Matrix Product Ansatz for Non-equilibrium Quantum Steady States

D. Karevski, V. Popkov and G.M. Schütz

Abstract We present a general construction of matrix product states for stationary density matrices of one-dimensional quantum spin systems kept out of equilibrium through boundary Lindblad dynamics. As an application we review the isotropic Heisenberg quantum spin chain which is closely related to the generator of the simple symmetric exclusion process. Exact and heuristic results as well as numerical evidence suggest a local quantum equilibrium and long-range correlations reminiscent of similar large-scale properties in classical stochastic interacting particle systems that can be understood in terms of fluctuating hydrodynamics.

Keywords Dissipative quantum spin chains · Lindblad equation
Matrix product ansatz · Nonequilibrium stationary states · Exact solution

1 The Quantum Master Equation

This article is concerned with stationary states of non-equilibrium quantum spin systems, addressing a mathematically minded readership. We spent some effort on recalling – in mathematical terms – relevant basic quantum mechanical notions as well as providing motivations from physics as to why quantum spin systems are of great current interest. Among them is, we feel, a striking analogy with some properties

D. Karevski
Institut Jean Lamour, Département P2M, Groupe de Physique Statistique,
Université de Lorraine, CNRS UMR 7198, B.P. 70239, 54506
Vandoeuvre Les Nancy Cedex, France
e-mail: dragi.karevski@univ-lorraine.fr

V. Popkov
Helmholtz-Institut Für Strahlen-und Kernphysik, Universität Bonn,
Nussallee 14-16, 53119 Bonn, Germany
e-mail: popkov@uni-bonn.de

G.M. Schütz (✉)
Institute of Complex Systems II, Forschungszentrum Jülich, 52425 Jülich, Germany
e-mail: g.schuetz@fz-juelich.de

P. Gonçalves and A.J. Soares (eds.), *From Particle Systems to Partial Differential Equations*, Springer Proceedings in Mathematics & Statistics 209,
DOI 10.1007/978-3-319-66839-0_11

of *classical* stochastic interacting particle systems [4, 10, 31] that we point out in the hope of stimulating further mathematically rigorous work.

Let $\mathfrak{H}$ be a separable complex Hilbert space. A concrete physical quantum system is mathematically defined by a specific self-adjoint (not necessarily bounded) linear operator H on $\mathfrak{H}$, called quantum Hamiltonian (in the following simply Hamiltonian). Vectors in $\mathfrak{H}$ are denoted by the ket-symbol $|\cdot\rangle$ and vectors in the dual space $\mathfrak{H}^*$ are denoted by the bra-symbol $\langle\cdot|$. The scalar product of two vectors $|\Psi\rangle = \sum_n c_n |n\rangle \in \mathfrak{H}$ and $|\Phi\rangle = \sum_n b_n |n\rangle \in \mathfrak{H}$ with coordinates $b_n, c_n \in \mathbb{C}$ in some orthonormal basis $|n\rangle$, $\langle n|$ of $\mathfrak{H}$ and its dual resp. is denoted $\langle\Phi|\Psi\rangle$ and defined to be linear in the *second* argument, i.e., $\langle\Phi|\Psi\rangle := \sum_n \bar{b}_n c_n$ where the bar denotes complex conjugation. We denote the unit operator on $\mathfrak{H}$ by $\mathbf{1}$. The Kronecker symbol $\delta_{a,b}$ is defined by $\delta_{a,b} = 1$ if $a = b$ and $\delta_{a,b} = 0$ else for a and b from any set.

The eigenvalues E_n of the Hamiltonian H are the physical energies measured in an experiment when the physical system is in an eigenstate n of H, defined by the corresponding eigenvector $|\Psi_n\rangle$. One normalizes these eigenvectors, which span the Hilbert space $\mathfrak{H}$, to satisfy the orthogonality relation $\langle\Psi_n|\Psi_m\rangle = \delta_{n,m}$. A spectral ray $|\Psi\rangle \in \mathfrak{H}$ normalized such that $||\Psi||^2 := \langle\Psi|\Psi\rangle = 1$ (i.e. a vector defined up to an arbitrary phase) is called a state vector. It represents the full information that one can have about a quantum system under the idealizing assumption that it is isolated (and has always been isolated) from its physical environment.[1] The modulus $|\psi_n|^2$ of the components of $|\Psi\rangle$ are the probabilities to find the physical system in eigenstate n.

In general, physically observable properties of a quantum system (e.g. particle positions, momenta and so on) are represented by self-adjoint linear operators O_i on $\mathfrak{H}$ which we call *observables*. The "fuzzy" and non-deterministic nature of quantum mechanics is reflected by the fact that the O_i are not all diagonal in some fixed basis of $\mathfrak{H}$ and that only the mean outcome of a large number (mathematically speaking, an infinite number) of measurements of such an observable is predictable. By the mean (or expected) value of an observable O in a general state vector $|\Psi\rangle$ we mean the scalar product $\langle O\rangle \equiv \langle\Psi|O|\Psi\rangle = \sum_{m,n} \bar{c}_m c_n \langle\Psi_m|O|\Psi_n\rangle$.

A self-adjoint positive definite linear operator on $\mathfrak{H}$ with unit trace is called a *density matrix* or *state* (not eigenstate!) of a physical system. Therefore a density matrix ρ with eigenvalues $\rho_n \in \mathbb{R}$ has the properties

$$\rho^\dagger = \rho, \quad \rho_n \geq 0, \quad \mathrm{Tr}(\rho) = 1 \tag{1}$$

where the dagger-symbol † denotes hermitian conjugation. For a given Hilbert space we denote the set of all density matrices by $\mathfrak{S}(\mathfrak{H})$. The mean value of an observable O_i in a state ρ is given by the Frobenius scalar product $\langle O_i\rangle := \mathrm{Tr}(O_i^\dagger \rho)$.

[1] Due to the quantum mechanical phenomenon of entanglement, a quantum subsystem that has interacted with its environment in the past (until some time t_0) cannot be considered isolated for $t \geq t_0$ even when there are no interactions from t_0 onwards.

Unlike a state vector describing a *single and isolated* quantum system, a density matrix contains the full information about a quantum system in either of the following three scenarios:

(1) A density matrix of the specific form

$$\rho = |\,\Psi\,\rangle\langle\,\Psi\,| \tag{2}$$

may describe a single isolated system.[2] In this case we say that ρ is a *pure* state. If a density matrix is not a pure state then there is no state vector $|\,\Psi\,\rangle$ such that $\mathrm{Tr}(O_i^\dagger \rho) = \langle\,\Psi\,|O|\,\Psi\,\rangle$ for all observables O_i.

(2) One describes an *ensemble* of identical isolated quantum systems. In particular, if for some $\beta \in \mathbb{R}_0^+$ the density matrix is of the form

$$\rho = \frac{1}{Z}\mathrm{e}^{-\beta H} \tag{3}$$

where $Z = \mathrm{Tr}\,(\exp(-\beta H))$ we say that the physical system defined by the Hamiltonian H is in thermal equilibrium at temperature $T = 1/\beta$ and the normalization factor Z is called the partition function. In this case the probability to find the system in an eigenstate n of H is proportional to the Boltzmann weight $\exp(-\beta E_n)$ analogous to classical thermodynamics.

(3) ρ describes a subsystem (or an ensemble thereof) of a larger physical system with which *it interacts* (or has interacted in the past).[3]

Pure states and equilibrium states have in common that they remain so when the physical system is isolated from its environment or becomes isolated from some time $t \geq t_0$ onwards. This follows from the time-evolution equation for the density matrix ρ_t of an isolated quantum system with quantum Hamiltonian H

$$\frac{\mathrm{d}}{\mathrm{d}t}\rho_t = -i[H, \rho_t] \tag{4}$$

where the commutator is defined by $[A, B] := AB - BA$. Therefore an equilibrium state is stationary. A pure state $\rho_0 = |\,\Psi(0)\,\rangle\langle\,\Psi(0)\,|$ is only stationary if $|\,\Psi(0)\,\rangle$ is an eigenstate of H, but generally remains a pure state since the evolution equation (4) is solved by the unitary transformation $\rho_t = \exp(-iHt)\rho_0 \exp(iHt)$ which gives $\rho_t = |\,\Psi(t)\,\rangle\langle\,\Psi(t)\,|$ with $|\,\Psi(t)\,\rangle = \exp(-iHt)|\,\Psi(0)\,\rangle$.

We are interested in open systems that are in contact with an environment. In the Markovian approach to open quantum systems [2, 7] the time evolution

---

[2]Following quantum mechanical convention we use the short hand $|\cdot\rangle\langle\cdot| \equiv |\cdot\rangle \otimes \langle\cdot|$ for the Kronecker product $\otimes$ of a state vector $|\cdot\rangle \in \mathfrak{H}$ and some dual state vector $\langle\cdot| \in \mathfrak{H}^*$. We stress that by the rules of tensor calculus one has $\langle\,\Psi\,| \otimes |\,\Phi\,\rangle = |\,\Psi\,\rangle \otimes \langle\,\Phi\,| \equiv |\,\Psi\,\rangle\langle\,\Phi\,|$ but $\langle\,\Psi\,| \otimes |\,\Phi\,\rangle \neq \langle\,\Psi\,|\,\Phi\,\rangle$ since $\langle\,\Psi\,|\,\Phi\,\rangle$ represents the scalar product.

[3]For this scenario, which we have in mind for applications, one often calls ρ the *reduced density matrix*, but we shall refrain doing so here.

$$\rho_t = \Lambda_t \rho_0 \tag{5}$$

is given by a one-parameter semigroup Λ_t of linear endomorphisms on the space $\mathfrak{S}(\mathfrak{H})$ of all density matrices [19]. Under some continuity conditions and for bounded H the Lindblad theorem [12, 21] asserts that the infinitesimal generator $\mathscr{L}$ of the semigroup Λ_t that preserves self-adjointness, positivity and unit trace is of the form

$$\mathscr{L}(\rho) = -i[H, \rho] + \mathscr{D}(\rho). \tag{6}$$

The commutator describes the unitary part of the time evolution (as in an isolated quantum system) and the dissipative part $\mathscr{D}(\rho) \in \mathfrak{End}(\mathfrak{S}(\mathfrak{H}))$, which encodes the physical properties of the coupling to the environment, is of the form

$$\mathscr{D}(\rho) = \sum_j \mathscr{D}_j(\rho), \quad \mathscr{D}_j(\rho) = D_j \rho D_j^\dagger - \frac{1}{2}\{\rho, D_j^\dagger D_j\} \tag{7}$$

with bounded operators $D_j \in \mathfrak{End}(\mathfrak{H})$ and the anticommutator $\{A, B\} := AB + BA$. The evolution equation (6) with dissipators (7) is called *quantum master equation*. The operators D_j that specify an individual dissipator are called Lindblad operators. In an open system a state that is initially pure or in equilibrium does not in general remain so as would be the case in the absence of dissipators in (6). This raises the question of stationary states in open systems.

In order to address existence we introduce the adjoint generator $\mathscr{L}^\dagger$ which is defined as follows [19]. Consider the Banach space $L^1(\mathfrak{H})$ over $\mathbb{R}$ of self-adjoint trace class linear operators $\sigma \in \mathfrak{H}$ with norm given by $||\sigma||_1 = \sup \sum_n |(x_n, \sigma y_n)|$ where the supremum is taken over all orthonormal and complete bases $\{x_n\}$ and $\{y_n\}$ of $\mathfrak{H}$. Then all linear, real and continuous functionals F on $L^1(\mathfrak{H})$ are of the form $\langle F, \sigma\rangle = \mathrm{Tr}(F^\dagger \sigma)$ where F is a bounded self-adjoint linear operator on $\mathfrak{H}$. The set of all such bounded observables F defines the space $L^\infty(\mathfrak{H})$ dual to $L^1(\mathfrak{H})$. Its norm is given by $||F||_\infty = \sup_{||\sigma||_1=1} |\langle F, \sigma\rangle| = \sup_{\Psi\in\mathfrak{H}} ||F\Psi||/||\Psi||$. Then the adjoint generator is given by

$$\mathscr{L}^\dagger(F) = -i[H, F] + \sum_j \left(D_j^\dagger F D_j - \frac{1}{2}\{F, D_j^\dagger D_j\}\right) \tag{8}$$

and one sees that $\mathscr{L}^\dagger(\mathbf{1}) = 0$. If $\mathfrak{H}$ is finite-dimensional then this guarantees the existence of a density matrix ρ such that

$$\mathscr{L}(\rho) = 0. \tag{9}$$

We call a density matrix satisfying (9) a *stationary state*, and, in particular, when $\rho \neq \mathrm{e}^{-\beta H}/Z$ for any $\beta \in \mathbb{R}_0^+$, we call ρ a *non-equilibrium steady state* (NESS) of the open quantum system with Hamiltonian H. For ergodicity and approach to stationarity, which are not our concern, we refer to [11]. For Lindblad operators of

the form $D_j = \Gamma L_j$ with a common coupling constant Γ the strong coupling limit $\Gamma \to \infty$ is called the *Zeno limit*.

Finally we remark that shifting the Lindblad operators by (in general complex) constants c_j generates an additional unitary term in the quantum master equation. More precisely, defining for some $c_j \in \mathbb{C}$ the self-adjoint operators

$$G_j = \frac{i}{2}\left(c_j D_j^\dagger - \bar{c}_j D_j\right), \quad \tilde{H} = H - \sum_j G_j, \tag{10}$$

one has

$$\mathscr{L}(\rho) = \tilde{\mathscr{L}}(\rho) \tag{11}$$

where $\tilde{\mathscr{L}}$ is defined by the modified Hamiltonian $\tilde{H}$ and shifted Lindblad operators

$$\tilde{D}_j := D_j - c_j. \tag{12}$$

Notice that $\tilde{G}_j = G_j$.

This paper deals with the construction of non-equilibrium stationary states ρ defined by (9) for a specific family of physical systems of great interest, viz. quantum spin chains coupled to environment at their boundaries, defined in Sect. 2. In Sect. 3 we generalize in mathematically rigorous form the matrix product ansatz (MPA) of Prosen [27, 29] with local divergence condition introduced by us in [16]. As an application (Sect. 4) we summarize recent progress that we made for the stationary non-equilibrium magnetization profiles in the isotropic spin-1/2 Heisenberg quantum spin chain [16, 17, 25] and discuss it in the light of very recent results [8] on correlation functions for this quantum system. The upshot is that there are substantial and perhaps somewhat unexpected similarities between quantum and classical stationary states of boundary-driven non-equilibrium systems.

2 Quantum Spin Chains

2.1 Why Quantum Spin Chains?

The prototypical model for the quantum mechanical description of magnetism in linear chains of atoms is the so-called Heisenberg quantum spin chain, proposed first in 1928 [13] as an improvement over the classical Ising model which was introduced a few years earlier by Lenz and solved by his student Ernst Ising in 1925 [15]. The simplest version of the Heisenberg model, the spin-1/2 chain defined below, is exactly solvable in the sense of quantum integrability [3]. Hence the equilibrium properties of the system, which were derived in the past decades in a vast body of literature, are rather well understood from a theoretical perspective and to some extent also

experimentally for various spin-chain materials which exhibit quasi one-dimensional interactions between neighbouring atoms.

In recent years, novel experimental Laser techniques involving single cold atoms in optical traps have made the investigation of spin chains *far from thermal equilibrium* feasible. The unique possibilities that the study of individual interacting atoms offers has triggered an immense experimental research activity. On the theoretical side, however, not much is known about non-equilibrium steady states of spin chains which are of particular interest in the case of *boundary driving*, since in this way one obtains information about anomalous transport properties. By boundary driving we mean a scenario where the two ends of a chain are forced into different states by some boundary interaction with the physical environment of the chain, thus inducing stationary currents of locally conserved quantities along the chain. The bulk of the system is considered to be effectively isolated from its physical environment, i.e., described by some quantum Hamiltonian H. The boundary interaction is described by Lindblad dissipators.

Exact results are scarce for chains with more than just a few atoms and there are, to our knowledge, no exact concrete results for specific quantum chains of arbitrary length kept far from thermal equilibrium by some kind of Lindblad boundary-drive. This state of affairs is in stark contrast to classical stochastic interacting particle systems whose Markov generators can be expressed in terms of (non-Hermitian) quantum spin chains [30] and for which many exact and rigorous results exist [6, 9, 18, 20, 30] and which are also amenable to generally applicable analytical approaches such as macroscopic fluctuation theory [5] and non-linear fluctuating hydrodynamics [32].

Nevertheless, a breakthrough in the study of quantum systems far from thermal equilibrium came a few years ago through the work of Prosen [26, 27] who devised a matrix product ansatz (MPA) somewhat reminiscent of the matrix product ansatz for classical stochastic interacting particle systems [6]. This MPA was subsequently developed by us, using a local divergence technique that reveals a link to quantum integrability and symmetries of the quantum system [16]. The MPA allowed for the derivation of recursion relations for mean values of physical observables from which stationary currents, magnetization profiles and correlations could be computed numerically exactly for *large* finite chains and analytically from a continuum approximation to these recursion relations [8, 17, 27]. As pointed out below, these results point to an interesting analogy with a well-known result in classical stochastic interacting particle systems [4, 10, 31].

2.2 Definitions and Notation

The set of integers $\{0, \ldots, n-1\}$ is denoted $\mathbb{S}_n$. We denote the canonical basis vectors of the n-dimensional complex vector space $\mathbb{C}^n$ by the symbol $|\alpha)$ with $\alpha \in \mathbb{S}_n$. Complex conjugation of some $z \in \mathbb{C}$ is denoted by $\bar{z}$. The canonical basis vectors of the dual space are denoted by $(\alpha|$. With the scalar product $(w|v) := \sum_\alpha \bar{w}_\alpha v_\alpha$ and

norm $||v|| = \sqrt{\sum_\alpha |v_\alpha|^2}$ the vector space $\mathbb{C}^n$ becomes a finite-dimensional Hilbert space which we shall call the *local physical space* and denote by $\mathfrak{p}$.

From the canonical basis vectors of $\mathbb{C}^n$ we construct the canonical basis of the space $\mathfrak{End}(\mathbb{C}^n)$ of endomorphisms $\mathbb{C}^n \to \mathbb{C}^n$ by the Kronecker products $E^{\alpha\beta} := |\alpha)(\beta| \equiv |\alpha) \otimes (\beta|$. Generally we shall somewhat loosely identify endomorphisms on some vector space with their matrix representation and sometimes call them operators. The n-dimensional matrices $E^{\alpha\beta}$ have matrix elements $(E^{\alpha\beta})_{jk} = \delta_{\alpha,j}\delta_{\beta,k}$ and they satisfy

$$E^{\alpha\beta}E^{\gamma\delta} = \delta_{\beta,\gamma}E^{\alpha\delta} \tag{13}$$

$$\mathrm{Tr}(E^{\alpha\beta}) = \delta_{\alpha,\beta}. \tag{14}$$

The n-dimensional unit matrix is denoted by $\mathbb{1}$. If a complex number appears as one term in any equation for matrices, then this complex number is understood to be a multiple of the unit matrix.

We construct a canonical basis of $\mathbb{C}^{n^N}$ by the tensor product $|\,\mathbf{a}\,\rangle = |\alpha_1) \otimes \cdots \otimes |\alpha_N)$ with the N-tuple $\mathbf{a} = (\alpha_1, \ldots, \alpha_N) \in \mathbb{S}_n^N$. A general vector in $\mathbb{C}^{n^N}$ with components $v_\mathbf{a}$ is then denoted by $|\,v\,\rangle$. We also define basis vectors $\langle\,\mathbf{a}\,|$ of the dual space $\mathbb{C}^{2^N *}$ (isomorphic to $\mathbb{C}^{2^N}$) and the scalar product $\langle\,w\,|\,v\,\rangle := \sum_{\mathbf{a}\in\mathbb{S}^N} \bar{w}_\mathbf{a} v_\mathbf{a}$ and norm $||v|| = \sqrt{\sum_\mathbf{a} |v_\mathbf{a}|^2}$. With these definitions $\mathbb{C}^{n^N}$ becomes a finite-dimensional Hilbert space which we shall call the *physical space* and denote by $\mathfrak{P}$. Here and below

$$\sum_\mathbf{a} := \sum_{\alpha_1\in\mathbb{S}} \cdots \sum_{\alpha_N\in\mathbb{S}} \tag{15}$$

is the N-fold sum over all indices in $\mathbb{S}$.

From arbitrary matrices $Q \in \mathfrak{End}(\mathbb{C}^n)$ we construct the local tensor operators

$$Q_k = \mathbb{1}^{\otimes(k-1)} \otimes Q \otimes \mathbb{1}^{\otimes(N-k)} \in \mathfrak{End}(\mathfrak{P}). \tag{16}$$

By convention $Q^{\otimes 0} := 1$ and $Q^{\otimes 1} := Q$ for any matrix Q. We denote the unit matrix acting on $\mathfrak{P}$ by $\mathbf{1}$, i.e., $\mathbf{1} = \mathbb{1}^{\otimes N}$. The set of products

$$\{E^{\mathbf{a},\mathbf{a}'}\} = \left\{ \prod_{j=1}^N E_j^{\alpha_j\alpha'_j} \right\} \tag{17}$$

for $\mathbf{a}, \mathbf{a}' \in \mathbb{S}_n^N$ forms a complete basis of $\mathfrak{End}(\mathfrak{P})$. Transposition of a matrix A is denoted by A^T. The adjoint of an operator is denoted $A^\dagger$ which in matrix form means $A^\dagger = \bar{A}^T$. Self-adjoint operators are called Hermitian. It is convenient to represent ket-vectors $|\,v\,\rangle$ as column vectors with components $v_\mathbf{a}$. Then $\langle\,v\,|$ is represented by a row vector with components $\bar{v}_\mathbf{a}$. Elements of a generic vector space $\mathfrak{V}$ (not Hilbert) over $\mathbb{C}$ are denoted by the double-ket symbol $|\cdot\rangle\rangle$ and elements of its dual $\mathfrak{V}^*$ by the double-bra symbol $\langle\langle\cdot|$. A linear form $\phi_W : \mathfrak{V} \to \mathbb{C}$ is denoted by $\langle\langle\,W\,|\cdot\rangle\rangle$.

With these conventions we are now in a position to define the objects of our investigation.

Definition 1 Let $h \in \mathfrak{End}(\mathbb{C}^{n^2})$ and $b^L, b^R \in \mathfrak{End}(\mathbb{C}^n)$ be self-adjoint and $b_1^L = b^L \otimes \mathbb{1}^{\otimes(N-1)}$, $b_N^R = \mathbb{1}^{\otimes(N-1)} \otimes b^R$, $h_{k,k+1} = \mathbb{1}^{\otimes(k-1)} \otimes h \otimes \mathbb{1}^{\otimes(N-k-1)}$. Then a homogeneous quantum spin chain with $N \geq 2$ sites with nearest-neighbour interaction h and boundary fields $b^{L,R}$ is defined by the Hamiltonian

$$H = b_1^L + b_N^R + \sum_{k=1}^{N-1} h_{k,k+1}. \tag{18}$$

A quantum spin system with one site is defined by a self-adjoint operator $b \in \mathfrak{End}(\mathbb{C}^n)$.

Definition 2 For $D^{\chi_k} \in \mathfrak{End}(\mathbb{C}^n)$ and a density matrix $\rho \in \mathfrak{S}(\mathfrak{P})$ the operator

$$\mathscr{D}_k(\rho) := D_k^{\chi_k} \rho D_k^{\chi_k\dagger} - \frac{1}{2}\left(\rho D_k^{\chi_k\dagger} D_k^{\chi_k} + D_k^{\chi_k\dagger} D_k^{\chi_k} \rho\right), \quad 1 \leq k \leq N, \quad N \geq 1 \tag{19}$$

is called dissipator at site k with local Lindblad operator D^{χ_k}, indexed by a symbol χ_k. For $N = 1$ the lower index $k = 1$ is dropped.

Definition 3 Let H be a quantum spin Hamiltonian with N sites according to Definition 1, $\mathscr{D}_1$ and $\mathscr{D}_N$ be dissipators with local Lindblad operators D^L and D^R resp. according to Definition 2 and let $\rho \in \mathfrak{S}(\mathfrak{P})$ be the solution of the equation

$$-i[H, \rho] + \mathscr{D}_1(\rho) + \mathscr{D}_N(\rho) = 0. \tag{20}$$

Then ρ is called a non-equilibrium stationary state of the boundary-driven quantum spin system defined by H.

We remark that the construction of matrix product states given below is straightforwardly generalized to more than one boundary dissipator at each edge of the chain.

3 Construction of Stationary Matrix Product States

3.1 Matrix Product Ansatz

In order to construct a solution of the stationary Lindblad equation of the form (20) we first make the following observations:

(a) For any density matrix $\rho \in \mathfrak{S}(\mathfrak{P})$ one can find a matrix $M \in \mathfrak{End}(\mathfrak{P})$ such that

$$\rho = MM^\dagger / Z \tag{21}$$

with the *partition function*

$$Z := \mathrm{Tr}(MM^\dagger). \tag{22}$$

Thus, given M one knows ρ.[4]

(b) One can expand M in the basis (17) of $\mathfrak{End}(\mathfrak{P})$ as

$$M = \sum_{\mathbf{a},\mathbf{a}'} M_{\mathbf{a},\mathbf{a}'} E_1^{\alpha_1,\alpha_1'} \dots E_N^{\alpha_N,\alpha_N'}. \tag{23}$$

The idea of the matrix product ansatz (MPA) is to write the matrix elements $M_{\mathbf{a},\mathbf{a}'}$ as the linear form [27, 29]

$$M_{\mathbf{a},\mathbf{a}'} = \langle\langle\, W \,|\Omega^{\alpha_1,\alpha_1'} \dots \Omega^{\alpha_N,\alpha_N'}|\, V \,\rangle\rangle \tag{24}$$

where $|\, V \,\rangle\rangle$ is a vector in some (generally infinite-dimensional) auxiliary space $\mathfrak{A}$, the n^2 matrices $\Omega^{\alpha,\alpha'}$ are suitably chosen endomorphisms of $\mathfrak{A}$ and $\langle\langle\, W \,|$ is a suitably chosen vector from the dual space $\mathfrak{A}^*$.

In order to use this MPA in applications we need to add some more structure. We define $\bar{\Omega}^{\alpha,\alpha'} \in \mathfrak{End}(\mathfrak{A})$ by complex conjugation of the matrix representation of $\Omega^{\alpha,\alpha'}$. Next we construct

$$\Omega := \sum_{\alpha,\alpha'} E^{\alpha\alpha'} \otimes \Omega^{\alpha\alpha'}, \quad \Omega^\star := \sum_{\alpha,\alpha'} E^{\alpha\alpha'} \otimes \bar{\Omega}^{\alpha'\alpha} \quad \in \mathfrak{End}(\mathbb{C}^n \otimes \mathfrak{A}) \tag{25}$$

$$\Omega^{\otimes_p N} := \sum_{\mathbf{a},\mathbf{a}'} E^{\alpha_1\alpha_1'} \otimes \dots \otimes E^{\alpha_N\alpha_N'} \otimes \Omega^{\alpha_1\alpha_1'} \dots \Omega^{\alpha_N\alpha_N'} \in \mathfrak{End}(\mathfrak{P} \otimes \mathfrak{A}) \tag{26}$$

and analogously $(\Omega^\star)^{\otimes_p N} = \left(\Omega^{\otimes_p N}\right)^\star$. The subscript p at the tensor symbol indicates that the tensor product is only taken over the local physical space $\mathfrak{p}$, i.e., the term $\Omega^{\alpha_1\alpha_1'} \dots \Omega^{\alpha_N\alpha_N'} \in \mathfrak{End}(\mathfrak{A})$ in (26) is the usual matrix product. The star $\star$ denotes the adjoint operation on the physical space $\mathfrak{P}$ only, not on the auxiliary space. This means that the matrix $\left(\Omega^{\otimes_p N}\right)^\star$ is obtained from the matrix $\Omega^{\otimes_p N}$ by transposition and complex conjugation of its components $\Omega^{\otimes_p N}_{\mathbf{a},\mathbf{a}'} = \Omega^{\alpha_1\alpha_1'} \dots \Omega^{\alpha_N\alpha_N'} \mapsto \bar{\Omega}^{\alpha_1'\alpha_1} \dots \bar{\Omega}^{\alpha_N'\alpha_N} = \left(\Omega^{\otimes_p N}\right)^\star_{\mathbf{a},\mathbf{a}'}$ as in the second definition in (25) *without* reversing the order of the matrix products and *without* transposing the matrices $\Omega^{\alpha_j\alpha_j'}$.

This construction immediately leads to the following lemma:

Lemma 1 *Let $\mathfrak{A}$ be a vector space, $\Omega^{\alpha,\alpha'} \in \mathfrak{End}(\mathfrak{A})$ for $\alpha, \alpha' \in \mathbb{S}_n$, $|\, V \,\rangle\rangle$, $|\, \overline{V} \,\rangle\rangle \in \mathfrak{A}$ and $\langle\langle\, W \,|$, $\langle\langle\, \overline{W} \,| \in \mathfrak{A}^*$ where the bar denotes complex conjugation of each vector component. Then M, $M^\dagger \in \mathfrak{End}(\mathfrak{P})$ defined by (23) and (24) can be written*

[4] M is not uniquely defined. For a given M and arbitrary unitary U the product MU gives the same ρ. This non-uniqueness seems to be exactly the point that makes M easier to treat than ρ.

$$M = \langle\langle\, W \,|\Omega^{\otimes_p N}|\, V \,\rangle\rangle, \quad M^\dagger = \langle\langle\, \overline{W} \,|\, \left(\Omega^\star\right)^{\otimes_p N} |\, \overline{V} \,\rangle\rangle \tag{27}$$

where the linear form $\langle\langle\, W \,|\cdot|\, V \,\rangle\rangle$ *on* $\mathfrak{A}$ *is taken on each component* $\Omega^{\alpha_1\alpha'_1} \ldots \Omega^{\alpha_N\alpha'_N}$ *of the endomorphism* $\Omega^{\otimes_p N}$ *on* $\mathfrak{P} \otimes \mathfrak{A}$.

Lemma 1 follows immediately from the expansion $\Omega = \sum_{\alpha,\alpha'} E^{\alpha\alpha'} \otimes \Omega^{\alpha\alpha'}$ and the multilinearity of the Kronecker product. It expresses the fact that $\Omega^{\otimes N}$ can be thought of as a matrix of dimension n^N (the dimension of the physical space $\mathfrak{P}$) whose matrix elements $(\mathbf{a}, \mathbf{a}')$ are the products $\Omega^{\alpha_1\alpha'_1} \ldots \Omega^{\alpha_N\alpha'_N}$ of (generally infinite-dimensional) matrices acting on the auxiliary space $\mathfrak{A}$. The linear form $\langle\langle\, W \,|\cdot|\, V \,\rangle\rangle$ maps each of these matrix products onto $\mathbb{C}$ so that M is indeed a usual matrix of dimension n^N.

The next technical idea is to double the auxiliary space. To this end we denote the unit operator on $\mathfrak{A}$ by I and define $\Omega_1^{\alpha\alpha'} := \Omega^{\alpha\alpha'} \otimes I$ and $\Omega_2^{\alpha\alpha'} := I \otimes \Omega^{\alpha\alpha'}$ which are endomorphisms of $\mathfrak{A}^2$. The multilinearity of the tensor product allows us to write $\Omega_1^{\alpha\alpha'}\Omega_2^{\beta\beta'} = \Omega^{\alpha\alpha'} \otimes \Omega^{\beta\beta'}$ for any $\alpha, \alpha', \beta, \beta' \in \mathbb{S}$. We also define in analogy to (25) the following endomorphisms of $\mathfrak{P} \otimes \mathfrak{A}^2$

$$\Omega_1 := \sum_{\alpha,\alpha'} E^{\alpha\alpha'} \otimes \Omega^{\alpha\alpha'} \otimes I, \quad \Omega_2 := \sum_{\alpha,\alpha'} E^{\alpha\alpha'} \otimes I \otimes \Omega^{\alpha\alpha'} \tag{28}$$

$$\Omega_1^\star := \sum_{\alpha,\alpha'} E^{\alpha\alpha'} \otimes \bar{\Omega}^{\alpha'\alpha} \otimes I, \quad \Omega_2^\star := \sum_{\alpha,\alpha'} E^{\alpha\alpha'} \otimes I \otimes \bar{\Omega}^{\alpha'\alpha}. \tag{29}$$

Lemma 2 *Let* $\mathfrak{A}$ *be a vector space and* $|\, V \,\rangle\rangle, |\, \overline{V} \,\rangle\rangle \in \mathfrak{A}$ *and* $\Omega^{\alpha\alpha'} \in \mathfrak{End}(\mathfrak{A})$ *for* $\alpha, \alpha' \in \mathbb{S}_n$ *and* $\langle\langle\, W \,|, \langle\langle\, \overline{W} \,| \in \mathfrak{A}^*$. *For some* $\Theta^{\alpha\alpha'} \in \mathfrak{End}(\mathfrak{A}^2)$ *define*

$$\Theta := \sum_{\alpha,\alpha'} E^{\alpha\alpha'} \otimes \Theta^{\alpha\alpha'} \in \mathfrak{End}(\mathbb{C}^2 \otimes \mathfrak{A}^2) \tag{30}$$

$$\Theta^{\otimes_p N} := \sum_{\mathbf{a},\mathbf{a}'} E^{\alpha_1\alpha'_1} \otimes \cdots \otimes E^{\alpha_N\alpha'_N} \otimes \Theta^{\alpha_1\alpha'_1} \ldots \Theta^{\alpha_N\alpha'_N} \in \mathfrak{End}(\mathfrak{P} \otimes \mathfrak{A}^2). \tag{31}$$

Then for

$$\Theta = \Omega_1\Omega_2^\star \tag{32}$$

a density matrix $\rho \in \mathfrak{S}(\mathfrak{P})$ *has the matrix product representation*

$$\rho = \langle\langle\, W, \overline{W} \,|\Theta^{\otimes_p N}|\, V, \overline{V} \,\rangle\rangle. \tag{33}$$

where the tensor products

$$|\, V, \overline{V} \,\rangle\rangle := |\, V \,\rangle\rangle \otimes |\, \overline{V} \,\rangle\rangle \in \mathfrak{A} \otimes \mathfrak{A}, \quad \langle\langle\, W, \overline{W} \,| := \langle\langle\, W \,| \otimes \langle\langle\, \overline{W} \,| \in \mathfrak{A}^* \otimes \mathfrak{A}^* \tag{34}$$

define a bilinear form $\phi_{W,\overline{W}} : \mathfrak{A} \otimes \mathfrak{A} \to \mathbb{C}$.

Proof We first note that for the scalar product on the physical space $\mathfrak{P}$ we have

$$\langle \mathbf{a} \,|\Theta^{\otimes_p N}|\, \mathbf{a}' \rangle = \Theta^{\alpha_1\alpha_1'} \ldots \Theta^{\alpha_N\alpha_N'}. \tag{35}$$

Furthermore, by the construction (32) for a single site and definition (28), one finds

$$\Theta^{\alpha\alpha'} = \sum_\beta (\alpha|\Omega_1|\beta)(\beta|\Omega_2^\star|\alpha') = \sum_\beta \Omega_1^{\alpha\beta}(\Omega_2^\star)^{\beta\alpha'} = \sum_\beta \Omega_1^{\alpha\beta}\bar{\Omega}_2^{\alpha'\beta} \tag{36}$$

and therefore with $\mathbf{b} := (\beta_1, \ldots, \beta_N) \in \mathbb{S}_n^N$

$$\begin{aligned}\Theta^{\alpha_1\alpha_1'} \ldots \Theta^{\alpha_N\alpha_N'} &= \sum_{\mathbf{b}} \Omega_1^{\alpha_1\beta_1}\bar{\Omega}_2^{\alpha_1'\beta_1} \ldots \Omega_1^{\alpha_N\beta_N}\bar{\Omega}_2^{\alpha_N'\beta_N} \\ &= \sum_{\mathbf{b}} \Omega^{\alpha_1\beta_1} \ldots \Omega^{\alpha_N\beta_N} \otimes \bar{\Omega}^{\alpha_1'\beta_1} \ldots \bar{\Omega}^{\alpha_N'\beta_N}.\end{aligned} \tag{37}$$

This shows that $\Theta^{\alpha_1\alpha_1'} \ldots \Theta^{\alpha_N\alpha_N'} \in \mathfrak{End}(\mathfrak{A}^2)$ is decomposable into a finite sum of endomorphisms of $\mathfrak{A} \otimes \mathfrak{A}$. Then the factorization property of the scalar product involving the tensor vectors (34) and the tensor operators (37) and Lemma 1 give

$$\begin{aligned}\langle\langle W, \overline{W} \,|\Theta^{\otimes_p N}|\, V, \overline{V} \rangle\rangle_{\mathbf{a}\mathbf{a}'} &= \langle\langle W, \overline{W} \,|\Theta^{\alpha_1\alpha_1'} \ldots \Theta^{\alpha_N\alpha_N'}|\, V, \overline{V} \rangle\rangle \\ &= \sum_{\mathbf{b}} \langle\langle W \,|\Omega^{\alpha_1\beta_1} \ldots \Omega^{\alpha_N\beta_N}|\, V \rangle\rangle \overline{\langle\langle W \,|\Omega^{\alpha_1'\beta_1} \ldots \Omega^{\alpha_N'\beta_N}|\, V \rangle\rangle} \\ &= \sum_{\mathbf{b}} M_{\mathbf{a}\mathbf{b}}\bar{M}_{\mathbf{a}'\mathbf{b}}\end{aligned} \tag{38}$$

The l.h.s. of the first equation is the matrix element ρ. Observing that $\bar{M}_{\mathbf{a}'\mathbf{b}} = M^\dagger_{\mathbf{b}\mathbf{a}'}$ and completeness of the basis (17) shows that the r.h.s. of the last equation is equal to $(MM^\dagger)_{\mathbf{a}\mathbf{a}'}$. Thus (33) is proved for each matrix element of ρ. □

The point of this lemma is the fact that a matrix product form of M induces a matrix product form for ρ which allows for a computation of physical observables in terms of the matrices $\Omega^{ss'}$. This is the content of the following proposition.

Proposition 1 *Let $\rho \in \mathfrak{S}(\mathfrak{P})$ be a density matrix with partition function Z (22) and $|\, V, \overline{V} \,\rangle\rangle$, $\langle\langle\, W, \overline{W} \,|$ as defined in (34). With*

$$\Theta_0 := \sum_\alpha \Theta^{\alpha\alpha} = \sum_{\alpha\beta} \Omega_1^{\alpha\beta}\bar{\Omega}_2^{\alpha\beta} \quad \in \mathfrak{End}\left(\mathfrak{A}^2\right) \tag{39}$$

one has

$$Z = \langle\langle\, W, \overline{W}\,|\Theta_0^N|\, V, \overline{V}\,\rangle\rangle \tag{40}$$

$$\begin{aligned}&\langle\, E_{k_1}^{\alpha_1\alpha_1'} E_{k_2}^{\alpha_2\alpha_2'} \dots E_{k_n}^{\alpha_n\alpha_n'}\,\rangle \\ &= \langle\langle\, W, \overline{W}\,|\Theta_0^{k_1-1}\Theta^{\alpha_1'\alpha_1}\Theta_0^{k_2-k_1-1}\Theta^{\alpha_2'\alpha_2}\dots\Theta^{\alpha_n'\alpha_n}\Theta_0^{N-k_n}|\, V, \overline{V}\,\rangle\rangle/Z\end{aligned} \tag{41}$$

Proof The equality following the definition in (39) follows from (36). By construction we have for the partition function (40)

$$\begin{aligned}Z &= \sum_{\mathbf{a},\mathbf{a}'} \mathrm{Tr}\left(E_1^{\alpha_1\alpha_1'}\dots E_N^{\alpha_N\alpha_N'}\right)\langle\langle\, W, \overline{W}\,|\Theta^{\alpha_1\alpha_1'}\dots\Theta^{\alpha_N\alpha_N'}|\, V, \overline{V}\,\rangle\rangle \\ &= \sum_{\mathbf{a},\mathbf{a}'}\left(\prod_{j=1}^{N}\mathrm{Tr}\left(E^{\alpha_j\alpha_j'}\right)\right)\langle\langle\, W, \overline{W}\,|\Theta^{\alpha_1\alpha_1'}\dots\Theta^{\alpha_N\alpha_N'}|\, V, \overline{V}\,\rangle\rangle\end{aligned} \tag{42}$$

where in the second equality we have used the factorization property of the trace for tensor products. The trace property (14) yields the expression (40) for the partition function Z. The expression (41) follows in similar fashion by noting that due to (13) one has $\mathrm{Tr}(E^{\alpha\alpha'}E^{\beta\beta'}) = \delta_{\alpha,\beta'}\delta_{\alpha',\beta}$. □

Remark 1 Since an observable $O_k \in \mathfrak{End}(\mathfrak{P})$ can be expanded $O_k = \sum_{\alpha\alpha'} O_k^{\alpha\alpha'} E_k^{\alpha\alpha'}$ with numerical coefficients of the form $O_k^{\alpha\alpha'} = \bar{O}_k^{\alpha'\alpha} \in \mathbb{C}$, Proposition 1 allows for computing averages of products of local observables in terms of matrix products involving the matrices $\Theta^{\alpha\alpha'}$ and Θ_0.

We note two useful corollaries of Lemma 2 which follow directly from (36).

Corollary 1 *Let ρ be a density matrix according to Lemma 2 and $D_k = \mathbb{1}^{\otimes(k-1)} \otimes D \otimes \mathbb{1}^{\otimes(N-k)}$ be a Lindblad operator acting non-trivially only on site k with some local Lindblad operator $D \in \mathfrak{End}(\mathbb{C}^n)$. Then for the local dissipator $\mathscr{D}_k$ with Lindblad operator D_k one has*

$$\mathscr{D}_k(\rho) = \frac{1}{Z}\langle\langle\, W, \overline{W}\,|\Theta^{\otimes(k-1)} \otimes \Delta \otimes \Theta^{\otimes(N-k)}|\, V, \overline{V}\,\rangle\rangle \tag{43}$$

with Z of Proposition 1 and

$$\Delta = \sum_{\beta}\sum_{\alpha\alpha'} \mathscr{D}\left(E^{\alpha\alpha'}\right) \otimes \Omega_1^{\alpha\beta}\bar{\Omega}_2^{\alpha'\beta} \tag{44}$$

where $\mathscr{D}$ is the dissipator with the local Lindblad operator D.

Corollary 2 *Let ρ be a density matrix according to Lemma 2 and $b_k = \mathbb{1}^{\otimes(k-1)} \otimes b \otimes \mathbb{1}^{\otimes(N-k)} \in \mathfrak{End}(\mathfrak{P})$ be a self-adjoint operator acting non-trivially only on site k with some local self-adjoint operator $b \in \mathfrak{End}(\mathbb{C}^n)$. Then for the unitary part of the time-evolution of the density matrix under b_k one has*

$$-i[b_k, \rho] = \frac{1}{Z}\langle\langle W, \overline{W}\,|\Theta^{\otimes(k-1)} \otimes \Gamma \otimes \Theta^{\otimes(N-k)}|\, V, \overline{V}\,\rangle\rangle \tag{45}$$

with Z of Proposition 1 and

$$\Gamma = -i \sum_{\beta} \sum_{\alpha\alpha'} \left[b, E^{\alpha\alpha'}\right] \otimes \Omega_1^{\alpha\beta} \bar{\Omega}_2^{\alpha'\beta}. \tag{46}$$

For $D = \sum_{\alpha\alpha'} D_{\alpha\alpha'} E^{\alpha\alpha'}$, $b = b^\dagger = \sum_{\alpha\alpha'} b_{\alpha\alpha'} E^{\alpha\alpha'}$ we note

$$\mathscr{D}(E^{\alpha\alpha'}) = \sum_{\beta\beta'} \left(D_{\beta\alpha} \bar{D}_{\beta'\alpha'} E^{\beta\beta'} - \frac{1}{2} D_{\beta\beta'} \bar{D}_{\beta\alpha'} E^{\alpha\beta'} - \frac{1}{2} D_{\beta'\alpha} \bar{D}_{\beta'\beta} E^{\beta\alpha'} \right) \tag{47}$$

$$\left[b, E^{\alpha\alpha'}\right] = \sum_{\beta} \left(b_{\beta\alpha} E^{\beta\alpha'} - \bar{b}_{\beta\alpha'} E^{\alpha\beta} \right) \tag{48}$$

which follows from (13) by straightforward computation and $b = b^\dagger$.

3.2 Main Result

The previous discussion is "abstract nonsense" in so far as we have provided no information about the matrices $\Omega^{\alpha\alpha'}$ and the vectors $\langle\langle W \,|$ and $|\, V \rangle\rangle$ from which a stationary density matrix ρ solving (20) could be constructed. In order to state a sufficient property of the $\Omega^{\alpha\alpha'}$ we define the local divergence condition which was first introduced for $n = 2$ in [16].

Definition 4 (*Local divergence condition*) Let H be a quantum spin Hamiltonian according to Definition 1 and with finite local physical space $\mathfrak{p}$ and let $\mathfrak{A}$ be a vector space with unit operator denoted by I. For $\Omega^{\alpha\alpha'}, \Xi^{\alpha\alpha'} \in \mathfrak{End}(\mathfrak{A})$ define $\Omega := \sum_{\alpha\alpha'} E^{\alpha\alpha'} \otimes \Omega^{\alpha\alpha'} \in \mathfrak{End}(\mathfrak{p} \otimes \mathfrak{A})$, $\Xi := \sum_{\alpha\alpha'} E^{\alpha\alpha'} \otimes \Xi^{\alpha\alpha'} \in \mathfrak{End}(\mathfrak{p} \otimes \mathfrak{A})$, and $\hat{h} := h \otimes I \in \mathfrak{End}(\mathfrak{p}^2 \otimes \mathfrak{A})$. We say that H satisfies a local divergence condition w.r.t. some non-zero Ω and Ξ if

$$\left[\hat{h}, \Omega \otimes_p \Omega\right] = \Xi \otimes_p \Omega - \Omega \otimes_p \Xi \tag{49}$$

where the tensor product $\otimes_p$ over the physical space is defined by $\Xi \otimes_p \Omega := \sum_{\alpha\alpha'} \sum_{\beta\beta'} E^{\alpha\alpha'} \otimes E^{\beta\beta'} \otimes (\Xi^{\alpha\alpha'} \Omega^{\beta\beta'})$.

Remark 2 The local divergence condition (49) defines a quadratic algebra [22] for $2n^2$ generators $\Omega^{\alpha\alpha'}$ and $\Xi^{\alpha\alpha'}$. Quadratic algebras arise e.g. as universal enveloping algebras of Lie algebras and also play an important role in the theory of quantum groups. They also arise in the study of invariant measures of stochastic interacting particle systems [1, 6]. The local divergence condition can be generalized to include

a term $\hat{T}\Omega \otimes_p \Omega - \hat{T}\Omega \otimes_p \Omega$ where $\hat{T} = \mathbb{1} \otimes \mathbb{1} \otimes T$ and $T \in \mathfrak{End}(\mathfrak{A})$ [24]. This extension gives rise to a cubic algebra.

Next we define the *Lindblad boundary matching condition* which underlies in some shape or form many concrete applications of the MPA [29], but which to our knowledge has never been stated as such and in full generality.

Definition 5 (*Lindblad boundary matching condition*) Let $\mathfrak{A}$ be a vector space. For $|\, V \,\rangle\rangle \in \mathfrak{A}$ and $\langle\langle\, W \,| \in \mathfrak{A}^*$ define the vectors $|\, V, \overline{V} \,\rangle\rangle := |\, V \,\rangle\rangle \otimes |\, \overline{V} \,\rangle\rangle$ and $\langle\langle\, W, \overline{W} \,| := \langle\langle\, W \,| \otimes \langle\langle\, \overline{W} \,|$ and for $\Omega^{\alpha\alpha'}, \bar{\Omega}^{\alpha\alpha'}, \Xi^{\alpha\alpha'}, \bar{\Xi}^{\alpha\alpha'} \in \mathfrak{End}(\mathfrak{A})$ define the endomorphisms

$$\Lambda^{\alpha\alpha'} := i \sum_{\beta} \left(\Omega^{\alpha\beta} \otimes \bar{\Xi}^{\alpha'\beta} - \Xi^{\alpha\beta} \otimes \bar{\Omega}^{\alpha'\beta} \right) \tag{50}$$

and for $B \in \{L, R\}$ with $b^B_{\alpha\alpha'} = \bar{b}^B_{\alpha'\alpha} \in \mathbb{C}$, $D^B_{\alpha\alpha'} \in \mathbb{C}$

$$\Gamma^{\alpha\alpha'}_B := -i \sum_{\beta\beta'} \left(b^B_{\alpha\beta} \Omega^{\beta\beta'} \otimes \bar{\Omega}^{\alpha'\beta'} - \bar{b}^B_{\alpha'\beta} \Omega^{\alpha\beta'} \otimes \bar{\Omega}^{\beta\beta'} \right) \tag{51}$$

$$\begin{aligned} \Delta^{\alpha\alpha'}_B := \sum_{\beta\beta'} \sum_{\gamma} \Big(& D^B_{\alpha\beta} \bar{D}^B_{\alpha'\beta'} \Omega^{\beta\gamma} \otimes \bar{\Omega}^{\beta'\gamma} \\ & - \frac{1}{2} D^B_{\beta\alpha'} \bar{D}^B_{\beta\beta'} \Omega^{\alpha\gamma} \otimes \bar{\Omega}^{\beta'\gamma} - \frac{1}{2} D^B_{\beta'\beta} \bar{D}^B_{\beta'\alpha} \Omega^{\beta\gamma} \otimes \bar{\Omega}^{\alpha'\gamma} \Big) . \end{aligned} \tag{52}$$

We say that vectors $|\, V \,\rangle\rangle \in \mathfrak{A}$ and $\langle\langle\, W \,| \in \mathfrak{A}^*$ satisfy the *Lindblad boundary matching condition* w.r.t. Ω and Ξ if for all $\alpha, \alpha' \in \mathbb{S}_n$

$$0 = \langle\langle\, X \,| \left(\Gamma^{\alpha\alpha'}_R + \Delta^{\alpha\alpha'}_R - \Lambda^{\alpha\alpha'} \right) |\, V, \overline{V} \,\rangle\rangle = \langle\langle\, W, \overline{W} \,| \left(\Gamma^{\alpha\alpha'}_L + \Delta^{\alpha\alpha'}_L + \Lambda^{\alpha\alpha'} \right) |\, Y \,\rangle\rangle \tag{53}$$

for all $\langle\langle\, X \,| \in \mathfrak{A}^{2*}$ and all $|\, Y \,\rangle\rangle \in \mathrm{span}(\Theta^{\alpha_2,\alpha'_2} \ldots \Theta^{\alpha_N,\alpha'_N} |\, V, \overline{V} \,\rangle\rangle)$ for $N \geq 2$.

Remark 3 Define $\Lambda_0 := \sum_\alpha \Lambda^{\alpha\alpha}$. It is easy to see that $0 = \sum_\alpha \Delta^{\alpha\alpha}_B = \sum_\alpha \Gamma^{\alpha\alpha}_B$. Hence (53) implies $0 = \langle\langle\, X \,| \Lambda_0 |\, V, \overline{V} \,\rangle\rangle = \langle\langle\, W, \overline{W} \,| \Lambda_0 |\, Y \,\rangle\rangle$. For the extended local divergence condition with operator T the Lindblad boundary matching condition acquires an extra term $\{T, \Omega^{\alpha\alpha'}\}$ in both brackets in (53).

With these preparations we are in a position to state the main result in terms of the original local divergence condition (49). The adaptation to the extended local divergence condition is trivial.

Theorem 1 *Given a quantum spin Hamiltonian*

$$H = H_b + H_s \tag{54}$$

according to Definition 1 with bulk part $H_b = \sum_{k=1}^{N-1} h_{k,k+1}$ *and surface part* $H_s = b_1^L + b_N^R$*, and given a vector space* $\mathfrak{A}$*, let* $\Omega^{\alpha\alpha'}$, $\Xi^{\alpha\alpha'} \in \mathfrak{End}(\mathfrak{A})$ *be representation matrices of the quadratic algebra* (49) *defined by h, and let* $|\, V \,\rangle$ *and* $|\, W \,\rangle$ *be vectors satisfying the Lindblad boundary matching condition* (53) *with coefficients* $L^B_{\alpha\alpha'} \in \mathbb{C}$ *and* $b^B_{\alpha\alpha'} = (\alpha|b^B|\alpha')$ *for* $B \in \{L, R\}$*. Then a density matrix* ρ *in the matrix product form* (33) *is a stationary solution of the quantum master equation* (20) *with Lindblad operators* L^B *given by* $L^B_{\alpha\alpha'} = (\alpha|L^B|\alpha')$*.*

This theorem breathes life into the matrix product form (33) of the stationary density matrix by providing sufficient (but not necessary!) conditions on the matrices $\Omega^{\alpha\alpha'}$, vectors $\langle\langle\, W\,|, |\, V\,\rangle\rangle$ and the auxiliary matrices $\Xi^{\alpha\alpha'}$. The basic idea of the proof is to split the quantum master equation into a bulk part and a boundary part. The bulk part comes from the unitary part of the evolution under the action of H_b and leads through the local divergence condition (49) to a quadratic algebra for the matrices $\Omega^{\alpha\alpha'}$, $\Xi^{\alpha\alpha'}$ plus some boundary terms. The boundary part, which involves (i) these boundary terms, (ii) the unitary evolution under the boundary fields, and (iii) the Lindblad dissipators then becomes a set of equations for the vectors $\langle\, W\,|$ and $|\, V\,\rangle$. Choosing a representation for the quadratic algebra and fixing these vectors to satisfy the Lindblad boundary matching condition then guarantees stationarity.

Proof We decompose $\rho = MM^\dagger/Z$ where $Z = \mathrm{Tr}(MM^\dagger) < \infty$ since $\dim(\mathfrak{P}) < \infty$. Hence it suffices to prove

$$\mathscr{L}(MM^\dagger) := -i\big[H, MM^\dagger\big] + \mathscr{D}_1(MM^\dagger) + \mathscr{D}_N(MM^\dagger) = 0 \tag{55}$$

for M and $M^\dagger$ given by Lemma 1.

We consider first the bulk part of the unitary evolution. By definition of the commutator one has $\big[H, MM^\dagger\big] = [H, M]M^\dagger + M\big[H, M^\dagger\big]$. The quadratic algebra (49) ensures validity of the local divergence condition according to Definition 4. The telescopic property of the sum in H_b then implies for $\hat{H}_b := H_b \otimes I \in \mathfrak{End}(\mathfrak{P} \otimes \mathfrak{A})$ the commutation relation

$$\Big[\hat{H}_b, \Omega^{\otimes_p N}\Big] = \Xi \otimes_p \Omega^{\otimes_p (N-1)} - \Omega^{\otimes_p (N-1)} \otimes_p \Xi, \tag{56}$$

and by transposition and complex conjugation in the physical space $\mathfrak{P}$

$$\Big[\hat{H}_b, (\Omega^\star)^{\otimes_p N}\Big] = (\Omega^\star)^{\otimes_p (N-1)} \otimes_p \Xi^\star - \Xi^\star \otimes_p (\Omega^\star)^{\otimes_p (N-1)} \tag{57}$$

where

$$\Xi^\star = \sum_{\alpha\alpha'} E^{\alpha\alpha'} \otimes \bar{\Xi}^{\alpha'\alpha}. \tag{58}$$

Therefore, with

$$N_L := \langle\langle\, W\,|\Xi \otimes_p \Omega^{\otimes_p (N-1)}|\, V\,\rangle\rangle, \quad N_R := \langle\langle\, W\,|\Omega^{\otimes_p (N-1)} \otimes_p \Xi|\, V\,\rangle\rangle \tag{59}$$

and consequently

$$N_L^\dagger = \langle\langle\, \overline{W}\,|\Xi^\star \otimes_p (\Omega^\star)^{\otimes_p(N-1)}|\, \overline{V}\,\rangle\rangle, \quad N_R^\dagger = \langle\langle\, \overline{W}\,|(\Omega^\star)^{\otimes_p(N-1)} \otimes_p \Xi^\star|\, \overline{V}\,\rangle\rangle \tag{60}$$

one has

$$[H_b, M] = N_L - N_R, \quad \left[H_b, M^\dagger\right] = N_R^\dagger - N_L^\dagger. \tag{61}$$

This yields

$$-i\left[H_b, MM^\dagger\right] = iM(N_L^\dagger - N_R^\dagger) - i(N_L - N_R)M^\dagger. \tag{62}$$

Now notice that

$$MN_L^\dagger = \langle\langle\, W, \overline{W}\,|\Omega_1\Xi_2^\star \otimes_p \Theta^{\otimes_p(N-1)}|\, V, \overline{V}\,\rangle\rangle \tag{63}$$

$$N_L M^\dagger = \langle\langle\, W, \overline{W}\,|\Xi_1\Omega_2^\star \otimes_p \Theta^{\otimes_p(N-1)}|\, V, \overline{V}\,\rangle\rangle \tag{64}$$

$$N_R M^\dagger = \langle\langle\, W, \overline{W}\,|\Theta^{\otimes_p(N-1)} \otimes_p \Xi_1\Omega_2^\star|\, V, \overline{V}\,\rangle\rangle \tag{65}$$

$$MN_R^\dagger = \langle\langle\, W, \overline{W}\,|\Theta^{\otimes_p(N-1)} \otimes_p \Omega_1\Xi_2^\star|\, V, \overline{V}\,\rangle\rangle. \tag{66}$$

Hence

$$-i\left[H_b, MM^\dagger\right] = \langle\langle\, W, \overline{W}\,|\Lambda \otimes_p \Theta^{\otimes_p(N-1)}|\, V, \overline{V}\,\rangle\rangle - \langle\langle\, W, \overline{W}\,|\Theta^{\otimes_p(N-1)} \otimes_p \Lambda|\, V, \overline{V}\,\rangle\rangle \tag{67}$$

with $\Lambda = i\left(\Omega_1\Xi_2^\star - \Xi_1\Omega_2^\star\right)$. Expanding Λ using (13) yields

$$\Lambda = \sum_{\alpha\alpha'} E^{\alpha\alpha'} \otimes \Lambda^{\alpha\alpha'} \tag{68}$$

with $\Lambda^{\alpha\alpha'}$ given by (50).

Next we consider the surface part of the unitary evolution. For the boundary fields we obtain from Corollary 2

$$-i\left[b_1^L, MM^\dagger\right] = \langle\langle\, W, \overline{W}\,|\Gamma_L \otimes_p \Theta^{\otimes_p(N-1)}|\, V, \overline{V}\,\rangle\rangle \tag{69}$$

$$-i\left[b_N^R, MM^\dagger\right] = \langle\langle\, W, \overline{W}\,|\Theta^{\otimes_p(N-1)} \otimes_p \Gamma_R|\, V, \overline{V}\,\rangle\rangle \tag{70}$$

with

$$\Gamma_B = -i\sum_\beta \sum_{\alpha\alpha'} \left[b^L, E^{\alpha\alpha'}\right] \otimes \Omega_1^{\alpha\beta}\bar{\Omega}_2^{\alpha'\beta}, \quad B \in \{L, R\}. \tag{71}$$

With (48) this yields

$$\Gamma_B = \sum_{\alpha\alpha'} E^{\alpha\alpha'} \otimes \Gamma_B^{\alpha\alpha'} \tag{72}$$

with $\Gamma_B^{\alpha\alpha'}$ defined by (51). Putting together the bulk and the surface contribution thus yields

$$-i\big[H, MM^\dagger\big] = \langle\langle\, W, \overline{W}\,|\,(\Gamma_L + \Lambda) \otimes_p \Theta^{\otimes_p(N-1)}\,|\, V, \overline{V}\,\rangle\rangle + \langle\langle\, W, \overline{W}\,|\Theta^{\otimes_p(N-1)} \otimes_p (\Gamma_R - \Lambda)\,|\, V, \overline{V}\,\rangle\rangle. \tag{73}$$

For the dissipator part of the generator $\mathscr{L}$ (55) we have from Corollary 1

$$\mathscr{D}_1(MM^\dagger) = \langle\langle\, W, \overline{W}\,|\Delta_L \otimes \Theta^{\otimes(N-k)}\,|\, V, \overline{V}\,\rangle\rangle \tag{74}$$

$$\mathscr{D}_N(MM^\dagger) = \langle\langle\, W, \overline{W}\,|\Theta^{\otimes(N-1)} \otimes \Delta_R\,|\, V, \overline{V}\,\rangle\rangle \tag{75}$$

with

$$\Delta_B = \sum_\beta \sum_{\alpha\alpha'} \mathscr{D}^B\left(E^{\alpha\alpha'}\right) \otimes \Omega_1^{\alpha\beta} \bar{\Omega}_2^{\alpha'\beta}, \quad B \in \{L, R\}. \tag{76}$$

Using (47) one finds after relabeling of indices

$$\Delta_B = \sum_{\alpha\alpha'} E^{\alpha\alpha'} \otimes \Delta_B^{\alpha\alpha'} \tag{77}$$

with $\Delta_B^{\alpha\alpha'}$ defined by (52). Thus

$$\mathscr{L}(MM^\dagger) = \langle\langle\, W, \overline{W}\,|\,(\Delta_L + \Gamma_L + \Lambda) \otimes_p \Theta^{\otimes_p(N-1)}\,|\, V, \overline{V}\,\rangle\rangle + \langle\langle\, W, \overline{W}\,|\Theta^{\otimes_p(N-1)} \otimes_p (\Delta_R + \Gamma_R - \Lambda)\,|\, V, \overline{V}\,\rangle\rangle = 0 \tag{78}$$

by the Lindblad boundary matching condition (53). □

4 The Heisenberg Ferromagnet

We have skirted the issue of existence of representations of the quadratic algebra arising from the local divergence condition and vectors satisfying the Lindblad boundary matching condition. In order to demonstrate that the matrix product construction of the previous section is not only non-empty but also allows for concrete non-trivial results we review the application to the isotropic Heisenberg ferromagnet [16, 17, 25]. Important other models where the matrix product construction has been employed include the one-dimensional Hubbard model [28] and the spin-1 Lai-Sutherland chain [14].

4.1 Definitions and Notation

It is expedient to introduce the Levi-Civita symbol $\varepsilon_{\alpha\beta\gamma}$ (defined $\alpha, \beta, \gamma \in \{1, 2, 3\}$) by $\varepsilon_{123} = 1$ and $\varepsilon_{\alpha\beta\gamma} = (-1)^\pi \varepsilon_{\pi(\alpha\beta\gamma)}$ for any permutation $\pi(\cdot)$. We also define $\zeta_{0\alpha\beta} = \zeta_{\alpha 0\beta} = \zeta_{\alpha\beta 0} = \delta_{\alpha,\beta}$ for $\alpha, \beta \in \{0, 1, 2, 3\}$ and $\zeta_{\alpha\beta\gamma} = i\varepsilon_{\alpha\beta\gamma}$ for $\alpha, \beta, \gamma \in$

$\{1, 2, 3\}$ and introduce the two-dimensional unit matrix and the Pauli matrices

$$\sigma^0 \equiv \mathbb{1} := \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \ \sigma^1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma^2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma^3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{79}$$

which form a complete basis of $\mathfrak{End}(\mathbb{C}^2)$. They satisfy

$$\sigma^\alpha \sigma^\beta = \sum_{\gamma=0}^{3} \zeta_{\alpha\beta\gamma} \sigma^\gamma. \tag{80}$$

For $\alpha \in \{1, 2, 3\}$ the matrices σ_k^α are related by a unitary transformation U with the property

$$U \sigma_k^\alpha U^\dagger = \sigma_k^{\alpha+1}, \quad \forall k \in \{1, \ldots, N\}, \quad \alpha \bmod 3. \tag{81}$$

Straightforward computation shows that this transformation is realized by the tensor product

$$U = u^{\otimes N} \tag{82}$$

with

$$u = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix} \tag{83}$$

which is unique up to a non-zero factor.

We shall also use the notation $\hat{n} \equiv E^{00} = (1 + \sigma^z)/2, \sigma^+ \equiv E^{01} = (\sigma^x + i\sigma^y)/2$, $\sigma^- \equiv E^{10} = (\sigma^x - i\sigma^y)/2$, $\hat{v} \equiv E^{11} = (1 - \sigma^z)/2$ and the representation of the local basis vectors as column vectors as

$$|0) := \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad |1) := \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \tag{84}$$

For later use we also introduce the notation $\sigma^x \equiv \sigma^1$, $\sigma^y \equiv \sigma^2$, $\sigma^z \equiv \sigma^3$ and the three-vectors $\boldsymbol{\sigma} = (\sigma^1, \sigma^2, \sigma^3)$ with the dot product $\mathbf{A} \cdot \mathbf{B} := \sum_{i=1}^3 A^i B^i$. Here the A_i and B_i can be real numbers or Pauli matrices. The reason for introducing this definition is the interpretation of the upper indices of the Pauli matrices as the components of the (quantum) angular momentum vector of an atom in the coordinate directions x, y, z of $\mathbb{R}^3$. If $\mathbf{A} \in \mathbb{R}^3$ is a vector of (Euclidean) length $\mathbf{A} \cdot \mathbf{A} = 1$, then the quantum expectation $\langle\, \mathbf{A} \cdot \boldsymbol{\sigma} \,\rangle$ is the mean of the projection of the angular momentum vector in the direction defined by the vector $\mathbf{A}$.

The Lie algebra $\mathfrak{gl}_2(\mathbb{C})$ with generators X^α, $\alpha \in \{0, 1, 2, 3\}$ is defined by Lie brackets

$$\left[X^0, X^\alpha\right] = 0 \tag{85}$$

$$\left[X^\alpha, X^\beta\right] = 2i \sum_{\gamma=1}^{3} \varepsilon_{\alpha\beta\gamma} X^\gamma, \quad \alpha, \beta \in \{1, 2, 3\}. \tag{86}$$

The two-dimensional unit matrix $\mathbb{1}$ and Pauli matrices σ^α (79) are representation matrices for $\mathfrak{gl}_2(\mathbb{C})$ with the Lie-bracket represented by the commutator. Since $\sigma_k^\alpha \sigma_l^\alpha = \sigma_l^\alpha \sigma_k^\alpha$ for $l \neq k$ it follows that also $\mathbf{1} \in \mathfrak{P}$ together with

$$S^\alpha = \sum_{k=1}^{N} \sigma_k^\alpha \in \mathfrak{P} \tag{87}$$

are representation matrices of $\mathfrak{gl}_2(\mathbb{C})$. We say that an endomorphism G on $\mathfrak{P}$ is $SU(2)$-symmetric if its representation matrix satisfies $[G, S^\alpha] = 0$ for $\alpha \in \{1, 2, 3\}$.

We also define the generators

$$X^\pm := \frac{1}{2}\left(X^1 \pm i X^2\right), \quad X^z := \frac{1}{2} X^3. \tag{88}$$

In terms of these generators the defining relations (85), (86) of $\mathfrak{gl}_2(\mathbb{C})$ read

$$\left[X^0, X^{\pm,z}\right] = 0 \tag{89}$$

$$\left[X^+, X^-\right] = 2X^z, \quad \left[X^z, X^\pm\right] = \pm X^\pm. \tag{90}$$

An infinite-dimensional family of representations $X^0 \mapsto I$, $X^{\pm,z} \mapsto S^{\pm,z}$ is given by matrices I, $S^{\pm,z}$ with matrix elements

$$I_{kl} = \delta_{k,l}, \quad S^+_{kl} = l\delta_{k+1,l}, \quad S^-_{kl} = (2p - l)\delta_{k,l+1}, \quad S^z_{kl} = (p - l)\delta_{k,l} \tag{91}$$

for the non-negative integers $k, l \in \mathbb{N}_0$ and parameter $p \in \mathbb{C}$.

4.2 Boundary-Driven Lindblad–Heisenberg Chain

We consider an open chain of $N \geq 2$ quantum spins in contact with boundary reservoirs for which we wish to construct the stationary density matrix defined by (20). For the unitary part of the time evolution we consider the isotropic spin-1/2 Heisenberg Hamiltonian [3, 13] defined with the dot-product by

$$H = \sum_{k=1}^{N-1} \boldsymbol{\sigma}_k \cdot \boldsymbol{\sigma}_{k+1} \tag{92}$$

for N quantum spins at positions k along the chain.

Before defining the boundary dissipators we point out that H is manifestly rotation invariant in $\mathbb{R}^3$ which due to the quantum nature of the spin is equivalent to the symmetry $[H, S^\alpha] = 0$ under the Lie-algebra $SU(2)$ with representation matrices (87). Thus the spin components are locally conserved with associated locally conserved currents j_k^α defined by (8) with $F = \sigma_k^\alpha$. For $1 < k < N$ the action of the adjoint generator (8) yields

$$\mathscr{L}^\dagger(\sigma_k^\alpha) = j_{k-1}^\alpha - j_k^\alpha \tag{93}$$

with

$$j_k^\alpha = 2\sum_{\beta=1}^{3}\sum_{\gamma=1}^{3} \varepsilon_{\alpha\beta\gamma}\sigma_k^\beta\sigma_{k+1}^\gamma, \quad 1 \le k < N. \tag{94}$$

In the steady state the current expectations $j^\alpha := \langle j_k^\alpha \rangle$ are position-independent.

We choose two boundary Lindblad operators $D^{L,R}$ to favour a relaxation of the boundary spins towards target states given by density matrices ρ_L, ρ_R satisfying $\mathscr{D}_1(\rho_L) = \mathscr{D}_N(\rho_R) = 0$. As target states we choose fully polarized states of one boundary spin

$$\rho_L = \frac{1}{2}(\mathbb{1} + \mathbf{n}_L \cdot \boldsymbol{\sigma}) \otimes \tilde{\rho}, \quad \rho_R = \tilde{\rho} \otimes \frac{1}{2}(\mathbb{1} + \mathbf{n}_R \cdot \boldsymbol{\sigma}) \tag{95}$$

where $|\mathbf{n}_L| = |\mathbf{n}_R| = 1$ and $\tilde{\rho}$ is an arbitrary reduced density matrix for the remaining $N-1$ spins. The reduced single-site boundary density matrix $\rho_B^{(1)} = \frac{1}{2}(\mathbb{1} + \mathbf{n}_B \cdot \boldsymbol{\sigma})$ is a pure state since for a projection direction given by

$$\mathbf{n}_B = (\sin(\phi_B)\cos(\theta_B), \sin(\phi_B)\sin(\theta_B), \cos(\phi_B)). \tag{96}$$

One has $\rho_B^{(1)} = |\psi_B) \otimes (\psi_B|$ with

$$|\psi_B) = \mathrm{e}^{i\alpha_B}\begin{pmatrix} \cos(\phi_B/2)\mathrm{e}^{-i\theta_B/2} \\ \sin(\phi_B/2)\mathrm{e}^{i\theta_B/2} \end{pmatrix} \tag{97}$$

and arbitrary phase $\alpha_B \in [0, 2\pi)$. The notion "full polarization" means that the expectation of the spin projection $\mathbf{n}_B \cdot \boldsymbol{\sigma}$ in the space-direction defined by $\mathbf{n}_B$ is given by $\langle\, \mathbf{n}_B \cdot \boldsymbol{\sigma}\, \rangle = 1$.

Due to the rotational symmetry (87) of H only the angle between the two boundary polarization vectors plays a role. Therefore we may, without loss of generality, choose $\phi_L = \phi_R = \pi/2$ and fix the coordinate frame in $\mathbb{R}^3$ such that the X–axis points in the $\mathbf{n}_L$ direction (corresponding to $\theta_L = 0$) and to let the XY-plane be spanned by the family vectors $\mathbf{n}_R(\theta)$, i.e.,

$$\mathbf{n}_L = (1, 0, 0), \quad \mathbf{n}_R = (\cos\theta, \sin\theta, 0), \quad 0 \le \theta \le \pi \tag{98}$$

corresponding to $\theta_R = \theta$.

It is easy to verify that there are two families of local Lindblad operators satisfying $\mathscr{D}_1[\rho_L] = 0$, viz. $D_1^R = a(\sigma_1^2 + i\sigma_1^3) + b(\mathbf{1} - \sigma_1^1)$ and $D_1^{R'} = a'\mathbf{1} + b'\sigma_1^1$. Following [16, 17] we choose D^R with $b = 0$ (so that $\mathrm{Tr}(D_1^R) = 0$) and coupling strength $a = \sqrt{\Gamma}$. Similarly, we choose for the right boundary site N the rotated projection to arrive at

$$D_1^R = \sqrt{\Gamma}(\sigma_1^2 + i\sigma_1^3), \quad D_N^L = \sqrt{\Gamma}(\sigma_N^2 \cos\theta - \sigma_N^1 \sin\theta + i\sigma_N^3). \tag{99}$$

Then in absence of the unitary term in (20) the boundary spins relax with characteristic times $\propto \Gamma^{-1}$ to approach ρ_L, ρ_R: Writing $\rho_L(t) = 1/2(\sigma_1^0 + x(t)\sigma_1^1 + y(t)\sigma_1^2 + z(t)\sigma_1^3) \otimes \tilde{\rho}$ one has $x(t) = 1 + (x(0) - 1)\exp(-4\Gamma t)$, $y(t) = y(0)\exp(-2\Gamma t)$, $z(t) = z(0)\exp(-2\Gamma t)$, and similarly for $\rho_R(t)$.

Remark 4 In the untwisted case $\mathbf{n}_L = \mathbf{n}_R := \mathbf{n}$ corresponding to $\theta = 0$ the Lindblad equation (20) for the stationary density matrix is trivially solved by [27]

$$\rho_N(\Gamma, 0) = \left(\frac{\mathbb{1} + \mathbf{n}\cdot\boldsymbol{\sigma}}{2}\right)^{\otimes N}. \tag{100}$$

This is a pure state of the form $\rho_N(\Gamma, 0) = |\,\Psi\,\rangle\langle\,\Psi\,|$ where $|\,\Psi\,\rangle = |\,\psi\,\rangle^{\otimes N}$ and

$$|\,\psi\,\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}. \tag{101}$$

This pure state is not of the form $\exp(-\beta H)/Z$ for any β and therefore not an equilibrium state.

4.3 Matrix Product Solution

From now on we exclude $\theta = 0$ so that the boundary coupling introduces a twist in the XY-plane, which drives the system perpetually out of equilibrium.

Theorem 2 *Let $I, S^{\pm,z} \in \mathfrak{End}(\mathfrak{A})$ be the infinite dimensional representation (91) of $\mathfrak{gl}_2(\mathbb{C})$ with representation parameter*

$$p = i\Gamma^{-1} \tag{102}$$

and let $\Omega^{00} = -\Omega^{11} = iS^z$, $\Omega^{01} = iS^+$, $\Omega^{10} = iS^-$. Furthermore, let

$$\langle\,\overline{W}, W\,| = \langle\,0\,|\otimes\langle\,0\,|, \quad |\,V, \overline{V}\,\rangle = \sum_{m,n=0}^{\infty}\left(-\cot\frac{\theta}{2}\right)^{m+n}\binom{2p}{m}\binom{2\bar{p}}{n}|\,m\,\rangle\otimes|\,n\,\rangle. \tag{103}$$

Then for ρ in matrix product from (33) and U defined by (81) the density matrix

$$\rho_N(\Gamma,\theta) = U\rho U^\dagger \tag{104}$$

is the unique solution of the quantum master equation (20) for the Heisenberg ferromagnet (92) with boundary dissipators (99).

Uniqueness is guaranteed by the structure of the Lindblad dissipators, see [29]. The proof of (104) follows from verifying the local divergence condition (49) with $\Xi^{00} = \Xi^{11} = iI$, $\Xi^{01} = \Xi^{10} = 0$ and the Lindblad boundary matching condition (53) by (somewhat lengthy but straightforward) explicit computation [16, 17]. Proposition 1 then yields for the non-equilibrium partition function (22)

$$Z_N(\Gamma,\theta) = \langle\, \overline{W}, W\,|\Theta_0^N|\, V, \overline{V}\,\rangle \tag{105}$$

with $\Theta_0 = 2S_1^zS_2^z + S_1^+S_2^+ + S_1^-S_2^-$ defined by (39).

We summarize the main conclusions of [16, 17, 25] drawn from Theorem 2 and the underlying quadratic algebra and Lindblad boundary matching property for $0 < \theta < \pi$.

(1) Dropping the arguments Γ, θ, the stationary magnetization currents are given by

$$j_N^x = -8ip\frac{Z_{N-1}}{Z_N}, \quad j_N^y = -\cot\frac{\theta}{2}j_N^x, \quad j_N^z = -4\frac{\frac{\mathrm{d}}{\mathrm{d}\theta}Z_{N-1}}{Z_N}. \tag{106}$$

Based on numerically exact computation up to $N = 100$ we conjectured that for any fixed coupling strength Γ one has [17]

$$\lim_{N\to\infty} N^2\frac{Z_{N-1}(\Gamma,\theta)}{Z_N(\Gamma,\theta)} = \frac{1}{4}\theta^2. \tag{107}$$

For the currents this result implies

$$\lim_{N\to\infty} N^2 j_N^x(\Gamma,\theta) = \frac{2\theta^2}{\Gamma}, \quad \lim_{N\to\infty} N j_N^z(\Gamma,\theta) = 2\theta. \tag{108}$$

Some rigorous results have been obtained for the Zeno limit $\Gamma \to \infty$ [25]. Rescaling the normalization factor yields a finite limit

$$\tilde{Z}_N(\theta) := \frac{1}{4}\lim_{\Gamma\to\infty}\Gamma^2 Z_N(\Gamma,\theta) \tag{109}$$

which was computed explicitly. Then for small twist angle $\theta = o(1/N)$ the conjecture (107) can be proved rigorously. For the currents one therefore finds

Theorem 3 *Let $\tilde{j}_N^\alpha(\theta) := \lim_{\Gamma\to\infty} j_N^\alpha(\Gamma,\theta)$ be the stationary currents of the Heisenberg chain in the Zeno limit. Then for any N one has*

$$\tilde{j}_N^x(\theta) = \tilde{j}_N^y(\theta) = 0 \quad \forall \theta \in [0, \pi[\tag{110}$$

and for any real $\varepsilon > 0$ *and real* $\theta_0 > 0$

$$\lim_{N\to\infty} N^{2+\varepsilon}\, \tilde{j}_N^z \left(\frac{\theta_0}{N^{1+\varepsilon}} \right) = 2\theta_0. \tag{111}$$

The first statement is a trivial consequence of the explicit expressions (106) and the result that $\tilde{Z}_N(\theta)$ is finite and non-zero. The second statement follows from the explicit form of $\tilde{Z}_N(\theta)$ given in [25].
(2) In terms of

$$B^x := \Theta^{01} + \Theta^{10}, \quad B^y := i\left(\Theta^{01} - \Theta^{10}\right), \quad B^z = \Theta^{00} - \Theta^{11} \tag{112}$$

the multiplication property (80) yields

$$\langle\, \sigma_k^\alpha \,\rangle_N = \frac{S_{k,N}^\alpha(\Gamma, \theta)}{Z_N(\Gamma, \theta)} \tag{113}$$

with

$$S_{k,N}^\alpha(\Gamma, \theta) = \langle\, \overline{W},\, W\, |\Theta_0^{k-1} B^\alpha \Theta_0^{N-k}|\, V, \overline{V}\,\rangle. \tag{114}$$

(3) The quadratic algebra implies that the operators Θ_0 and B^α satisfy the remarkable *cubic* relation

$$[\Theta_0, [\Theta_0, B^\alpha]] + 2\{\Theta_0, B^\alpha\} - 8p^2 B^\alpha = 0 \tag{115}$$

which was found earlier for a specific representation by using computer algebra [27]. This relation induces recursion relations for the unnormalized correlation functions $Z_N \langle\, \sigma_{k_1}^{\alpha_1} \ldots \sigma_{k_n}^{\alpha_n} \,\rangle$. In particular, with

$$\begin{aligned} B^x &= S_1^+ S_2^+ - S_1^- S_2^-, \quad B^y = S_1^z(S_2^- - S_2^+) + (S_1^- - S_1^+)S_2^z, \\ B^z &= i\, S_1^z(S_2^- + S_2^+) - i(S_1^- + S_1^+)S_2^z. \end{aligned} \tag{116}$$

one finds for the unnormalized one-point function (dropping the arguments)

$$S_{k+2,N+1}^\alpha + S_{k,N+1}^\alpha - 2S_{k,N}^\alpha + 2(S_{k,N}^\alpha + S_{k+1,N}^\alpha) - 8p^2 S_{k,N-1}^\alpha = 0. \tag{117}$$

By setting $r = k/N$ and taking the continuum limit $k, N \to \infty$ such that the macroscopic coordinate r remains fixed this recursion together with (107) yields the simple ordinary differential equation $m''(r) + \theta^2 m(r) = 0$ for the large-scale magnetization profile $m^\alpha(r) := \lim_{k,N\to\infty} \langle\, \sigma_k^\alpha \,\rangle_N$. The boundary conditions are given by the microscopic complete polarizations so that

$$m^x(r) = \cos(\theta r), \quad m^y(r) = \sin(\theta r), \quad m^z(r) = 0, \quad 0 \le r \le 1 \tag{118}$$

corresponding to a spin helix state [25]. This implies a strongly sub-diffusive current $0 = \lim_{N\to\infty} N j_N^x = \lim_{N\to\infty} N j_N^y$ inside the twist-plane.

For maximal twist $\theta = \pi$ one has by symmetry $j_N^y(\Gamma, \pi) = j_N^z(\Gamma, \pi) = 0$ for all N, Γ [23]. Magnetization profiles and correlation functions were computed in [8, 27] using the cubic relation (115) and the resulting continuum approximation, see also the review [29]. Remarkably, the correlations along the twist axis are of a form reminiscent of what was obtained for the symmetric simple exclusion process with open boundaries, using the fluctuating hydrodynamics approach [31]. This similarity suggest that also the boundary driven quantum problem may be understood in terms of fluctuating hydrodynamics.

Acknowledgements VP and GMS thank T. Prosen for useful discussions and DFG for financial support.

References

1. Alcaraz, F.C., Dasmahapatra, S., Rittenberg, V.: N-species stochastic models with boundaries and quadratic algebras. Phys. A **257**, 1 (1998)
2. Attal, S., Joye, A., Pillet, C.-A. (eds.): Open Quantum Systems II. The Markovian Approach. Springer, Berlin (2006)
3. Baxter, R.J.: Exactly Solved Models in Statistical Mechanics. Academic, New York (1982)
4. Bertini, L., De Sole, A., Gabrielli, D., Jona Lasinio, G., Landim, C.: Macroscopic fluctuation theory for stationary non-equilibrium states. J. Stat. Phys. **107**, 635–675 (2002)
5. Bertini, L., De Sole, A., Gabrielli, D., Jona Lasinio, G., Landim, C.: Macroscopic fluctuation theory. Rev. Mod. Phys. **87**, 593–636 (2015)
6. Blythe, R.A., Evans, M.R.: Nonequilibrium steady states of matrix-product form: a solver's guide. J. Phys. A: Math. Theor. **40**, R333–R441 (2007)
7. Breuer, H.-P., Petruccione, F.: The Theory of Open Quantum Systems. Oxford University Press, Oxford (2002)
8. Buča, B., Prosen, T.: Connected correlations, fluctuations and current of magnetization in the steady state of boundary driven XXZ spin chains. J. Stat. Mech. 023102 (2016)
9. Derrida, B.: An exactly soluble non-equilibrium system: the asymmetric simple exclusion process. Phys. Rep. **301**, 65–83 (1998)
10. Derrida, B., Lebowitz, J.L., Speer, E.R.: Large deviation of the density profile in the steady state of the open symmetric simple exclusion process. J. Stat. Phys. **107**, 599–634 (2002)
11. Frigerio, A., Spohn, H.: Stationary states of quantum dynamical semigroups and applications. In: Accardi, L., Gorini, V., Paravicini, G. (eds.) Proceedings of Mathematical Problems in the Theory of Quantum Irreversible Processes, Laboratoria di Cibernetica del CNR, pp. 115–135 (1978)
12. Gorini, V., Kossakowski, A., Sudarshan, E.C.G.: Completely positive dynamical semigroups of N-level systems. J. Math. Phys. **17**(5), 821–825 (1976)
13. Heisenberg, W.: Zur Theorie des Ferromagnetismus. Z. Phys. **49**, 619–636 (1928)
14. Ilievski, E., Prosen, T.: Exact steady state manifold of a boundary driven spin-1 Lai-Sutherland chain. Nucl. Phys. B **882**, 485 (2014)
15. Ising, E.: Beitrag zur Theorie des Ferromagnetismus. Z. Phys. **31**, 253–258 (1925)
16. Karevski, D., Popkov, V., Schütz, G.M.: Exact matrix product solution for the boundary-driven Lindblad XXZ chain. Phys. Rev. Lett. **110**, 047201 (2013)
17. Karevski, D., Popkov, V., Schütz, G.M.: Driven isotropic Heisenberg spin chain with arbitrary boundary twisting angle: exact results. Phys. Rev. E **88**, 062118 (2013)

18. Kipnis, C., Landim, C.: Scaling Limits of Interacting Particle Systems. Springer, Berlin (1999)
19. Kossakowski, A.: On quantum statistical mechanics of non-Hamiltonian systems. Rep. Math. Phys. **3**(4), 247–274 (1972)
20. Liggett, T.M.: Stochastic Interacting Systems: Contact, Voter and Exclusion Processes. Springer, Berlin (1999)
21. Lindblad, G.: On the generators of quantum dynamical semigroups. Commun. Math. Phys. **48**(2), 119–130 (1976)
22. Polishchuk, A., Positselski, L.: Quadratic Algebras. University Lecture Series, vol. 37. American Mathematical Society, Providence (2005)
23. Popkov, V., Livi, R.: Manipulating energy and spin currents in non-equilibrium systems of interacting qubits. New J. Phys. **15**, 023030 (2013)
24. Popkov, V., Prosen, T.: Infinitely dimensional Lax structure for one-dimensional Hubbard model. Phys. Rev. Lett. **114**, 127201 (2015)
25. Popkov, V., Schütz, G.M.: Solution of the Lindblad equation for spin helix states. Phys. Rev. E **95**, 042128 (2017)
26. Prosen, T.: Open XXZ spin chain: nonequilibrium steady state and a strict bound on Ballistic transport. Phys. Rev. Lett. **106**, 217206 (2011)
27. Prosen, T.: Exact nonequilibrium steady state of a strongly driven open XXZ chain. Phys. Rev. Lett. **107**, 137201 (2011)
28. Prosen, T.: Exact nonequilibrium steady state of an open Hubbard chain. Phys. Rev. Lett. **112**, 030603 (2014)
29. Prosen, T.: Matrix product solutions of boundary driven quantum chains. J. Phys. A: Math. Theor. **48**, 373001 (2015)
30. Schütz, G.M.: Exactly solvable models for many-body systems far from equilibrium. In: Domb, C., Lebowitz, J. (eds.) Phase Transitions and Critical Phenomena, vol. 19, pp. 1–251. Academic Press, London (2001)
31. Spohn, H.: Long-range correlations for stochastic lattice gases in a non-equilibrium steady state. J. Phys. A: Math. Gen. **16**, 4275–4291 (1983)
32. Spohn, H.: Nonlinear fluctuating hydrodynamics for anharmonic chains. J. Stat. Phys. **154**, 1191–1227 (2014)