On a quantum phase transition in a steady state out of equilibrium

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Abstract

Within the rigorous axiomatic framework for the description of quantum mechanical systems with a large number of degrees of freedom, we show that the nonequilibrium steady state, constructed in the quasifree fermionic system corresponding to the isotropic XY chain in which a finite sample, coupled to two thermal reservoirs at different temperatures, is exposed to a local external magnetic field, is breaking translation invariance and exhibits a strictly positive entropy production rate. Moreover, we prove that there exists a second-order nonequilibrium quantum phase transition with respect to the strength of the magnetic field as soon as the system is truly out of equilibrium.

1 Introduction

"As useful as the characterization of equilibrium states by thermostatic theory has proven to be, it must be conceded that our primary interest is frequently in processes rather than in states. In biology, particularly, it is the life process that captures our imagination rather than the eventual equiilbrium [sic] state to which each organism inevitably proceeds."

<div align="right">H. B. Callen [11, p. 283]</div>

A precise analysis of quantum mechanical systems having a large, i.e., often, in physically idealized terms, an infinite number of degrees of freedom is most effectively carried

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out within the mathematically rigorous framework of operator algebras. As a matter of fact, having been heavily used in the 1960s for the description of quantum mechanical systems in thermal equilibrium, the benefits of this framework have again started to unfold more recently in the physically much more general situation of open quantum systems out of equilibrium. In the latter field, vast by its very nature, most of the mathematically rigorous results have been obtained for a particular family of states out of equilibrium, namely for the so-called nonequilibrium steady states (NESS) introduced in [17, p. 6] as the large time limit of the averaged trajectory of some initial state along the full time evolution. Beyond the challenging construction of this central object of interest in physically interesting situations, the derivation, from first principles, of fundamental transport and quantum phase transition properties for thermodynamically nontrivial systems out of equilibrium has also come within reach.

In both quantum statistical mechanics in and out of equilibrium, an important role is played by the so-called quasifree fermionic systems, and this is true not only with respect to the mathematical accessibility but also when it comes to real physical applications. Namely, from a mathematical point of view, such systems allow for a simple and powerful description by means of scattering theory restricted to the underlying one-particle Hilbert space over which the fermionic algebra of observables is constructed. This restriction of the dynamics to the one-particle Hilbert space opens the way for a rigorous mathematical analysis of many properties which are of fundamental physical interest. On the other hand, they also constitute a class of systems which are indeed realized in nature. One of the most prominent representatives of this class is the so-called XY spin chain introduced in 1961 in [13, p. 409] where a specific equivalence of this spin model with a quasifree fermionic system has been established. Already in the 1960s, the first real physical candidate has been identified in [12, p. 459] (see, for example, [15] for a survey of the rich interplay between the experimental and theoretical research activity in the very dynamic field of low-dimensional magnetic systems).

In the present paper, we analyze transport and quantum phase transition properties for the quasifree fermionic system over the two-sided discrete line corresponding, in the spin picture, to the special case of the so-called isotropic XY spin chain. In order to model the desired nonequilibrium situation as in [7, p. 3431], we first fix

$$\nu \in \mathbb{N}_0, \tag{1}$$

and cut the finite piece of length $2\nu + 1$,

$$\mathbb{Z}_S := \{x \in \mathbb{Z} \,|\, |x| \leq \nu\}, \tag{2}$$

out of the two-sided discrete line. This piece plays the role of the configuration space of the confined sample, whereas the remaining parts,

$$\mathbb{Z}_L := \{x \in \mathbb{Z} \,|\, x \leq -(\nu + 1)\}, \tag{3}$$
$$\mathbb{Z}_R := \{x \in \mathbb{Z} \,|\, x \geq \nu + 1\}, \tag{4}$$

act as the configuration spaces of the infinitely extended thermal reservoirs. Furthermore, over these configuration spaces, an initial decoupled state is prepared as the product of

three thermal equilibrium states carrying the corresponding inverse temperatures

$$0 = \beta_S < \beta_L < \beta_R < \infty. \tag{5}$$

Finally, the NESS is constructed with respect to the full time evolution which not only recouples the sample and the reservoirs but also introduces a one-site magnetic field of strength

$$\lambda \in \mathbb{R} \tag{6}$$

at the origin.

As a first result, we show that there exists a unique quasifree NESS, which we call the magnetic NESS, whose translation invariance is broken as soon as the local magnetic field strength λ is switched on. This property contrasts with the translation invariance of the NESS constructed in [9, p. 1158] for the anisotropic XY model with spatially constant magnetic field (see also Remark 3 below). Moreover, we explicitly determine the NESS expectation value of the extensive energy current observable describing the energy flow through the sample from the left to the right reservoir. The form of this current immediately yields that the entropy production rate, the first fundamental physical quantity for systems out of equilibrium, is strictly positive. Finally, we show that the system also exhibits what we call a second-order nonequilibrium quantum phase transition, i.e., in the case at hand, a logarithmic divergence of the second derivative of the entropy production rate with respect to the magnetic field strength at the origin.

The present paper is organized as follows.
Section 2 specifies the nonequilibrium setting, i.e., it introduces the observables, the quasifree dynamics, and the quasifree initial state.
Section 3 contains the construction of the magnetic NESS and the proof of the breaking of translation invariance for nonvanishing magnetic field strength.
Section 4 introduces the notions of energy current and entropy production rate. It also contains the determination of the heat flow and the strict positivity of the entropy production rate.
Section 5 displays the last result, i.e., the proof of the existence of a second-order nonequilibrium quantum phase transition.
Finally, the *Appendix* collects some ingredients used in the foregoing sections pertaining to the spectral theory of the magnetic Hamiltonian, the structure of the XY NESS, and the action of the magnetic wave operators on completely localized wave functions.

2 Nonequilibrium setting

Remember that, in the operator algebraic approach to quantum statistical mechanics, a physical system is specified by an algebra of observables, a group of time evolution automorphisms, and a normalized positive linear state functional on this observable algebra (see, for example, the standard references [10] for more details).

In the Definition 1, 2, and 5 below, part *(a)* recalls the general formulation for quasifree fermionic systems and part *(b)* specializes to the concrete situation from [7, p. 3431] which we are interested in in the present paper.

In the following, the commutator and the anticommutator of two elements a and b in the corresponding sets in question read as usual as $[a,b] := ab - ba$ and $\{a,b\} := ab + ba$, respectively.

Definition 1 (Observables)

(a) Let $\mathfrak{h}$ be the one-particle Hilbert space of the physical system. The observables are described by the elements of the unital canonical anticommutation algebra $\mathfrak{A}$ over $\mathfrak{h}$ generated by the identity 1 and elements $a(f)$ for all $f \in \mathfrak{h}$, where $a(f)$ is antilinear in f and, for all $f, g \in \mathfrak{h}$, we have the canonical anticommutation relations

$$\{a(f), a(g)\} = 0, \tag{7}$$
$$\{a(f), a^*(g)\} = (f, g)\, 1, \tag{8}$$

where $(\cdot, \cdot)$ denotes the scalar product of $\mathfrak{h}$.

(b) Let the configuration space of the physical system be given by the two-sided infinite discrete line $\mathbb{Z}$ and let

$$\mathfrak{h} := \ell^2(\mathbb{Z}) \tag{9}$$

be the one-particle Hilbert space over this configuration space.

The second ingredient is the time evolution. In order to define a quasifree dynamics, it is sufficient, by definition, to specify its one-particle Hamiltonian, i.e., the generator of the time evolution on the one-particle Hilbert space $\mathfrak{h}$. In general, a one-particle Hamiltonian is an unbounded selfadjoint operator on $\mathfrak{h}$ (which is typically bounded from below though). Such an action on the one-particle Hilbert space can be naturally lifted to the observable algebra $\mathfrak{A}$, becoming a group of automorphisms of $\mathfrak{A}$.

In the following, the set of $(*-)$automorphisms of $\mathfrak{A}$ will be written as $\mathrm{Aut}(\mathfrak{A})$ and we denote by $\mathcal{L}(\mathfrak{h})$ and $\mathcal{L}^0(\mathfrak{h})$ the bounded operators and the finite rank operators on $\mathfrak{h}$, respectively. Moreover, for all $r, q \in \mathbb{R}$, the Kronecker symbol is defined as usual by $\delta_{rq} := 1$ if $r = q$ and $\delta_{rq} := 0$ if $r \neq q$. Furthermore, for all $a \in \mathcal{L}(\mathfrak{h})$, we define the real part and the imaginary part of a by $\mathrm{Re}(a) := (a + a^*)/2$ and $\mathrm{Im}(a) := (a - a^*)/(2\mathrm{i})$, respectively. Finally, we set $a^0 := 1 \in \mathcal{L}(\mathfrak{h})$, and, if a is invertible, we use the notation $a^{-n} := (a^{-1})^n$ for all $n \in \mathbb{N}$.

Definition 2 (Quasifree dynamics)

(a) Let h be a Hamiltonian on $\mathfrak{h}$. The quasifree dynamics generated by h is the automorphism group defined, for all $t \in \mathbb{R}$ and all $f \in \mathfrak{h}$, by

$$\tau^t(a(f)) := a(\mathrm{e}^{\mathrm{i}th} f), \tag{10}$$

and suitably extended to the whole of $\mathfrak{A}$.

(b) *The right translation $u \in \mathcal{L}(\mathfrak{h})$ and the localization projection $p_0 \in \mathcal{L}^0(\mathfrak{h})$ are defined, for all $f \in \mathfrak{h}$ and all $x \in \mathbb{Z}$, by*

$$(uf)(x) := f(x-1), \tag{11}$$

$$p_0 f := f(0)\,\delta_0, \tag{12}$$

where the elements of the usual completely localized orthonormal Kronecker basis $\{\delta_y\}_{y \in \mathbb{Z}}$ of $\mathfrak{h}$ are given by $\delta_y(x) := \delta_{xy}$ for all $x \in \mathbb{Z}$. Moreover, let $\lambda \in \mathbb{R}$ denote the magnetic field strength and define the one-particle Hamiltonians $h, h_{\mathrm{d}}, h_\lambda \in \mathcal{L}(\mathfrak{h})$ by

$$h := \mathrm{Re}(u), \tag{13}$$

$$h_{\mathrm{d}} := h - (v_L + v_R), \tag{14}$$

$$h_\lambda := h + \lambda v, \tag{15}$$

where the local external magnetic field $v \in \mathcal{L}^0(\mathfrak{h})$ and the decoupling operators $v_L, v_R \in \mathcal{L}^0(\mathfrak{h})$ read

$$v := p_0, \tag{16}$$

$$v_L := \mathrm{Re}(u^{-\nu} p_0 u^{\nu+1}), \tag{17}$$

$$v_R := \mathrm{Re}(u^{\nu+1} p_0 u^{-\nu}). \tag{18}$$

The operators h, h_{d}, and h_λ will be called the XY Hamiltonian, the decoupled Hamiltonian, and the magnetic Hamiltonian, respectively. The corresponding time evolution automorphisms of $\mathfrak{A}$ are given by (10) and will be denoted by τ^t, τ_{d}^t, and τ_λ^t for all $t \in \mathbb{R}$.

Remark 3 As mentioned in the Introduction, the model specified by Definition 1 and 2 has its origin in the XY spin chain whose formal Hamiltonian reads

$$H = -\frac{1}{4} \sum_{x \in \mathbb{Z}} \left\{ (1+\gamma)\, \sigma_1^{(x)} \sigma_1^{(x+1)} + (1-\gamma)\, \sigma_2^{(x)} \sigma_2^{(x+1)} + 2\mu \sigma_3^{(x)} \right\}, \tag{19}$$

where $\gamma \in (-1, 1)$ represents the anisotropy, $\mu \in \mathbb{R}$ the spatially homogeneous magnetic field, and $\sigma_1, \sigma_2, \sigma_3$ are the usual Pauli matrices. Indeed, using the so-called Araki-Jordan-Wigner transformation introduced in [5, p. 279] (see also Remark 14), the Hamiltonian from (13) corresponds to the case of the so-called isotropic XY chain without magnetic field, i.e., to the case with $\gamma = \mu = 0$ in (19). In order to treat the anisotropic case $\gamma \neq 0$, one uses the so-called selfdual quasifree setting developed in [4, p. 386]. In this most natural framework, one works in the doubled one-particle Hilbert space $\mathfrak{h} \oplus \mathfrak{h}$ and the generator of the truly anisotropic XY dynamics has nontrivial off-diagonal blocks on $\mathfrak{h} \oplus \mathfrak{h}$ (which vanish for $\gamma = 0$). In many respects, the truly anisotropic XY model is substantially more complicated than the isotropic one (this is true, a fortiori, if the magnetic field μ is switched on whose contribution to the generator acts diagonally on $\mathfrak{h} \oplus \mathfrak{h}$ though).

Remark 4 For all $\alpha \in \{L, S, R\}$, let us define the Hilbert space

$$\mathfrak{h}_\alpha := \ell^2(\mathbb{Z}_\alpha) \tag{20}$$

over the sample and reservoir configuration spaces $\mathbb{Z}_\alpha$ defined in (2), (3), and (4), respectively. Moreover, for all $\alpha \in \{L, S, R\}$, we define the map $i_\alpha : \mathfrak{h}_\alpha \to \mathfrak{h}$, for all $f \in \mathfrak{h}_\alpha$ and all $x \in \mathbb{Z}$, by

$$(i_\alpha f)(x) := \begin{cases} f(x), & x \in \mathbb{Z}_\alpha, \\ 0, & x \in \mathbb{Z} \setminus \mathbb{Z}_\alpha, \end{cases} \tag{21}$$

and we note that its adjoint $i_\alpha^* : \mathfrak{h} \to \mathfrak{h}_\alpha$ is the operator acting by restriction to $\mathfrak{h}_\alpha$. With the help of these natural injections, we define the unitary operator $w : \mathfrak{h} \to \mathfrak{h}_L \oplus \mathfrak{h}_S \oplus \mathfrak{h}_R$, for all $f \in \mathfrak{h}$, by

$$wf := i_L^* f \oplus i_S^* f \oplus i_R^* f, \tag{22}$$

and we observe that its inverse $w^{-1} : \mathfrak{h}_L \oplus \mathfrak{h}_S \oplus \mathfrak{h}_R \to \mathfrak{h}$ is given by $w^{-1}(f_L \oplus f_S \oplus f_R) = i_L f_L + i_S f_S + i_R f_R$ for all $f_L \oplus f_S \oplus f_R \in \mathfrak{h}_L \oplus \mathfrak{h}_S \oplus \mathfrak{h}_R$. Then, using (22), we can write

$$w v_L w^{-1} = \frac{1}{2} \begin{bmatrix} 0 & (i_S^* \delta_{-\nu}, \cdot\,) i_L^* \delta_{-(\nu+1)} & 0 \\ (i_L^* \delta_{-(\nu+1)}, \cdot\,) i_S^* \delta_{-\nu} & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \tag{23}$$

$$w v_R w^{-1} = \frac{1}{2} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & (i_R^* \delta_{\nu+1}, \cdot\,) i_S^* \delta_\nu \\ 0 & (i_S^* \delta_\nu, \cdot\,) i_R^* \delta_{\nu+1} & 0 \end{bmatrix}, \tag{24}$$

where we used the same notation for the scalar products on $\mathfrak{h}_L$, $\mathfrak{h}_S$, and $\mathfrak{h}_R$ and for the one on $\mathfrak{h}$. Computing $w h w^{-1}$ and using (23) and (24), we find that the decoupling operators v_L and v_R indeed decouple the sample from the reservoirs in the sense that

$$w h_{\mathrm{d}} w^{-1} = h_L \oplus h_S \oplus h_R, \tag{25}$$

where, for all $\alpha \in \{L, S, R\}$, the Hamiltonians $h_\alpha \in \mathcal{L}(\mathfrak{h}_\alpha)$ are defined by

$$h_\alpha := i_\alpha^* h i_\alpha. \tag{26}$$

The last ingredient are the states, i.e., the normalized positive linear functionals on the observable algebra $\mathfrak{A}$. As discussed in the Introduction, we are interested in quasifree states, i.e., in states whose many-point correlation functions factorize in determinantal form.

In the following, $E_{\mathfrak{A}}$ stands for the set of states on $\mathfrak{A}$. Moreover, for all $n \in \mathbb{N}$, the $n \times n$ matrix with entries $a_{ij} \in \mathbb{C}$ for all $i, j \in \{1, \ldots, n\}$ is denoted by $[a_{ij}]_{i,j=1}^n$.

Definition 5 (Quasifree states)

(a) *Let $s \in \mathcal{L}(\mathfrak{h})$ be an operator satisfying $0 \leq s \leq 1$. A state $\omega_s \in E_{\mathfrak{A}}$ is called a quasifree state induced by s if, for all $n, m \in \mathbb{N}$, all $f_1, \ldots, f_n \in \mathfrak{h}$, and all $g_1, \ldots, g_m \in \mathfrak{h}$, we have*

$$\omega_s(a^*(f_n) \ldots a^*(f_1) a(g_1) \ldots a(g_m)) = \delta_{nm} \det([(g_i, sf_j)]_{i,j=1}^n). \tag{27}$$

The operator s is called the two-point operator of the quasifree state ω_s.

(b) *The decoupled initial state is defined to be the quasifree state $\omega_{\mathrm{d}} \in E_{\mathfrak{A}}$ induced by the two-point operator $s_{\mathrm{d}} \in \mathcal{L}(\mathfrak{h})$ of the form*

$$s_{\mathrm{d}} := \rho(\beta_L i_L h_L i_L^* + \beta_R i_R h_R i_R^*), \tag{28}$$

where, for all $r \in \mathbb{R}$, the Planck density function $\rho_r : \mathbb{R} \to \mathbb{R}$ is defined, for all $e \in \mathbb{R}$, by

$$\rho_r(e) := \frac{1}{1 + \mathrm{e}^{re}}, \tag{29}$$

and, in (28), we used the simplified notation $\rho := \rho_1$.

Remark 6 In the selfdual quasifree setting mentioned in Remark 3, the quasifreeness of a state is expressed by means of a pfaffian of the two-point correlation matrix with respect to the generators of the selfdual canonical anticommutation algebra (see, for example, [7, p. 3447]).

Remark 7 Using the unitarity of $w \in \mathcal{L}(\mathfrak{h}, \mathfrak{h}_L \oplus \mathfrak{h}_S \oplus \mathfrak{h}_R)$ from (22), the unitary invariance of the spectrum, the uniqueness of the continuous functional calculus, and

$$w i_L h_L i_L^* w^{-1} = h_L \oplus 0 \oplus 0, \tag{30}$$
$$w i_R h_R i_R^* w^{-1} = 0 \oplus 0 \oplus h_R, \tag{31}$$

the two-point operator of the decoupled quasifree initial state can be written as

$$\begin{aligned}
w s_{\mathrm{d}} w^{-1} &= w\rho(\beta_L i_L h_L i_L^* + \beta_R i_R h_R i_R^*) w^{-1} \\
&= \rho(w(\beta_L i_L h_L i_L^* + \beta_R i_R h_R i_R^*) w^{-1}) \\
&= \rho(\beta_L h_L \oplus 0 \oplus \beta_R h_R) \\
&= \rho_{\beta_L}(h_L) \oplus \tfrac{1}{2} 1 \oplus \rho_{\beta_R}(h_R),
\end{aligned} \tag{32}$$

i.e., the two-point operator s_{d} does not couple the sample and the reservoir subsystems as required by our nonequilibrium setting.

One of the main motivations for introducing the magnetic Hamiltonian (15) in [7, p. 3432] was to study the effect of the breaking of translation invariance. For quasifree states as given in Definition 5 *(a)*, this property can be defined as follows.

Definition 8 (Translation invariance) *A quasifree state $\omega_s \in E_\mathfrak{A}$ induced by the two-point operator $s \in \mathcal{L}(\mathfrak{h})$ is called translation invariant if*

$$[s, u] = 0, \tag{33}$$

where $u \in \mathcal{L}(\mathfrak{h})$ is the right translation from (11).

Remark 9 By using the translation automorphism $\tau_u \in \mathrm{Aut}(\mathfrak{A})$ defined by $\tau_u(a(f)) := a(uf)$ for all $f \in \mathfrak{h}$ and suitably extended to the whole of $\mathfrak{A}$, we note that a quasifree state $\omega_s \in E_\mathfrak{A}$ is translation invariant if and only if $\omega_s \circ \tau_u = \omega_s$.

3 Nonequilibrium steady state

The definition of a nonequilibrium steady state (NESS) below stems from [17, p. 6]. We immediately specialize it to the case at hand.

In the following, if nothing else is explicitly stated, we will always use the assumptions $0 = \beta_S < \beta_L < \beta_R < \infty$ and $\lambda \in \mathbb{R}$ from (5) and (6). Moreover, we will also use the notation

$$\delta := \frac{\beta_R - \beta_L}{2}, \tag{34}$$

$$\beta := \frac{\beta_R + \beta_L}{2}. \tag{35}$$

Definition 10 (Magnetic NESS) *The state $\omega_\lambda \in E_\mathfrak{A}$, defined, for all $A \in \mathfrak{A}$, by*

$$\omega_\lambda(A) := \lim_{t \to \infty} \omega_\mathrm{d}(\tau_\lambda^t(A)), \tag{36}$$

is called the magnetic NESS associated with the decoupled quasifree initial state $\omega_\mathrm{d} \in E_\mathfrak{A}$ and the magnetic dynamics $\tau_\lambda^t \in \mathrm{Aut}(\mathfrak{A})$ for all $t \in \mathbb{R}$.

Remark 11 The more general definition in [17, p. 6] defines a NESS as a weak-$*$ limit point for $T \to \infty$ of

$$\frac{1}{T} \int_0^T \mathrm{d}t \; \omega_\mathrm{d} \circ \tau_\lambda^t. \tag{37}$$

This averaging procedure implies, in general, the existence of a limit point. In particular, in the quasifree setting, it allows to treat a nonvanishing contribution to the point spectrum of the one-particle Hamiltonian generating the full time evolution. In the present case, since, due to Proposition 31 *(c)* from Appendix A, the Hamiltonian h_λ has a single eigenvalue, (36) is sufficient to extract a limit from the point spectrum subspace (see (49) below).

In [7, p. 3436], we found that the magnetic NESS is a quasifree state induced by a two-point operator $s_\lambda \in \mathcal{L}(\mathfrak{h})$ whose form could be determined with the help of scattering theory on the one-particle Hilbert space $\mathfrak{h}$. In particular, we made use of the wave operator $w(h_\mathrm{d}, h_\lambda) \in \mathcal{L}(\mathfrak{h})$ defined by

$$w(h_\mathrm{d}, h_\lambda) := \mathrm{s} - \lim_{t \to \infty} \mathrm{e}^{-ith_\mathrm{d}} \mathrm{e}^{ith_\lambda} 1_\mathrm{ac}(h_\lambda), \tag{38}$$

where $1_\mathrm{ac}(h_\lambda) \in \mathcal{L}(\mathfrak{h})$ denotes the spectral projection onto the absolutely continuous subspace of the magnetic Hamiltonian h_λ. Moreover, we will also need the spectral projection $1_\mathrm{pp}(h_\lambda) \in \mathcal{L}(\mathfrak{h})$ onto the pure point subspace of h_λ. All the spectral properties of the magnetic Hamiltonian h_λ which we will use in the following are summarized in Appendix A.

Theorem 12 (Magnetic two-point operator) *The magnetic NESS ω_λ is the quasifree state induced by the two-point operator $s_\lambda \in \mathcal{L}(\mathfrak{h})$ given by*

$$s_\lambda = w^*(h_\mathrm{d}, h_\lambda) s_\mathrm{d} w(h_\mathrm{d}, h_\lambda) + 1_\mathrm{pp}(h_\lambda) s_\mathrm{d} 1_\mathrm{pp}(h_\lambda). \tag{39}$$

Moreover, if $\lambda \neq 0$, the pure point subspace of $h_\lambda \in \mathcal{L}(\mathfrak{h})$ is one-dimensional.

Remark 13 For all $\gamma \in (-1, 1)$ and all $\mu \in \mathbb{R}$ in (19), the so-called XY NESS has been constructed in [9, p. 1170] using time dependent scattering theory (see Theorem 32 of Appendix B for the XY NESS with $\gamma = \mu = 0$). The two-point operator of the XY NESS for $\gamma = \mu = 0$ coincides with the two-point operator of the magnetic NESS for $\lambda = 0$.

Remark 14 For the special case $\gamma = \mu = 0$, the XY NESS has also been found in [6] with the help of asymptotic approximation methods. The construction of the XY NESS in [6] and [9] is carried out within the mathematically rigorous axiomatic framework of operator algebras for the description of quantum mechanical systems having an infinite number of degrees of freedom. Due to the two-sidedness of the present nonequilibrium setting, the passage from the spin algebra to the canonical anticommutation algebra relies on the so-called Araki-Jordan-Wigner transformation introduced in [5, p. 279]. In contrast to the case of the usual Jordan-Wigner transformation for finite or infinite one-sided systems, the direct correspondence between these two algebras breaks down in the thermodynamic limit of an infinite chain which extends in both directions.

Remark 15 In [9, p. 1158], we observed that the XY NESS can be written, formally, as an equilibrium state specified by the inverse temperature β and an effective Hamiltonian which differs from the original XY Hamiltonian by conserved long-range multi-body charges (in [14, p. 914], it has been proved though that, if $\beta_L \neq \beta_R$, there exists no strongly continuous one-parameter automorphism group of the spin algebra with respect to which the XY NESS is an equilibrium [KMS] state). The Lagrange multiplier approach of [3, p. 168] (see also [2, p. 5186]), set up for a chain of finite length, directly defines a NESS as the ground state of an effective Hamiltonian which differs from the original Hamiltonian by the conserved macroscopic energy current observable. As formally discussed in [16, p. 168], the effective Hamiltonian constructed in this way is substantially different from the one corresponding to

the XY NESS in that it only contains a finite subfamily of the infinite family of all the charges present in the latter situation. Moreover, since the XY NESS consists of left movers and right movers carrying the inverse temperatures β_R and β_L of the right and left reservoirs, respectively (cf. [9, p. 1171]), the exponential decay of the transversal spin-spin correlation function (cf. [8, p. 10]) contrasts with its weak power law behavior in the Lagrange multiplier approach.

For the sake of completeness, we display the proof of Theorem 12 given in [7, p. 3437].

Proof. Since $\mathfrak{A}$ is generated by the identity 1 and the elements $a(f)$ for all $f \in \mathfrak{h}$, since $|\omega_{\mathrm{d}}(\tau_\lambda^t(A))| \le \|A\|$ for all $t \in \mathbb{R}$ and all $A \in \mathfrak{A}$, and since ω_{d} satisfies the determinantal factorization property (27), it is enough to study, for all $n \in \mathbb{N}$, the large time limit of

$$\omega_{\mathrm{d}}(\tau_\lambda^t(a^*(f_n) \ldots a^*(f_1) a(g_1) \ldots a(g_n))) = \det(\Omega(t)), \tag{40}$$

where the map $\Omega : \mathbb{R} \to \mathrm{Mat}(n, \mathbb{C})$ is defined, for all $t \in \mathbb{R}$ and all $i, j \in \{1, \ldots, n\}$, by

$$\Omega_{ij}(t) := (\mathrm{e}^{ith_\lambda} g_i, s_{\mathrm{d}} \mathrm{e}^{ith_\lambda} f_j), \tag{41}$$

and $\mathrm{Mat}(n, \mathbb{C})$ stands for the set of complex $n \times n$ matrices. Moreover, since, due to Proposition 31 *(a)* from Appendix A, the singular continuous spectrum of h_λ is empty, we have $1 = 1_{\mathrm{ac}}(h_\lambda) + 1_{\mathrm{pp}}(h_\lambda)$. Thus, inserting 1 between the propagator and the wave function on both sides of the scalar product in (41), we can write, for all $t \in \mathbb{R}$ and all $i, j \in \{1, \ldots, n\}$, that

$$\Omega_{ij}(t) = \Omega_{ij}^{\mathrm{aa}}(t) + \Omega_{ij}^{\mathrm{ap}}(t) + \Omega_{ij}^{\mathrm{pa}}(t) + \Omega_{ij}^{\mathrm{pp}}(t), \tag{42}$$

where the maps $\Omega^{\mathrm{aa}}, \Omega^{\mathrm{ap}}, \Omega^{\mathrm{pa}}, \Omega^{\mathrm{pp}} : \mathbb{R} \to \mathrm{Mat}(n, \mathbb{C})$ are defined, for all $t \in \mathbb{R}$ and all $i, j \in \{1, \ldots, n\}$, by

$$\Omega_{ij}^{\mathrm{aa}}(t) := (\mathrm{e}^{ith_\lambda} 1_{\mathrm{ac}}(h_\lambda) g_i, s_{\mathrm{d}} \mathrm{e}^{ith_\lambda} 1_{\mathrm{ac}}(h_\lambda) f_j), \tag{43}$$

$$\Omega_{ij}^{\mathrm{ap}}(t) := (\mathrm{e}^{ith_\lambda} 1_{\mathrm{ac}}(h_\lambda) g_i, s_{\mathrm{d}} \mathrm{e}^{ith_\lambda} 1_{\mathrm{pp}}(h_\lambda) f_j), \tag{44}$$

$$\Omega_{ij}^{\mathrm{pa}}(t) := (\mathrm{e}^{ith_\lambda} 1_{\mathrm{pp}}(h_\lambda) g_i, s_{\mathrm{d}} \mathrm{e}^{ith_\lambda} 1_{\mathrm{ac}}(h_\lambda) f_j), \tag{45}$$

$$\Omega_{ij}^{\mathrm{pp}}(t) := (\mathrm{e}^{ith_\lambda} 1_{\mathrm{pp}}(h_\lambda) g_i, s_{\mathrm{d}} \mathrm{e}^{ith_\lambda} 1_{\mathrm{pp}}(h_\lambda) f_j). \tag{46}$$

Term $\Omega_{ij}^{\mathrm{aa}}$
Using that $[h_{\mathrm{d}}, s_{\mathrm{d}}] = 0$ which follows from (25) and (32), the large time limit of (43) yields the wave operator contribution to s_λ in (39) since, for all $i, j \in \{1, \ldots, n\}$, we have

$$\lim_{t \to \infty} \Omega_{ij}^{\mathrm{aa}}(t) = \lim_{t \to \infty} (\mathrm{e}^{-ith_{\mathrm{d}}} \mathrm{e}^{ith_\lambda} 1_{\mathrm{ac}}(h_\lambda) g_i, s_{\mathrm{d}} \mathrm{e}^{-ith_{\mathrm{d}}} \mathrm{e}^{ith_\lambda} 1_{\mathrm{ac}}(h_\lambda) f_j)$$

$$= (g_i, w^*(h_{\mathrm{d}}, h_\lambda) s_{\mathrm{d}} w(h_{\mathrm{d}}, h_\lambda) f_j). \tag{47}$$

Terms $\Omega_{ij}^{\mathrm{ap}}$ and $\Omega_{ij}^{\mathrm{pa}}$
The large time limit of (44) behaves, for all $i, j \in \{1, \ldots, n\}$, like

$$\lim_{t \to \infty} |\Omega_{ij}^{\mathrm{ap}}(t)| \le \lim_{t \to \infty} \|1_{\mathrm{pp}}(h_\lambda) s_{\mathrm{d}} \mathrm{e}^{ith_\lambda} 1_{\mathrm{ac}}(h_\lambda) g_i\| \|f_j\|$$

$$= 0, \tag{48}$$

where we used the Riemann-Lebesgue lemma and the fact from Proposition 31 *(c)* of Appendix A that $1_{\mathrm{pp}}(h_\lambda) \in \mathcal{L}^0(\mathfrak{h})$. The estimate from (48) also holds true for the term (45), of course.

Term $\Omega_{ij}^{\mathrm{pp}}$

Since, if $\lambda \neq 0$, the subspace $\mathrm{ran}\,(1_{\mathrm{pp}}(h_\lambda))$ is spanned by the normalized eigenfunction $f_\lambda \in \mathfrak{h}$ corresponding to the eigenvalue e_λ given in Proposition 31 *(c)* of Appendix A, we have $\mathrm{e}^{ith_\lambda}1_{\mathrm{pp}}(h_\lambda) = \mathrm{e}^{ite_\lambda}1_{\mathrm{pp}}(h_\lambda)$ for all $t \in \mathbb{R}$. This implies, for all $t \in \mathbb{R}$ and all $i, j \in \{1, \ldots, n\}$, that (46) reads as

$$\Omega_{ij}^{\mathrm{pp}}(t) := (g_i, 1_{\mathrm{pp}}(h_\lambda)s_{\mathrm{d}}1_{\mathrm{pp}}(h_\lambda)f_j). \tag{49}$$

Finally, since the map $\det : \mathrm{Mat}(n, \mathbb{C}) \to \mathbb{C}$ is continuous, we arrive at the conclusion. $\qquad\square$

We next show that, as soon as the magnetic field strength is nonvanishing, the magnetic NESS breaks translation invariance. In order to do so, we switch to momentum space

$$\widehat{\mathfrak{h}} := L^2([-\pi, \pi]; \tfrac{\mathrm{d}k}{2\pi}) \tag{50}$$

by means of the unitary Fourier transform $\mathfrak{f} : \mathfrak{h} \to \widehat{\mathfrak{h}}$ which is defined, as usual, by $\mathfrak{f}f := \sum_{x \in \mathbb{Z}} f(x)\mathrm{e}_x$ for all $f \in \mathfrak{h}$, and for all $x \in \mathbb{Z}$, the plane wave function $\mathrm{e}_x : [-\pi, \pi] \to \mathbb{C}$ is given by $\mathrm{e}_x(k) := \mathrm{e}^{ikx}$ for all $k \in [-\pi, \pi]$.

In the following, we will also use the notation $\widehat{a} := \mathfrak{f}a\mathfrak{f}^* \in \mathcal{L}(\widehat{\mathfrak{h}})$ for all $a \in \mathcal{L}(\mathfrak{h})$. Hence, in momentum space, the XY Hamiltonian $\widehat{h}$ acts through multiplication by the dispersion relation function $\epsilon : [-\pi, \pi] \to \mathbb{R}$ defined, for all $k \in [-\pi, \pi]$, by

$$\epsilon(k) := \cos(k). \tag{51}$$

The function introduced next will capture the effect of a nonvanishing strength of the local external magnetic field. Its action will also be particularly visible in the description of the heat flux in Theorem 24 below.

Definition 16 (Magnetic correction function) *The function* $\Delta_\lambda : [-1, 1] \to \mathbb{R}$*, defined, for all* $e \in [-1, 1]$*, by*

$$\Delta_\lambda(e) := \begin{cases} \frac{1-e^2}{1-e^2+\lambda^2}, & \lambda \neq 0, \\ 1, & \lambda = 0, \end{cases} \tag{52}$$

is called the magnetic correction function (see Figure 1).

Remark 17 The magnetic correction function also plays an important role in the mechanism which regularizes the symbol of the Toeplitz operator describing a certain class of nonequilibrium correlation functions in the magnetic NESS (see [7, p. 3441]).
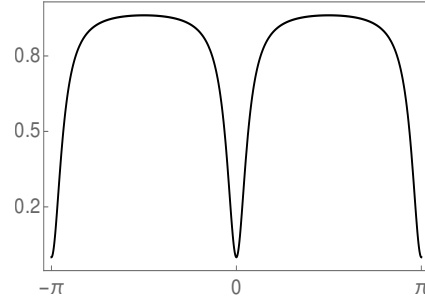
Figure 1: The magnetic correction function $[-\pi, \pi] \ni k \mapsto \Delta_\lambda(\epsilon(k)) \in \mathbb{R}$ for $\lambda = \frac{1}{5}$.

Proposition 18 (Broken translation invariance) *If $\lambda \neq 0$, the magnetic NESS ω_λ is breaking translation invariance.*

In order to carry out the proof, we will frequently refer to the results contained in the Appendices A, B, and C.

Proof. Due to Definition 8, it is sufficient to show that $[s_\lambda, u] \neq 0$ for all $\lambda \in \mathbb{R} \setminus \{0\}$. To this end, we will separately study the commutators of the absolutely continuous and the pure point contributions to the two-point operator s_λ from (39).

Term $1_{\mathrm{ac}}(h_\lambda)$
We want to take advantage of the fact used in [7, p. 3439] that the chain rule for wave operators allows us to write

$$w^*(h_{\mathrm{d}}, h_\lambda) s_{\mathrm{d}} w(h_{\mathrm{d}}, h_\lambda) = w^*(h, h_\lambda) w^*(h_{\mathrm{d}}, h) s_{\mathrm{d}} w(h_{\mathrm{d}}, h) w(h, h_\lambda)$$
$$= w^*(h, h_\lambda) s w(h, h_\lambda), \tag{53}$$

where s is the so-called XY two-point operator, i.e., the two-point operator inducing the XY NESS from Theorem 32 of Appendix B and discussed in Remark 13. Moreover, we also know from this theorem that $\widehat{s}$ acts in momentum space $\widehat{\mathfrak{h}}$ through multiplication by an explicit function θ given in (100). Hence, in order to compute the matrix elements of the commutator of (53) with u with respect to the Kronecker basis $\{\delta_x\}_{x \in \mathbb{Z}}$ of $\mathfrak{h}$, we switch to momentum space and get, for all $x, y \in \mathbb{Z}$, that

$$(\delta_x, [w^*(h, h_\lambda) s w(h, h_\lambda), u]\delta_y) = (\widehat{w}(h, h_\lambda)\mathrm{e}_x, \widehat{s}\widehat{w}(h, h_\lambda)\mathrm{e}_{y+1})$$
$$- (\widehat{w}(h, h_\lambda)\mathrm{e}_{x-1}, \widehat{s}\widehat{w}(h, h_\lambda)\mathrm{e}_y). \tag{54}$$

Using the action of the wave operator $\widehat{w}(h, h_\lambda)$ from (101) in Proposition 33 of Appendix C

on the plane wave functions $e_x = \mathfrak{f}\delta_x$ for all $x \in \mathbb{Z}$, we find, for all $x, y \in \mathbb{Z}$, that

$$(\widehat{w}(h, h_\lambda)e_x, \widehat{s}\widehat{w}(h, h_\lambda)e_y) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \theta(k) e^{ik(y-x)}$$

$$+ i\lambda \int_{-\pi}^{\pi} \frac{dk}{2\pi} \theta(k) \frac{\sin(|k|)}{\sin^2(k) + \lambda^2} \left(e^{i(|ky|-kx)} - e^{i(ky-|kx|)} \right)$$

$$- \lambda^2 \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{\theta(k)}{\sin^2(k) + \lambda^2} \left(e^{i(|ky|-kx)} + e^{i(ky-|kx|)} - e^{i|k|(|y|-|x|)} \right).$$

(55)

We next plug $x = 0$ and $y = 1$ into (54). Separating the positive and negative momentum contributions in (55), regrouping with respect to the temperature dependence of θ, and re-assembling the terms over the whole momentum interval with the help of the evenness of ϵ from (51), we find, for all $\lambda \in \mathbb{R} \setminus \{0\}$, that

$$(\delta_0, [w^*(h, h_\lambda)sw(h, h_\lambda), u]\delta_1) = i\lambda \int_{-\pi}^{\pi} \frac{dk}{2\pi} \theta(k) \frac{\sin(|k|)}{\sin^2(k) + \lambda^2} \left(e^{2i|k|} - e^{2ik} \right)$$

$$- \lambda^2 \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{\theta(k)}{\sin^2(k) + \lambda^2} e^{2ik}$$

$$- i\lambda \int_{-\pi}^{\pi} \frac{dk}{2\pi} \theta(k) \frac{\sin(|k|)}{\sin^2(k) + \lambda^2} \left(e^{i(|k|+k)} - e^{i(k-|k|)} \right)$$

$$+ \lambda^2 \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{\theta(k)}{\sin^2(k) + \lambda^2} \left(e^{i(|k|+k)} + e^{i(k-|k|)} - 1 \right)$$

$$= \lambda \int_{-\pi}^{\pi} \frac{dk}{2\pi} \epsilon(k)[\rho_{\beta_L}(\epsilon(k)) - \rho_{\beta_R}(\epsilon(k))] \Delta_\lambda(\epsilon(k)).$$

(56)

  Term $1_{\mathrm{pp}}(h_\lambda)$

Due to Proposition 31 *(c)* of Appendix A, we know that the pure point subspace of the magnetic Hamiltonian is spanned by the exponentially localized eigenfunction $f_\lambda \in \mathfrak{h}$ given in (99). Hence, for all $x, y \in \mathbb{Z}$, we can write

$$(\delta_x, [1_{\mathrm{pp}}(h_\lambda)s_d 1_{\mathrm{pp}}(h_\lambda), u]\delta_y) = (f_\lambda, s_d f_\lambda)[f_\lambda(x)f_\lambda(y+1) - f_\lambda(x-1)f_\lambda(y)].$$

(57)

Plugging $x = 0$ and $y = 1$ into (57) and using the form of f_λ from (99), we get that

$$(\delta_0, [1_{\mathrm{pp}}(h_\lambda)s_d 1_{\mathrm{pp}}(h_\lambda), u]\delta_1) = 0.$$

(58)

Hence, with the help of (56), (52), and (58), we arrive at the conclusion. $\square$

Remark 19 Since $1/(1+e^x) - 1/(1+e^y) = \sinh[(y-x)/2]/(\cosh[(y-x)/2] + \cosh[(y+x)/2])$ for all $x, y \in \mathbb{R}$, the difference of the Planck density functions in (56) reads, for all $x \in \mathbb{R}$, as

$$\rho_{\beta_L}(x) - \rho_{\beta_R}(x) = \frac{\sinh(\delta x)}{\cosh(\delta x) + \cosh(\beta x)},$$

(59)

where we used the definitions (34) and (35).

4 Entropy production

One of the central physical notions for systems out of equilibrium is the well-known entropy production rate being a bilinear form in the affinities, driving the system out of equilibrium, and in the fluxes, describing the response to these applied forces. In the present situation, these quantities correspond to the differences between the inverse temperature of each reservoir and the inverse temperature of the sample and to the corresponding heat fluxes (see, for example, [17, p. 8] and [9, p. 1159], and references therein). Hence, we are led to the following definition.

Definition 20 (Energy current observable) *Let $\alpha \in \{L, R\}$. The one-particle energy current observable $\varphi_\alpha \in \mathcal{L}(\mathfrak{h})$, describing the energy flow from reservoir α into the sample, is defined by*

$$\varphi_\alpha := - \left. \frac{\mathrm{d}}{\mathrm{d}t} \right|_{t=0} \mathrm{e}^{\mathrm{i}th_\lambda} i_\alpha h_\alpha i_\alpha^* \mathrm{e}^{-\mathrm{i}th_\lambda}. \tag{60}$$

Moreover, the extensive energy current observable $\Phi_\alpha := \mathrm{d}\Gamma(\varphi_\alpha)$ is the usual second quantization of φ_α.

The entropy production rate then reads as follows.

Definition 21 (Entropy production rate) *The entropy production rate in the magnetic NESS ω_λ is defined by*

$$\sigma_\lambda := - \sum_{\alpha \in \{L,R\}} \beta_\alpha J_{\lambda,\alpha}, \tag{61}$$

where the NESS expectation value of the extensive energy current observable, the so-called heat flux, has been denoted, for all $\alpha \in \{L, R\}$, by

$$J_{\lambda,\alpha} := \omega_\lambda(\Phi_\alpha). \tag{62}$$

Remark 22 Since, for all $\alpha \in \{L, R\}$, we have $\varphi_\alpha = -\mathrm{i}[h_\lambda, i_\alpha h_\alpha i_\alpha^*] = -\mathrm{i}[h, i_\alpha h_\alpha i_\alpha^*]$, we see that φ_α is independent of λ and that

$$\varphi_L = \frac{1}{2} \mathrm{Im}(u^{-\nu} p_0 u^{\nu+2}), \tag{63}$$

$$\varphi_R = \frac{1}{2} \mathrm{Im}(u^\nu p_0 u^{-(\nu+2)}), \tag{64}$$

i.e., $\varphi_\alpha \in \mathcal{L}^0(\mathfrak{h})$ which implies that $\Phi_\alpha \in \mathfrak{A}(\mathfrak{h})$ (the latter statement also holds in the more general case of trace class operators in the selfdual setting, see [4, p. 410, 412]). Hence, σ_λ is well-defined.

Remark 23 Using that $\sum_{\alpha \in \{L,R\}} i_\alpha h_\alpha i_\alpha^* = h - i_S h_S i_S^* - (v_L + v_R)$, we can write

$$\sum_{\alpha \in \{L,R\}} \varphi_\alpha = \mathrm{i}[h_\lambda, q], \tag{65}$$

where we set $q := i_S h_S i_S^* + v_L + v_R + \lambda v$. Hence, since $q \in \mathcal{L}^0(\mathfrak{h})$, we can write

$$\sum_{\alpha \in \{L,R\}} \Phi_\alpha = \mathrm{d}\Gamma(\mathrm{i}[h_\lambda, q])$$

$$= \frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} \tau_\lambda^t(\mathrm{d}\Gamma(q)). \tag{66}$$

Taking the NESS expectation value of (66) and using that, due to (36), ω_λ is τ_λ^t-invariant for all $t \in \mathbb{R}$, we find the first law of thermodynamics, i.e.,

$$\sum_{\alpha \in \{L,R\}} J_{\lambda,\alpha} = 0. \tag{67}$$

Due to (61) and (67), we restrict ourselves to the study of the NESS expectation value of the extensive energy current describing the energy flow from the left reservoir into the sample, and we will use the simplified notation $J_\lambda := J_{\lambda,L}$ in the following.

Theorem 24 (Heat flux) *The heat flux, i.e., the NESS expectation value of the extensive energy current observable describing the energy flow from the left reservoir into the sample has the form*

$$J_\lambda = \frac{1}{2} \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \; j(\epsilon(k)) \, \Delta_\lambda(\epsilon(k)), \tag{68}$$

where the density function $j : [-1, 1] \to \mathbb{R}$ is defined, for all $e \in [-1, 1]$, by

$$j(e) := e\sqrt{1 - e^2} \left[\rho_{\beta_L}(e) - \rho_{\beta_R}(e)\right], \tag{69}$$

and the functions $\rho_{\beta_L}, \rho_{\beta_R}$, ϵ, and Δ_λ are given in (29), (51), and (52), respectively (see Figure 2).

Remark 25 Since, due to the proof of Theorem 28 *(a)* below, we have that $(j\Delta_\lambda) \circ \epsilon \in L^1([-\pi, \pi]; \mathrm{d}k)$, the integral (68) is well-defined.

Remark 26 Note that (68) is independent of the sample size parameter ν.

Proof. The case $\lambda = 0$ is treated in [9, p. 1160] (see Remark 3 above) and corresponds to the triviality of the magnetic correction function $\Delta_0 = 1$ in (68).

In the following, we thus discuss the case $\lambda \neq 0$. Using (39) and the fact that $\omega_\lambda(\mathrm{d}\Gamma(\varphi)) = \mathrm{tr}(s_\lambda \varphi)$ for all $\varphi \in \mathcal{L}^0(\mathfrak{h})$ (a similar statement also holds in the more general case of trace
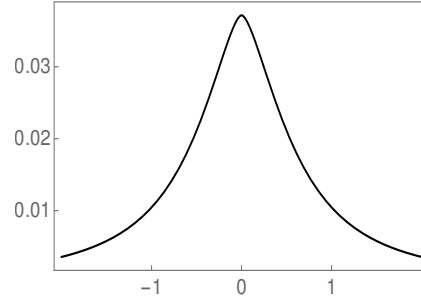
Figure 2: The heat flux $\mathbb{R} \ni \lambda \mapsto J_\lambda \in \mathbb{R}$ as a function of the strength of the local external magnetic field for $\beta_L = 1$ and $\beta_R = 2$.

class operators in the selfdual setting, see [4, p. 410, 412]), the NESS expectation value of the extensive energy current observable describing the energy flow from the left reservoir into the sample can be written in the form

$$
\begin{aligned}
J_\lambda &= \omega_\lambda(\Phi_L) \\
&= \omega_\lambda(\mathrm{d}\Gamma(\varphi_L)) \\
&= \mathrm{tr}(s_\lambda \varphi_L) \\
&= J_{\lambda,\mathrm{ac}} + J_{\lambda,\mathrm{pp}},
\end{aligned}
\tag{70}
$$

where we make the definitions

$$
J_{\lambda,\mathrm{ac}} := \mathrm{tr}(w^*(h_\mathrm{d}, h_\lambda) s_\mathrm{d} w(h_\mathrm{d}, h_\lambda) \varphi_L), \tag{71}
$$

$$
J_{\lambda,\mathrm{pp}} := \mathrm{tr}(1_\mathrm{pp}(h_\lambda) s_\mathrm{d} 1_\mathrm{pp}(h_\lambda) \varphi_L). \tag{72}
$$

We next discuss the two terms (71) and (72) separately.

   Term $J_{\lambda,\mathrm{ac}}$

Using (53), (63), the Kronecker basis $\{\delta_x\}_{x \in \mathbb{Z}}$ of $\mathfrak{h}$ and the fact that the two-point operator s is selfadjoint, we can write

$$
\begin{aligned}
J_{\lambda,\mathrm{ac}} &= \frac{1}{2} \mathrm{tr}(w^*(h, h_\lambda) s w(h, h_\lambda) \mathrm{Im}(u^{-\nu} p_0 u^{\nu+2})) \\
&= \frac{1}{2} \mathrm{Im}[(w(h, h_\lambda)\delta_{-(\nu+2)}, s w(h, h_\lambda)\delta_{-\nu})].
\end{aligned}
\tag{73}
$$

In order to compute (73), we proceed as in the proof of Proposition 18 and switch to momentum space $\hat{\mathfrak{h}}$. Using (55) for $x = -(\nu + 2)$ and $y = -\nu$, we then get

$$
(\widehat{w}(h, h_\lambda)\mathrm{e}_{-(\nu+2)}, \widehat{s}\,\widehat{w}(h, h_\lambda)\mathrm{e}_{-\nu}) = \sum_{i=1}^{3} z_i, \tag{74}
$$

where we make the definitions

$$z_1 := \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \, \theta(k) \, \mathrm{e}^{2\mathrm{i}k} \tag{75}$$

$$z_2 := \mathrm{i}\lambda \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \, \theta(k) \, \frac{\sin(|k|)}{\sin^2(k) + \lambda^2} \left(\mathrm{e}^{\mathrm{i}(|k|\nu + k(\nu+2))} - \mathrm{e}^{-\mathrm{i}(k\nu + |k|(\nu+2))} \right) \tag{76}$$

$$z_3 := -\lambda^2 \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \, \frac{\theta(k)}{\sin^2(k) + \lambda^2} \left(\mathrm{e}^{\mathrm{i}(|k|\nu + k(\nu+2))} + \mathrm{e}^{-\mathrm{i}(k\nu + |k|(\nu+2))} - \mathrm{e}^{-2\mathrm{i}|k|} \right), \tag{77}$$

and we recall that θ is given in (100) of Theorem 32 in Appendix B. Separating the positive and negative momentum contributions (which directly leads to (79)), regrouping with respect to the temperature dependence of θ, and reassembling the terms over the whole momentum interval with the help of the evenness of ϵ, the imaginary parts take the form

$$\mathrm{Im}(z_1) = \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \, \cos(k)|\sin(k)|[\rho_{\beta_L}(\cos(k)) - \rho_{\beta_R}(\cos(k))], \tag{78}$$

$$\mathrm{Im}(z_2) = 0, \tag{79}$$

$$\mathrm{Im}(z_3) = -\lambda^2 \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \, \cos(k)|\sin(k)|[\rho_{\beta_L}(\cos(k)) - \rho_{\beta_R}(\cos(k))] \frac{1}{\sin^2(k) + \lambda^2}. \tag{80}$$

Therefore, (78), (79), and (80) lead us to

$$J_{\lambda,\mathrm{ac}} = \frac{1}{2} \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \, \cos(k)|\sin(k)|[\rho_{\beta_L}(\cos(k)) - \rho_{\beta_R}(\cos(k))] \frac{\sin^2(k)}{\sin^2(k) + \lambda^2}. \tag{81}$$

Term $J_{\lambda,\mathrm{pp}}$
Since the one-particle energy current observable $\varphi_L = -\mathrm{i}[h_\lambda, i_L h_L i_L^*]$ has the form of a commutator, the cyclicity of the trace implies that

$$\begin{aligned} J_{\lambda,\mathrm{pp}} &= \mathrm{tr}(s_\mathrm{d} 1_\mathrm{pp}(h_\lambda) \varphi_L 1_\mathrm{pp}(h_\lambda)) \\ &= -\mathrm{i}\,\mathrm{tr}(s_\mathrm{d} 1_\mathrm{pp}(h_\lambda)[h_\lambda, i_L h_L i_L^*] 1_\mathrm{pp}(h_\lambda)) \\ &= -\mathrm{i}\,\mathrm{tr}(s_\mathrm{d} 1_\mathrm{pp}(h_\lambda)[e_\lambda 1, i_L h_L i_L^*] 1_\mathrm{pp}(h_\lambda)) \\ &= 0, \end{aligned} \tag{82}$$

where e_λ is the unique eigenvalue of the magnetic Hamiltonian h_λ given in Proposition 31 *(c)* of Appendix A.

Hence, using (81), (82), (52), and (69), we arrive at the conclusion. □

Corollary 27 (Strict positivity of the entropy production) *The heat flux is flowing through the sample from the hotter to the colder reservoir. Moreover, the entropy production rate is strictly positive,*

$$\sigma_\lambda > 0. \tag{83}$$

Proof. It immediately follows from (68) and the form of the functions (52) and (69) that $J_\lambda > 0$. Moreover, using (61) and (67), the entropy production can be written as

$$\sigma_\lambda = (\beta_R - \beta_L)J_\lambda. \tag{84}$$

Hence, we arrive at the conclusion. $\square$

5   Nonequilibrium quantum phase transition

Going beyond Ehrenfest's classification proposition not only with respect to the nature of the singularity, as it is usually done in the modern classification schemes, but also with respect to the nature of the state considered, we define a nonequilibrium quantum phase transition to be a point of (higher-order) non-differentiability of the entropy production rate with respect to an external physical parameter of interest. In the case at hand, the parameter which we are interested in is the local external magnetic field λ.

   In the following, J_λ' will denote the derivative of J_λ with respect to λ.

Theorem 28 (Second-order nonequilibrium quantum phase transition) *The heat flux* $\mathbb{R} \ni \lambda \mapsto J_\lambda \in \mathbb{R}$ *has the following properties:*

  (a) It belongs to $C^1(\mathbb{R}) \cap C^\infty(\mathbb{R} \setminus \{0\})$.

  (b) Its second derivative with respect to the local external magnetic field does not exist at the origin, i.e., for $\lambda \to 0$, *we have*

$$J_\lambda' = C\lambda \log(|\lambda|) + \mathcal{O}(\lambda), \tag{85}$$

   where we set $C := (4/\pi)[\rho(\beta_L) - \rho(\beta_R)]$.

Remark 29 In [1, p. 4], an interesting study of a class of nonequilibrium quantum phase transitions in the NESS constructed in [9, p. 1158] has been carried out. In particular, it has been shown that current type correlation functions in this NESS have a discontinuous first and third derivative with respect to the spatially homogeneous external magnetic field μ (at different (γ, μ)-values on the so-called nonequilibrium critical line) as soon as the anisotropy γ is nonvanishing (cf. Remark 3).

Remark 30 In the Lagrange multiplier approach discussed in Remark 15, the expectation value of the macroscopic energy current observable in the ground state of the effective Hamiltonian defines a phase diagram in the effective field-magnetic field plane (cf. [3, p. 169]) separating the equilibrium phase, in which the heat flux is zero, from the nonequilibrium phase of nonvanishing heat flux (in the latter phase, the spin-spin correlations in

the x direction also exhibit an oscillatory behavior dominated by a slowly decaying amplitude). This interpretation contrasts with Theorem 28 which yields a point of second-order non-differentiability of the always strictly positive entropy production rate.

Proof. We start off by noting that the function $f : \mathbb{R} \times [-\pi, \pi] \to \mathbb{R}$, defined, for all $\lambda \in \mathbb{R}$ and all $k \in [-\pi, \pi]$, by

$$
\begin{aligned}
f(\lambda, k) &:= j(\epsilon(k)) \, \Delta_\lambda(\epsilon(k)) \\
&= j(\cos(k)) \cdot
\begin{cases}
\frac{\sin^2(k)}{\sin^2(k)+\lambda^2}, & \lambda \neq 0, \\
1, & \lambda = 0,
\end{cases}
\end{aligned}
\tag{86}
$$

is integrable in k over $[-\pi, \pi]$ for any fixed $\lambda \in \mathbb{R}$ since $|j(\cos(k))| \leq 2$ for all $k \in [-\pi, \pi]$ and since $\sin^2(k)/(\sin^2(k) + \lambda^2) \leq 1$ for all $\lambda \neq 0$ and all $k \in [-\pi, \pi]$.

Using Lebesgue's dominated convergence theorem, we can now proceed to study the regularity of the heat flux.

(a) $J. \in C(\mathbb{R})$

We first want to show that $f(\,\cdot\,, k) \in C(\mathbb{R})$ for any fixed $k \in [-\pi, \pi]$. In order to do so, we note that, since $j(\cos(k)) = 0$ and $\Delta_\lambda(\cos(k)) = \delta_{0\lambda}$ for all $k \in \{0, \pm\pi\}$ and all $\lambda \in \mathbb{R}$, we get that $f(\,\cdot\,, k) = 0$ for all $k \in \{0, \pm\pi\}$, i.e., $f(\,\cdot\,, k) \in C(\mathbb{R})$ for all $k \in \{0, \pm\pi\}$. Moreover, (86) immediately implies that $f(\,\cdot\,, k) \in C(\mathbb{R})$ for all $k \in [-\pi, \pi] \setminus \{0, \pm\pi\}$. Second, since we have from above that $|f(\lambda, k)| \leq 2 \in L^1([-\pi, \pi]; \mathrm{d}k)$ for all $\lambda \in \mathbb{R}$ and all $k \in [-\pi, \pi]$, Lebesgue's dominated convergence theorem implies that $J. \in C(\mathbb{R})$.

$J. \in C^1(\mathbb{R})$

Again, first, we immediately get that $f(\,\cdot\,, k) \in C^1(\mathbb{R})$ for all $k \in \{0, \pm\pi\}$ and $f(\,\cdot\,, k) \in C^1(\mathbb{R} \setminus \{0\})$ for all $k \in [-\pi, \pi] \setminus \{0, \pm\pi\}$. Moreover, for any fixed $k \in [-\pi, \pi] \setminus \{0, \pm\pi\}$, we have $\lim_{\lambda \to 0}(f(\lambda, k) - f(0, k))/\lambda = 0$. Therefore, for all $k \in [-\pi, \pi] \setminus \{0, \pm\pi\}$ and all $\lambda \in \mathbb{R}$, we get

$$
\frac{\partial f}{\partial \lambda}(\lambda, k) = -2\lambda j(\cos(k)) \, \frac{\sin^2(k)}{(\sin^2(k) + \lambda^2)^2},
\tag{87}
$$

which implies that $f(\,\cdot\,, k) \in C^1(\mathbb{R})$ for all $k \in [-\pi, \pi] \setminus \{0, \pm\pi\}$. Second, since $0 \leq (|\sin(k)| - |\lambda|)^2 = \sin^2(k) - 2|\lambda||\sin(k)| + \lambda^2$ for all $\lambda \in \mathbb{R}$ and all $k \in [-\pi, \pi]$, we can write $2|\lambda||\sin(k)|^3 \leq (\sin^2(k) + \lambda^2)^2$ for all $\lambda \in \mathbb{R}$ and all $k \in [-\pi, \pi]$. Hence, since $|j(\cos(k))| \leq 2|\cos(k)||\sin(k)|$ for all $k \in [-\pi, \pi]$, it follows, for all $k \in [-\pi, \pi] \setminus \{0, \pm\pi\}$ and all $\lambda \in \mathbb{R}$, that

$$
\left| \frac{\partial f}{\partial \lambda}(\lambda, k) \right| \leq 2 \, |\cos(k)| \, \frac{2|\lambda||\sin(k)|^3}{(\sin^2(k) + \lambda^2)^2},
\tag{88}
$$

which leads to $|\frac{\partial f}{\partial \lambda}(\lambda, k)| \leq 2 \in L^1([-\pi, \pi]; \mathrm{d}k)$ for all $\lambda \in \mathbb{R}$ and all $k \in [-\pi, \pi]$. Hence, Lebesgue's dominated convergence theorem implies that $J. \in C^1(\mathbb{R})$.
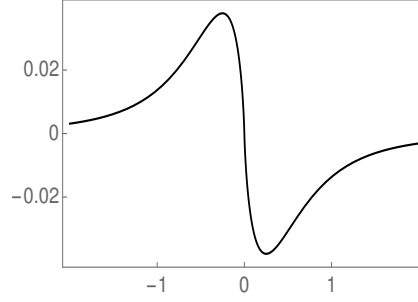
Figure 3: The first derivative of the heat flux with respect to the strength of the local external magnetic field $\mathbb{R} \ni \lambda \mapsto J'_\lambda \in \mathbb{R}$ for $\beta_L = 1$ and $\beta_R = 2$.

$J. \in C^\infty(\mathbb{R} \setminus \{0\})$
Since (86) tells us that, for all $k \in [-\pi, \pi]$, the derivatives of any order of $f(\,\cdot\,, k)$ with respect to λ exist and are bounded by a constant for all $k \in [-\pi, \pi]$ and all points in a sufficiently small neighborhood of any $\lambda \neq 0$, Lebesgue's dominated convergence theorem also yields that $J. \in C^\infty(\mathbb{R} \setminus \{0\})$.

(b) Using *(a)*, (87), (69), and (59), we get, for all $\lambda \in \mathbb{R}$, that

$$
\begin{aligned}
J'_\lambda &= -2\lambda \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \; \cos(k)|\sin(k)|[\rho_{\beta_L}(\cos(k)) - \rho_{\beta_R}(\cos(k))] \frac{\sin^2(k)}{(\sin^2(k) + \lambda^2)^2} \\
&= -8\lambda \int_0^{\frac{\pi}{2}} \frac{\mathrm{d}k}{2\pi} \; \frac{\cos(k)\,\sinh(\delta\cos(k))}{\cosh(\delta\cos(k)) + \cosh(\beta\cos(k))} \frac{\sin^3(k)}{(\sin^2(k) + \lambda^2)^2},
\end{aligned}
\tag{89}
$$

where, in the second equality, we reduced the integration interval from $[-\pi, \pi]$ to $[0, \pi]$ and then from $[0, \pi]$ to $[0, \pi/2]$ by using the coordinate transformations $k \mapsto -k$ and $k \mapsto \pi - k$, respectively (see Figure 3). Next, using the coordinate transformation $\arcsin : [0, 1] \to [0, \frac{\pi}{2}]$ in (89), we can write, for all $\lambda \in \mathbb{R} \setminus \{0\}$, that (see Figure 4)

$$
-\frac{\pi}{4} \frac{J'_\lambda}{\lambda} = \int_0^1 \mathrm{d}x \; f(x) \frac{x^3}{(x^2 + \lambda^2)^2},
\tag{90}
$$

where the function $f : [0, 1] \to \mathbb{R}$ is defined, for all $x \in [0, 1]$, by

$$
f(x) := \frac{\sinh(\delta\sqrt{1 - x^2})}{\cosh(\delta\sqrt{1 - x^2}) + \cosh(\beta\sqrt{1 - x^2})}.
\tag{91}
$$

In order to extract the logarithmic divergence at the origin, we make the decomposition

$$
\int_0^1 \mathrm{d}x \; f(x) \frac{x^3}{(x^2 + \lambda^2)^2} = F_1(\lambda) + F_2(\lambda),
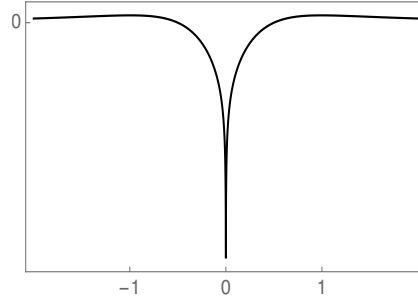\tag{92}
$$

Figure 4: The second derivative of the heat flux with respect to the strength of the local external magnetic field $\mathbb{R} \setminus \{0\} \ni \lambda \mapsto J''_\lambda \in \mathbb{R}$ for $\beta_L = 1$ and $\beta_R = 2$.

where the functions $F_1, F_2 : \mathbb{R} \setminus \{0\} \to \mathbb{R}$ are defined, for all $\lambda \in \mathbb{R} \setminus \{0\}$, by

$$F_1(\lambda) := f(0) \int_0^1 \mathrm{d}x \, \frac{x^3}{(x^2 + \lambda^2)^2}, \tag{93}$$

$$F_2(\lambda) := \int_0^1 \mathrm{d}x \, [f(x) - f(0)] \frac{x^3}{(x^2 + \lambda^2)^2}. \tag{94}$$

Term $F_1(\lambda)$
Using the primitive of its integrand, the first integral reads, for all $\lambda \in \mathbb{R} \setminus \{0\}$, as

$$F_1(\lambda) = -\frac{\sinh(\delta)}{\cosh(\delta) + \cosh(\beta)} \log(|\lambda|)$$
$$- \frac{1}{2} \frac{\sinh(\delta)}{\cosh(\delta) + \cosh(\beta)} \left(\frac{1}{1 + \lambda^2} - \log(1 + \lambda^2) \right), \tag{95}$$

and the second term on the right hand side of (95) is obviously defined and bounded in any neighborhood of the origin.

Term $F_2(\lambda)$
In order to treat the term (94), we use that $|f(x) - f(0)| \leq \int_0^x \mathrm{d}t \, |f'(t)|$ for all $x \in [0,1]$ and that the derivative of f can be estimated, for all $t \in [0,1)$, as

$$|f'(t)| = \frac{ct}{\sqrt{1 - t^2}}, \tag{96}$$

where we set $c := [\delta + \delta \cosh(\delta) \cosh(\beta) + \beta \sinh(\delta) \sinh(\beta)]/4$. It then follows from (96) that $|f(x) - f(0)| \leq cx^2/(1 + \sqrt{1 - x^2})$ for all $x \in [0,1]$. Hence, (94) can be bounded, for all $\lambda \in \mathbb{R} \setminus \{0\}$, by

$$|F_2(\lambda)| \leq c \int_0^1 \mathrm{d}x \, \frac{x^4}{(x^2 + \lambda^2)^2}$$
$$\leq c. \tag{97}$$

Finally, using the same estimates, Lebesgue's dominated convergence theorem also implies that F_2 has a continuous extension to the origin, the latter being again bounded by c in any neighborhood of the origin.

Hence, we arrive at the conclusion. $\square$

A   Magnetic Hamiltonian

In this appendix, we summarize the spectral theory of $h_\lambda \in \mathcal{L}(\mathfrak{h})$ needed in the previous sections. To this end, we recall that $\mathrm{spec}_{\mathrm{sc}}(h_\lambda)$, $\mathrm{spec}_{\mathrm{ac}}(h_\lambda)$, and $\mathrm{spec}_{\mathrm{pp}}(h_\lambda)$ stand for the singular continuous, the absolutely continuous, and the point spectrum of h_λ, respectively.

Proposition 31 (Magnetic spectrum) *The magnetic Hamiltonian $h_\lambda \in \mathcal{L}(\mathfrak{h})$ has the following spectral properties:*

(a) $\mathrm{spec}_{\mathrm{sc}}(h_\lambda) = \emptyset$

(b) $\mathrm{spec}_{\mathrm{ac}}(h_\lambda) = [-1, 1]$

(c) $\mathrm{spec}_{\mathrm{pp}}(h_\lambda) = \begin{cases} \emptyset, & \lambda = 0 \\ \{e_\lambda\}, & \lambda \neq 0 \end{cases}$

Here, the eigenvalue is given by

$$e_\lambda := \begin{cases} \sqrt{1 + \lambda^2}, & \lambda > 0, \\ -\sqrt{1 + \lambda^2}, & \lambda < 0. \end{cases} \tag{98}$$

Moreover, we have $\mathrm{ran}\left(1_{\mathrm{pp}}(h_\lambda)\right) = \mathrm{span}\{f_\lambda\}$, and the normalized eigenfunction $f_\lambda \in \mathfrak{h}$ is defined, for all $x \in \mathbb{Z}$, by

$$f_\lambda(x) := \frac{\mathrm{e}^{-\alpha_\lambda |x|}}{\nu_\lambda} \cdot \begin{cases} 1, & \lambda > 0, \\ (-1)^x, & \lambda < 0, \end{cases} \tag{99}$$

where the inverse decay rate and the square of the normalization constant are given by $\alpha_\lambda := \log(\sqrt{1 + \lambda^2} + |\lambda|)$ and $\nu_\lambda^2 := \sqrt{1 + \lambda^2}/|\lambda|$, respectively.

Proof. See [7, p. 3449] for the case $\lambda > 0$. An analogous straightforward calculation also yields the eigenvalue and the eigenfunction for the case $\lambda < 0$ (the case $\lambda = 0$ corresponds to the Laplacian on the discrete line). $\square$

B   XY NESS

In [9], we constructed the unique translation invariant NESS, called the XY NESS, in the sense of (36) for the general XY model briefly discussed in Remark 3. For simplicity, we restrict the formulation of the following assertion to the case at hand for which the XY NESS with $\gamma = \mu = 0$ corresponds to the limit (36) with $\lambda = 0$.

Theorem 32 (XY two-point operator) *The XY NESS is the quasifree state induced by the two-point operator $s = w^*(h_\mathrm{d}, h)s_\mathrm{d}w(h_\mathrm{d}, h)$. In momentum space, $\widehat{s}$ acts through multiplication by the function $\theta : [-\pi, \pi] \to \mathbb{C}$ given by*

$$\theta(k) := \begin{cases} \rho_{\beta_R}(\epsilon(k)), & k \in [-\pi, 0], \\ \rho_{\beta_L}(\epsilon(k)), & k \in (0, \pi], \end{cases} \tag{100}$$

and we recall that $\epsilon(k) = \cos(k)$ for all $k \in [-\pi, \pi]$.

Proof. See [9, p. 1171]. □

C   Scattering theory

In [7], we determined the action in momentum space of the wave operator (38) on the completely localized orthonormal Kronecker basis $\{\delta_x\}_{x \in \mathbb{Z}}$ of $\mathfrak{h}$ using the stationary scheme of scattering theory and the weak abelian form of the wave operator. Recall that the plane wave function is related to the Kronecker function by $e_x = \mathfrak{f}\delta_x$ for all $x \in \mathbb{Z}$, where we used the notations introduced after (50).

Proposition 33 (Wave operator) *In momentum space, the action of the wave operator $w(h, h_\lambda)$ on the elements of the completely localized Kronecker basis $\{\delta_x\}_{x \in \mathbb{Z}}$ reads, for all $x \in \mathbb{Z}$ and all $k \in [-\pi, \pi]$, as*

$$(\widehat{w}(h, h_\lambda)\mathrm{e}_x)(k) = \mathrm{e}_x(k) + \mathrm{i}\lambda \, \frac{\mathrm{e}_{|x|}(|k|)}{\sin(|k|) - \mathrm{i}\lambda}. \tag{101}$$

Proof. See [7, p. 3439]. □

Remark 34 The action (101) relates to the action of the wave operator for the one-center δ-interaction on the continuous line by replacing $\sin(|k|)$ by $|k|$.

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