Driven isotropic Heisenberg spin chain with arbitrary boundary twisting angle: exact results

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We consider an open isotropic Heisenberg quantum spin chain, coupled at the ends to boundary reservoirs polarized in different directions, which sets up a twisting gradient across the chain. Using a matrix product ansatz, we calculate the exact magnetization profiles and magnetization currents in the nonequilibrium steady state of a chain with $N$ sites. The magnetization profiles are harmonic functions with a frequency proportional to the twisting angle $\theta$. The currents of the magnetization components lying in the twisting plane and in the orthogonal direction behave qualitatively differently: In-plane steady state currents scale as $1/N^2$ for fixed and sufficiently large boundary coupling, and vanish as the coupling increases, while the transversal current increases with the coupling and saturates to $20/N$.

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The Heisenberg quantum spin chain is a fundamental and one of the most well-studied quantum models of statistical mechanics. However, not much is known about the Heisenberg chain in a nonequilibrium setting where the chain is maintained in a strongly non-equilibrium state by e.g. a coupling to the ends to boundary reservoirs at different chemical potential or different polarization. The boundary gradient drives a quantum system towards a nonequilibrium steady state (NESS), typically characterized by various nonvanishing currents of energy, magnetization etc. The open quantum system is canonically described by the celebrated quantum master equation for the reduced density matrix in the Lindblad form (Lindblad Master Equation, or LME) [1,2].

The full LME evolution of an open system of $N$ spins is described by a $2^N \times 2^N$ reduced density matrix $\rho(t)$, which has $2^{2N} - 1$ independent real entries. It is clear that the usage of even most powerful numerical methods is restricted due to exponentially growing complexity of the problem. However, many fundamental properties like conductivity, universality classes and critical behaviour are the properties of thermodynamically large systems and hence require the development of analytic non-perturbative methods. In spin chain materials like SrCuO$_2$ many transport characteristics are measurable experimentally [3, 4].

The purpose of the present paper is to investigate in detail the NESS of a simply formulated, and analytically treatable, open quantum many-body system. Namely, we consider an open nonequilibrium isotropic Heisenberg spin chain, coupled to boundary reservoirs, which tend to polarize spins at the edges along arbitrary directions $\vec{n}_R, \vec{n}_L$ on the right and on the left end, see Fig. 1. Due to the bulk isotropy, the NESS depends on two scalar parameters: the angle $\theta$ between the unit vectors $\vec{n}_L, \vec{n}_R$, $\cos \theta = (\vec{n}_L, \vec{n}_R)$, and the ratio between the boundary coupling strength and bulk exchange interaction. Except for the case of an ideal alignment $\theta = 0$, the boundary coupling induces twisting gradient gradients and nonvanishing steady state currents.

During last few years, the open nonequilibrium Heisenberg spin chain with local dissipative action at the boundaries has become a paradigmatic reference model in the field, due to its conceptual simplicity and recently discovered powerful non-perturbative methods [3,7]. The NESS for the case with antiparallel alignment $\vec{n}_L = (0,0,1), \vec{n}_R = (0,0,-1)$, so that $\theta = \pi$ was formulated as a matrix product ansatz (MPA) and solved for a more general XXZ quantum model. Further generalizations of the basic model [7] were proposed, in which additional incoherent hopping processes or bulk dephasing processes were included [8,9].

The model with twisting boundary gradients was introduced and studied in [10, 11] in a slightly more general setting with exchange $Z$–anisotropy, while twisting was applied in the perpendicular $XY$-plane. However, previous studies were limited to small system sizes, and could not provide reliable information on scaling behaviour. Using LME symmetries [10], one can at most make general qualitative predictions about the nature of the steady state and admissibility of certain observables [12]. E.g., based on a particular odd-even size alternating symmetry argument, the possibility of a ballistic magnetization current in XXZ-model with XY-twisting gradient at $\theta = \pi/2$ was ruled out [10].

In our recent study [6] it was shown that the isotropic XXX-model is exactly solvable by an MPA for any twisting angle $\theta$. Here we go further and compute analytically various steady-state observables for finite systems and in
thermodynamic limit, namely the magnetization profiles and the steady state magnetization energy currents, as functions of the twisting angle $\theta$ and the coupling strength $\Gamma$. Due to the isotropy projections of the total magnetization on all three axes are individually conserved in the steady state. We find drastically different scalings (with system size $N$ and with coupling) of the magnetization current components within the plane on which the twisting boundary gradient is imposed, and the magnetization current $j_\perp$ in the perpendicular direction. Moreover, for $j_\perp$ we find an intriguing non-commutativity of the limits $N \to \infty$ and $\theta \to \pi$.

The plan of the paper is the following: In Sec. I we introduce the model and outline the Matrix Product Ansatz method. In Sec. II we calculate the magnetization profiles, and in Sec. III the magnetization currents. Appendix A contains some necessary technical details.

I. THE MODEL

We consider an open chain of $N$ quantum spins in contact with boundary reservoirs, the time evolution of which is given by a quantum Master equation in the Lindblad form \[1, 2, 14\] (we set $\hbar = 1$)

$$\frac{\partial \rho}{\partial t} = -i[H, \rho] + 4\Gamma(\mathcal{L}_L[\rho] + \mathcal{L}_R[\rho]).$$

Here $\rho$ is the reduced density matrix, $H$ is the isotropic spin-1/2 Heisenberg Hamiltonian

$$H_{XXX} = \sum_{k=1}^{N-1} \left(\sigma^x_k \sigma^x_{k+1} + \sigma^y_k \sigma^y_{k+1} + \sigma^z_k \sigma^z_{k+1}\right),$$

$\Gamma$ an effective coupling with the reservoirs, and $\mathcal{L}_L$ and $\mathcal{L}_R$ are Lindblad dissipators which favour a relaxation of the leftmost and the rightmost spins towards target states $\rho_L, \rho_R$, so that $\mathcal{L}_L[\rho_L] = \mathcal{L}_R[\rho_R] = 0$. As target states we choose fully polarized states of one spin $\rho_L = \frac{1}{2} + \frac{1}{2} \sum n_k^\alpha \sigma^\alpha$, $\rho_R = \frac{1}{2} + \frac{1}{2} \sum n_R^\alpha \sigma^\alpha$, $|\bar{n}_L| = |\bar{n}_R| = 1$. To fix the coordinate frame, we choose the $XY$-plane as the plane spanned by the vectors $\bar{n}_L, \bar{n}_R$ and the $X^-$ axis to point in the $\bar{n}_L$ direction,

$$\bar{n}_L = (1, 0, 0)$$

$$\bar{n}_R = (\cos \theta, \sin \theta, 0),$$

the angle $\theta$ between $\bar{n}_L, \bar{n}_R$ taking values $0 \leq \theta \leq \pi$. A canonical, although not the most general, form of the Lindblad action satisfying $\mathcal{L}_L[\rho_L] = \mathcal{L}_R[\rho_R] = 0$, is

$$\mathcal{L}_{L,R}[\rho] = X_{L,R} \rho X_{L,R}^+ - \frac{1}{2} \left\{ \rho, X_{L,R}^+ X_{L,R} \right\},$$

where

$$X_L = \frac{1}{2}(\sigma^y + i\sigma^z), \quad X_R = \frac{1}{2}(\sigma^y \cos \theta + i\sigma^z - \sigma^z \sin \theta)$$

are polarization targeting Lindblad operators. Indeed, in absence of the unitary term in (1) the boundary spins relax with a characteristic time $\Gamma^{-1}$ to states $\rho_L, \rho_R$. Consequently, the boundary coupling introduces a twist in $XY$ plane across the whole system, which constantly drives the system out of equilibrium. Eq. (1) describes the exact time evolution of a reduced density matrix, provided that the coupling to reservoir is rescaled appropriately with the time interval between consecutive interactions of the system with the reservoirs, see [14].

Our setting is shown schematically in Fig. 1. A model with a twist [6] with right twisting angle $\theta = \pi/2$ in $XY$-plane and more general anisotropic $XXZ$-Hamiltonian $H_{XXX} = \sum_{k=1}^{N-1} \left(\sigma^x_k \sigma^x_{k+1} + \sigma^y_k \sigma^y_{k+1} + \Delta \sigma^z_k \sigma^z_{k+1}\right)$ was introduced in [10], and the respective NESS $\rho_{NESS}(\Delta)$ was shown to possess intriguing properties. The existence of a duality transformation between $\rho_{NESS}(\Delta)$ and $\rho_{NESS}(-\Delta)$, of a different form for even and odd $N$, allowed to conclude that the $j^{\perp}$ magnetization current alternates its sign with system size $10$. For large $\Gamma \gg \infty$ and for an adequate choice of the anisotropy $|\Delta^*(N)| < 1$, which depends on system size $N$, one can generate a NESS arbitrarily close to a pure state, $1 - Tr[\rho_{NESS}^{\perp}(\Delta^*)] < \varepsilon [13]$. For small $\Gamma \ll 1$ the NESS $\rho_{NESS}(\Delta)$ was shown to have an anomaly peaked around the isotropic point $\Delta = 1$, the anomaly turning into a singularity at $\Delta = 1$ in the limit $\Gamma \to 0 [10]$. While some of above features were proved with general symmetry arguments, others were conjectured by extrapolating the analytic behaviour of the system for small sizes $N < 10$ onto larger sizes. However, many important
questions concerning scaling behaviour or finite-size corrections crucial for determining the universality, could not be answered.

In the present work we obtain exact results for the model with a boundary twist for the thermodynamic limit $N \gg 1$ by using a Matrix Product Ansatz (MPA). Our study treats the isotropic Heisenberg chain $\Delta = 1$, but an arbitrary twisting angle $\theta$ between the targeted polarizations at the ends. Our calculations are based on the following observation: The unnormalized NESS of the model (1), (5) can be written in the form (6)

$$\rho_{NESS} = US_N(US_N)^\dagger$$

(7)

$$S_N = \langle 0 | \Omega^{\otimes N} | R_\theta \rangle$$

(8)

$$U = U^{\otimes N}$$

where $\Omega$ is a $2 \times 2$ matrix with operator-valued entries $\Omega(p) = S_z(p)\sigma^z + S_z(p)\sigma^+ + S_z(p)\sigma^-$, which satisfy the $SU(2)$ algebra $[S^z, S^\pm] = \pm S^z$, $[S^+, S^-] = 2S^z$ for any $p$. The representation parameter $p$ is defined by the action of $S_z$ on the lowest weight vector of $SU(2)$, $|0\rangle S_z = p |0\rangle$, and is connected to the coupling constant $\Gamma$ through $p = i/\Gamma$. More precisely, the operators $S_z(p), S^x(p)$ operate on a semi-infinite set of states $\{|n\rangle\}_{n=0}^{\infty}$, as

$$S_z(p) = \sum_{n=0}^\infty (p - n) |n\rangle \langle n|$$

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

$$S^- = \sum_{n=0}^\infty (2p - n) |n + 1\rangle \langle n|.$$

Finally, the vector $|R_\theta\rangle$ is a coherent state, parametrized by the twisting angle $\theta$

$$|R_\theta(p)\rangle = \sum_{n=0}^\infty (-\cot \theta)^n (S^-)^n |0\rangle = \sum_{n=0}^\infty (-\cot \theta)^n (2p)^n |n\rangle,$$

(9)

where $\binom{2p}{n}$ is a generalized binomial coefficient.

Note that the Lindblad operators (5) differ from the ones considered in (6) by a cyclic permutation $\sigma^z, \sigma^+, \sigma^- \rightarrow \sigma^x, \sigma^y, \sigma^z$, accounted for by introducing a unitary matrix $U$ which performs a cyclic permutation on the basis of Pauli matrices,

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -i \\ 1 & i \end{pmatrix},$$

(10)

i.e. $U\sigma^zU^\dagger = \sigma^y, U\sigma^yU^\dagger = \sigma^z, U\sigma^zU^\dagger = \sigma^x$.

Some care should be taken in distinguishing the physical Hilbert space $\mathbb{C}^2$ in which the matrices $\Omega(p)$ and $U$ are acting, and an auxiliary space $\mathbb{R}$ spanned by the vectors $\{|n\rangle\}_{n=0}^{\infty}$, in which $S_z(p), S^x(p)$ are acting. The result of the operation (8) $\langle 0 | \Omega^{\otimes N} | R_\theta \rangle$ is a scalar in the auxiliary space and is a matrix in the full Hilbert space for $N$ spins $(\mathbb{C}^2)^{\otimes N}$. For the following it is convenient to rewrite the (7) in the form

$$\rho_{NESS} = \langle 0, 0 | \Omega(p)^{\otimes N} | R_\theta, R_\theta^* \rangle$$

(11)

where the matrix

$$\Omega(p) = U\Omega(p) \otimes_{au} \Omega^T(-p)U^\dagger$$

(12)
acts in $\mathbb{C}^2 \otimes \mathbb{R} \otimes \mathbb{R}$ such that $\otimes_{au}$ is a tensor product in the auxiliary space, and transposition $\Omega^T$ is done in the physical space only. Notation simplifies by embedding the matrices $\Omega(p)$ and $\Omega^T(-p)$ in $\mathbb{C}^2 \otimes \mathbb{R} \otimes \mathbb{R}$ through the redefinitions $\sigma^a \rightarrow \sigma^a \otimes I \otimes I$, $S_a \rightarrow I \otimes S_a \otimes I$, where the $I$ are the unit operators on the respective subspaces in the tensor space $\mathbb{C}^2 \otimes \mathbb{R} \otimes \mathbb{R}$ and by introducing operators $T_a \equiv I \otimes I \otimes T_a$ where the operators $T_x, T_\pm$ also satisfy $SU(2)$ and the representation for $T_a(p)$ are obtained from those for $S_a(p)$ by the replacement $p \rightarrow -p$. With these definitions one has $\Omega(p) = S_z(p)\sigma^z + S_+(p)\sigma^+ + S_-(p)\sigma^-, \Omega^T(-p) = T_z(p)\sigma^z + T_+(p)\sigma^+ + T_-(p)\sigma^-$ and (12) can be written without the tensor product symbol over the auxiliary space in the simpler form

$$\Omega(p) = U\Omega(p)U^T.$$

(13)

The vector $\langle 0, 0 \rangle = \langle 0 \rangle \otimes \langle 0 \rangle$ in (11) is a tensor product of two lowest weight vectors $\langle 0, 0 \rangle, T_- = 0, 0 \rangle$, and the vector $|R_\theta, R_\theta^*\rangle = |R_\theta^*\rangle \otimes |R_\theta\rangle$ is a tensor product of two coherent states (9).

$$|R_\theta, R_\theta^*\rangle = \sum_{n, m=0}^{\infty} \left(\cot \frac{\theta}{2}\right)^{n+m} \frac{(2p)^n}{n!} \frac{(-2p)^m}{m!} |n, m\rangle.$$

(14)

II. STEADY STATE MAGNETIZATION PROFILES

Steady state expectations are found by the usual prescription, e.g. one-point correlations are

$$\langle \sigma^a_m \rangle = \frac{Tr(\sigma^a_m \rho_{NESS})}{Z(N, \theta)}$$

(15)

where $Z(N, \theta) = Tr(\rho_{NESS})$. It is convenient to introduce operators $B_\alpha(p) = Tr(\sigma^a \Omega(p))$,

$$B_0 = 2S_0 T_0 + S_+ T_+ + S_- T_-,$$
$$B_x = S_+ T_+ - S_- T_-,$$
$$B_y = S_z (T_- - T_+) + T_z (S_- - S_+),$$
$$B_z = i (S_0 (T_+ + T_-) - T_z (S_+ + S_-)),$$

(16) (17) (18) (19)

which act in the auxiliary space $\mathbb{R} \otimes \mathbb{R}$ (here and below we omit the argument $p$ for simplicity). Note that by construction $|S_\alpha, T_\beta\rangle = 0$ for any $\alpha, \beta$. In terms of the $B$-operators, the normalization factor becomes

$$Z(N, \theta) = Tr(\rho_{NESS}) = Tr \langle 0, 0 | \Omega(p) \otimes N | R_\theta, R_\theta^* \rangle =$$

$$= \langle 0, 0 | (Tr(\Omega(p)))^N | R_\theta, R_\theta^* \rangle =$$
$$= \langle 0, 0 | Tr(\sigma^a \Omega(p))^N | R_\theta, R_\theta^* \rangle =$$
$$= \langle 0, 0 | B_0^N | R_\theta, R_\theta^* \rangle$$

(20) (21) (22) (23)

Analogously, the one-point expectations (15) are expressed in terms of $B_\alpha$ as

$$M_{\alpha, N}^\alpha = \langle \sigma^\alpha_m \rangle = \frac{\langle 0, 0 | B_0^{k-1} B_\alpha B_0^N - k | R_\theta, R_\theta^* \rangle}{\langle 0, 0 | B_0^N | R_\theta, R_\theta^* \rangle}.$$

(24)

Using the $SU(2)$ commutation rules for $S_\alpha$ and $T_\alpha$, we obtain, with some effort:

$$[B_0 [B_0, B_x]] + 2\{B_0, B_x\} = 4(C_S + C_T)B_x,$$

(25)

where $C_S$ and $C_T$ are $SU(2)$ Casimir operators $C_S = S_z(S_z - I) + S_+ S_-; C_T = T_z(T_z - I) + T_+ T_-$. From the representations we readily find $C_S = p(p + 1), C_T = p(p - 1)$, so that the Eq. (25) becomes $[B_0 [B_0, B_x]] + 2\{B_0, B_x\} = 8p^2 B_x$. Due to the rotational isotropy of the XXX model, this relation is also valid for other spin components,

$$[B_0 [B_0, B_\alpha]] + 2\{B_0, B_\alpha\} = 8p^2 B_\alpha, \quad \alpha = x, y, z.$$

(26)

Another important relation is derived by analyzing the behaviour of the quantity

$$\lim_{r \rightarrow \infty} \frac{Z(N + 1, \theta)}{Z(N, \theta)} = \frac{4}{9} N^2 + O(N)$$

(27)
for $N \gg 1$, see Appendix A. Multiplying (26) by $(0, 0 | B_{0}^{k-1})$ from the left and by $B_{0}^{N-k-1} | R_{\theta}, R_{\theta}^{*})$ from the right, and using (27), (24), we obtain

\begin{align*}
(-2M_{k+1,N+1}^{\alpha} + M_{k+2,N+1}^{\alpha} + M_{k,N+1}^{\alpha}) \frac{Z(N + 1, \theta)}{Z(N, \theta)} \\
+ 2(M_{k,N}^{\alpha} + M_{k+1,N}^{\alpha}) = 8p^2 M_{k,N-1}^{\alpha} \frac{Z(N - 1, \theta)}{Z(N, \theta)}.
\end{align*}

Taking the continuum limit, we substitute $k/N = x, M_{k,N}^{\alpha}, M_{k+1,N}^{\alpha} \to M_{\alpha}(x), M_{\alpha}(x + \frac{1}{N})$ in the above and expand in Taylor series in $1/N$. In the lowest order of expansion, we can neglect the right-hand side of (28) and obtain using (27),

$$
\frac{\partial^2 M_{\alpha}(x)}{\partial x^2} + \theta^2 M_{\alpha}(x) = 0,
$$

provided that

$$
\Gamma \gg \Gamma^* = \frac{1}{N}.
$$

Integrating (29) with the boundary conditions $M_{\alpha}(0) = \sigma^{\alpha}_{\text{target}(L)}$, $M_{\alpha}(1) = \sigma^{\alpha}_{\text{target}(R)}$ where $\sigma^{\alpha}_{\text{target}(L,R)}$ are targeted boundary magnetizations,

\begin{align*}
\sigma^{x}_{\text{target}(L)} = 1; \quad \sigma^{y}_{\text{target}(L)} = \sigma^{z}_{\text{target}(L)} = 0, \\
\sigma^{x}_{\text{target}(R)} = \cos \theta; \quad \sigma^{y}_{\text{target}(R)} = \sin \theta; \quad \sigma^{z}_{\text{target}(R)} = 0,
\end{align*}

we obtain stationary density profiles

\begin{align*}
M^{x}(x) &= \cos \theta x \\
M^{y}(x) &= \sin \theta x \\
M^{z}(x) &= 0,
\end{align*}

interpolating between the left and right boundary values, see Fig. 2. In a finite chain these asymptotic results can be approximated by

\begin{align*}
\langle \sigma^{x}_{k} \rangle &= \cos \left( \frac{\theta}{N} \left( k - \frac{1}{2} \right) \right), \\
\langle \sigma^{y}_{k} \rangle &= \sin \left( \frac{\theta}{N} \left( k - \frac{1}{2} \right) \right),
\end{align*}

see Fig. 2. Note that for $\theta = \pi$ the Eqs (29) reproduce the results obtained in [5].

Numerical evidence as well as the leading behaviour of the normalization (27) suggest that $\theta^2/N$ is a good scaling variable. For small $\Gamma$ of order of $\theta^2/N$, there are corrections to the asymptotic formula (33). In particular the $M^{z}(x)$ profile becomes harmonic as well $M^{z}(x) = -f_1(\Gamma) \sin((x - \frac{1}{2}) \omega(\Gamma))$ see Fig. 2(b). It is quite remarkable that the stationary magnetization profile for NESS satisfies a simple harmonic equation (29) for all magnetization components. However we were not able to derive the (29) in a shorter way. Note that the NESS is formed with highly excited states, since the magnetization is not alternating in space as would be expected for a ground state of an antiferromagnet [3]. Reversing the sign of the spin exchange interaction $H \to -H$ amounts, for the NESS, to reversing the sign $\Gamma$, see (1). We find that $M^{x}(x)$ and $M^{y}(x)$ are invariant under $\Gamma \to -\Gamma$ exchange, while $M^{z}(x)$ reverses its sign, $M^{z}(x) \to -M^{z}(x)$. As a consequence, the limiting harmonic shape of the magnetization profile for $\Gamma \gg \Gamma^* = \frac{1}{N}$, given by (33), does not depend on whether the bulk Hamiltonian is antiferromagnetic or ferromagnetic one, as long as it stays isotropic [12]. Note also that harmonic density profile leads to diffusive $1/N$ scaling of the trasversal magnetization current, see discussion after (52).
III. MAGNETIZATION CURRENTS

The XXX-model, due to its isotropy, has three independent local magnetization currents defined by the time derivative of the respective local magnetization components, \( \frac{d\sigma^\alpha_n}{dt} = \hat{3}^\alpha_n \), where

\[
\hat{j}_n^\alpha = 2\varepsilon_{\alpha\beta\gamma} \sigma_n^\beta \sigma_{n+1}^\gamma,
\]

with the Levi-Civita symbol \( \varepsilon_{\alpha\beta\gamma} \). In the steady state the current expectations \( j^\alpha(\theta) := \langle \hat{j}_n^\alpha \rangle \) are position-independent.

Some important conclusions can be drawn on the base of LME symmetries, and the uniqueness of the steady state \( \Sigma \). Parallel boundary driving \( \theta = 0 \) does not create any gradient, and therefore all currents vanish, \( j^\alpha(0) = 0 \). For the antiparallel alignment \( \theta = \pi \), the magnetization currents \( j^x, j^y \) vanish, but not \( j^z \). \( j^z(\pi) = j^z(0) = 0 \). To see this, note that for \( \theta = \pi \) the NESS has a symmetry \( \rho_{NESS} = \Sigma_x \rho_{NESS} \Sigma_x \), where \( \Sigma_x = (\sigma_x)^{\otimes N} \). The operators \( \hat{j}_n^x, \hat{j}_n^y \) change sign under the action of the symmetry \( : \Sigma_x \hat{j}_n^x \Sigma_x = -\hat{j}_n^x, \Sigma_x \hat{j}_n^y \Sigma_x = -\hat{j}_n^y \). Since \( Tr(\hat{j}_n^z \rho_{NESS}) = -Tr(\Sigma_x \hat{j}_n^z \rho_{NESS} \Sigma_x) = -Tr(\hat{j}_n^{z*} \rho_{NESS}) \), the current suppression follows, see \([10, 13]\) for more details.

In terms of the MPA the steady magnetization currents are given by

\[
\langle \hat{j}_n^\alpha \rangle = \frac{2\varepsilon_{\alpha\beta\gamma} \langle 0, 0 | B_0^{k-1} B_3 B_0^{N-k-1} | R_\theta, \rho_\theta \rangle}{Z(N, \theta)}.
\]

Using the algebra, we find

\[
[B_y, B_z] = 2i(T_z - S_z)B_0 \quad (38)
\]
\[
[B_z, B_y] = B_0 I_1 = B_0 (S_+ - S_- + T_+ - T_-) \quad (39)
\]
\[
i[B_z, B_x] = B_0 I_2 = B_0 (S_+ + S_- - T_+ - T_-) \quad (40)
\]

Operators \( (T_z - S_z), I_1, I_2 \) commute with \( B_0 \), which manifests the local conservation of the magnetizations \( \sigma_n^x, \sigma_n^y, \sigma_n^z \) respectively, so that current expectations values \( \langle \hat{j}_n^\alpha \rangle = j^\alpha \) are indeed position-independent. We readily derive the exact expressions for the \( x \)-magnetization current as

\[
\hat{j}^x(N) = -8i\rho \frac{Z(N - 1, \theta)}{Z(N, \theta)},
\]

which has a characteristic bell-shaped form, see Fig.8.

For \( N = 2, 3, 4 \) the exact expressions for \( \hat{j}^x \) are

\[
\hat{j}^x(2) = \frac{16\Gamma \sin^2 \left( \frac{\theta}{2} \right) (3 + \cos \theta)}{8 \Gamma^2 + 19 + 12 \cos \theta + 8 \cos \theta}
\]
\[
\hat{j}^x(3) = \frac{16\Gamma \sin^2 \left( \frac{\theta}{2} \right) (8\Gamma^2 + 19 + 12 \cos \theta + 8 \cos \theta)}{48\Gamma^4 + 208\Gamma^2 + 216 + (16\Gamma^4 + 112\Gamma^2 + 111) \cos \theta + 18 \cos 2\theta + 8 \cos 3\theta}
\]

Figure 2: (Color online) Exact steady state magnetization profiles from the MPA for the XXX-chain of \( N = 40 \) sites and \( \theta = -\pi/2 \). The three components are \( x \) (top), \( y \) (bottom) and \( z \) (middle). The continuous lines shows analytic results \([34, 35]\) valid for large \( \Gamma N \). Panel (a): \( \Gamma = 4 \), Panel (b): \( \Gamma = 0.2 \).
Note that the applicability of the asymptotic formula (45), as well as of other asymptotics (52), (27), (34), (35) depends on the value of the coupling $\Gamma$ which should be much larger than a characteristic value $\Gamma^*$, see (30). For small values of $\Gamma \ll \Gamma^*$, we find linear growth of $j^x$ with $\Gamma$ of the form
\[
j^x(N) \approx \frac{2}{\Gamma N^2} + O\left(N^{-3}\right)
\]
valid for all $N \geq 2$. Finally, for intermediate $\Gamma$ values, $\Gamma = O(\Gamma^*)$ the function $j^x$ has a maximum in $\Gamma$, see Fig. 3 which scales as $1/N$. The value of $\Gamma$ which maximizes $j^x$ is well-approximated by $\Gamma_{\text{max}} = 2/N$, for $N \gg 1$, data not shown. The amplitude of the maximum can be approximated as $j^x(N)|_{\Gamma=\Gamma_{\text{max}}} = \theta^2/(2N)$.

The $j^y(N)$ current has the same scaling $1/N^2$ for $\Gamma \gg \Gamma^*$ as the current $j^x$ as it is simply proportional to the $j^x$ current, with a proportionality coefficient $(-\cot \theta/2)$. Indeed, e.g. for $\theta = \pm \pi/2$ it follows from the properties of the coherent state that $I_2 |R_\theta, \hat{R}_\theta\rangle = \mp 4p |R_\theta, \hat{R}_\theta\rangle$, and we obtain from (44), (47) that $j^y(\theta = \pm \pi/2) = \mp j^x(\theta = \pm \pi/2)$. For arbitrary $\theta$, $I_2 |R_\theta, \hat{R}_\theta\rangle = (2p \cot \theta/2 + \cot^{-1} \theta/2)I + (\cot \theta/2 - \cot^{-1} \theta/2)(S - T)|R_\theta, \hat{R}_\theta\rangle$ and after a straightforward calculation we obtain
\[
j^y(N, \theta) = 8ip \frac{Z(N-1, \theta)}{Z(N, \theta)} \cot \frac{\theta}{2} = -\cot \frac{\theta}{2} \times j^x(N, \theta).
\]

On the contrary, the scaling and qualitative behaviour of the $j^z$ current is different, in two respects: It scales as $1/N$ and is a monotonically increasing function of $\Gamma$, see Fig. 3. Using properties of coherent states one obtains the following exact expression
\[
j^z(N, \theta) = \frac{4}{\sin \theta} \frac{\langle 0, 0 | B_{\theta}^{N-1}(-S_z - T_z) | R_\theta, \hat{R}_\theta\rangle}{Z(N, \theta)}
\]

For $N = 2, 3, 4$ explicit expressions for $j^z(N)$ are
\[
j^z(2) = \frac{16\Gamma^2 \sin \theta}{8\Gamma^2 + 19 + 12 \cos \theta + \cos 2\theta}
\]
Making use of the exact expressions (33), we have density profiles (33) if one neglects the connected part of the two-point correlations, as ≪ small coupling Γ

\[ j^z(3) = \frac{64 \Gamma^2 \sin \theta \left( \Gamma^2 + 3 + \cos \theta \right)}{48 \left( \Gamma^2 + 126 \right) \cos \theta + 18 \cos 2\theta + \cos 3\theta} \]

\[ j^z(4) = \frac{32 \Gamma^2 \sin \theta \left( 20 \Gamma^4 + 92 \Gamma^2 + 57 + 4 \Gamma^4 + 28 \Gamma^2 + 36 \right) \cos \theta + 3 \cos 2\theta}{\beta_0 + \beta_1 \cos \theta + \beta_2 \cos 2\theta + 24 \cos 3\theta + \cos 4\theta} \]

where \( \beta_0 = 688 \Gamma^6 + 3584 \Gamma^4 + 3616 \Gamma^2 + 867, \beta_1 = 448 \Gamma^6 + 2560 \Gamma^4 + 3200 \Gamma^2 + 936, \beta_2 = 4 \Gamma^6 + 128 \Gamma^4 + 352 \Gamma^2 + 220. \)

For \( \theta = \pi/2, \) the above expressions reduce to those obtained by direct diagonalization in [10], \( j^z(2) = \frac{8 \Gamma^2}{117}, \)

\( j^z(3) = \frac{16 \Gamma^2 (1^2 + 3^2)}{121 + 52 \Gamma^2 + 27}, \)

\( j^z(4) = \frac{8 \Gamma^2 (101^4 + 46 \Gamma^2 + 27)}{3 \left( 28 \Gamma^6 + 144 \Gamma^4 + 136 \Gamma^2 + 27 \right)}. \)

For small values of \( \Gamma \ll \Gamma^*, \) we find quadratic growth of \( j^z \) with \( \Gamma \) of the form

\[ j^z(N)_{\Gamma \ll \Gamma^*} = \frac{8 \sin \theta}{(3 + \cos \theta)^2} (N - 1) \Gamma^2 + O \left( \Gamma^4 \right), \]

for all \( N \geq 2. \) So,

For \( \theta = \pi/2 \) Eq (51) reduces to obtained in [16] by direct diagonalization. Finally, for large \( \Gamma, N, \) (47) reduces to a very simple expression,

\[ j^z(N)_{\Gamma \gg \Gamma^*, N \gg 1} = \frac{2 \theta}{N} + O \left( \frac{1}{N^2} \right) \]

see Appendix A. Note that unlike the currents \( j^x, j^y \) which decrease with the coupling as \( 1/\Gamma, \) the current \( j^z \) increases with \( \Gamma \) and takes a finite value \( \frac{2 \theta}{N} \) as \( \Gamma \to \infty, \) see also Fig. 4. The finiteness of the magnetization current \( j^z \) at \( \Gamma \to \infty \) also emerges from an analysis of a perturbative expansion of NESS for small systems in 1/\( \Gamma, \) for arbitrary spin exchange \( Z- \) anisotropy \( \Delta \neq 0 \) [10]. Note also that an increase of system size \( N \) results in increase of \( j^z(N) \) for small coupling \( \Gamma \ll \Gamma^* \) due to (51), and in decrease of \( j^z(N) \) for \( \Gamma \gg \Gamma^* \) due to (52).

Interestingly, the leading term in the asymptotic expression (52) for the current \( j^z \) can be obtained from the exact density profiles (53) if one neglects the connected part of the two-point correlations, as

\[ j_{MF}^x(N) = 2 \langle \sigma_{n+1}^x \rangle - 2 \langle \sigma_n^y \rangle \langle \sigma_{n+1}^x \rangle. \]

Making use of the exact expressions (53), we have \( \langle \sigma_n^x \rangle = \cos \left( \frac{\theta n}{N} \right), \)

\( \langle \sigma_{n+1}^y \rangle = \sin \left( \frac{\theta n+1}{N} \right). \) \( \) The Eq. (52) is then obtained in the first non-vanishing order of the Taylor expansion of (53) in \( \frac{1}{N}. \)

Another surprising property consists in the fact that for large \( N \) the maximum of the \( j^z(N, \theta) \) current is observed for \( \theta = \pi - O(N^{-1}). \) On the other hand, see the discussion after (36), \( j^z(N, \pi) = 0 \) for any \( N. \) Consequently, the
limits $N \to \infty$ and $\theta \to \pi$ do not commute, namely

\[
\lim_{\theta \to \pi} \lim_{N \to \infty} N j^z(N) = 2\pi \tag{54}
\]
\[
\lim_{N \to \infty} \lim_{\theta \to \pi} N j^z(N) = 0, \tag{55}
\]

see Fig. 5. The reason for the non-commutativity of the limits is the presence of an additional symmetry at $\theta = \pi$ as discussed after (36).

\[NJ^Z_{NESS}(N)\]

Figure 5: (Color online) Function $N j^z(N)$ versus $\theta$, for $N = 10, 20, 100$ (lower, middle, upper curves). In all cases, $\frac{\theta}{N} \ll 1$. The dotted line shows the asymptotics (52) for $N \to \infty$.

IV. CONCLUSIONS

We have investigated open driven XXZ model where boundary spins are pumped in two different directions, with an arbitrary twisting angle between them. We find explicit expressions for one- and two-point observables (magnetization currents and magnetization profiles) in the steady state, and investigate various asymptotic regimes. We find scaling of the magnetization current to be qualitatively different in the direction parallel to the twisting plane, and in the orthogonal direction. We find explicit dependencies on the twisting angle, and retrieve known cases. At the point of antiparallel driving $\theta = \pi$ we find a non-analyticity of the transversal magnetization current in the thermodynamic limit.

It is instructive to compare our findings with previous results on spin transport in the isotropic Heisenberg chain. For $\theta = \pi$, we retrieve an anomalous scaling of the current $1/N^2$ [15], obtained in [5] (note that our $j^x$ current then corresponds to the $j^z$ current of [4]). For $\theta = \pi$, and small driving (i.e. small amplitude of the targeted boundary values, another scaling form was obtained, $j = \text{const}/\sqrt{N}$ [18]. In both cases the current decreases as $1/\Gamma$ with coupling which was attributed to a quantum Zeno effect.

Our study shows that already by an infinitesimal perturbation of the antiparallel boundary alignment $\theta \to \pi - \varepsilon$ in the isotropic model an additional current appears, pointing in the direction perpendicular to the twisting plane, which has yet another scaling form $1/N$ [52]. This new current does not decrease with coupling, but, on the contrary, saturates to its maximal value at $\Gamma \to \infty$.

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Appendix A: Computation of the $Z(N, \theta)$

$Z(N, \theta)$ is given by Eq. (23). The operator $B_0$, restricted to the basis of vectors $V = \{|n, n\rangle\}_{n=0}^{\infty}$, has the form

\[
B_0|_{V} = \sum_{n=0}^{\infty} 2s_n t_n |n, n\rangle \langle n, n| + s_{n+1}^+ t_{n+1}^+ |n, n\rangle \langle n + 1, n + 1| + s_{n}^- t_{n}^- |n + 1, n + 1\rangle \langle n, n|,
\]
where \( s_n = p - n; s_n^+ = n; s_n^- = n - 2p \) and expressions for \( t_n, t_n^\pm \) are obtained from \( s_n, s_n^\pm \) by replacing \( p \to p^* = -p \).

Let us introduce functions \( F_n^{(N)}(p) \) defined as

\[
\langle 0, 0 \rangle B_0^N = \sum_{n=0}^N F_n^{(N)}(p) \langle n, n \rangle \tag{A1}
\]

through which the normalization factor is expressed as \( Z(N, \theta) = \sum_{n=0}^{\infty} F_n^{(N)}(p) \langle n, n \rangle R_{\theta}, R_{\theta}^* \), or,

\[
Z(N, \theta) = \sum_{n=0}^N F_n^{(N)}(p) \left( \cot \frac{\theta}{2} \right)^{2n} \left( \frac{2p}{n} \right) \left( -2p \right) \tag{A2}
\]

**Limit of small \( p \to 0 \).** For \( p \to 0 \), in the lowest order in \( p \) we obtain

\[
Z(N + 1, \theta) = -4p^2 \left( F_1^{(N)}(0) + \sum_{n=1}^{N+1} F_n^{(N+1)}(0) \left( \cot \frac{\theta}{2} \right)^{2n} \sum_{n=1}^{N} \frac{1}{n^2} \right) + o(p^2). \tag{A3}
\]

On the other hand, from the \( (A1) \) the recursion relations for \( F_{n+1}^{(N+1)}(0) \) read

\[
F_{n+1}^{(N+1)}(0) = n^2 \left( 2 F_{n}^{(N)}(0) + F_{n+1}^{(N)}(0) + F_{n+1}^{(N)}(0) \right) \tag{A4}
\]

with the initial condition \( F_{n}^{(1)}(0) = \delta_{n,1} \). Substituting the recursion in the \( (A3) \), and noting that \( F_k^{(N)} = 0 \) for \( k > N \), we obtain

\[
\lim_{p \to 0} \frac{Z(N + 1, \theta)}{p^2} = -16 \sum_{n=1}^{N} F_n^{(N)}(0) \tag{A5}
\]

Here below we treat the case \( \theta = \pi/2 \) in more detail, for which the quantity \( Z(N + 1, \theta) \) becomes

\[
\lim_{p \to 0} \frac{Z(N + 1, \pi/2)}{p^2} = -16 \sum_{n=1}^{N} F_n^{(N)}(0) \tag{A6}
\]

and the recursion relations for \( F_{n}^{(N)}(0) \) are given by \( (A4) \). For further analysis, fix notation as follows: (i) \( F_{n}^{(N)} := F_{n}^{(N)}(0) \), (ii) \( F^{(N)} = \sum_{n=0}^{N} F_{n}^{(N)} \). The conjecture is \( \lim_{N \to \infty} 1/N^y F^{(N+1)}/F^{(N)} = c^{-2} \) with \( y = 2 \) and \( c = 4/\pi \). This implies that asymptotically \( F^{(N)} = F(cN)^{2N} \) with some undetermined constant \( F \). Solving the recursion explicitly for \( n \) close to \( N \) yields the following exact expressions:

\[
F_{N+1}^{(N)} = 0, \tag{A7}
\]

\[
F_{N}^{(N)}/(N!)^2 = 1, \tag{A8}
\]

\[
F_{N-1}^{(N)}/[(N-1)!]^2 = 2 \sum_{k=1}^{N-1} k^2 \sim \frac{2N^3}{3}, \tag{A9}
\]

\[
F_{N-2}^{(N)}/[(N-2)!]^2 = 4 \sum_{k=1}^{N-2} k^2 \sum_{m=1}^{k} m^2 + \sum_{k=1}^{N-2} k^2 (k+1)^2 \sim \frac{1}{2!} \left( \frac{2N^3}{3} \right)^2, \tag{A10}
\]

\[
F_{N-3}^{(N)}/[(N-3)!]^2 = 8 \sum_{k=1}^{N-3} k^2 \sum_{m=1}^{k} m^2 \sum_{n=1}^{m} n^2 + 2 \sum_{k=1}^{N-3} k^2 \sum_{m=1}^{k} m^2 (m+1)^2 \sum_{n=1}^{m} n^2 \sim \frac{1}{3!} \left( \frac{2N^3}{3} \right)^3. \tag{A11}
\]

Here \( \sim \) means up to order \( 1/N \). Hence for fixed \( k \) we obtain the large \( N \) behaviour

\[
\lim_{N \to \infty} N^{-k} F_{N-k}/[(N-k)!]^2 = \frac{2^k}{3^k k!}. \tag{A12}
\]
However, these terms grow strongly with \( k \) and do not dominate the sum over \( m \). To study the behaviour for \( m \propto N \) we make the ansatz

\[
F_m^{(N)}/F^{(N)} = \frac{1}{\sqrt{4\pi bN}} e^{-\frac{(m-aN)^2}{2bN N}}
\]

(A13)

This solves the recursion (A4) with \( a = c/2, b = c^2/8 \) and any \( m - aN \) of the order \( \sqrt{N} \) solves the recursion (A4) up to corrections of order \( 1/N \) for any (positive) value of \( c \). This can be seen by setting \( m = aN + \sqrt{N} \) and plugging this into the recursion (A4).

The l.h.s. yields

\[
F_m^{(N+1)} = F_{m+1}^{(N+1)} \frac{1}{\sqrt{4\pi b(N+1)}} e^{-\frac{(m-an(N+1))^2}{2b(N+1) N}}
\]

\[
= F_{m+1}^{(N+1)} \frac{1}{\sqrt{1 + N^{-1}}} \frac{1}{\sqrt{4\pi bN}} e^{-\frac{(m-an)^2}{2bN N}} + O(N^{-1})
\]

Comparing terms up to order \( N^{-1} \) one gets for \( \theta \)

\[
\left. \frac{\exp \{- (m-a\theta N)^2/2b\theta N \}}{\exp \{- (m-a\theta N^2)^2/2b\theta N \}} \right|_{\theta = 0}
\]

we make the the ansatz

\[
\alpha(m) = \frac{2}{\pi b} \sqrt{\frac{2}{m}}
\]

with \( \alpha(m) \) being a factor of order \( \sqrt{m} \) for \( m \ll 1 \). We are interested in the lowest order in \( p \), for which the "diagonal" part of the vector \( |R_\theta, R_\theta^*\rangle \) becomes

\[
|R_\theta, R_\theta^*\rangle = |0, 0\rangle - 4p^2 \sum_{n=1}^{\infty} \frac{(\cot \frac{\theta}{2})^{2n}}{n^2} |n, n\rangle + O(p^3) + \text{nondiag. terms}
\]

This yields the recursion (A4) up to corrections of order \( 1/N \) for any (positive) value of \( c \). This agrees to the values we found for \( N = 100 \) from numerically exact computation using Mathematica, apart from finite-size corrections. So we have proved the scaling exponent \( y = 2 \) and also found the asymptotic form of \( F_m^{(N)} \) except for the amplitude \( F^{(N)} \).

For arbitrary twisting angle \( \theta \) we assume, analogously to (A13),

\[
\frac{F_m^{(N)}(\cot \frac{\theta}{2})^{2n}}{\sum_{m=0}^{N} F_m^{(N)}(\cot \frac{\theta}{2})^{2n}} = \frac{1}{\sqrt{4\pi b\theta N}} \exp \left( -\frac{(m-a(\theta)N)^2}{2b(\theta) N} \right).
\]

(A14)

Comparing terms up to order \( N^{-1/2} \) yields \( F_m^{(N+1)}/F^{(N)} = (2aN)^2 \) and \( b = a^2/2 \). With the definition of \( c = 4/\pi \) this yields \( a = c/2 = 2/\pi \approx 0.637 \) and \( b = 2/\pi^2 \approx 0.203 \). This agrees to the values we found for \( N = 100 \) from numerically exact computation using Mathematica, apart from finite-size corrections. So we have proved the scaling exponent \( y = 2 \) and also found the asymptotic form of \( F_m^{(N)} \) except for the amplitude \( F^{(N)} \).

\[\text{Current } J^z. \] Let us denote \( Q^{(N)} = \langle 0, 0| B_0^N (-S_z - T_z) |R_\theta, R_\theta^*\rangle \) so that

\[
j^z(N, \theta) = \frac{4}{\sin \theta} Q^{(N-1)} \quad \text{and} \quad \lim_{p \to 0} \frac{Z(N+1, \theta)}{Z(N, \theta)} = \frac{4}{\sin \theta} a(\theta)^2 N^2
\]

(A15)

(A16)

Current \( J^z. \) We start from the expression (A17). Let us denote \( Q^{(N)} = \langle 0, 0| B_0^N (-S_z - T_z) |R_\theta, R_\theta^*\rangle \) so that

\[
j^z(N, \theta) = \frac{4}{\sin \theta} Q^{(N-1)} \quad \text{and} \quad \lim_{p \to 0} \frac{Z(N+1, \theta)}{Z(N, \theta)} = \frac{4}{\sin \theta} a(\theta)^2 N^2
\]

(A15)
Using the above, \((-S_z - T_z)|n,n\rangle = 2n|n,n\rangle\), \((A1)\), and the recursion \((A1)\), we obtain for small \(p\)

\[
Q^{(N-1)} = -8p^2 \sum_{n=1}^{N-1} \frac{(\cot \frac{\theta}{2})^{2n}}{n} F_n^{(N-1)} =
\]

\[
= -8p^2 \sum_{n=1}^{N-1} \left( \frac{\cot \frac{\theta}{2}}{2} \right)^{2n} n \left( 2F_n^{(N-2)} + F_{n-1}^{(N-2)} + F_{n+1}^{(N-2)} \right) =
\]

\[
= -32p^2 \frac{1}{\sin^2 \theta} \left( \sum_{n=1}^{N-2} n \left( \frac{\cot \frac{\theta}{2}}{2} \right)^{2n} F_n^{(N-2)} + \frac{\sin \theta}{4} F_1^{(N-2)} \left( \frac{\cot \frac{\theta}{2}}{2} \right)^4 \right)
\]

The last term on the rhs is of lower order in \(N\) and can be neglected. Substituting \(Q^{(N-1)}\) in \((A17)\), and using \((A15)\), \((A5)\), we obtain

\[
j^2(N,\theta) = \frac{8}{\sin \theta} \sum_{n=1}^{N-2} n \left( \frac{\cot \frac{\theta}{2}}{2} \right)^{2n} \frac{F_n^{(N-2)}}{Z(N-2,\theta)} \frac{Z(N-1,\theta)}{Z(N-2,\theta)} =
\]

\[
= \frac{2\sin \theta}{a(\theta)^2 N^2} \langle n \rangle,
\]

where \(\langle n \rangle = \sum_{n=1}^{N-2} n \left( \frac{\cot \frac{\theta}{2}}{2} \right)^{2n} F_n^{(N-2)} / Z(N-2,\theta)\). Using the Ansatz \((A14)\), we get \(\langle n \rangle = a(\theta) N\), to yield

\[
j^2(N,\theta) = \frac{2\sin \theta}{a(\theta) N} + O \left( \frac{1}{N^2} \right).
\]

The only unknown parameter \(a(\theta)\), corresponding to the maximum of the distribution \((A14)\), on the basis of numerical evidence is conjectured to be

\[
a(\theta) = \frac{\sin \theta}{\theta},
\]

(A19)

up to corrections of order \(O(N^{-1})\). Substituting the \((A19)\) into \((A18)\) and \((A15)\), we obtain \((27)\), and then, all steady state density profiles and steady currents \((33), (45), (52)\).

[12] That the isotropy of the Hamiltonian is important for harmonicity of the magnetization profile, is seen in an integrable example of XXZ model with antiparallel twisting \((\theta = \pi)\): outside the isotropic point \(\Delta = 1\), magnetization profiles are either flat or domain-wall like \([\text{3}]\).
[17] Note that our definition of \(\theta\) is related to the one in \([\text{2}]\) by replacement \(\theta \to \pi - \theta\).