generated by a Hamiltonian H, we would like to construct a discrete–time map

$$\rho_{t+1} = \mathcal{U}\rho_t\mathcal{U}^\dagger, \tag{2}$$

with $\mathcal{U}$ being a unitary propagator, so that in the appropriate limit, the original continuous dynamics (1) are recovered. The propagator $\mathcal{U}$ should be expressed in terms of a finite sequence of operators U acting locally on the spin chain. Moreover, it should commute with some extensive family

of local operators, $\{Q_k\}$, generated by a transfer matrix, so that we can declare the model to be integrable. From a mathematical point of view, the advantage of such Trotterization would be that the return amplitudes $\langle\psi|\mathcal{U}^n|\psi\rangle$ could be interpreted as partition functions of some vertex models, e.g., with domain wall boundary conditions [16], for which a lot of computational techniques have already been developed.

As an example, we consider a specific nontrivial SU(2)-invariant spin-1/2 model, although the construction should easily be generalizable to other Yang-Baxter integrable models. For the local propagator U, acting on any two neighboring spins of the chain, take the $\check{R}$ matrix of the XXX model [17],

$$U_{j,j+1} = \check{R}_{j,j+1}(\delta), \qquad \check{R}(\lambda) = \frac{1 + i\lambda P}{1 + i\lambda}. \tag{3}$$

Indices denote the spins acted upon by the operator, while P denotes a permutation. If we denote Pauli matrices by $\boldsymbol{\sigma} = (\sigma^x, \sigma^y, \sigma^z)$ and the identity by 1, the latter can be written as $P_{j,j+1} = \frac{1}{2}(1 + \boldsymbol{\sigma}_j \cdot \boldsymbol{\sigma}_{j+1})$. Real parameter δ can be interpreted as a spin coupling constant and is crucial in recovering the continuous dynamics. The particular choice of the normalization of $\check{R}$ ensures unitarity. U, chosen in this way, appears as one of the simplest unitary operations on a pair of spins-1/2 one can think of—it swaps the spins with a probability amplitude proportional to the coupling parameter δ. It can be interpreted as an elementary quantum gate.

Suppose now that N is an even integer. The full unitary propagator acting on the whole chain of N spins-1/2 can be defined as

$$\mathcal{U} = \mathcal{U}_{\text{even}}\mathcal{U}_{\text{odd}} = \prod_{j=1}^{N/2} U_{2j-1,2j} \prod_{k=1}^{N/2} U_{2k,2k+1}. \tag{4}$$

We have imposed periodic boundary conditions so that the sites $N + 1$ and 1 are equivalent. The full propagator $\mathcal{U}$ can be interpreted as two-step discrete-time Floquet dynamics or a quantum cellular automaton, see Fig. 1. The first step is carried by the action of $\mathcal{U}_{\text{odd}}$, which updates all even-odd numbered spins, while in the same manner, the second step $\mathcal{U}_{\text{even}}$ updates spins on odd–even sites.

From the construction of $\mathcal{U}$ it is easy to realize that in the infinitesimal coupling limit, $\delta = -J\Delta t$, with $\Delta t = t/n$ and n being very large, we get $U_{1,2} \sim 1 - i\Delta t\, h_{12}$, where $h_{12} = JP_{12}$ is the local Hamiltonian density of the XXX spin-1/2 chain and

$$\lim_{n\to\infty} \mathcal{U}^n = \exp(-itH). \tag{5}$$

As expected, this is just the Trotter formula for the Hamiltonian of the XXX spin-1/2 model

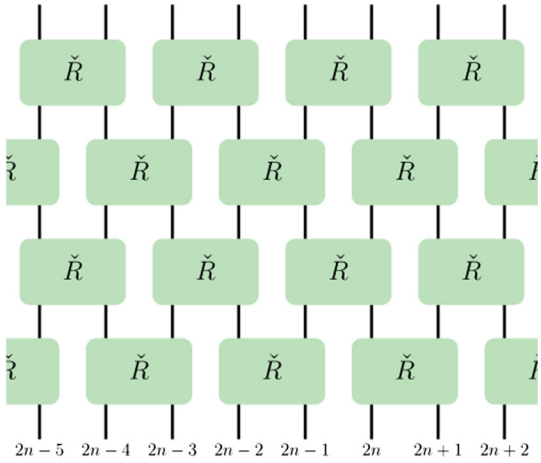

FIG. 1. Time evolution of the model. Each time step consists of two half steps. In the first one, we apply gates $U_{2j-2,2j-1}$, and in the second one, $U_{2j-1,2j}$. The protocol thus shifts for one site each half step.

$$H = \frac{J}{2}\sum_{j=1}^{N}(1 + \boldsymbol{\sigma}_j \cdot \boldsymbol{\sigma}_{j+1}). \tag{6}$$

A similar Trotterization scheme, using the quantum transfer matrix method has been used for computing quantum dynamics for a particular subset of initial states [18], or to simplify computation of dynamical correlation functions [11]. It also corresponds to the row-transfer matrix Floquet integrability as defined in [19].

Since we have taken an $\check{R}$ matrix for the local propagator (3), the integrability of this Trotterization scheme is not surprising. It stems from a family of inhomogeneous (staggered) transfer operators $T(\lambda)$ that are in involution, $[T(\lambda), T(\mu)] = 0$, for all values of the spectral parameters λ and μ. This involution is described in Appendix A of the Supplemental Material [20]. The inhomogeneous transfer operators act on the whole spin chain and can be expressed as

$$T(\lambda) = \mathrm{tr}_0\left(\prod_{1\le j\le N}^{\leftarrow} R_{0,j}\left(\lambda - (-1)^j\frac{\delta}{2}\right)\right), \tag{7}$$

where we have denoted $R(\lambda) = P\check{R}(\lambda)$. The trace is taken over the auxiliary space, which is a copy of a spin-1/2 space, used to facilitate the matrix-product formalism. Elementary evaluation of the transfer operator at two particular points, $\delta/2$ and $-\delta/2$, now yields the following expression for the unitary propagator (4)

$$\mathcal{U} = \left[T\left(-\frac{\delta}{2}\right)\right]^{-1} T\left(\frac{\delta}{2}\right). \tag{8}$$

In particular, this implies the integrability of this model.

In lattice discretizations of continuous field theories, see, e.g., [13–15], the time evolution can generically be put into such a perspective. One example is the sine-Gordon field theory and its discretized version—the quantum Hirota equation [13]. It is a Trotterization of the quantum Volterra model [14]. The entire hierarchy of conservation laws, which we are going to present now, can also be constructed in that case [21].

Local integrals of motion.—The transfer operators (7) generate local integrals of motion through the logarithmic differentiation. Because of the inhomogeneity, we have two families of such local conservation laws, given by evaluating the logarithmic derivatives at the points $\delta/2$ and $-\delta/2$, respectively,

$$Q_n^+ = \frac{d^n}{d\lambda^n}\log T(\lambda)\Big|_{\lambda=\frac{\delta}{2}}, \quad Q_n^- = \frac{d^n}{d\lambda^n}\log T(\lambda)\Big|_{\lambda=-\frac{\delta}{2}}. \tag{9}$$

Conservation laws are invariant under the translation for two lattice sites. Explicit computation shows that the local terms of $Q_n^\pm$ act nontrivially on $2n+1$ neighboring sites. Terms of Q_n^- are, however, shifted for one lattice site to the right, with respect to those of Q_n^+. Explicitly, we can write, for example,

$$Q_1^+ = \sum_{n=1}^{N/2} q^{[1,+]}_{2n-2,2n-1,2n}, \quad Q_1^- = \sum_{n=1}^{N/2} q^{[1,-]}_{2n-1,2n,2n+1}, \tag{10}$$

with the three-site local densities being

$$q^{[1,\pm]}_{1,2,3} = \frac{i}{2(1+\delta^2)}[\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 + \boldsymbol{\sigma}_2\cdot\boldsymbol{\sigma}_3 + \delta^2\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_3 \mp \mp \delta\boldsymbol{\sigma}_1\cdot(\boldsymbol{\sigma}_2\times\boldsymbol{\sigma}_3)]. \tag{11}$$

We have subtracted the trivial terms proportional to the identity. We have also computed the densities of $Q_2^\pm$, which are written in Appendix C of [20]. At this point we would like to stress, that in the continuous–time limit, $\delta \to 0$, both of the derivatives (9) become the same and converge to the standard charges of XXX model [22]. In particular, $\lim_{\delta\to 0} Q_1^\pm \propto H$; i.e., the first pair of charges become the Hamiltonian of the XXX model.

Both sets of conservation laws, Q_n^+ and Q_n^-, can now be equipped with the boost operation—a ladder mapping that transforms lower-order conservation laws into higher-order ones and thus facilitates their computation. In our case, it takes the form

$$[B, Q_n^\pm] = Q_{n+1}^\pm, \tag{12}$$

$$B = \sum_{n=1}^{N/2}\left(n \mod \frac{N}{2}\right)\mathbb{R}'_{2n-3,2n-2|2n-1,2n}(0), \tag{13}$$

with B being the boost operator. In Eq. (13), $f'(0)$ denotes the derivative with respect to λ at the point $\lambda = 0$, while $\mathbb{R}_{12|34}(\lambda) = \check{R}_{23}(\lambda-\delta)\check{R}_{12}(\lambda)\check{R}_{34}(\lambda)\check{R}_{23}(\lambda+\delta)$ is the four-point R matrix. The factor n has been considered modulo $N/2$ due to periodic boundary conditions. The local terms of the boost operator can also be explicitly written in terms of three-site SU(2) invariant products of vectors of Pauli matrices

$$\mathbb{R}'_{12|34}(0) = \frac{i}{2(1+\delta^2)}[\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_2 + \boldsymbol{\sigma}_3\cdot\boldsymbol{\sigma}_4 + 2\boldsymbol{\sigma}_2\cdot\boldsymbol{\sigma}_3 + \delta^2\boldsymbol{\sigma}_2\cdot\boldsymbol{\sigma}_4 + \delta^2\boldsymbol{\sigma}_1\cdot\boldsymbol{\sigma}_3 + \delta\boldsymbol{\sigma}_1\cdot(\boldsymbol{\sigma}_2\times\boldsymbol{\sigma}_3) - \delta\boldsymbol{\sigma}_2\cdot(\boldsymbol{\sigma}_3\times\boldsymbol{\sigma}_4)], \tag{14}$$

where the identity component has been subtracted as it does not affect the boost procedure. Again note that, in the limit $\delta \to 0$, the boost operator becomes the first moment of the XXX model's Hamiltonian, in accordance with [22]. For the derivation of the boost relation, which is similar as in the case of a homogeneous transfer operator [22], see Appendix B of [20].

Dissipative boundaries.—We now wish to study the behavior of the model when a dissipative protocol is performed at the boundaries. The goal is to write a discrete time version of the Lindblad equation with local dissipators located at the first and the last site of an open chain and to find the steady state of the protocol that it defines. For convenience, the length N of the chain is now taken to be an odd integer. The dissipative boundaries can be modeled by two pairs of Kraus operators

$$K_0 = \frac{\mathbb{1}+\sigma_1^z}{2} + \sqrt{1-\gamma_L}\frac{\mathbb{1}-\sigma_1^z}{2}, \quad K_1 = \sqrt{\gamma_L}\sigma_1^+ \tag{15}$$

for the left boundary, and

$$\bar{K}_0 = \frac{\mathbb{1}-\sigma_N^z}{2} + \sqrt{1-\gamma_R}\frac{\mathbb{1}+\sigma_N^z}{2}, \quad \bar{K}_1 = \sqrt{\gamma_R}\sigma_N^- \tag{16}$$

for the right one. Note that, they satisfy the trace preservation conditions, $\sum_{j=0}^1 K_j^\dagger K_j = \mathbb{1}$, $\sum_{j=0}^1 \bar{K}_j^\dagger \bar{K}_j = \mathbb{1}$. We write the dynamics of the density matrix as a two-step discrete-time protocol

$$\rho_{t+1} = \hat{\mathcal{M}}\rho_t, \qquad \hat{\mathcal{M}} = \hat{\mathcal{M}}_{\text{odd}}\hat{\mathcal{M}}_{\text{even}}, \tag{17}$$

where $\hat{\mathcal{M}}_{\text{even}}$ and $\hat{\mathcal{M}}_{\text{odd}}$ are two *completely-positive maps* defined as

$$\hat{\mathcal{M}}_{\text{even}}\rho = \sum_{j=0}^{1} \bar{K}_j \mathcal{U}_{\text{even}} \rho \mathcal{U}_{\text{even}}^{\dagger} \bar{K}_j^{\dagger}$$

$$\hat{\mathcal{M}}_{\text{odd}}\rho = \sum_{j=0}^{1} K_j \mathcal{U}_{\text{odd}} \rho \mathcal{U}_{\text{odd}}^{\dagger} K_j^{\dagger}. \tag{18}$$

The unitary propagators $\mathcal{U}_{\text{even}}$ and $\mathcal{U}_{\text{odd}}$ are defined similarly as in the periodic case, but this time with additional boundary magnetic fields, represented in terms of unitary matrices $B_1 = \exp(ib_L\sigma_1^z)$ and $\bar{B}_N = \exp(ib_R\sigma_N^z)$,

$$\mathcal{U}_{\text{even}} = \prod_{j=1}^{[(N-1)/2]} U_{2j-1,2j}\bar{B}_N,$$

$$\mathcal{U}_{\text{odd}} = B_1 \prod_{j=1}^{[(N-1)/2]} U_{2j,2j+1}. \tag{19}$$

Parameters b_L and b_R correspond to the strengths of magnetic fields at the left and the right edges of the chain, respectively. This process has a very natural interpretation in terms of a repeated interaction protocol [23,24] where, periodically, in each half time step, the left-most (right-most) spin is brought into interaction with a fresh up (down) polarized spin (see Appendix D of [20] for an explicit description). As such, the protocol probably has a more straightforward experimental implementation than the corresponding boundary driven Lindblad equation [3,25,26], which is obtained in the continuum limit $\delta \to 0$.

As is shown in Appendix E of [20], the stationary problem $\rho_\infty = \hat{\mathcal{M}}\rho_\infty$ can be solved exactly for the stationary state ρ_∞. We will see that the structure of the stationary state remarkably resembles that of the inhomogeneous transfer matrix introduced in the previous section. Let us state the ansatz and the result. The stationary state is searched for in the Cholesky form as

$$\rho_\infty = \frac{\Omega^\dagger\Omega}{\text{tr}(\Omega^\dagger\Omega)}, \tag{20}$$

where Ω is a triangular matrix built in an inhomogeneous (staggered) matrix–product form

$$\Omega = D^{\otimes N}\langle 0|L_{a,1}(\lambda,s)L_{a,2}(\lambda-\delta,s)\cdots \times L_{a,N-1}(\lambda-\delta,s)L_{a,N}(\lambda,s)|0\rangle. \tag{21}$$

By D, we have denoted a diagonal matrix that acts on the spin-1/2 space and depends on some arbitrary real parameter χ, while $L(\lambda,s)$ is the well known Lax matrix of the isotropic spin-1/2 Heisenberg model,

$$D = \chi^{\frac{1}{4}\sigma^z}, \qquad L(\lambda,s) = \begin{bmatrix} i\lambda + S^z & S^- \\ S^+ & i\lambda - S^z \end{bmatrix}. \tag{22}$$

In the matrix-product expression (21), Lax matrices are equipped with two indices. The second index denotes the position of the spin in the chain, upon which $L(\lambda,s)$ acts, while the letter a denotes the auxiliary space. The latter is now an infinite-dimensional space with basis $\{|k\rangle\}_{k=0}^{\infty}$, upon which operators S^z and $S^\pm$ act. These operators satisfy sl_2 algebraic relations $[S^z, S^\pm] = \pm S^\pm$ and $[S^+, S^-] = 2S^z$ and can take the following explicit form

$$S^z = \sum_{k=0}^{\infty}(s-k)|k\rangle\langle k|$$

$$S^+ = \sum_{k=0}^{\infty}(k+1)|k\rangle\langle k+1|$$

$$S^- = \sum_{k=0}^{\infty}(2s-k)|k+1\rangle\langle k|. \tag{23}$$

For s being an integer or a half integer, we recover the standard $2s+1$ dimensional unitary spin-s representation from these relations. However, in our case, s and the other two parameters, λ and χ, are complex and real numbers set by the boundary conditions,

$$\lambda = \frac{\delta}{2}\left(\frac{1}{1-e^{-2ib_R}\sqrt{1-\gamma_R}} - \frac{e^{2ib_L}\sqrt{1-\gamma_L}}{1-e^{2ib_L}\sqrt{1-\gamma_L}}\right)$$

$$s = \frac{i\delta}{2}\left(\frac{1}{1-e^{-2ib_R}\sqrt{1-\gamma_R}} + \frac{e^{2ib_L}\sqrt{1-\gamma_L}}{1-e^{2ib_L}\sqrt{1-\gamma_L}}\right)$$

$$\chi = \frac{\gamma_L}{\gamma_R}\frac{2[1-\cos(2b_R)\sqrt{1-\gamma_R}]-\gamma_R}{2[1-\cos(2b_L)\sqrt{1-\gamma_L}]-\gamma_L}. \tag{24}$$

For the derivation of this exact solution, see Appendix E of [20].

Note that, the stationary state shares a lot of common features with the solution of the similar continuous-time model, i.e., the Lindblad-driven XXX spin-1/2 chain (the most general one presented in the review [3]). An important difference to our discrete-time case is the introduction of the inhomogeneous (staggered) structure of the matrix–product ansatz. This is needed in order to deal with the two-step discrete-time dynamics. A conceptually similar procedure is used to write the steady state and Markov eigenvectors of the classical, boundary driven Bobenko cellular automaton—see [27].

Quasilocal charges and Floquet GGE.—Following the procedure outlined in [28,29], we can now propose a family of quasilocal conservation laws for our discrete-time model with periodic boundary conditions. Take $t \in \mathbb{R}$ and let the auxiliary space correspond to a $2s+1$ dimensional spin $s \in \frac{1}{2}\mathbb{Z}$ representation (23). One can generalize the transfer operator (7) as $T_s(\lambda) = \text{tr}_a(\prod_{1\le j\le N}^{\leftarrow} L_{a,j}[\lambda-(-1)^j(\delta/2),s])$. Integrability dictates $[T(\lambda), T_s(\lambda)] = 0$ and

$$X_s(t) = \frac{T_s(t-\frac{i}{2})T'_s(t+\frac{i}{2})}{[\tau_s(t-\frac{\delta}{2})\tau_s(t+\frac{\delta}{2})]^{N/2}}, \tag{25}$$

with $\tau_s(t) = -t^2 - (s+\frac{1}{2})^2$, are the quasilocal conservation laws. For the details, see Appendix F in [20]. We conjecture that $X_s(t)$ form a complete set of quasilocal charges and describe a Floquet generalized Gibbs ensemble (see, e.g., [30,31] for the analogous concept for free systems), which should fully describe relaxation after a quantum quench in analogy to [32].

Conclusion.—We have discussed a method of constructing an integrable real-time Trotterization scheme of interacting lattice models, with both the time evolution and the local conservation laws generated by an inhomogeneous transfer matrix. The discussion related to the hierarchy of local conservation laws can be understood in a wider context—it relies solely on the existence of a unitary solution $R(\lambda)$ of the Yang-Baxter equation, which generates the cellular automaton through the inhomogeneous transfer matrix.

The time evolution of our system is a sequence of local quantum gates and can be understood either as a Floquet driven system or a quantum cellular automaton. As a particular example, we have studied, in detail, a Trotterized XXX spin-1/2 model. For the periodic lattice, we have considered local, as well as quasi-local, integrals of motion and derived the boost operator for the inhomogeneous transfer operator. In the continuous time limit, these conservation laws become those of the XXX model. Apart from that, we have exactly solved a steady state of a boundary driven problem, which is described by the Trotterization scheme in the bulk, while being coupled with a pair of spin reservoirs at the boundaries.

From the point of view of a field theorist, these results provide a method to treat dissipative boundary conditions in a light-cone discretization, while for an experimentalist, the described discrete-time quantum protocol could become a simple paradigm of a spin chain simulator realized by subsequent application of SWAP-like quantum gates, corresponding to the local propagator and additional boundary dissipative processes [33,34].

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