Heat flux in general quasifree fermionic right mover/left mover systems

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Abstract

With the help of time-dependent scattering theory on the observable algebra of infinitely extended quasifree fermionic chains, we introduce a general class of so-called right mover/left mover states which are inspired by the nonequilibrium steady states for the prototypical nonequilibrium configuration of a finite sample coupled to two thermal reservoirs at different temperatures. Under the assumption of spatial translation invariance, we relate the 2-point operator of such a right mover/left mover state to the asymptotic velocity of the system and prove that the system is thermodynamically nontrivial in the sense that its entropy production rate is strictly positive. Our study of these not necessarily gauge-invariant systems covers and substantially generalizes well-known quasifree fermionic chains and opens the way for a more systematic analysis of the heat flux in such systems.

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1 Introduction

The rigorous study, from first principles, of open quantum systems is of fundamental importance for a deepened understanding of their thermodynamic properties in and out of equilibrium. Since, by definition, open quantum systems have a very large number of degrees of freedom and since the finite accuracy of any feasible experiment does not allow an empirical distinction between an infinite system and a finite system with sufficiently many degrees of freedom, a powerful strategy consists in approximating (in a somewhat reversed

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sense) the actual finite system by an idealized one with infinitely many degrees of freedom (see [26] for an extensive discussion of this idealization and its implications). Furthermore, it is conceptually more appealing and often mathematically more rigorous to treat the idealized system from the outset in a framework designed for infinite systems rather than taking the thermodynamic limit at an intermediate or the final stage.

One of the most important axiomatic frameworks for the study of such idealized infinite systems is the so-called algebraic approach to quantum mechanics based on operator algebras. Indeed, after having been heavily used from as early as the 1960s on, in particular for the quantum statistical description of quantum systems in thermal equilibrium (see, for example, [16, 28, 14]), 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. Although the most interesting phenomena which emerge on the macroscopic level are not restricted to systems in thermal equilibrium but, quite the contrary, often occur out of equilibrium, our general theoretical understanding of nonequilibrium order and phase transitions is substantially less developed since, in particular, the effect of the dynamics becomes much more important out of equilibrium.

Most of the rather scarce mathematically rigorous results have been obtained for the so-called nonequilibrium steady states (NESSs) introduced by Ruelle in [27] by means of scattering theory on the algebra of observables. An important role in the construction of such NESSs is played by the so-called quasifree fermionic systems, and this is true not only because of their mathematical accessibility but also when it comes to real physical applications. Indeed, from a mathematical point of view, these systems allow for a simple and powerful representation independent description since scattering theory on the fermionic algebra of observables boils down to scattering theory on the underlying 1-particle Hilbert space over which the fermionic algebra is constructed. This restriction of the dynamics to the 1-particle sector opens the way for a rigorous mathematical analysis of many purely quantum mechanical properties which are of fundamental physical interest. But, beyond their importance due to their mathematical accessibility, quasifree fermionic systems effectively describe nature: aside from the various electronic systems in their independent electron approximation, they also play an important role in the rigorous approach to physically realizable spin systems. An important member of the family of Heisenberg spin chains is the so-called XY model, introduced in 1961 in [21] (see also [24] for the so-called isotropic case), for which a physical realization has already been identified in the late 1960s (see [15] for example). The impact of the XY model on the experimental, numerical, theoretical, and mathematical research activity in the field of low-dimensional magnetic systems is ongoing ever since (see [23] for example).

In the present paper, we consider a 1-dimensional quantum mechanical system whose configuration space is the 2-sided infinite discrete line $\mathbb{Z}$ and whose algebra of observables is the CAR (canonical anticommutation relations) algebra over the 1-particle Hilbert space of the square-summable functions over $\mathbb{Z}$. Using scattering theory on the 1-particle Hilbert space, we then introduce a class of states over the CAR algebra which we call the class of right mover/left mover states (R/L movers). For a given Hamiltonian on the 1-particle Hilbert space, an R/L mover is specified by a 2-point operator whose main part consists of a mixture of two independent species stemming from the asymptotic right and left side of $\mathbb{Z}$, carrying the inverse temperatures β_R and β_L, respectively, of the right and left reservoir with configuration spaces

$$\mathbb{Z}_R := \{x \in \mathbb{Z} \,|\, x \geq x_R + 1\}, \tag{1}$$
$$\mathbb{Z}_L := \{x \in \mathbb{Z} \,|\, x \leq x_L - 1\}, \tag{2}$$

where $x_R, x_L \in \mathbb{Z}$ are fixed and satisfy $x_L \leq x_R$. Moreover, the finite piece

$$\mathbb{Z}_S := \{x \in \mathbb{Z} \,|\, x_L \leq x \leq x_R\}, \tag{3}$$

containing $n_S := x_R - x_L + 1 \geq 1$ sites, plays the role of the configuration space of the confined sample. The prototypical example of such an R/L-mover is the NESS constructed as the large time limit of the averaged trajectory of a time-evolved initial state which is the decoupled product of three thermal equilibrium states over the corresponding configuration spaces (as somewhat degenerate examples, thermal equilibrium states and ground states are also covered by our setting). The first rigorous construction of such a NESS by means of time-dependent scattering theory has been carried out in [11] for the XY model (see also [5] for the special case of the so-called isotropic XY model [or XX model] using different asymptotic approximation methods) and, to the best of our knowledge, very few models have been rigorously studied within the framework of Ruelle's scattering approach since then (see, for example, [22, 10, 7, 8, 9]). The setting of the present paper, being thus kept, at various places, at a mathematically rather general level in order to highlight the structural dependence on the different ingredients (and in view of future generalizations), allows for the study of more general and not necessarily gauge-invariant fermionic systems covering and generalizing several well-known models of spin chains (as, for example, the NESS for the XY model from [11], the Suzuki model, etc.). Furthermore, under the additional assumption of translation invariance of the Hamiltonian (whose breaking will be studied elsewhere, but see also [7, 8, 9]) and substantially generalizing the approach of [11], the 2-point operator of the R/L mover is explicitly linked to the asymptotic velocity of the system allowing for a rigorous and detailed study of the heat flux in general quasifree R/L mover systems whose sample is coupled to the reservoirs through short range forces across the boundaries. As a consequence of the structural form of the heat flux, we obtain strict positivity of the entropy production, i.e., thermodynamical nontriviality, for the whole class of such quasifree R/L mover systems.

The paper is organized as follows.

Section 2 (Infinite fermionic systems) We introduce the framework for the systems to be studied, i.e., the CAR algebra of observables, its selfdual generalization, the quasifree dynamics generated by selfdual Hamiltonians, and the states on the observable algebra with their corresponding 2-point operators.

Section 3 (Right mover/left mover states) In order to be able to define R/L movers, we introduce the asymptotic projections for the underlying right/left geometry and general Fermi functions. The class of R/L mover 2-point operators is defined under simple assumptions on the selfdual Hamiltonian and for general so-called initial 2-point operators. We also discuss thermal equilibrium and ground states with respect to this framework and the special case of states with gauge-invariant 2-point operators which frequently occurs in practice.

Section 4 (Nonequilibrium steady states) This section is devoted to the definition and the construction of NESSs, in the nonequilibrium setting at hand, using Ruelle's time-dependent scattering approach. This class of states serves as the main motivation for the introduction of the R/L movers of Section 3.

Section 5 (Asymptotic velocity) Using the fundamental assumption of translation invariance for the selfdual Hamiltonian, we rigorously determine the asymptotic velocity of the system. The latter is the key ingredient of the so-called R/L mover generator which, together with the selfdual Hamiltonian, determines the main part of the 2-point operator of the R/L mover.

Section 6 (Heat flux) We introduce the notion of heat flux and entropy production rate in the R/L mover state. Under the additional assumption that the range of the selfdual Hamiltonian is bounded by the size of the sample, i.e., that there is no direct coupling between the two reservoirs, the R/L mover heat flux is explicitly determined in general and for typical special cases appearing in practice. We also provide examples of several well-known models of spin chains covered by the formalism and explicitly determine instances of new ones. Moreover, under suitable monotonicity conditions on the Fermi function, we prove that the R/L mover heat flux is nonvanishing and the entropy production strictly positive, i.e., that the system under consideration is thermodynamically nontrivial.

Appendix A (Spectral theory) We present a brief summary of the somewhat different approach to spectral theory used in the main body of the paper. Due to the attempt to be, at least conceptually, self-contained, we rather explicitly carry out most of the necessary arguments in this appendix (and also in the main body of the text).

Appendix B (Matrix multiplication operators) Based on Appendix A, we study the functional calculus for the matrix multiplication operators describing selfdual translation invariant observables and derive a criterion for their absolute continuity.

Appendix C (Real trigonometric polynomials) We carry out the computations in the ring of real trigonometric polynomials which, in particular, are needed in the study of the examples in Section 6.

Appendix D (Heat flux contributions) This appendix contains some of the lengthy computations from the proof of the main theorem.

Appendix E (Hamiltonian densities) We display the selfdual second quantization of the local first, second, and third Pauli coefficient of H in the fermionic and the spin picture (the selfdual second quantization of the zeroth Pauli coefficient of H is given in the main body of the paper).

2 Infinite fermionic systems

In this section, we introduce the operator algebraic setting used to describe the fermionic system under consideration whose extension is infinite. Recall that, in the operator algebraic approach to quantum statistical mechanics, the three fundamental ingredients of a physical system, i.e., the observables, the time evolution, and the states, are given by a C^*-algebra, by a 1-parameter group of $*$-automorphisms, and by normalized positive linear functionals on the observable algebra, respectively (see [16, 28, 14] for example). In order to introduce the notation, let $\mathcal{H}$ be any separable complex Hilbert space and let $\mathcal{L}(\mathcal{H})$ stand for the bounded linear operators on $\mathcal{H}$. Moreover, $\mathcal{L}^\infty(\mathcal{H})$, $\mathcal{L}^1(\mathcal{H})$, and $\mathcal{L}^0(\mathcal{H})$ denote the compact operators, the trace class operators, and the operators of finite rank on $\mathcal{H}$, respectively, and $\|\cdot\|_1$ stands for the trace norm on $\mathcal{L}^1(\mathcal{H})$. Furthermore, if $a_{ij} \in \mathcal{L}(\mathcal{H})$ for all $i,j \in \langle 1,2\rangle$, we denote by $A := [a_{ij}]_{i,j\in\langle 1,2\rangle} \in \mathcal{L}(\mathcal{H}\oplus\mathcal{H})$ the operator on $\mathcal{H}\oplus\mathcal{H}$ whose entries are given by a_{ij}, where here and in the following, for all $x,y\in\mathbb{Z}$ with $x\leq y$, we set

$$\langle x,y\rangle := \begin{cases}\{x,x+1,\ldots,y\}, & x<y,\\ \{x\}, & x=y.\end{cases} \tag{4}$$

Instead of using the standard basis, it is often useful to expand with respect to the Pauli matrices, i.e., if $a_\alpha \in \mathcal{L}(\mathcal{H})$ for all $\alpha\in\langle 0,3\rangle$, we define the operator $A\in\mathcal{L}(\mathcal{H}\oplus\mathcal{H})$ by

$$A := a_0\sigma_0 + a\sigma, \tag{5}$$

where $\{\sigma_0,\sigma_1,\sigma_2,\sigma_3\}\subseteq\mathbb{C}^{2\times 2}$ stands for the Pauli basis of $\mathbb{C}^{2\times 2}$ which consists of the usual Pauli matrices $\sigma_1,\sigma_2,\sigma_3\in\mathbb{C}^{2\times 2}$ and the identity $\sigma_0\in\mathbb{C}^{2\times 2}$,

$$\sigma_0 := \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix},\quad \sigma_1 := \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix},\quad \sigma_2 := \begin{bmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{bmatrix},\quad \sigma_3 := \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}. \tag{6}$$

Here and in the following, for all $n\in\mathbb{N}:=\{1,2,\ldots\}$, we denote by $\mathbb{C}^{n\times n}$ the complex $n\times n$ matrices and by $\mathbb{C}^{n\times n}_a$ the skew-symmetric complex $n\times n$ matrices. Moreover, $a\in\mathcal{L}(\mathcal{H})^3$ and $\sigma\in(\mathbb{C}^{2\times 2})^3$ are written as $a:=[a_1,a_2,a_3]$ and $\sigma:=[\sigma_1,\sigma_2,\sigma_2]$, and we set $a\sigma := a_1\sigma_1+a_2\sigma_2+a_3\sigma_3$, where, for all $b\in\mathcal{L}(\mathcal{H})$ and all $M\in\mathbb{C}^{2\times 2}$ having entries m_{ij} with $i,j\in\langle 1,2\rangle$, the operator $bM\in\mathcal{L}(\mathcal{H}\oplus\mathcal{H})$ is defined by $(bM)_{ij} := m_{ij}b$ for all $i,j\in\langle 1,2\rangle$ (and we have $(bM)(cN)=(bc)(MN)$ for all $b,c\in\mathcal{L}(\mathcal{H})$ and $M,N\in\mathbb{C}^{2\times 2}$). Conversely, any $A\in\mathcal{L}(\mathcal{H}\oplus\mathcal{H})$ can be written uniquely in the form (5) which we call the Pauli expansion of A. Moreover, if $A,B\in\mathcal{L}(\mathcal{H}\oplus\mathcal{H})$ have the Pauli expansions $A=a_0\sigma_0+a\sigma$ and $B=b_0\sigma_0+b\sigma$, respectively, their product has the Pauli expansion

$$AB = (a_0b_0+ab)\sigma_0 + (a_0b+ab_0+\mathrm{i}a\wedge b)\sigma, \tag{7}$$

where we set $ab := a_1b_1+a_2b_2+a_3b_3$, $a_0b := [a_0b_1, a_0b_2, a_0b_3]$, $ab_0 := [a_1b_0,a_2b_0,a_3b_0]$, and the vector $a\wedge b\in\mathcal{L}(\mathcal{H})^3$ is given by $(a\wedge b)_i := \sum_{j,k\in\langle 1,3\rangle}\varepsilon_{ijk}\,a_jb_k$ for all $i\in\langle 1,3\rangle$, and ε_{ijk} with $i,j,k\in\langle 1,3\rangle$ is the usual Levi-Civita symbol. Of course, all the foregoing considerations can be analogously applied to the case of antilinear operators which we denote by $\bar{\mathcal{L}}(\mathcal{H})$. Finally, $\ell^2(\mathbb{Z})$ will stand for the usual separable complex Hilbert space of square-summable complex-valued functions on $\mathbb{Z}$, and for elements A and B in the various sets in question below, the commutator and the anticommutator of A and B are denoted as usual by $[A,B]:=AB-BA$ and $\{A,B\}:=AB+BA$, respectively.

In the following, we will make use of the so-called selfdual setting. For our case, the 1-particle Hilbert space in the selfdual setting is the direct sum of the usual 1-particle Hilbert space with itself. Here and there, we will make brief remarks about this underlying general framework.

Definition 1 (Observables)

(a) *The 1-particle position Hilbert space and its doubling are defined by*

$$\mathfrak{h} := \ell^2(\mathbb{Z}), \tag{8}$$
$$\mathfrak{H} := \mathfrak{h} \oplus \mathfrak{h}. \tag{9}$$

Abusing notation, the usual scalar products, the corresponding induced norms (as well as the corresponding operator norms) on both $\mathfrak{h}$ and $\mathfrak{H}$ are all denoted by $(\cdot,\cdot)$ and $\|\cdot\|$, respectively.

(b) *Let the map $\zeta \in \bar{\mathcal{L}}(\mathfrak{h})$ be given by $\zeta f := \bar{f}$ for all $f \in \mathfrak{h}$, where $\bar{f}$ is the usual complex conjugation of f. The antiunitary involution $\Gamma \in \bar{\mathcal{L}}(\mathfrak{H})$, defined by the block anti-diagonal lifting of ζ to $\mathfrak{H}$ as*

$$\Gamma := \zeta\sigma_1, \tag{10}$$

is called the conjugation of $\mathfrak{H}$.

(c) *The algebra of observables, denoted by $\mathfrak{A}$, is defined to be the CAR algebra over $\mathfrak{h}$,*

$$\mathfrak{A} := \mathrm{CAR}(\mathfrak{h}). \tag{11}$$

The generators are denoted, as usual, by 1, $a(f)$, and $a^*(f)$ for all $f \in \mathfrak{h}$ (and the C^*-norm of $\mathfrak{A}$, as many other norms within their context, by $\|\cdot\|$).

(d) *The complex linear map $B : \mathfrak{H} \to \mathfrak{A}$, defined, for all $F := f_1 \oplus f_2 \in \mathfrak{H}$, by*

$$B(F) = a^*(f_1) + a(\zeta f_2), \tag{12}$$

satisfies the selfdual CARs

$$B^*(F) = B(\Gamma F), \tag{13}$$
$$\{B^*(F), B(G)\} = (F, G)1. \tag{14}$$

The elements $B(F)$ for all $F \in \mathfrak{H}$ are called the selfdual generators of $\mathfrak{A}$.

(e) *The complex linear map $b : \mathcal{L}^1(\mathfrak{H}) \to \mathfrak{A}$, called the selfdual second quantization, is defined, for all $A \in \mathcal{L}^0(\mathfrak{H})$, by*

$$b(A) := \sum_{i=1}^{m} B(G_i)B^*(F_i), \tag{15}$$

where $m \in \mathbb{N}$ and $\{F_i, G_i\}_{i\in\langle 1,m\rangle} \subseteq \mathfrak{H}$ are such that $A := \sum_{i=1}^{m}(F_i, \cdot)G_i$. Moreover, for all $A \in \mathcal{L}^1(\mathfrak{H})$, the selfdual second quantization is defined by

$$b(A) := \lim_{n\to\infty} b(A_n), \tag{16}$$

where the sequence $(A_n)_{n\in\mathbb{N}}$ in $\mathcal{L}^0(\mathfrak{H})$ is such that $\lim_{n\to\infty} \|A - A_n\|_1 = 0$.

Remark 2 The algebra of observables $\mathfrak{A}$ is $*$-isomorphic to $\overline{\mathrm{SDC}}(\mathfrak{H}, \Gamma)$, the completed (with respect to the C^*-norm) selfdual CAR algebra over $\mathfrak{H}$ and Γ. The selfdual setting is a very useful general framework which has been introduced and developed in [1, 2, 4] for general $\mathfrak{H}$ and Γ not necessarily of the form (9) and (10) (see there for a more detailed description of the selfdual objects used in the following). In particular, the selfdual setting allows for the description of general non gauge-invariant quasifree fermionic systems such as, for example, the prominent XY model from [21] whose Hamiltonian density has the form

$$(1+\gamma)\,\sigma_1^{(x)}\sigma_1^{(x+1)} + (1-\gamma)\,\sigma_2^{(x)}\sigma_2^{(x+1)}, \tag{17}$$

where the superscripts denote the sites in $\mathbb{Z}$ of the local Hilbert space of the spin chain on which the Pauli matrices act. In order to establish a bridge between the spin picture and the fermionic picture, the generalization from [3] of the Jordan-Wigner transformation for 1-dimensional systems whose configuration space extends infinitely in both directions makes use of the so-called crossed product of the algebra $\mathfrak{P}$ of the Pauli spins over $\mathbb{Z}$ (a Glimm or UHF [i.e., uniformly hyperfinite] algebra as is $\mathfrak{A}$) by the involutive automorphism $\alpha \in \mathrm{Aut}(\mathfrak{P})$ describing the rotation around the 3-axis by an angle of π of the observables on the nonpositive sites (and, thereby, makes it mathematically rigorous for the Jordan-Wigner transformation to be anchored at minus infinity). Up to $*$-isomorphism equivalence, it is given by the C^*-subalgebra

$$\left\{ \begin{bmatrix} A & B \\ \alpha(B) & \alpha(A) \end{bmatrix} \middle| A, B \in \mathfrak{P} \right\} \subseteq \mathfrak{P}^{2\times 2}, \tag{18}$$

where $\mathfrak{P}^{2\times 2}$ stands for the C^*-algebra of all 2×2 matrices with entries in $\mathfrak{P}$ (with respect to the naturally generalized matrix operations and the Hilbert C^*-module norm). Using this bridge, (17) can be expressed in the fermionic picture and becomes (up to a global prefactor)

$$a_x^* a_{x+1} + a_{x+1}^* a_x + \gamma(a_x^* a_{x+1}^* + a_{x+1} a_x), \tag{19}$$

where we set $a_x := a(\delta_x)$ and $a_x^* := a^*(\delta_x)$ for all $x \in \mathbb{Z}$. In order to treat the anisotropic case $\gamma \neq 0$, i.e., the case in which there is an asymmetry between the first and the second term in (17), the selfdual setting is most natural since gauge invariance is broken in (19). Hence, due to the presence of the γ-term, the anisotropy Hamiltonian acquires non-diagonal components with respect to $\mathfrak{H} = \mathfrak{h} \oplus \mathfrak{h}$ (see Example 67 in Section 6). In many respects, the truly anisotropic XY model is substantially more complicated than the isotropic one (see [9] for example).

Remark 3 For all $F \in \mathfrak{H}$, the selfdual generator $B(F) \in \mathfrak{A}$ has the norm (see [4])

$$\|B(F)\| = \frac{1}{\sqrt{2}} \sqrt{\|F\|^2 + \sqrt{\|F\|^4 - |(F, \Gamma F)|^2}}, \tag{20}$$

from which we can infer that

$$\frac{1}{\sqrt{2}} \|F\| \leq \|B(F)\| \leq \|F\|. \tag{21}$$

Furthermore, the selfdual second quantization (15) is well-defined since $b(A)$ does not depend on the choice of the functions $F_1, \ldots, G_m \in \mathfrak{H}$ which represent $A \in \mathcal{L}^0(\mathfrak{H})$. As to (16), the limit exists and is independent of the sequence $(A_n)_{n\in\mathbb{N}}$ in $\mathcal{L}^0(\mathfrak{H})$ which approximates $A \in \mathcal{L}^1(\mathfrak{H})$ in the trace norm (such a sequence exists since $\mathcal{L}^0(\mathfrak{H})$ is dense in $\mathcal{L}^1(\mathfrak{H})$ with respect to the trace norm). Moreover, for all $A \in \mathcal{L}^1(\mathfrak{H})$, it holds that $b(A)^* = b(A^*)$ (and $\mathcal{L}^1(\mathfrak{H})$ is a 2-sided $*$-ideal of $\mathcal{L}(\mathfrak{H})$). If $A \in \mathcal{L}^1(\mathfrak{H})$ satisfies the condition $\Gamma A \Gamma = -A^*$, we have

$$\frac{1}{4} \|A\|_1 \leq \|b(A)\| \leq \|A\|_1. \tag{22}$$

If, in addition, A is selfadjoint, we even have $\|b(A)\| = \|A\|_1$.

In the following, the set of $*$-automorphisms on the algebra of observables $\mathfrak{A}$ is denoted by $\mathrm{Aut}(\mathfrak{A})$.

The so-called Bogoliubov $*$-automorphism to be defined next play an important role in the theory of quasifree fermionic systems.

Definition 4 (Bogoliubov $*$-automorphism)

(a) A unitary operator $U \in \mathcal{L}(\mathfrak{H})$ is called a Bogoliubov operator if $[U, \Gamma] = 0$.

(b) Let $U \in \mathcal{L}(\mathfrak{H})$ be a Bogoliubov operator. The $*$-automorphism $\tau_U \in \mathrm{Aut}(\mathfrak{A})$ defined, for all $F \in \mathfrak{H}$, by

$$\tau_U(B(F)) := B(UF), \tag{23}$$

and suitably extended to the whole of $\mathfrak{A}$, is called the Bogoliubov $*$-automorphism (induced by U).

Remark 5 Note that τ_U preserves the properties of Definition 1 *(d)*, i.e., $B' := \tau_U \circ B : \mathfrak{H} \to \mathfrak{A}$ is complex linear and satisfies the selfdual CARs (13)-(14).

The following 1-particle Hilbert space isometries will be frequently used in the sequel.

Definition 6 (Isometries)

(a) The (right) translation $\theta \in \mathcal{L}(\mathfrak{h})$ is defined by $(\theta f)(x) := f(x-1)$ for all $f \in \mathfrak{h}$ and all $x \in \mathbb{Z}$. Its lifting to $\mathfrak{H}$ is given by the Bogoliubov operator $\Theta := \theta\sigma_0 \in \mathcal{L}(\mathfrak{H})$.

(b) The parity $\xi \in \mathcal{L}(\mathfrak{h})$ *is defined by* $(\xi f)(x) := f(-x)$ *for all* $f \in \mathfrak{h}$ *and all* $x \in \mathbb{Z}$*.*

(c) For all $\varphi \in \mathbb{R}$*, the Bogoliubov operator* $U_\varphi \in \mathcal{L}(\mathfrak{H})$ *defined by*

$$U_\varphi := \mathrm{e}^{\mathrm{i}\varphi} 1 \oplus \mathrm{e}^{-\mathrm{i}\varphi} 1, \tag{24}$$

is called a gauge transformation.

In the following, the map $\tau : \mathbb{R} \to \mathrm{Aut}(\mathfrak{A})$, written as $t \to \tau^t$, is called a dynamics on $\mathfrak{A}$ if it is a group homomorphism between the additive group $\mathbb{R}$ and the group $\mathrm{Aut}(\mathfrak{A})$ (with respect to composition) and if, for all $A \in \mathfrak{A}$, the map $\mathbb{R} \ni t \mapsto \tau^t(A) \in \mathfrak{A}$ is continuous with respect to the C^*-norm on $\mathfrak{A}$ (the pair $(\mathfrak{A}, \tau)$ is a sometimes called a C^*-dynamical system).

Definition 7 (Quasifree dynamics)

(a) An operator $H \in \mathcal{L}(\mathfrak{H})$ *is called a selfdual observable if*

$$H^* = H, \tag{25}$$

$$\Gamma H \Gamma = -H. \tag{26}$$

(b) Let $H \in \mathcal{L}(\mathfrak{H})$ *be a selfdual observable. The dynamics* $\tau : \mathbb{R} \to \mathrm{Aut}(\mathfrak{A})$ *defined, for all* $t \in \mathbb{R}$ *and all* $F \in \mathfrak{H}$*, by*

$$\tau^t(B(F)) := B(\mathrm{e}^{\mathrm{i}tH} F), \tag{27}$$

and suitably extended to the whole of $\mathfrak{A}$*, is called the quasifree dynamics (generated by* H*) and* H *is called a Hamiltonian.*

Remark 8 Due to (25)-(26), the map $\mathbb{R} \ni t \mapsto \tau^t \in \mathrm{Aut}(\mathfrak{A})$ given by (27) is a 1-parameter group of Bogoliubov $*$-automorphisms induced by the 1-parameter group of Bogoliubov operators $\mathbb{R} \ni t \mapsto \mathrm{e}^{\mathrm{i}tH} \in \mathcal{L}(\mathfrak{H})$ (see (50) in the proof of Proposition 17 *(b)* below).

The following class of operators characterizes the expectation values of all the quadratic observables in the states we are interested in. The set of states over the observable algebra $\mathfrak{A}$ is denoted by $\mathcal{E}_{\mathfrak{A}}$.

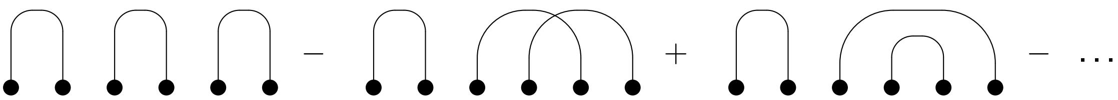
Definition 9 (2-point operator) *An operator* $T \in \mathcal{L}(\mathfrak{H})$ *having the properties*

$$T^* = T, \tag{28}$$

$$\Gamma T \Gamma = 1 - T, \tag{29}$$

$$0 \leq T \leq 1, \tag{30}$$

is called a 2-point operator.



$\pi = (123456)$ $\pi = (123546)$ $\pi = (123645)$

Figure 1: Some of the 15 pairings for $m = 3$. The total number of intersections I relates to the signature of the permutation π as $\mathrm{sgn}(\pi) = (-1)^I$.

Remark 10 Since, by definition, a state $\omega \in \mathcal{E}_{\mathfrak{A}}$ is a normalized positive linear functional on $\mathfrak{A}$, (21) yields $|\omega(B^*(F)B(G))| \le \|F\|\|G\|$ for all $F, G \in \mathfrak{H}$. Hence, the map $\mathfrak{H} \times \mathfrak{H} \ni (F, G) \mapsto \omega(B^*(F)B(G)) \in \mathbb{C}$ is a bounded sesquilinear form on $\mathfrak{H} \times \mathfrak{H}$ and Riesz's lemma implies that there exists a unique $T \in \mathcal{L}(\mathfrak{H})$ such that, for all $F, G \in \mathfrak{H}$, we have

$$\omega(B^*(F)B(G)) = (F, TG). \tag{31}$$

Moreover, due to the positivity of ω, we get $T \ge 0$ and, hence, $T^* = T$. Since ω is normalized, (13)-(14) yield $\Gamma T \Gamma = 1 - T$. Finally, since $T \ge 0$, we have $\Gamma T \Gamma \ge 0$, i.e., $1 - T \ge 0$, and it follows that the operator T which characterizes the 2-point function in (31) is a 2-point operator. If $\omega \in \mathcal{E}_{\mathfrak{A}}$ satisfies (31) for a 2-point operator $T \in \mathcal{L}(\mathfrak{H})$, we use the notation ω_T.

We next introduce the class of quasifree states, i.e., the states in $\mathcal{E}_{\mathfrak{A}}$ whose many-point correlation functions factorize in Pfaffian form. For this purpose, recall that, for all $m \in \mathbb{N}$, the Pfaffian $\mathrm{pf} : \mathbb{C}^{2m\times 2m} \to \mathbb{C}$ is defined, for all $A \in \mathbb{C}^{2m\times 2m}$, by

$$\mathrm{pf}(A) := \sum_{\pi \in \mathcal{P}_{2m}} \mathrm{sgn}(\pi) \prod_{i \in \langle 1, m\rangle} A_{\pi(2i-1)\pi(2i)}, \tag{32}$$

where the sum is running over all the $(2m)!/(2^m m!)$ pairings of the set $\langle 1, 2m\rangle$, i.e., $\mathcal{P}_{2m} := \{\pi \in \mathcal{S}_{2m} \,|\, \pi(2i{-}1) < \pi(2i{+}1)$ for all $i \in \langle 1, m{-}1\rangle$ and $\pi(2i{-}1) < \pi(2i)$ for all $i \in \langle 1, m\rangle\}$, and $\mathcal{S}_{2m}$ stands for the symmetric group on $\langle 1, 2m\rangle$, i.e., the set of all bijections (permutations) $\langle 1, 2m\rangle \to \langle 1, 2m\rangle$, see Figure 1. Moreover, for all $n \in \mathbb{N}$, we denote by $A = [a_{ij}]_{i,j\in\langle 1,n\rangle}$ the matrix $A \in \mathbb{C}^{n\times n}$ with entries $a_{ij} \in \mathbb{C}$ for all $i, j \in \langle 1, n\rangle$.

Definition 11 (Quasifree state) *Let $\omega_T \in \mathcal{E}_{\mathfrak{A}}$ be a state with 2-point operator $T \in \mathcal{L}(\mathfrak{H})$. If, for all $n \in \mathbb{N}$ and all $\{F_i\}_{i\in\langle 1,n\rangle} \subseteq \mathfrak{H}$, it holds that*

$$\omega_T\Big(\prod\nolimits_{i\in\langle 1,n\rangle} B(F_i)\Big) = \begin{cases} \mathrm{pf}\big([\omega_T(B(F_i)B(F_j))]_{i,j\in\langle 1,n\rangle}\big), & n \text{ even}, \\ 0, & n \text{ odd}, \end{cases} \tag{33}$$

the state ω_T is called the quasifree state (induced by T).

3 Right mover/left mover states

In this section, we introduce the R/L mover states whose definition is based on the geometric decomposition of the configuration space into a right part, a central part, and a left part. To begin with, this decomposition gives rise to the so-called R/L mover generator whose role is to specify the temperatures carried by the R/L movers stemming from the corresponding reservoirs.

In the following, let $\ell^\infty(\mathbb{Z})$ stand for the usual complex Banach space of bounded complex-valued functions on $\mathbb{Z}$. For all $u \in \ell^\infty(\mathbb{Z})$, the multiplication operator $m[u] \in \mathcal{L}(\mathfrak{h})$ is defined, for all $f \in \mathfrak{h}$, by

$$m[u]f := uf. \tag{34}$$

In view of the Pauli expansion (5), we also write $m[v] := [m[v_1], m[v_2], m[v_3]] \in \mathcal{L}(\mathfrak{h})^3$ for all $v := [v_1, v_2, v_3] \in \ell^\infty(\mathbb{Z})^3$. Moreover, for all $M \subseteq \mathbb{R}$, we denote by 1_M the usual characteristic function of M, and we use the abbreviations $1_L := 1_{\mathbb{Z}_L}$, $1_S := 1_{\mathbb{Z}_S}$, and $1_R := 1_{\mathbb{Z}_R}$, and $1_\lambda := 1_{\{\lambda\}}$ for all $\lambda \in \mathbb{R}$. Finally, for all $n \in \mathbb{N}$, the family $\{P_1, \ldots, P_n\} \subseteq \mathcal{L}(\mathfrak{H})$ is called an orthogonal family of projections if $P_iP_j = \delta_{i,j}P_i$ for all $i, j \in \langle 1, n\rangle$, where, for all $r, s \in \mathbb{R}$, we denote by $\delta_{r,s}$ the usual Kronecker symbol. If, in addition, $\sum_{i=1}^n P_i = 1$, the family is said to be complete.

Definition 12 (1-sided projections) *The operators $q_L, q_R \in \mathcal{L}(\mathfrak{h})$ defined by*

$$q_L := m[1_L], \tag{35}$$
$$q_R := m[1_R], \tag{36}$$

and their liftings to $\mathfrak{H}$ by $Q_L := q_L\sigma_0$ and $Q_R := q_R\sigma_0$ are called the 1-sided projections.

Remark 13 Setting $q_S := m[1_S] \in \mathcal{L}(\mathfrak{h})$ and $Q_S := q_S\sigma_0$, it follows that $\{Q_L, Q_S, Q_R\} \subseteq \mathcal{L}(\mathfrak{H})$ is a complete orthogonal family of orthogonal projections.

In the following, if $H \in \mathcal{L}(\mathfrak{H})$ is a Hamiltonian, we denote by $1_{sc}(H), 1_{ac}(H), 1_{pp}(H) \in \mathcal{L}(\mathfrak{H})$ the orthogonal projections onto the singularly continuous, the absolutely continuous, and the pure point subspace of H, respectively. Moreover, we denote by $\operatorname{spec}(H)$ and $\operatorname{eig}(H)$ the spectrum and the set of all eigenvalues of H. Finally, for all $\kappa, \lambda \in \{L, S, R\}$, we write

$$H_\kappa := Q_\kappa H Q_\kappa, \tag{37}$$
$$H_{\kappa\lambda} := Q_\kappa H Q_\lambda. \tag{38}$$

In the course of our study, one or several of the following conditions on the Hamiltonian of the system will be used. For the case of a translation invariant system, i.e., if Assumption 14 *(b)* holds, we will also rely on further conditions which we will discuss in Section 5.

Assumption 14 (Hamiltonian) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian.*

(a) $1_{sc}(H) = 0$
(b) $[H, \Theta] = 0$
(c) $H_{LR} \in \mathcal{L}^1(\mathfrak{H})$
(d) $H_{LR} = 0$
(e) $H \neq z1$ *for all* $z \in \mathbb{C}$

Remark 15 If Assumption 14 *(e)* does not hold, i.e., if there exists $z \in \mathbb{C}$ such that $H = z1$, (25)-(26) imply that $z = 0$.

In the following, $\mathrm{s} - \lim$ stands for the limit with respect to the strong operator topology on $\mathcal{L}(\mathfrak{H})$.

In order to define the R/L mover states, we make use of the large time asymptotic behavior of the 1-sided projections.

Definition 16 (Asymptotic projections) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (c) and let $\beta_L, \beta_R \in \mathbb{R}$ be the inverse reservoir temperatures.*

(a) The operators $P_L, P_R \in \mathcal{L}(\mathfrak{H})$, defined by

$$P_L := \mathrm{s} - \lim_{t \to \infty} \mathrm{e}^{-\mathrm{i}tH} Q_L \mathrm{e}^{\mathrm{i}tH} 1_{ac}(H), \tag{39}$$

$$P_R := \mathrm{s} - \lim_{t \to \infty} \mathrm{e}^{-\mathrm{i}tH} Q_R \mathrm{e}^{\mathrm{i}tH} 1_{ac}(H), \tag{40}$$

are called the asymptotic projections (for H).

(b) The operator $\Delta \in \mathcal{L}(\mathfrak{H})$, defined by

$$\Delta := \beta_L P_R + \beta_R P_R, \tag{41}$$

is called the R/L mover generator (for H and β_L, β_R).

In the following, we call Kronecker basis of $\mathfrak{h}$ the complete orthonormal system $\{\delta_y\}_{y \in \mathbb{Z}} \subseteq \mathfrak{h}$, where, for all $y \in \mathbb{Z}$, the function $\delta_y \in \mathfrak{h}$ is defined by $\delta_y(x) := \delta_{x,y}$ for all $x, y \in \mathbb{Z}$. We also define $p_{x,y} \in \mathcal{L}^0(\mathfrak{H})$ by $p_{x,y} := (\delta_x, \cdot\,)\, \delta_y \in \mathcal{L}^0(\mathfrak{h})$ for all $x, y \in \mathbb{Z}$. Moreover, the domain, the range, and the kernel of a given map will be denoted by $\mathrm{dom}, \mathrm{ran}\,, \ker$, respectively. For any separable complex Hilbert space $\mathcal{H}$, the commutant of any $\mathcal{A} \subseteq \mathcal{L}(\mathcal{H})$ is defined by $\mathcal{A}' := \{A \in \mathcal{L}(\mathcal{H}) \,|\, [A, B] = 0$ for all $B \in \mathcal{A}\}$. Furthermore, $\mathcal{B}(\mathbb{R})$ stands for the Borel functions and $\mathcal{M}(\mathbb{R})$ for the Borel sets on $\mathbb{R}$ as given in Definition 75 *(c)* (we frequently refer to the appendices in the following). For any $M \in \mathcal{M}(\mathbb{R})$, we denote by $|M|$ the (non-complete) Borel-Lebesgue measure of M. Finally, for all $M \subseteq \mathbb{R}$, we set $-M := \{-x \,|\, x \in M\}$.

Proposition 17 (Asymptotic projections) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (c). Then:*

(a) The asymptotic projections $P_L, P_R \in \mathcal{L}(\mathfrak{H})$ exist. Moreover, $\{P_L, P_R\}$ is a (not necessarily complete) orthogonal family of orthogonal projections satisfying

$$P_L + P_R = 1_{ac}(H). \tag{42}$$

(b) For all $\kappa \in \{L, R\}$, we have

$$[P_\kappa, H] = 0, \tag{43}$$
$$[P_\kappa, \Gamma] = 0. \tag{44}$$

(c) If, in addition, Assumption 14 (b) is satisfied, we also have

$$[P_\kappa, \Theta] = 0. \tag{45}$$

Proof. (a) Let $\mathrm{dom}(\mu_H) := \{A \in \mathcal{L}(\mathfrak{H}) \mid \mathrm{s}-\lim_{t\to\infty} \mathrm{e}^{-\mathrm{i}tH} A\, \mathrm{e}^{\mathrm{i}tH} 1_{ac}(H)$ exists$\}$ be the so-called wave algebra (see [12] for example) and let the so-called the wave morphism $\mu_H : \mathrm{dom}(\mu_H) \subseteq \mathcal{L}(\mathfrak{H}) \to \mathcal{L}(\mathfrak{H})$ be defined, for all $A \in \mathrm{dom}(\mu_H)$, by

$$\mu_H(A) := \mathrm{s}-\lim_{t\to\infty} \mathrm{e}^{-\mathrm{i}tH} A\, \mathrm{e}^{\mathrm{i}tH} 1_{ac}(H). \tag{46}$$

Due to Remark 13, we can write

$$H = H_L + H_S + H_R + H_{LS} + H_{SL} + H_{RS} + H_{SR} + H_{LR} + H_{RL}, \tag{47}$$

from which it follows that $Q_L H = H_L + H_{LS} + H_{LR}$ and $H Q_L = H_L + H_{SL} + H_{RL}$. Hence, due to Assumption 14 *(c)* (and since $\mathcal{L}^0(\mathfrak{H})$ is a 2-sided $*$-ideal of $\mathcal{L}(\mathfrak{H})$, too), we get

$$\begin{aligned}[Q_L, H] &= H_{LS} + H_{LR} - (H_{SL} + H_{RL}) \\ &\in \mathcal{L}^1(\mathfrak{H}),\end{aligned} \tag{48}$$

where we used that $H_{LS} \in \mathcal{L}^0(\mathfrak{H})$ since $Q_S \in \mathcal{L}^0(\mathfrak{H})$ (and analogously for $[Q_R, H] \in \mathcal{L}^1(\mathfrak{H})$). Hence, the Kato-Rosenblum theorem from the trace class approach to scattering theory implies that $Q_L, Q_R \in \mathrm{dom}(\mu_H)$, i.e., we get the first conclusion of part *(a)*.

We next show that $\{P_L, P_R\} \subseteq \mathcal{L}(\mathfrak{H})$ is an orthogonal family of orthogonal projections (which, in general, is incomplete). For this purpose, we note that, since $Q_\kappa^2 = Q_\kappa^* = Q_\kappa$ for all $\kappa \in \{L, R\}$ due to Remark 13, since μ_H is an algebra homomorphism, and since $\mu_H(A^*) = \mu_H(A)^*$ for all $A \in \mathrm{dom}(\mu_H)$ for which $A^* \in \mathrm{dom}(\mu_H)$ (note that, in general, μ_H is not a $*$-algebra homomorphism because $\mathrm{dom}(\mu_H)$ is not a $*$-algebra), we find that $P_\kappa = \mu_H(Q_\kappa)$ is an orthogonal projection for all $\kappa \in \{L, R\}$. Moreover, since $Q_L Q_R = 0$, we also get

$P_L P_R = 0$. Finally, since $Q_L + Q_R = 1 - Q_S$ and since $\mu_H(Q_S) = 0$ because we know that $Q_S \in \mathcal{L}^0(\mathfrak{H}) \subseteq \mathcal{L}^\infty(\mathfrak{H}) \subseteq \ker(\mu_H)$, we get

$$\begin{aligned} P_L + P_R &= \mu_H(1) - \mu_H(Q_S) \\ &= 1_{ac}(H). \end{aligned} \tag{49}$$

(b) If $B \in \operatorname{ran}(\mu_H)$, there exists $A \in \mathcal{L}(\mathfrak{H})$ such that $B = \mu_H(A)$ and, since the strong limit is translation invariant, we get $B = \mu_H(\mathrm{e}^{-\mathrm{i}sH} A \mathrm{e}^{\mathrm{i}sH})$ for all $s \in \mathbb{R}$. Hence, $\mathrm{e}^{-\mathrm{i}sH} B \mathrm{e}^{\mathrm{i}sH} = \mathrm{e}^{-\mathrm{i}sH} \mu_H(A) \mathrm{e}^{\mathrm{i}sH} = \mu_H(\mathrm{e}^{-\mathrm{i}sH} A \mathrm{e}^{\mathrm{i}sH}) = B$ for all $s \in \mathbb{R}$ and it follows that $\operatorname{ran}(\mu_H) \subseteq \{H\}'$ (we actually know that $\operatorname{ran}(\mu_H) = \{B \in \{H\}' \,|\, 1_{ac}(H) B = B 1_{ac}(H) = B\}$), i.e., we get (43). As for (44), we first note that Lemma 83 *(a)* and Remark 85 yield $\Gamma E_H(\mathrm{e}_t)\Gamma = E_{\Gamma H \Gamma}(\zeta \mathrm{e}_t) = E_{-H}(\mathrm{e}_{-t}) = E_H(\mathrm{e}_t)$ for all $t \in \mathbb{R}$, where, for all $t \in \mathbb{R}$, the function $\mathrm{e}_t \in \mathcal{B}(\mathbb{R})$ is defined by $\mathrm{e}_t(x) := \mathrm{e}^{\mathrm{i}tx}$ for all $x \in \mathbb{R}$ (and E_A stands for resolution of the identity of the selfadjoint operator A as discussed in Appendix A), i.e., we get, for all $t \in \mathbb{R}$,

$$[\mathrm{e}^{\mathrm{i}tH}, \Gamma] = 0. \tag{50}$$

Moreover, we also note that, for all $\kappa \in \{L, R\}$,

$$[Q_\kappa, \Gamma] = 0. \tag{51}$$

Finally, since the absolutely continuous subspace of H is given by $\operatorname{ran}(1_{ac}(H)) = \{F \in \mathfrak{H} \,|\, (F, 1_M(H) F) = 0 \text{ for all } M \in \mathcal{M}(\mathbb{R}) \text{ with } |M| = 0\}$, since, again due to Lemma 83 *(a)* and Remark 85, we can write that $(\Gamma F, 1_M(H)\Gamma F) = (\Gamma E_H(1_M)\Gamma F, F) = (F, 1_{-M}(H) F)$ for all $M \in \mathcal{M}(\mathbb{R})$ and all $F \in \mathfrak{H}$, and since the Borel-Lebesgue measure is reflexion invariant, i.e., since $-M \in \mathcal{M}(\mathbb{R})$ and $|-M| = |M|$ for all $M \in \mathcal{M}(\mathbb{R})$, we get $\Gamma F \in \operatorname{ran}(1_{ac}(H))$ for all $F \in \operatorname{ran}(1_{ac}(H))$. This implies that $1_{ac}(H)\Gamma 1_{ac}(H) = \Gamma 1_{ac}(H)$, and since the (anti-linear) adjoints of $1_{ac}(H)\Gamma 1_{ac}(H), \Gamma 1_{ac}(H) \in \bar{\mathcal{L}}(\mathfrak{H})$ are given by $1_{ac}(H)\Gamma 1_{ac}(H)$ and $1_{ac}(H)\Gamma$, respectively, we get

$$[1_{ac}(H), \Gamma] = 0. \tag{52}$$

Hence, using (50)-(52), we arrive at (44).

(c) We first note that Assumption 14 *(b)* and the proof of Lemma 83 *(d)* imply that $[\chi(H), \Theta] = 0$ for all $\chi \in \mathcal{B}(\mathbb{R})$. Hence, since $\mathrm{e}_t \in \mathcal{B}(\mathbb{R})$ for all $t \in \mathbb{R}$ and since we know that $1_{ac}(H) = E_H(1_{M_{ac}})$ for some $M_{ac} \in \mathcal{M}(\mathbb{R})$, we get $[\mathrm{e}^{\mathrm{i}tH}, \Theta] = 0$ for all $t \in \mathbb{R}$ and $[1_{ac}(H), \Theta] = 0$. This implies that, for all $\kappa \in \{L, R\}$,

$$[P_\kappa, \Theta] = \mu_H([Q_\kappa, \Theta]). \tag{53}$$

Now, since $[Q_\kappa, \Theta] = [q_\kappa, \theta]\sigma_0$ for all $\kappa \in \{L, R\}$ and since $[q_L, \theta] = -p_{x_L - 1, x_L} \in \mathcal{L}^0(\mathfrak{h})$ and $[q_R, \theta] = p_{x_R, x_R + 1} \in \mathcal{L}^0(\mathfrak{h})$, we get $[Q_\kappa, \Theta] \in \mathcal{L}^0(\mathfrak{H}) \subseteq \ker(\mu_H)$ as in part *(a)*. □

In the following, we also denote by ξ the parity operation from Definition 6 *(b)* when applied to a function $\chi : M \to \mathbb{C}$, where $M \subseteq \mathbb{R}$ satisfies $M = -M$. Moreover, the even and odd parts of such a χ are written as

$$\mathrm{Ev}(\chi) := \frac{1}{2}(\chi + \xi\chi), \tag{54}$$

$$\mathrm{Od}(\rho) := \frac{1}{2}(\chi - \xi\chi). \tag{55}$$

In order to define our L/R mover states, we introduce the following class of functions.

Definition 18 (Fermi function) *If $\rho \in \mathcal{B}(\mathbb{R})$ has the properties*

$$\rho \geq 0, \tag{56}$$

$$\mathrm{Ev}(\rho) = \frac{1}{2}, \tag{57}$$

it is called a Fermi function.

Remark 19 Since $\rho = \mathrm{Ev}(\rho) + \mathrm{Od}(\rho)$ for all $\rho \in \mathcal{B}(\mathbb{R})$ and since $\mathcal{B}(\mathbb{R})$ is a $*$-algebra due to Definition 75 *(b)*, ρ is a Fermi function if and only if there exists an odd function $\mu \in \mathcal{B}(\mathbb{R})$ with $-1 \leq \mu \leq 1$ such that $\rho = (1+\mu)/2$.

The following assumption will be used at the end of Section 6.

Assumption 20 (Strict positivity) *Let $\rho \in \mathcal{B}(\mathbb{R})$ be a Fermi function and let $\beta_L, \beta_R \in \mathbb{R}$ be the inverse reservoir temperatures.*

(a) $\rho(x) > \rho(y)$ *for all* $x, y \in \mathbb{R}$ *with* $x > y$
(b) $\rho'(x) \geq c$ *for some* $c > 0$ *and almost all* $x \in \mathbb{R}$
(c) $\beta_L < \beta_R$

Remark 21 Due to Lebesgue's theorem on the differentiability of monotone functions, ρ' exists almost everywhere on $\mathbb{R}$ if Assumption 20 *(a)* holds.

For the following, recall that, since $\mathfrak{H}$ is a separable Hilbert space, $\mathrm{eig}(H)$ is a countable subset of $\mathbb{R}$, and we write

$$\mathrm{eig}(H) = \{\lambda_i\}_{i \in I}, \tag{58}$$

where the index set I is empty, finite, or countably infinite (in the following notations, we stick to the case of a countably infinite number of eigenvalues, i.e., we set $I = \mathbb{N}$). Also recall Definition 16 *(b)* for the R/L generator Δ.

With the help of the asymptotic projections and the class of Fermi functions, we next define what we call the R/L mover states.

Definition 22 (R/L mover state) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (a) and (c). Moreover, let $T_0 \in \mathcal{L}(\mathfrak{H})$ be a 2-point operator, called the initial 2-point operator, let $\rho \in \mathcal{B}(\mathbb{R})$ be a Fermi function, and let $\beta_L, \beta_R \in \mathbb{R}$ be the inverse reservoir temperatures.*

(a) An operator $T \in \mathcal{L}(\mathfrak{H})$ of the form $T := T_{ac} + T_{pp}$, where $T_{ac}, T_{pp} \in \mathcal{L}(\mathfrak{H})$ are given by

$$T_{ac} := \rho(\Delta H) 1_{ac}(H), \tag{59}$$

$$T_{pp} := \sum_{\lambda \in \mathrm{eig}(H)} 1_\lambda(H) T_0 1_\lambda(H), \tag{60}$$

is called an R/L mover 2-point operator (for H, T_0, ρ, and β_L, β_R). Moreover, the right hand side of (60) *is defined by* $\mathrm{s}-\lim_{N\to\infty} \sum_{n\in\langle 1,N\rangle} 1_{\lambda_n}(H) T_0 1_{\lambda_n}(H)$.

(b) A state whose 2-point operator is an R/L mover 2-point operator is called an R/L mover state.

Remark 23 First, note that (59) is well-defined since, due to Proposition 17 *(a)* and (43), we have $\Delta^* = \Delta$ and $[\Delta, H] = 0$, i.e., ΔH is selfadjoint. As for (60), since, for all $N \in \mathbb{N}$, we have $\chi_N := 1_{\{\lambda_1,\ldots,\lambda_N\}} \in \mathcal{B}(\mathbb{R})$ and $|\chi_N|_\infty \le 1$, we get $\mathcal{B}-\lim_{N\to\infty} \chi_N = 1_{\mathrm{eig}(H)} \in \mathcal{B}(\mathbb{R})$ and, hence, Proposition 76 *(b)* yields

$$\mathrm{s}-\lim_{N\to\infty} \chi_N(H) = 1_{\mathrm{eig}(H)}(H). \tag{61}$$

Moreover, since $\chi_N(H) = \sum_{i\in\langle 1,N\rangle} 1_{\lambda_i}(H)$ and since $\{1_{\lambda_i}(H)\}_{i\in\mathbb{N}}$ is an orthogonal family of orthogonal projections, we can write $\|\chi_N(H)F - \chi_M(H)F\|^2 = \sum_{i\in\langle M+1,N\rangle} \|1_{\lambda_i}(H)F\|^2$ for all $N, M \in \mathbb{N}$ with $N > M$ and all $F \in \mathfrak{H}$. Hence, due to (61), $\sum_{i\in\langle M+1,N\rangle} \|1_{\lambda_i}(H)F\|^2$ vanishes for sufficiently large N and M, i.e., the series $\sum_{i\in\mathbb{N}} \|1_{\lambda_i}(H)F\|^2 := \lim_{N\to\infty} \sum_{i\in\langle 1,N\rangle} \|1_{\lambda_i}(H)F\|^2$ converges absolutely and, hence, unconditionally. Settting $S_N^\pi := \sum_{i\in\langle 1,N\rangle} 1_{\lambda_{\pi(i)}}(H) T_0 1_{\lambda_{\pi(i)}}(H) \in \mathcal{L}(\mathfrak{H})$ for all $N \in \mathbb{N}$ and all $\pi \in \mathcal{S}_\mathbb{N}$, where $\mathcal{S}_\mathbb{N}$ denotes the symmetric group of $\mathbb{N}$, we can write, for all $N, M \in \mathbb{N}$ with $N > M$, all $\pi \in \mathcal{S}_\mathbb{N}$, and all $F \in \mathfrak{H}$, that

$$\begin{aligned}\|S_N^\pi F - S_M^\pi F\|^2 &= \sum_{i\in\langle M+1,N\rangle} \|1_{\lambda_{\pi(i)}}(H) T_0 1_{\lambda_{\pi(i)}}(H) F\|^2 \\ &\le \|T_0\|^2 \sum_{i\in\langle M+1,N\rangle} \|1_{\lambda_{\pi(i)}}(H) F\|^2,\end{aligned} \tag{62}$$

where we used that, for all $\pi \in \mathcal{S}_\mathbb{N}$, the family $\{1_{\lambda_{\pi(i)}}(H)\}_{i\in\mathbb{N}}$ is again an orthogonal family of orthogonal projections. Since the series $\sum_{i\in\mathbb{N}} \|1_{\lambda_i}(H)F\|^2$ is unconditionally convergent, the right hand side of (62) vanishes for sufficiently large N and M. Hence, the strong limit of $(S_N^\pi)_{N\in\mathbb{N}}$ exists for all $\pi \in \mathcal{S}_\mathbb{N}$. Since, in addition, we know that it is independent of π, the notation on the right hand side of (60) is well-motivated.

Remark 24 Due to Proposition 17 *(a)*, (43), and (361) in the proof of Lemma 83 *(c)*, we can write $\rho(\Delta H) = \rho(\beta_L H P_L + \beta_R H P_R) = \rho(\beta_L H) P_L + \rho(\beta_R H) P_R + \rho(0)(1 - 1_{ac}(H))$. Hence, we get

$$T_{ac} - \rho(\Delta H) = -\frac{1}{2} 1_{pp}(H), \tag{63}$$

where we used Assumption 14 *(a)*, the fact that the family $\{1_{pp}(H), 1_{ac}(H), 1_{sc}(H)\}$ is a complete orthogonal family of orthogonal projections, and $\rho(0) = 1/2$ from (57).

Proposition 25 (R/L mover 2-point operator) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (a) and (c), $T_0 \in \mathcal{L}(\mathfrak{H})$ an initial 2-point operator, $\rho \in \mathcal{B}(\mathbb{R})$ a Fermi function, and $\beta_L, \beta_R \in \mathbb{R}$ the inverse reservoir temperatures. Moreover, let $T \in \mathcal{L}(\mathfrak{H})$ be the R/L mover 2-point operator for H, T_0, ρ, and β_L, β_R. Then:*

(a) *T is a 2-point operator.*

(b) $[T, H] = 0$

Proof. *(a)* We have to verify (28)-(30) for $T = T_{ac} + T_{pp}$, where T_{ac} and T_{pp} are defined in (59) and (60), respectively. As for (28), we first note that, due to (357) from Lemma 83 *(d)*,

$$[1_{ac}(H), \rho(\Delta H)] = 0, \tag{64}$$

where we used that $1_{ac}(H) = E_H(1_{M_{ac}})$ for some $M_{ac} \in \mathcal{M}(\mathbb{R})$ as in the proof of Proposition 17 *(b)* (and that $[\Delta, H] = 0$ as discussed at the beginning of Remark 23). Hence, we get $T_{ac}^* = 1_{ac}(H)\rho(\Delta H) = T_{ac}$. As for the selfadjointness of T_{pp}, since $T_{pp} = \mathrm{s} - \lim_{N\to\infty} S_N$, where $S_N := \sum_{i\in\langle 1,N\rangle} 1_{\lambda_i}(H) T_0 1_{\lambda_i}(H) \in \mathcal{L}(\mathfrak{H})$ for all $N \in \mathbb{N}$, and since $S_N^* = S_N$ for all $N \in \mathbb{N}$, we have $(T_{pp}^* F, G) = (F, T_{pp} G) = \lim_{N\to\infty}(S_N F, G) = (T_{pp} F, G)$ for all $F, G \in \mathfrak{H}$, i.e., $T_{pp}^* = T_{pp}$. Hence, T satisfies (28). As for (29), using Lemma 83 *(a)*, Remark 85, and applying (44) and (56)-(57), we get $\Gamma\rho(\Delta H)\Gamma = E_{\Gamma\Delta H\Gamma}(\zeta\rho) = E_{-\Delta H}(\rho) = E_{\Delta H}(1-\rho) = 1 - \rho(\Delta H)$. Hence, with the help of (52), we get

$$\Gamma T_{ac} \Gamma = 1_{ac}(H) - T_{ac}. \tag{65}$$

As for the contribution T_{pp}, since we know that $1_{pp}(H) = E_H(1_{\mathrm{eig}(H)})$, (61) yields

$$1_{pp}(H) = \sum_{\lambda\in\mathrm{eig}(H)} 1_\lambda(H), \tag{66}$$

where we used the notation $\sum_{\lambda\in\mathrm{eig}(H)} 1_\lambda(H) := \mathrm{s} - \lim_{N\to\infty} \sum_{i\in\langle 1,N\rangle} 1_{\lambda_i}(H)$ (and, as in Remark 23, we note that the strong convergence of the corresponding series is unconditional). Next, using again Lemma 83 *(a)* and *(b)*, we get, for all $\lambda \in \mathrm{eig}(H)$,

$$\Gamma 1_\lambda(H) \Gamma = 1_{-\lambda}(H). \tag{67}$$

Moreover, since $H(\Gamma F) = -\Gamma H F = -\lambda(\Gamma F)$ for all $F \in \operatorname{ran}(1_\lambda(H))$ with $F \neq 0$ (and, hence, $\Gamma F \neq 0$ because $\|\Gamma F\| = \|F\|$ for all $F \in \mathfrak{H}$), we find

$$\operatorname{eig}(H) = -\operatorname{eig}(H). \tag{68}$$

Therefore, using (67), the property (29) for T_0, (68), and (66), we get

$$\begin{aligned} \Gamma T_{pp} \Gamma &= \mathrm{s}-\lim_{N\to\infty} \sum_{i \in \langle 1,N \rangle} 1_{-\lambda_i}(H)(1-T_0)1_{-\lambda_i}(H) \\ &= 1_{pp}(H) - T_{pp}. \end{aligned} \tag{69}$$

Due to Assumption 14 *(a)*, we have $1 = 1_{ac}(H) + 1_{pp}(H)$ and, hence, T also satisfies (29). Finally, we turn to (30). Using (64), we get, for all $F \in \mathfrak{H}$,

$$(F, T_{ac}F) = (1_{ac}(H)F, \rho(\Delta H)1_{ac}(H)F), \tag{70}$$

$$(F, T_{pp}F) = \lim_{N\to\infty} \sum_{i \in \langle 1,N \rangle} (1_{\lambda_i}(H)F, T_0 1_{\lambda_i}(H)F). \tag{71}$$

Hence, with the help of (56) and Proposition 76 *(a)* for $\rho(\Delta H)$ in (70), and (30) for T_0 in (71), we arrive at $T \geq 0$. Furthermore, since, as shown above, (28) and (29) hold for T, we can write $(F,(1-T)F) = (F, \Gamma T \Gamma F) = (T\Gamma F, \Gamma F) = (\Gamma F, T \Gamma F) \geq 0$ for all $F \in \mathfrak{H}$, i.e., we also find $T \leq 1$.

(b) With the help of the first part in the proof of Lemma 83 *(d)*, we can write $[T_{ac}, H] = \rho(\Delta H)[1_{ac}(H), H] + [\rho(\Delta H), H]1_{ac}(H) = 0$. Moreover, for all $\lambda \in \operatorname{eig}(H)$, Remark 85 yields $H1_\lambda(H) = E_H(\kappa_1 1_{\mathrm{spec}(H)} 1_\lambda) = \lambda 1_\lambda(H)$ and $[H, 1_\lambda(H)] = 0$ and, hence, for all $F \in \mathfrak{H}$, we get

$$\begin{aligned} [T_{pp}, H]F &= \lim_{N\to\infty} \sum_{i \in \langle 1,N \rangle} [1_{\lambda_i}(H)T_0 1_{\lambda_i}(H), H]F \\ &= \lim_{N\to\infty} \sum_{i \in \langle 1,N \rangle} [1_{\lambda_i}(H)T_0 1_{\lambda_i}(H), \lambda_i 1]F \\ &= 0. \end{aligned} \tag{72}$$

□

We next give some examples of important states which fit into the foregoing framework of R/L mover states. However, the prototypical example of a non degenerate R/L mover state will be treated separately in Section 4.

Example 26 (Thermal equilibrium state) *Let H be a Hamiltonian satisfying Assumption 14 (a) and (c). Moreover, set $\beta_L := \beta$ and $\beta_R := \beta$ for some $\beta \in \mathbb{R}$, let ρ be a Fermi function, and let the initial 2-point operator be defined by $T_0 := \rho(\beta H)$ (it can be verified as in the proof of Proposition 25 (a) that T_0 is indeed a 2-point operator). Then, the R/L mover 2-point operator T (for H, T_0, ρ, and β_L, β_R) has the form*

$$T = \rho(\beta H), \tag{73}$$

where we made use of Lemma 83 (c) yielding $T_{ac} = E_{\beta H 1_{ac}(H)}(\rho)1_{ac}(H) = \rho(\beta H)1_{ac}(H)$*. Moreover, with the help of Lemma 83 (d) and* (66)*, we get* $T_{pp} = \rho(\beta H)1_{pp}(H)$*. The so-called* (τ, β)*-KMS state, or thermal equilibrium state, where* τ *is the quasifree dynamics generated by* H *from Definition 7 (b) and where* β *plays the role of an inverse physical temperature (if* $\beta > 0$ *and the Boltzmann constant* k_B *set to unity), is the quasifree state whose 2-point operator has the form* (73) *and the Fermi function is given, for all* $x \in \mathbb{R}$*, by the classical Fermi-Dirac (Pauli) distribution*

$$\rho(x) := \frac{1}{1+\mathrm{e}^{-x}}. \tag{74}$$

Moreover, the (τ, β)*-KMS state is unique if* $1_0(H) = 0$ *(see [2] for the foregoing and other sufficient conditions).*

Note that, in contrast to the gauge-invariant case discussed next (which frequently occurs in practice), there is a minus sign in (74) (see Lemma 28 *(d)* below).

Definition 27 (Gauge invariance) *A state* $\omega \in \mathcal{E}_{\mathfrak{A}}$ *is called gauge-invariant if it is invariant under the 1-parameter group of Bogoliubov* $*$*-automorphisms* $\mathbb{R} \ni \varphi \mapsto \tau_{U_\varphi} \in \mathrm{Aut}(\mathfrak{A})$ *induced by the 1-parameter group of Bogoliubov operators* $\mathbb{R} \ni \varphi \mapsto U_\varphi \in \mathcal{L}(\mathfrak{H})$ *given in Definition 6 (c), i.e., if* $\omega \circ \tau_{U_\varphi} = \omega$ *for all* $\varphi \in \mathbb{R}$*.*

Gauge invariance leads to the following properties.

Lemma 28 (Gauge-invariant 2-point operator) *Let* $T \in \mathcal{L}(\mathfrak{H})$*. Then:*

(a) If $\omega \in \mathcal{E}_{\mathfrak{A}}$ *is a gauge-invariant state with 2-point operator* T*, we have, for all* $\varphi \in \mathbb{R}$*,*

$$[T, U_\varphi] = 0. \tag{75}$$

Any $T \in \mathcal{L}(\mathfrak{H})$ *satisfying* (75) *is called gauge-invariant.*

(b) T *is a gauge-invariant 2-point operator if and only if there exists an operator* $s \in \mathcal{L}(\mathfrak{h})$ *with* $0 \leq s \leq 1$ *such that*

$$T = (1-s) \oplus \zeta s \zeta. \tag{76}$$

(c) If $\omega \in \mathcal{E}_{\mathfrak{A}}$ *is a state with 2-point operator* T *and if* $\eta \in \mathcal{E}_{\mathfrak{A}}$ *satisfies, for some* $s \in \mathcal{L}(\mathfrak{h})$ *with* $0 \leq s \leq 1$ *and all* $f, g \in \mathfrak{h}$*,*

$$\eta(a^*(f)a(g)) = (g, sf), \tag{77}$$

we have, for all $F, G \in \mathfrak{H}$*,*

$$\omega(B^*(F)B(G)) = \eta(B^*(F)B(G)), \tag{78}$$

if and only if T *has the form* (76)*.*

(d) Let $T=\rho(\beta H)$, where $\rho\in\mathcal{B}(\mathbb{R})$ has the form (74)*, $H\in\mathcal{L}(\mathfrak{H})$ is a Hamiltonian, and $\beta\in\mathbb{R}\setminus\{0\}$. If T is gauge invariant, there exists $h\in\mathcal{L}(\mathfrak{h})$ with $h^*=h$ such that*

$$H=h\oplus(-\zeta h\zeta). \tag{79}$$

Moreover, if (79) *holds, T has the form* (76) *and*

$$s=\rho(-\beta h). \tag{80}$$

Remark 29 Note that, if $s\in\mathcal{L}(\mathfrak{h})$ with $0\le s\le 1$ and if $\omega_s\in\mathcal{E}_{\mathfrak{A}}$ is a state having the property $\omega_s(a^*(f)a(g))=(g,sf)$ for all $f,g\in\mathfrak{h}$, we have, for all $F,G\in\mathfrak{H}$, that

$$\omega_s(B^*(F)B(G))=\omega_T(B^*(F)B(G)), \tag{81}$$

where $\omega_T\in\mathcal{E}_{\mathfrak{A}}$ is a state whose 2-point operator $T\in\mathcal{L}(\mathfrak{H})$ has the form (76).

Proof. (a) Since $\omega(\tau_{U_\varphi}(B^*(F)B(G)))=\omega(B^*(F)B(G))$ for all $\varphi\in\mathbb{R}$ and all $F,G\in\mathfrak{H}$, (31) yields $[T,U_\varphi]=0$ for all $\varphi\in\mathbb{R}$.

(b) If we write $T=[t_{ij}]_{i,j\in\langle 1,2\rangle}$, where $t_{ij}\in\mathcal{L}(\mathfrak{h})$ for all $i,j\in\langle 1,2\rangle$, (75) is equivalent to

$$t_{12}=0, \tag{82}$$
$$t_{21}=0, \tag{83}$$

since $[T,U_\varphi]=2\mathrm{i}\sin(\varphi)\begin{bmatrix}0 & -t_{12}\\ t_{21} & 0\end{bmatrix}$ for all $\varphi\in\mathbb{R}$. Moreover, since T is a 2-point operator, it satisfies (28), (29), and (30), respectively equivalent to $t_{11}^*=t_{11}$, $t_{22}^*=t_{22}$, and $t_{12}^*=t_{21}$, to

$$t_{22}=1-\zeta t_{11}\zeta, \tag{84}$$
$$t_{21}=-\zeta t_{21}\zeta, \tag{85}$$

and to the two conditions that, for all $f_1,f_2\in\mathfrak{h}$,

$$0\le(f_1,t_{11}f_1+t_{12}f_2)+(f_2,t_{21}f_1+t_{22}f_2), \tag{86}$$
$$0\le(f_1,(1-t_{11})f_1-t_{12}f_2)-(f_2,t_{21}f_1-(1-t_{22})f_2). \tag{87}$$

Hence, setting $s:=1-t_{11}\in\mathcal{L}(\mathfrak{h})$, (82)-(85) are equivalent to $T=(1-s)\oplus\zeta s\zeta$. Moreover, (86) and (87) are equivalent to $0\le s\le 1$.

(c) Note that (78) is equivalent to the condition that, for all $f_1,f_2,g_1,g_2\in\mathfrak{h}$,

$$(f_1,t_{11}g_1+t_{12}g_2)+(f_2,t_{21}g_1+t_{22}g_2)=(f_1,(1-s)g_1)+(\zeta g_2,s\zeta f_2), \tag{88}$$

where we used the same notation as in part *(b)*. Hence, plugging $f_2=g_2=0$ into (88), we get $t_{11}=1-s$, and (84) implies that $t_{22}=\zeta s\zeta$. Moreover, plugging $f_2=g_1=0$ into (88), we get $t_{12} = 0$, and (85) yields $t_{21} = 0$. Conversely, if T has the form (76), since $s^* = s$ and $(f, \zeta g) = (g, \zeta f)$ for all $f, g \in \mathfrak{h}$, (88) is satisfied.

(d) If T satisfies (75), part *(b)* implies that there exists $s \in \mathcal{L}(\mathfrak{h})$ with $0 \leq s \leq 1$ such that T has the form (76). Next, note that $\rho : \mathbb{R} \to (0,1)$ is strictly monotonically increasing and let $\rho^{-1} : (0,1) \to \mathbb{R}$ be its inverse function (i.e., $\rho^{-1}(x) = \log(x/(1-x))$ for all $x \in (0,1)$). Since $1 = E_{\beta H}(1_{\mathrm{spec}(\beta H)})$ and since $\mathrm{spec}(\beta H) \subseteq [-|\beta| r, |\beta| r]$, where $r := \|H\|$, we can write $T = E_{\beta H}(\rho 1_{[-|\beta| r, |\beta| r]})$. Defining $\psi \in \mathcal{B}(\mathbb{R})$ by $\psi(x) := \rho^{-1}(x)$ for all $x \in [\rho(-|\beta| r), \rho(|\beta| r)]$ and $\psi(x) := 0$ for all $x \in \mathbb{R} \setminus [\rho(-|\beta| r), \rho(|\beta| r)]$, Lemma 83 *(b)* yields, on one hand,

$$\begin{aligned} \psi(T) &= E_{\beta H}(\psi \circ (\rho 1_{[-|\beta| r, |\beta| r]})) \\ &= \beta H, \end{aligned} \tag{89}$$

where we used that $\psi \circ (\rho 1_{[-|\beta| r, |\beta| r]}) = \kappa_1 1_{[-|\beta| r, |\beta| r]}$. On the other hand, since, for all $\chi \in \mathcal{B}(\mathbb{R})$ and all selfadjoint $a, b \in \mathcal{L}(\mathfrak{h})$, we have $\chi(a \oplus b) = \chi(a) \oplus \chi(b)$ (which can be proven as, for example, in the proof of Lemma 83 *(c)*), we get $\psi(T) = \psi((1-s) \oplus \zeta s \zeta) = \psi(1-s) \oplus \psi(\zeta s \zeta)$, i.e., H is block diagonal. Hence, writing $H = [h_{ij}]_{i,j \in \langle 1,2 \rangle}$ and setting $h := h_{11} \in \mathcal{L}(\mathfrak{h})$, the fact that $H^* = H$ implies that $h^* = h$. Moreover, since $\Gamma H \Gamma = -H$ (which is equivalent to $h_{22} = -\zeta h_{11} \zeta$ and $h_{21} = -\zeta h_{12} \zeta$), we get $h_{22} = -\zeta h \zeta$, i.e., H has the form (79).

Moreover, if H is given by (79) for some $h \in \mathcal{L}(\mathfrak{h})$ with $h^* = h$, (56)-(57) imply

$$\begin{aligned} T &= E_{\beta h}(\rho) \oplus E_{-\beta \zeta h \zeta}(\rho) \\ &= E_{\beta h}(1 - \xi\rho) \oplus E_{-\beta \zeta h \zeta}(\rho) \\ &= (1 - E_{\beta h}(\xi\rho)) \oplus \zeta E_{-\beta h}(\rho) \zeta \\ &= (1 - E_{-\beta h}(\rho)) \oplus \zeta E_{-\beta h}(\rho) \zeta, \end{aligned} \tag{90}$$

where we used that $\zeta \chi(a) \zeta = (\zeta \chi)(\zeta a \zeta)$ for all selfadjoint $a \in \mathcal{L}(\mathfrak{h})$ and all $\chi \in \mathcal{B}(\mathbb{R})$ (which follows from Lemma 83 *(a)* for the case $A = a \oplus 0$) and Remark 85 for $\xi\rho = \rho_{-1}$. $\square$

Example 30 (Ground state) *Let H be as in Example 26. The so-called τ-ground state is the quasifree state whose 2-point operator has the form* (73) *(with $\beta = 1$), where the Fermi function, denoted by ρ_∞, is given by*

$$\rho_\infty := 1_{(0,\infty)} + \frac{1}{2} 1_0. \tag{91}$$

Moreover, the τ-ground state is unique if $1_0(H) = 0$ (if $1_0(H) \neq 0$, a 2-point operator of the form $T = 1_{(0,\infty)}(H) + 1_0(H) S 1_0(H)$, where $S \in \mathcal{L}(\mathfrak{H})$ is any 2-point operator, specifies a τ-ground state, see [6]). Furthermore, note that $\mathcal{B} - \lim_{\beta \to \infty} \rho(\beta\,\cdot) = \rho_\infty$, where ρ is given by (74)*. Hence, Proposition 76 (b) yields*

$$\mathrm{s} - \lim_{\beta \to \infty} \rho(\beta H) = \rho_\infty(H), \tag{92}$$

i.e., if $1_0(H) = 0$, the 2-point operator of the unique (τ, β)-KMS state converges strongly to the 2-point operator of the unique τ-ground state.

4 Nonequilibrium steady states

In this section, we construct a special class of R/L movers, the so-called nonequilibrium steady states (NESSs) discussed in the introduction. They serve as the main motivation for the introduction of the R/L mover states in the foregoing section.

For the following, recall the definitions (37)-(38) from Section 3.

Definition 31 (Initial system) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian, let $\rho \in \mathcal{B}(\mathbb{R})$ be a Fermi function, and let $\beta_L, \beta_R \in \mathbb{R}$ the inverse reservoir temperatures. Moreover, let $\beta_S \in \mathbb{R}$ be the inverse sample temperature.*

(a) The operator $H_0 \in \mathcal{L}(\mathfrak{H})$, defined by

$$H_0 := H_L + H_S + H_R, \tag{93}$$

is called the initial Hamiltonian (for H).

(b) The quasifree dynamics generated by $H_0 \in \mathcal{L}(\mathfrak{H})$ is called the initial dynamics.

(c) The quasifree state $\omega_0 \in \mathcal{E}_{\mathfrak{A}}$ whose 2-point operator $T_0 \in \mathcal{L}(\mathfrak{H})$ has the form

$$T_0 := \rho(\Delta_0 H_0), \tag{94}$$

where $\Delta_0 \in \mathcal{L}(\mathfrak{H})$ is defined by

$$\Delta_0 := \beta_L Q_L + \beta_S Q_S + \beta_R Q_R, \tag{95}$$

is called the initial state (for ρ and $\beta_L, \beta_S, \beta_R$).

Remark 32 Since, due to Remark 13, the family $\{Q_L, Q_S, Q_R\} \subseteq \mathcal{L}(\mathfrak{H})$ is a complete orthogonal family of orthogonal projections and since $[Q_\kappa, \Gamma] = 0$ for all $\kappa \in \{L, S, R\}$, the operators H_L, H_S, H_R, and H_0 are selfdual observables. Moreover, $\Delta_0 H_0 \in \mathcal{L}(\mathfrak{H})$ is selfadjoint and, as in the proof of Proposition 25 *(a)*, property (57), Definition 77, Lemma 83 *(a)*, and Remark 85 yield that T_0 is a 2-point operator.

For the setting at hand, the NESS discussed in the introduction is defined as follows.

Definition 33 (NESS) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian, let $\rho \in \mathcal{B}(\mathbb{R})$ be a Fermi function, and let $\beta_L, \beta_R \in \mathbb{R}$ be the inverse reservoir temperatures. Moreover, let $\beta_S \in \mathbb{R}$ be the inverse sample temperature, let $\omega_0 \in \mathcal{E}_{\mathfrak{A}}$ be the initial state for ρ and $\beta_L, \beta_S, \beta_R$, and let $\mathbb{R} \ni t \mapsto \tau^t \in \mathrm{Aut}(\mathfrak{A})$ be the quasifree dynamics generated by H. The state $\omega \in \mathcal{E}_{\mathfrak{A}}$ defined, for all $A \in \mathfrak{A}$, by*

$$\omega(A) := \lim_{t\to\infty} \frac{1}{t} \int_0^t \mathrm{d}s\ \omega_0(\tau^s(A)), \tag{96}$$

is called the NESS (for H, ρ, and $\beta_L, \beta_S, \beta_R$).

Remark 34 The general definition stems from [27] and defines the NESSs as the limit points in the weak-$*$ topology of the net defined by the ergodic mean between 0 and $t > 0$ of the given initial state time-evolved by the dynamics of interest (note that, due to the Banach-Alaoglu theorem, the set of such NESSs is not empty). In general, the averaging procedure enables us to treat a nonvanishing contribution to the point spectrum of the Hamiltonian which generates the full time evolution (see Theorem 36 below).

The following ingredients from the time-dependent approach to Hilbert space scattering theory will be used for the construction of our NESS.

Definition 35 (Wave operators) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (c) and let $H_0 \in \mathcal{L}(\mathfrak{H})$ be the initial Hamiltonian for H.*

(a) The operator $W \in \mathcal{L}(\mathfrak{H})$, defined by

$$W := \mathrm{s} - \lim_{t\to\infty} \mathrm{e}^{-\mathrm{i}tH_0}\mathrm{e}^{\mathrm{i}tH}1_{\mathrm{ac}}(H), \tag{97}$$

is called the wave operator (for H and H_0).

(b) The operators $W_L, W_R \in \mathcal{L}(\mathfrak{H})$, defined by

$$W_L := \mathrm{s} - \lim_{t\to\infty} \mathrm{e}^{-\mathrm{i}tH_L}Q_L\mathrm{e}^{\mathrm{i}tH}1_{\mathrm{ac}}(H), \tag{98}$$

$$W_R := \mathrm{s} - \lim_{t\to\infty} \mathrm{e}^{-\mathrm{i}tH_R}Q_R\mathrm{e}^{\mathrm{i}tH}1_{\mathrm{ac}}(H), \tag{99}$$

are called the partial wave operators (for H and H_L, and H and H_R, respectively).

For the following, let us denote by $AP(\mathbb{R})$ the complex-valued functions on $\mathbb{R}$ which are almost-periodic (in the sense of H. Bohr). Also recall the definitions of the asymptotic projections P_L, P_R and of the R/L mover generator Δ from Definition 16. Moreover, for all $A = [a_{ij}]_{i,j\in\langle 1,n\rangle} \in \mathbb{C}^{n\times n}$, the Euclidean matrix norm is denoted by $|A|_2 := (\sum_{i,j\in\langle 1,n\rangle} |a_{ij}|^2)^{1/2}$.

Theorem 36 (NESS) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (a) and (c), let $\rho \in \mathcal{B}(\mathbb{R})$ be a Fermi function, and let $\beta_L, \beta_R \in \mathbb{R}$ be the inverse reservoir temperatures. Moreover, let $\beta_S \in \mathbb{R}$ be the inverse sample temperature, let $\omega_0 \in \mathcal{E}_{\mathfrak{A}}$ be the initial state for ρ and $\beta_L, \beta_S, \beta_R$, and let $\mathbb{R} \ni t \mapsto \tau^t \in \mathrm{Aut}(\mathfrak{A})$ be the quasifree dynamics generated by H. Then:*

(a) The NESS $\omega \in \mathcal{E}_{\mathfrak{A}}$ for H, ρ, and $\beta_L, \beta_S, \beta_R$ exists.

(b) The 2-point operator $T \in \mathcal{L}(\mathfrak{H})$ of ω is given by

$$T = T_{ac} + T_{pp}, \tag{100}$$

where $T_{ac}, T_{pp} \in \mathcal{L}(\mathfrak{H})$ are defined by

$$T_{ac} := \rho(\Delta H)1_{ac}(H), \tag{101}$$

$$T_{pp} := \sum_{\lambda\in\mathrm{eig}(H)} 1_\lambda(H)T_0\,1_\lambda(H). \tag{102}$$

Proof. (a) We start off by studying (96) for elements of $\mathfrak{A}$ of the form $\prod_{i\in\langle 1,2n\rangle} B(F_i)$ for all $n\in\mathbb{N}$ and all $\{F_i\}_{i\in\langle 1,2n\rangle}\subseteq\mathfrak{H}$. Since ω_0 is quasifree, the expectation value with respect to ω_0 of such elements propagated in time by means of the quasifree dynamics generated by H has the Pfaffian factorization property from Definiton 11, i.e.,

$$\omega_0\Big(\prod\nolimits_{i\in\langle 1,2n\rangle}\tau^t\big(B(F_i)\big)\Big)=\mathrm{pf}(\Omega(t)), \tag{103}$$

where, for all $n\in\mathbb{N}$ and all $\{F_i\}_{i\in\langle 1,2n\rangle}\subseteq\mathfrak{H}$, the entries of the matrix-valued map $\Omega:\mathbb{R}\to\mathbb{C}^{2n\times 2n}$ are defined, for all $i,j\in\langle 1,2n\rangle$ and all $t\in\mathbb{R}$, by

$$\Omega_{ij}(t):=(\Gamma\mathrm{e}^{\mathrm{i}tH}F_i,T_0\mathrm{e}^{\mathrm{i}tH}F_j). \tag{104}$$

In the following, let $n\in\mathbb{N}$ and $\{F_i\}_{i\in\langle 1,2n\rangle}\subseteq\mathfrak{H}$ be fixed. Since, due to Assumption 14 *(a)*, we can write $1=1_{ac}(H)+1_{pp}(H)\in\mathcal{L}(\mathfrak{H})$, we have, for all $i,j\in\langle 1,2n\rangle$ and all $t\in\mathbb{R}$, that

$$\Omega_{ij}(t)=\Omega_{ij}^{aa}(t)+\Omega_{ij}^{ap}(t)+\Omega_{ij}^{pa}(t)+\Omega_{ij}^{pp}(t), \tag{105}$$

where the entries of the matrix-valued maps $\Omega^{aa},\Omega^{ap},\Omega^{pa},\Omega^{pp}:\mathbb{R}\to\mathbb{C}^{2n\times 2n}$ are defined, for all $i,j\in\langle 1,2n\rangle$ and all $t\in\mathbb{R}$, by

$$\Omega_{ij}^{aa}(t):=(\mathrm{e}^{\mathrm{i}tH}1_{ac}(H)\Gamma F_i,T_0\mathrm{e}^{\mathrm{i}tH}1_{ac}(H)F_j), \tag{106}$$
$$\Omega_{ij}^{ap}(t):=(\mathrm{e}^{\mathrm{i}tH}1_{ac}(H)\Gamma F_i,T_0\mathrm{e}^{\mathrm{i}tH}1_{pp}(H)F_j), \tag{107}$$
$$\Omega_{ij}^{pa}(t):=(\mathrm{e}^{\mathrm{i}tH}1_{pp}(H)\Gamma F_i,T_0\mathrm{e}^{\mathrm{i}tH}1_{ac}(H)F_j), \tag{108}$$
$$\Omega_{ij}^{pp}(t):=(\mathrm{e}^{\mathrm{i}tH}1_{pp}(H)\Gamma F_i,T_0\mathrm{e}^{\mathrm{i}tH}1_{pp}(H)F_j), \tag{109}$$

and we used (50) and (52). We next study the large time averages of (106)-(109).

As for (106), since the family $\{Q_L,Q_S,Q_R\}\subseteq\mathcal{L}(\mathfrak{H})$ is complete, we can insert $1=Q_L+Q_S+Q_R$ in front of the propagators on both sides of (106). Hence, for all $i,j\in\langle 1,2n\rangle$ and all $t\in\mathbb{R}$, we get

$$\Omega_{ij}^{aa}(t)=\sum_{\kappa\in\{L,S,R\}}\Omega_{ij}^{aa,\kappa}(t), \tag{110}$$

where, for all $\kappa\in\{L,S,R\}$, the entries of the matrix-valued maps $\Omega^{aa,\kappa}:\mathbb{R}\to\mathbb{C}^{2n\times 2n}$ are defined, for all $i,j\in\langle 1,2n\rangle$ and all $t\in\mathbb{R}$, by

$$\Omega_{ij}^{aa,\kappa}(t):=(Q_\kappa\mathrm{e}^{\mathrm{i}tH}1_{ac}(H)\Gamma F_i,T_0Q_\kappa\mathrm{e}^{\mathrm{i}tH}1_{ac}(H)F_j), \tag{111}$$

and we used that, since $[Q_\kappa,\Delta_0H_0]=[Q_\kappa,\beta_LH_L+\beta_SH_S+\beta_RH_R]=0$ for all $\kappa\in\{L,S,R\}$, Lemma 83 *(d)* yields $[Q_\kappa,T_0]=0$ for all $\kappa\in\{L,S,R\}$. In order to determine the large time limit of $\Omega^{aa,L}$, we note that, again due to Lemma 83 *(d)*, we have $[\mathrm{e}^{-\mathrm{i}tH_0},T_0]=0$ for all $t\in\mathbb{R}$ since $[H_0,\Delta_0H_0]=0$. Hence, for all $i,j\in\langle 1,2n\rangle$ and all $t\in\mathbb{R}$, we can write

$$\begin{aligned}\Omega_{ij}^{aa,L}(t)&=(\mathrm{e}^{-\mathrm{i}tH_0}Q_L\mathrm{e}^{\mathrm{i}tH}1_{ac}(H)\Gamma F_i,T_0\mathrm{e}^{-\mathrm{i}tH_0}Q_L\mathrm{e}^{\mathrm{i}tH}1_{ac}(H)F_j)\\&=(\mathrm{e}^{-\mathrm{i}tH_L}Q_L\mathrm{e}^{\mathrm{i}tH}1_{ac}(H)\Gamma F_i,\rho(\beta_LH_L)\mathrm{e}^{-\mathrm{i}tH_L}Q_L\mathrm{e}^{\mathrm{i}tH}1_{ac}(H)F_j),\end{aligned} \tag{112}$$

where we used that $\rho(\Delta_0 H_0)Q_L = \rho(\beta_L H_L)Q_L$ which follows from Lemma 83 *(c)*. Since, due to Assumption 14 *(c)*, we have

$$H_L Q_L - Q_L H = -(H_{LS} + H_{LR}) \\ \in \mathcal{L}^1(\mathfrak{H}), \tag{113}$$

the Kato-Rosenblum theorem guarantees the existence of the partial wave operator W_L as in the proof of Proposition 17 *(a)*. Moreover, the Kato-Rosenblum theorem also implies the existence of the wave operator $W_L' \in \mathcal{L}(\mathfrak{H})$ given by

$$W_L' := \mathrm{s}-\lim_{t\to\infty} \mathrm{e}^{-\mathrm{i}tH} Q_L \mathrm{e}^{\mathrm{i}tH_L} 1_{\mathrm{ac}}(H_L). \tag{114}$$

Hence, since the adjoint property for wave operators yields $W_L^* = W_L'$, since Remark 85 and the intertwining property for wave operators imply that $W_L' \rho(\beta_L H_L) = \rho(\beta_L H) W_L'$, and since the chain rule for wave operators results in $W_L' W_L = P_L$, we get, for all $i, j \in \langle 1, 2n\rangle$,

$$\begin{aligned} \lim_{t\to\infty} \Omega_{ij}^{aa,L}(t) &= (W_L \Gamma F_i, \rho(\beta_L H_L) W_L F_j) \\ &= (\Gamma F_i, W_L' \rho(\beta_L H_L) W_L F_j) \\ &= (\Gamma F_i, \rho(\beta_L H) W_L' W_L F_j) \\ &= (\Gamma F_i, \rho(\beta_L H) P_L F_j). \end{aligned} \tag{115}$$

Interchanging L and R, we also get $\lim_{t\to\infty} \Omega_{ij}^{aa,R}(t) = (\Gamma F_i, \rho(\beta_R H) P_R F_j)$ for all $i, j \in \langle 1, 2n\rangle$. Moreover, since, for all $i, j \in \langle 1, 2n\rangle$ and all $t \in \mathbb{R}$, we have

$$|\Omega_{ij}^{aa,S}(t)| \leq \|T_0 Q_S \mathrm{e}^{\mathrm{i}tH} 1_{ac}(H) F_j\| \|F_i\|, \tag{116}$$

and since $T_0 Q_S \in \mathcal{L}^0(\mathfrak{H})$, we know that $\lim_{t\to\infty} \Omega_{ij}^{aa,S}(t) = 0$ for all $i, j \in \langle 1, 2n\rangle$. Therefore, (110), (115), and the foregoing arguments yield, for all $i, j \in \langle 1, 2n\rangle$,

$$\begin{aligned} \lim_{t\to\infty} \Omega_{ij}^{aa}(t) &= (\Gamma F_i, (\rho(\beta_L H) P_L + \rho(\beta_R H) P_R) F_j) \\ &= (\Gamma F_i, \rho(\Delta H) 1_{ac}(H) F_j), \end{aligned} \tag{117}$$

where, in the last equality, we used Lemma 83 *(c)* and (42).

We next turn to (107). First, we note that, since $\mathfrak{H}$ is separable, there exists a sequence $(\eta_N)_{N\in\mathbb{N}} \subseteq \mathcal{L}^0(\mathfrak{H})$ of orthogonal projections satisfying $[\eta_N, H] = 0$ for all $N \in \mathbb{N}$ and $\mathrm{s}-\lim_{N\to\infty} \eta_N = 1_{pp}(H)$ (pick an orthonormal basis $\{E_n\}_{n\in\mathbb{N}}$ of eigenvectors of H for the closed subspace $\mathrm{ran}\,(1_{pp}(H))$ of $\mathfrak{H}$ and set $\eta_N := \sum_{n\in\langle 1,N\rangle} (E_n, \cdot) E_n \in \mathcal{L}^0(\mathfrak{H})$ for all $N \in \mathbb{N}$). Inserting $1 = \eta_N + (1 - \eta_N)$ for any $N \in \mathbb{N}$ after the second propagator on the right hand side of (107), we get, for all $i, j \in \langle 1, 2n\rangle$, all $t \in \mathbb{R}$, and all $N \in \mathbb{N}$,

$$\Omega_{ij}^{ap}(t) = \Omega_{ij}^{ap,N}(t) + \Omega_{ij}^{ap,N_\perp}(t), \tag{118}$$

where the entries of the matrix-valued maps $\Omega^{ap,N}, \Omega^{ap,N_\perp}\colon \mathbb{R} \to \mathbb{C}^{2n\times 2n}$ are defined, for all $i,j \in \langle 1, 2n\rangle$, all $N \in \mathbb{N}$, and all $t \in \mathbb{R}$, by

$$\Omega_{ij}^{ap,N}(t) := (\mathrm{e}^{\mathrm{i}tH} 1_{ac}(H)\Gamma F_i, T_0 \mathrm{e}^{\mathrm{i}tH}\eta_N 1_{pp}(H)F_j), \tag{119}$$

$$\Omega_{ij}^{ap,N_\perp}(t) := (\mathrm{e}^{\mathrm{i}tH} 1_{ac}(H)\Gamma F_i, T_0 \mathrm{e}^{\mathrm{i}tH}(1-\eta_N) 1_{pp}(H)F_j). \tag{120}$$

Using that $[\eta_N, H] = 0$ for all $N \in \mathbb{N}$ and Lemma 83 *(d)* for (119), we get, for all $i,j \in \langle 1, 2n\rangle$, all $N \in \mathbb{N}$, and all $t \in \mathbb{R}$,

$$|\Omega_{ij}^{ap,N}(t)| \le \|\eta_N T_0 \mathrm{e}^{\mathrm{i}tH} 1_{ac}(H)\Gamma F_i\| \|F_j\|, \tag{121}$$

$$|\Omega_{ij}^{ap,N_\perp}(t)| \le \|(1-\eta_N)1_{pp}(H)F_j\| \|T_0\| \|F_i\|. \tag{122}$$

As above, since $\eta_N T_0 \in \mathcal{L}^0(\mathfrak{H})$ for all $N \in \mathbb{N}$, (121) implies that $\lim_{t\to\infty} \Omega_{ij}^{ap,N}(t) = 0$ for all $i,j \in \langle 1, 2n\rangle$ and all $N \in \mathbb{N}$. Moreover, $\lim_{N\to\infty} \Omega_{ij}^{ap,N_\perp}(t) = 0$ for all $i,j \in \langle 1, 2n\rangle$ and all $t \in \mathbb{R}$ due to (122). Hence, for all $i,j \in \langle 1, 2n\rangle$, we get

$$\lim_{t\to\infty} \Omega_{ij}^{ap}(t) = 0. \tag{123}$$

The term (108) is treated analogously leading to $\lim_{t\to\infty} \Omega_{ij}^{pa}(t) = 0$ for all $i,j \in \langle 1, 2n\rangle$.

We finally turn to (109). Setting $\chi_N := \sum_{n\in\langle 1,N\rangle} 1_{\lambda_n}(H)$ for all $N \in \mathbb{N}$, we know from (61) in Remark 23 and from $1_{pp}(H) = 1_{\mathrm{eig}(H)}(H)$ that $\mathrm{s}-\lim_{N\to\infty}\chi_N = 1_{pp}(H)$. Next, we define the entries of the matrix-valued map $\Omega^{pp,N}\colon \mathbb{R} \to \mathbb{C}^{2n\times 2n}$, for all $i,j \in \langle 1, 2n\rangle$, all $N \in \mathbb{N}$, and all $t \in \mathbb{R}$, by

$$\Omega_{ij}^{pp,N}(t) := (\mathrm{e}^{\mathrm{i}tH}\chi_N \Gamma F_i, T_0 \mathrm{e}^{\mathrm{i}tH}\chi_N F_j), \tag{124}$$

and we note $\Omega_{ij}^{pp,N} \in AP(\mathbb{R})$ for all $i,j \in \langle 1, 2n\rangle$ and all $N \in \mathbb{N}$ because (124) defines a trigonometric polynomial on $\mathbb{R}$ due to the fact that $\mathrm{e}^{\mathrm{i}tH}1_\lambda(H) = \mathrm{e}^{\mathrm{i}t\lambda}1_\lambda(H)$ for all $t \in \mathbb{R}$ and all $\lambda \in \mathrm{eig}(H)$. Moreover, since, for all $i,j \in \langle 1, 2n\rangle$, all $N \in \mathbb{N}$, and all $t \in \mathbb{R}$, we have

$$|\Omega_{ij}^{pp,N}(t) - \Omega_{ij}^{pp}(t)| \le \|T_0\| \|\chi_N F_j\| \|(\chi_N - 1_{pp}(H))F_i\| + \|T_0\| \|F_i\| \|(\chi_N - 1_{pp}(H))F_j\|, \tag{125}$$

and since the sequence $(\|\chi_N F\|)_{N\in\mathbb{N}}$ is bounded for all $F \in \mathfrak{H}$, we get, for all $i,j \in \langle 1, 2n\rangle$,

$$\lim_{N\to\infty} |\Omega_{ij}^{pp,N} - \Omega_{ij}^{pp}|_\infty = 0, \tag{126}$$

which implies that $\Omega_{ij}^{pp} \in AP(\mathbb{R})$ for all $i,j \in \langle 1, 2n\rangle$ since $AP(\mathbb{R})$ is closed with respect to the norm $|\cdot|_\infty$ (given in (344) of Appendix A). Since the argument of the Pfaffian on the right hand side of (103) has the form $\Omega(t) = \Lambda^{aa} + \Omega^{pp}(t)$ for all $t \in \mathbb{R}$, where the entries of the matrix $\Lambda^{aa} \in \mathbb{C}^{2n\times 2n}$ are defined by the right hand side of (117), i.e., for all $i,j \in \langle 1, 2n\rangle$, by

$$\Lambda_{ij}^{aa} := (\Gamma F_i, \rho(\Delta H) 1_{ac}(H) F_j), \tag{127}$$

since the Pfaffian is a polynomial function of the entries of the matrix on which it acts, and since $AP(\mathbb{R})$ is an algebra (with respect to the usual pointwise addition, scalar multiplication, and multiplication), the function $\vartheta : \mathbb{R} \to \mathbb{C}$, defined by $\vartheta(t) := \mathrm{pf}(\Lambda^{aa} + \Omega^{pp}(t))$ for all $t \in \mathbb{R}$, satisfies $\vartheta \in AP(\mathbb{R})$. Therefore, we know that the large time average $\lim_{t\to\infty} \int_0^t \mathrm{d}s\, \vartheta(s)/t$ exists, and we want to show that it is equal to the large time average of (103). To this end, let the entries of the range of the linear map $\mathbb{C}^{2n\times 2n} \ni A = [a_{ij}]_{i,j\in\langle 1,2n\rangle} \mapsto A^a \in \mathbb{C}_a^{2n\times 2n}$ be defined, for all $i,j \in \langle 1,2n\rangle$, by $[A^a]_{ij} := a_{ij}$ if $i<j$, $[A^a]_{ii} := 0$, and $[A^a]_{ij} := -a_{ji}$ if $i>j$. Using Hadamard's inequality $|\det(A)| \le \prod_{i\in\langle 1,n\rangle}(\sum_{j\in\langle 1,n\rangle} |a_{ij}|^2)^{1/2}$ for all $A \in \mathbb{C}^{n\times n}$ and the Cayley-Muir lemma $(\mathrm{pf}(A))^2 = \det(A)$ for all $A \in \mathbb{C}_a^{2n\times 2n}$, we get $|\mathrm{pf}(A)| \le |A|_2^n$ for all $A \in \mathbb{C}_a^{2n\times 2n}$. Hence, since the function $[0,\infty) \ni r \mapsto r^n \in \mathbb{R}$ is monotonically increasing, we know that $|\mathrm{pf}(A) - \mathrm{pf}(B)| \le |A-B|_2(|A|_2 + |B|_2 + 1)^n$ for all $A, B \in \mathbb{C}_a^{2n\times 2n}$ (see [29] for example). Moreover, we note that $\mathrm{pf}(A) = \mathrm{pf}(A^a)$ due to (32) and that $|A^a|_2^2 = 2\sum_{i,j\in\langle 1,2n\rangle, i<j} |a_{ij}|^2 \le 2|A|_2^2$ for all $A \in \mathbb{C}^{2n\times 2n}$. Hence, since, for all $t \in \mathbb{R}$, we have $|\Omega(t)|_2 \le C_1$ and $|\Lambda^{aa} + \Omega^{pp}(t)|_2 \le C_2$, where $C_1 := \|T_0\|(\sum_{i,j\in\langle 1,2n\rangle} \|F_i\|^2\|F_j\|^2)^{1/2}$ and $C_2 := \sqrt{2}(\sum_{i,j\in\langle 1,2n\rangle} |\Lambda_{ij}^{aa}|^2 + C_1^2)^{1/2}$, we get, for all $t \in \mathbb{R}$,

$$|\mathrm{pf}(\Omega(t)) - \mathrm{pf}(\Lambda^{aa} + \Omega^{pp}(t))| \le C(|\Omega^{aa}(t) - \Lambda^{aa}|_2 + |\Omega^{ap}(t)|_2 + |\Omega^{pa}(t)|_2), \tag{128}$$

where $C := \sqrt{2}(1 + \sqrt{2}(C_1 + C_2))^n$. Therefore, since the right hand side of (128) vanishes for $t \to \infty$, its large time average also vanishes and we get

$$\begin{aligned} \lim_{t\to\infty} \frac{1}{t}\int_0^t \mathrm{d}s\, \omega_0\Big(\prod\nolimits_{i\in\langle 1,2n\rangle} \tau^s\big(B(F_i)\big)\Big) &= \lim_{t\to\infty} \frac{1}{t}\int_0^t \mathrm{d}s\, \mathrm{pf}(\Omega(s)) \\ &= \lim_{t\to\infty} \frac{1}{t}\int_0^t \mathrm{d}s\, \mathrm{pf}(\Lambda^{aa} + \Omega^{pp}(s)). \end{aligned} \tag{129}$$

Finally, we have to show that the limit on the right hand side of (96) exists for all $A \in \mathfrak{A}$. Let $A \in \mathfrak{A}$ be fixed. Since, by definition, $\mathfrak{A}$ is the completion (with respect to the C^*-norm $\|\cdot\|$) of the $*$-algebra generated by the selfdual generators from Definition 1 *(d)*, there exists a sequence $(P_n)_{n\in\mathbb{N}}$ of polynomials in these generators such that $\lim_{n\to\infty} \|A - P_n\| = 0$. For all $B \in \mathfrak{A}$, defining the function $F_B : (0,\infty) \to \mathbb{C}$ by $F_B(t) := \int_0^t \mathrm{d}s\, \omega_0(\tau^s(B))/t$ for all $t \in (0,\infty)$ and noting that $|\omega_0(\tau^t(B))| \le \|B\|$ for all $t \in \mathbb{R}$ and all $B \in \mathfrak{A}$, we get, for all $t, t' \in \mathbb{R}$ and all $n \in \mathbb{N}$,

$$|F_A(t) - F_A(t')| \le 2\|A - P_n\| + |F_{P_n}(t) - F_{P_n}(t')|. \tag{130}$$

Hence, since the limit for $t \to \infty$ of $F_{P_n}(t)$ exists for all $n \in \mathbb{N}$ due to (129), (130) implies the existence of the desired limit on the right hand side of (96).

(b) Let $F_1, F_2 \in \mathfrak{H}$ be fixed. Due to (96), (129), and (31), we have

$$\begin{aligned} (\Gamma F_1, T F_2) &= \omega(B(F_1)B(F_2)) \\ &= \lim_{t\to\infty} \frac{1}{t}\int_0^t \mathrm{d}s\, \omega_0(\tau^s(B(F_1)B(F_2))) \\ &= (\Gamma F_1, \rho(\Delta H) 1_{ac}(H) F_2) + \lim_{t\to\infty} \frac{1}{t}\int_0^t \mathrm{d}s\, \Omega_{12}^{pp}(s), \end{aligned} \tag{131}$$

where we recall that Ω_{12}^{pp} from (109) satisfies $\Omega_{12}^{pp} \in AP(\mathbb{R})$ and that the limit on the right hand side of (131) thus exists. Moreover, we have, for all $t \in \mathbb{R}^+ := (0,\infty)$ and all $N \in \mathbb{N}$,

$$\begin{aligned}\frac{1}{t}\int_0^t \mathrm{d}s\, \Omega_{12}^{pp,N}(t) &= \sum_{n\in\langle 1,N\rangle} (\Gamma F_1, 1_{\lambda_n}(H)T_0 1_{\lambda_n}(H)F_2)\\ &\quad + \sum_{\substack{n,m\in\langle 1,N\rangle\\ n\neq m}} \frac{\mathrm{e}^{\mathrm{i}t(\lambda_m-\lambda_n)}-1}{\mathrm{i}t(\lambda_m-\lambda_n)}(\Gamma F_1, 1_{\lambda_n}(H)T_0 1_{\lambda_m}(H)F_2), \qquad (132)\end{aligned}$$

from which it follows that, for all $N \in \mathbb{N}$,

$$\lim_{t\to\infty}\frac{1}{t}\int_0^t \mathrm{d}s\, \Omega_{12}^{pp,N}(s) = \Big(\Gamma F_1, \sum\nolimits_{n\in\langle 1,N\rangle} 1_{\lambda_n}(H)T_0 1_{\lambda_n}(H)F_2\Big). \qquad (133)$$

Hence, due to (133), and since (126) implies that the sequence of functions $\mathbb{R}^+ \ni t \mapsto \int_0^t \mathrm{d}s\, \Omega_{12}^{pp,N}(s)/t$ converges, for $N \to \infty$, uniformly in $t \in \mathbb{R}^+$ to the function $\mathbb{R}^+ \ni t \mapsto \int_0^t \mathrm{d}s\, \Omega_{12}^{pp}(s)/t$, the limit operations for $t \to \infty$ and $N \to \infty$ can be interchanged and the second term on the right hand side of (131) becomes

$$\begin{aligned}\lim_{t\to\infty}\frac{1}{t}\int_0^t \mathrm{d}s\, \Omega_{12}^{pp}(s) &= \lim_{t\to\infty}\frac{1}{t}\int_0^t \mathrm{d}s\, \lim_{N\to\infty}\Omega_{12}^{pp,N}(s)\\ &= \lim_{t\to\infty}\lim_{N\to\infty}\frac{1}{t}\int_0^t \mathrm{d}s\, \Omega_{12}^{pp,N}(s)\\ &= \lim_{N\to\infty}\lim_{t\to\infty}\frac{1}{t}\int_0^t \mathrm{d}s\, \Omega_{12}^{pp,N}(s)\\ &= \lim_{N\to\infty}\Big(\Gamma F_1, \sum\nolimits_{n\in\langle 1,N\rangle} 1_{\lambda_n}(H)T_0 1_{\lambda_n}(H)F_2\Big)\\ &= \Big(\Gamma F_1, \sum\nolimits_{\lambda\in\mathrm{eig}(H)} 1_{\lambda}(H)T_0 1_{\lambda}(H)F_2\Big), \qquad (134)\end{aligned}$$

where, in the last equality, we used Definition 22 *(a)*. □

Remark 37 Due to Assumption 14 *(c)*, we have $H - H_0 = H_{LS} + H_{SL} + H_{RS} + H_{SR} + H_{LR} + H_{RL} \in \mathcal{L}^1(\mathfrak{H})$. Hence, the Kato-Rosenblum theorem again implies the existence of the wave operator $W \in \mathcal{L}(\mathfrak{H})$ from Definition 35 *(a)*. Moreover, as in the proof of Theorem 36 *(b)* (or by noting that $W = W_L + W_R$ and by using Lemma 83 *(c)*), inserting $1 = \mathrm{e}^{\mathrm{i}tH_0}\mathrm{e}^{-\mathrm{i}tH_0}$ for all $t \in \mathbb{R}$ in front of T_0 in (106) and using that $[\mathrm{e}^{-\mathrm{i}tH_0}, T_0] = 0$ for all $t \in \mathbb{R}$ directly leads to

$$T_{ac} = W^* T_0 W. \qquad (135)$$

5 Asymptotic velocity

In this section, we implement translation invariance and study its consequences. In particular, we construct the so-called asymptotic velocity and derive the action of the R/L generator as a matrix multiplication operator.

In the following, we will resort to the usual Fourier Hilbert space isomorphism $\mathfrak{f}$ between the 1-particle position Hilbert space $\mathfrak{h}$ over $\mathbb{Z}$ and the 1-particle momentum Hilbert space $\hat{\mathfrak{h}}$ over $\mathbb{T} := [-\pi, \pi]$ defined by

$$\hat{\mathfrak{h}} := L^2(\mathbb{T}). \tag{136}$$

Here and in the following, for all $p \in \mathbb{R}$ with $p \geq 1$, we denote by $L^p(\mathbb{T})$ the space of equivalence classes of functions $\varphi : \mathbb{T} \to \mathbb{C}$ which are measurable with respect to $\mathcal{M}(\mathbb{T})$ and for which $|\varphi|^p$ is integrable with respect to the Borel-Lebesgue measure (and analogously if $\mathbb{T}$ is replaced by another subinterval of $\mathbb{R}$). As usual, the equivalence relation identifies functions which coincide almost everywhere with respect to the Borel-Lebesgue measure (i.e., on the complement of a subset of a set of Borel-Lebesgue measure zero). Moreover, $\mathcal{M}(\mathbb{T})$ is defined to be the restriction of $\mathcal{M}(\mathbb{R})$ to $\mathbb{T}$, i.e., we have $\mathcal{M}(\mathbb{T}) := \{M \cap \mathbb{T} \,|\, M \in \mathcal{M}(\mathbb{R})\} = \{M \subseteq \mathbb{T} \,|\, M \in \mathcal{M}(\mathbb{R})\}$, and we recall that $\mathcal{M}(\mathbb{R})$ is given in Definition 75 *(c)*. Abusing notation, for all $M \in \mathcal{M}(\mathbb{T})$, we write $|M|$ for the (restriction to $\mathcal{M}(\mathbb{T})$ of the) Borel-Lebesgue measure of M. Moreover, we denote by $L^\infty(\mathbb{T})$ the space of equivalence classes of functions $\varphi : \mathbb{T} \to \mathbb{C}$ which are measurable with respect to $\mathcal{M}(\mathbb{T})$ and almost everywhere bounded on $\mathbb{T}$, and the norm on $L^\infty(\mathbb{T})$ is denoted by $\|\cdot\|_\infty$.

For all $f \in \mathfrak{h}$, the Fourier transform is given by the limit (in $\hat{\mathfrak{h}}$) $\mathfrak{f}f := \lim_{N\to\infty} \sum_{|x|\leq N} f(x)\mathrm{e}_x$, where, for all $x \in \mathbb{Z}$, the plane wave functions $\mathrm{e}_x \in \hat{\mathfrak{h}}$ are given by $\mathrm{e}_x(k) := \mathrm{e}^{\mathrm{i}kx}$ for all $k \in \mathbb{T}$. Furthermore, for all $f \in \mathfrak{h}$ and all $a \in \mathcal{L}(\mathfrak{h})$, we set $\hat{f} := \mathfrak{f}f \in \hat{\mathfrak{h}}$ and $\hat{a} := \mathfrak{f}a\mathfrak{f}^* \in \mathcal{L}(\hat{\mathfrak{h}})$ and, sometimes, we also write $\check{\varphi} := \mathfrak{f}^*\varphi$ for all $\varphi \in \hat{\mathfrak{h}}$. On $\mathfrak{H} = \mathfrak{h} \oplus \mathfrak{h}$, we define $\mathfrak{F} := \mathfrak{f}\sigma_0 : \mathfrak{H} \to \widehat{\mathfrak{H}}$, where the doubled 1-particle momentum Hilbert space is given by

$$\widehat{\mathfrak{H}} := \hat{\mathfrak{h}} \oplus \hat{\mathfrak{h}}, \tag{137}$$

and we set $\widehat{F} := \mathfrak{F}F \in \widehat{\mathfrak{H}}$ for all $F \in \mathfrak{H}$ and $\widehat{A} := \mathfrak{F}A\mathfrak{F}^* \in \mathcal{L}(\widehat{\mathfrak{H}})$ for all $A \in \mathcal{L}(\mathfrak{H})$ (the usual scalar products and the corresponding induced norms and operator norms, on both $\hat{\mathfrak{h}}$ and $\widehat{\mathfrak{H}}$, are again all denoted by $(\cdot,\cdot)$ and $\|\cdot\|$, respectively).

Furthermore, similarly to (34) on position space, for all $u \in L^\infty(\mathbb{T})$, the multiplication operator $m[u] \in \mathcal{L}(\hat{\mathfrak{h}})$ on momentum space is defined by $m[u]\varphi := u\varphi$ for all $\varphi \in \hat{\mathfrak{h}}$. Moreover, for all $u := [u_1, u_2, u_3] \in L^\infty(\mathbb{T})^3$, we define $m[u] \in \mathcal{L}(\hat{\mathfrak{h}})^3$ by

$$m[u] := [m[u_1], m[u_2], m[u_3]], \tag{138}$$

and we note that, for all $\Phi \in \widehat{\mathfrak{H}}$ on which it is defined, the operator $U := m[u_0]\sigma_0 + m[u]\sigma$ (using the same matrix operator notation as the one introduced in (5)) satisfies the bound

$$\|U\Phi\| \leq C_U\|\Phi\|, \tag{139}$$

where we set $C_U := \sum_{\alpha\in\langle 0,3\rangle} \|u_\alpha\|_\infty$ (in particular, if U is defined on the whole of $\widehat{\mathfrak{H}}$, we have $U \in \mathcal{L}(\widehat{\mathfrak{H}})$). Finally, for all $u \in L^\infty(\mathbb{T})$, we denote the real, imaginary, even, and odd part of u (defined almost everywhere) by $\mathrm{Re}(u)$, $\mathrm{Im}(u)$, $\mathrm{Ev}(u)$, and $\mathrm{Od}(u)$, respectively.

We next determine the properties of the Pauli coefficients specifying a translation invariant Hamiltonian in momentum space.

Proposition 38 (Translation invariance) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (b).Then:*

(a) There exist $u_0 \in L^\infty(\mathbb{T})$ and $u = [u_1, u_2, u_3] \in L^\infty(\mathbb{T})^3$ such that

$$\widehat{H} = m[u_0]\sigma_0 + m[u]\sigma. \tag{140}$$

(b) For all $\alpha \in \langle 0, 3\rangle$, we have

$$\mathrm{Im}(u_\alpha) = 0. \tag{141}$$

Moreover, the even and odd parts have the properties, for all $\alpha \in \langle 0, 2\rangle$,

$$\mathrm{Ev}(u_\alpha) = 0, \tag{142}$$

$$\mathrm{Od}(u_3) = 0. \tag{143}$$

Proof. (a) Let us first note that, since the Hamiltonian can be written in the form $H = h_0\sigma_0 + h\sigma$ with the Pauli coefficients $h_0 \in \mathcal{L}(\mathfrak{h})$ and $h := [h_1, h_2, h_3] \in \mathcal{L}(\mathfrak{h})^3$, (25) and (26) respectively yield, for all $\alpha \in \langle 0, 3\rangle$,

$$h_\alpha^* = h_\alpha, \tag{144}$$

$$\zeta h_\alpha \zeta = \begin{cases} -h_\alpha, & \alpha \in \langle 0, 2\rangle, \\ \ \ h_\alpha, & \alpha = 3. \end{cases} \tag{145}$$

On the other hand, Assumption 14 *(b)* implies, for all $\alpha \in \langle 0, 3\rangle$, that

$$[h_\alpha, \theta] = 0. \tag{146}$$

Hence, we know (see [13] for example) that, for all $\alpha \in \langle 0, 3\rangle$, there exist $u_\alpha \in L^\infty(\mathbb{T})$ with

$$\hat{h}_\alpha = m[u_\alpha], \tag{147}$$

i.e., we can write $\widehat{H} = m[u_0]\sigma_0 + m[u]\sigma$, where we set $u := [u_1, u_2, u_3] \in L^\infty(\mathbb{T})^3$.

(b) Using (144) and (147), we have $\bar{u}_\alpha = u_\alpha$ for all $\alpha \in \langle 0, 3\rangle$, where $\bar{\varphi}$ is the complex conjugation of $\varphi \in \hat{\mathfrak{h}}$. Moreover, since $\mathfrak{f}\zeta f = \hat{\xi}\,\bar{\hat{f}}$ for all $f \in \mathfrak{h}$, we get, for all $\alpha \in \langle 0, 3\rangle$,

$$\hat{\xi} u_\alpha = \begin{cases} -u_\alpha, & \alpha \in \langle 0, 2\rangle, \\ \ \ u_\alpha, & \alpha = 3, \end{cases} \tag{148}$$

and we note that $(\hat{\xi}\varphi)(k) = \varphi(-k)$ for all $\varphi \in \hat{\mathfrak{h}}$ and almost all $k \in \mathbb{T}$. □

Remark 39 Let $\alpha \in \langle 0, 3\rangle$. Due to a theorem by Bernstein, if, and only if, (the 2π-periodic extension of) u_α is real-analytic, there exist constants $C, a > 0$ such that, for all $x \in \mathbb{Z}$,

$$|\check{u}_\alpha(x)| \leq C\mathrm{e}^{-a|x|}. \tag{149}$$

Moreover, under these conditions, the number of zeros of u_α on $\mathbb{T}$ is finite. In Section 6, we will study the special case for which $\check{u}_\alpha$ has finite support.

In the following, for all functions $\mathbb{T} \ni k \mapsto u(k) \in \mathbb{C}$ and all $k_0 \in \mathbb{T}$, we denote by $u'(k_0)$ not only the derivative of u with respect to k at the point k_0 if $k_0 \in \mathbb{T} \setminus \{\pm\pi\}$ but also the one-sided derivatives if $k_0 \in \{\pm\pi\}$ (if all the derivatives in question exist). In this sense, for all $m \in \mathbb{N}$, we denote by $C^m(\mathbb{T})$ the m times continuously differentiable complex-valued functions on $\mathbb{T}$. Moreover, $C(\mathbb{T})$ stands for the continuous and $C^\infty(\mathbb{T})$ for the infinitely differentiable complex-valued functions on $\mathbb{T}$. The analogous notations are used if $\mathbb{T}$ is replaced by $\mathbb{R}$ and/or the target space $\mathbb{C}$ by another Banach space (which is then explicitly indicated).

The following conditions will be used at various places in the sequel.

Assumption 40 (Pauli coefficient functions) *Let $u_\alpha \in L^\infty(\mathbb{T})$ for all $\alpha \in \langle 0, 3\rangle$.*

(a) $\mathrm{Im}(u_\alpha) = 0$ *for all* $\alpha \in \langle 0, 3\rangle$

(b) $u_\alpha \in C^1(\mathbb{T})$ *with* $u_\alpha(\pi) = u_\alpha(-\pi)$ *and* $u'_\alpha(\pi) = u'_\alpha(-\pi)$ *for all* $\alpha \in \langle 0, 3\rangle$

In the following, for all $m \in \mathbb{N}$ and all $u := [u_1, \ldots, u_m] \in L^\infty(\mathbb{T})^m$ with real-valued entries, we define the Euclidean norm function $|u| \in L^\infty(\mathbb{T})$ by $|u| := \sqrt{\sum_{i\in\langle 1,m\rangle} u_i^2}$ and the generalized zero set $\mathcal{Z}_u \in \mathcal{M}(\mathbb{T})$ (up to subsets of sets of Borel-Lebesgue measure zero) by

$$\mathcal{Z}_u := \{k \in \mathbb{T} \,|\, |u|(k) = 0\} \tag{150}$$

$$= \bigcap_{i\in\langle 1,m\rangle} \mathcal{Z}_{u_i}, \tag{151}$$

and we use the notation $\mathcal{Z}_u^c := \mathbb{T} \setminus \mathcal{Z}_u \in \mathcal{M}(\mathbb{T})$. Moreover, for all $i \in \langle 1, m\rangle$, the functions $\tilde{u}_i \in L^\infty(\mathbb{T})$ are defined by

$$\tilde{u}_i := \begin{cases} \dfrac{u_i}{|u|}, & \text{on } \mathcal{Z}_u^c, \\ 0, & \text{on } \mathcal{Z}_u, \end{cases} \tag{152}$$

and we set $\tilde{u} := [\tilde{u}_1, \ldots, \tilde{u}_m] \in L^\infty(\mathbb{T})^m$. Moreover, for all $u := [u_1, \ldots, u_m] \in L^\infty(\mathbb{T})^m$ and $v := [v_1, \ldots, v_m] \in L^\infty(\mathbb{T})^m$ with real-valued entries, the Euclidean scalar product function $uv \in L^\infty(\mathbb{T})$ is defined by $uv := \sum_{i\in\langle 1,m\rangle} u_i v_i$ and we set $u^2 := uu$. Finally, for all $u_0 \in L^\infty(\mathbb{T})$ and all $u := [u_1, \ldots, u_m] \in L^\infty(\mathbb{T})^m$, we set $u_0 u := [u_0 u_1, \ldots, u_0 u_m] \in L^\infty(\mathbb{T})^m$.

The following functions are the basic ingredients in the diagonalization of the Hamiltonian (see Proposition 86 and Remark 87).

Definition 41 (Eigenvalue functions) *Let $u_0 \in L^\infty(\mathbb{T})$ and $u := [u_1, u_2, u_3] \in L^\infty(\mathbb{T})^3$ satisfy Assumption 40 (a) and (b). The eigenvalue functions $e_\pm \in C(\mathbb{T}) \cap C^1(\mathcal{Z}_u^c)$ are defined by*

$$e_\pm := u_0 \pm |u|. \tag{153}$$

Moreover, we define the set $\mathcal{Z}_\pm \in \mathcal{M}(\mathbb{T})$ by

$$\mathcal{Z}_\pm := \{k \in \mathcal{Z}_u^c \,|\, e'_\pm(k) = 0\}, \tag{154}$$

and, on $\mathcal{Z}_u^c$, we have $e'_\pm = u'_0 \pm \tilde{u}u'$.

Remark 42 Since, due to Assumption 40 *(b)*, we have $u_\alpha \in C(\mathbb{T})$ for all $\alpha \in \langle 1, 3\rangle$, the set $\mathcal{Z}_u$ is closed relative to $\mathbb{T}$ (and $\mathbb{R}$) and, hence, $\mathcal{Z}_u^c$ is open relative to $\mathbb{T}$.

In the following, whenever the symbol $\pm$ appears several times in the same equation, the latter stands for two equations, one of which corresponds to all the upper signs and the other one to all the lower signs (no cross terms).

The following conditions will be used in Section 6 and Appendix B.

Assumption 43 (Zero sets) *Let $u_0 \in L^\infty(\mathbb{T})$ and $u := [u_1, u_2, u_3] \in L^\infty(\mathbb{T})^3$ satisfy Assumption 40 (a) and (b) and let $M \in \mathcal{M}(\mathbb{R})$.*

(a) $|\mathcal{Z}_u \cap e_\pm^{-1}(M)| = 0$
(b) $|\mathcal{Z}_\pm \cap e_\pm^{-1}(M)| = 0$

In the following, $\ell^0(\mathbb{Z})$ stands for the subspace of $\mathfrak{h}$ of all the complex-valued functions on $\mathbb{Z}$ with finite support. Moreover, let $\mathrm{dom}(q)$ be the subspace of $\mathfrak{h}$ defined by

$$\mathrm{dom}(q) := \Big\{ f \in \mathfrak{h} \,\Big|\, \sum\nolimits_{x\in\mathbb{Z}} x^2 |f(x)|^2 < \infty \Big\}, \tag{155}$$

and note that $\mathrm{dom}(q)$ is dense in $\mathfrak{h}$ since the Kronecker basis satisfies $\{\delta_x\}_{x\in\mathbb{Z}} \subseteq \ell^0(\mathbb{Z}) \subseteq \mathrm{dom}(q)$. Moreover, let $q : \mathrm{dom}(q) \subseteq \mathfrak{h} \to \mathfrak{h}$ stand for the usual position operator on the position space $\mathfrak{h}$ whose action is given, for all $f \in \mathrm{dom}(q)$ and all $x \in \mathbb{Z}$, by

$$(qf)(x) := xf(x). \tag{156}$$

Recall that q is unbounded since, if, for any $f \in \mathrm{dom}(q)$ with $f \notin \ell^0(\mathbb{Z})$, we set $f_n := (f - 1_{\langle -n,n\rangle} f)/\|f - 1_{\langle -n,n\rangle} f\| \in \mathrm{dom}(q)$ for all $n \in \mathbb{N}$, we have $\|qf_n\| \geq n+1$ for all $n \in \mathbb{N}$. Moreover, since $f/(\kappa_1 \pm \mathrm{i}) \in \mathrm{dom}(q)$ for all $f \in \mathfrak{h}$, where $\kappa_1(x) = x$ for all $x \in \mathbb{R}$ stems from (346), we have $\mathrm{ran}\,(q \pm \mathrm{i}1) = \mathfrak{h}$. Hence, since, due to (156), q is symmetric, the standard criterion for selfadjointness implies that $q^* = q$. Furthermore, its lifting to the doubled 1-particle Hilbert space $\mathfrak{H}$ is defined by

$$\mathrm{dom}(Q) := \mathrm{dom}(q) \oplus \mathrm{dom}(q), \tag{157}$$

$$Q := q\sigma_0, \tag{158}$$

where, for the case of unbounded operators, we use the same matrix operator notation as the one introduced in (5) for the bounded operators (but acting on the domain of definition of the unbounded operator in question). From the foregoing considerations for q, we obtain that $\mathrm{dom}(Q)$ is a dense subspace of $\mathfrak{H}$ and that $Q^* = Q$.

Next, let $\mathrm{dom}(p)$ be the subspace of $\hat{\mathfrak{h}}$ defined by

$$\mathrm{dom}(p) := \{\varphi \in AC(\mathbb{T}) \,|\, \varphi' \in \hat{\mathfrak{h}} \text{ and } \varphi(\pi) = \varphi(-\pi)\}, \tag{159}$$

where $AC(\mathbb{T})$ stands for the complex-valued absolutely continuous functions on $\mathbb{T}$. Recall that if $\varphi \in AC(\mathbb{T})$, then $\varphi'(k)$ exists for almost all $k \in \mathbb{T}$, $\varphi' \in L^1(\mathbb{T})$, and $\varphi(k) = \varphi(-\pi) + \int_{[-\pi,k]} \mathrm{d}s\, \varphi'(s)$ for all $k \in \mathbb{T}$. Conversely, if $\psi \in L^1(\mathbb{T})$, then the function $\mathbb{T} \ni k \to \varphi(k) := \int_{[-\pi,k]} \mathrm{d}s\, \psi(s)$ satisfies $\varphi \in AC(\mathbb{T})$ and $\varphi'(k) = \psi(k)$ for almost all $k \in \mathbb{T}$. Now, note that $\mathfrak{f}^*\varphi \in \mathrm{dom}(q)$ for all $\varphi \in \mathrm{dom}(p)$ since, for all $\varphi \in \mathrm{dom}(p)$ and all $x \in \mathbb{Z}$, we have

$$x(\mathfrak{f}^*\varphi)(x) = -\mathrm{i}(\mathfrak{f}^*\varphi')(x), \tag{160}$$

where we used partial integration in $AC(\mathbb{T})$ (and, for example, that $C^1(\mathbb{T}) \subseteq AC(\mathbb{T})$). Moreover, we also have $\mathfrak{f}f \in \mathrm{dom}(p)$ for all $f \in \mathrm{dom}(q)$ because, on one hand, $\mathfrak{f}f \in W^{1,2}(\mathbb{T})$ due to the fact that $\{\varphi \in \hat{\mathfrak{h}} \,|\, \mathfrak{f}^*\varphi \in \mathrm{dom}(q)\} = W^{1,2}(\mathbb{T})$ ((160) also holds for $\varphi \in W^{1,2}(\mathbb{T})$), where $W^{1,2}(\mathbb{T})$ stands for the usual (periodic) Sobolev space, and, on the other hand, since we know that $W^{1,2}(\mathbb{T}) = \mathrm{dom}(p)$. Hence, since $\mathfrak{f}^*\varphi \in \mathrm{dom}(q)$ for all $\varphi \in \mathrm{dom}(p)$ and since $\mathfrak{f}f \in \mathrm{dom}(p)$ for all $f \in \mathrm{dom}(q)$, the restriction of the unitary operator $\mathfrak{f} : \mathfrak{h} \to \hat{\mathfrak{h}}$ to $\mathrm{dom}(q)$ is a bijection between $\mathrm{dom}(q)$ and $\mathrm{dom}(p)$. Therefore, $\mathrm{dom}(p)$ being a dense subspace of $\hat{\mathfrak{h}}$, we define the position operator on momentum space $p : \mathrm{dom}(p) \subseteq \hat{\mathfrak{h}} \to \hat{\mathfrak{h}}$, for all $\varphi \in \mathrm{dom}(p)$, by

$$p\varphi := -\mathrm{i}\varphi'. \tag{161}$$

Moreover, due to (160), we can write $p\varphi = \mathfrak{f}q\mathfrak{f}^*\varphi$ for all $\varphi \in \mathrm{dom}(p)$ which implies that p is an unbounded selfadjoint operator on momentum space. Finally, as for Q above, the lifting to the doubled 1-particle momentum space $\widehat{\mathfrak{H}}$ is defined by

$$\mathrm{dom}(P) := \mathrm{dom}(p) \oplus \mathrm{dom}(p), \tag{162}$$

$$P := p\sigma_0, \tag{163}$$

and we again get that $\mathrm{dom}(P)$ is a dense subspace of $\widehat{\mathfrak{H}}$ and that $P^* = P$. Moreover, $\mathfrak{F}$ is a bijection between $\mathrm{dom}(Q)$ and $\mathrm{dom}(P)$ and $P\Phi = \mathfrak{F}Q\mathfrak{F}^*\Phi$ for all $\Phi \in \mathrm{dom}(P)$.

We now arrive at the definition of the asymptotic velocity of the system.

Definition 44 (Asymptotic velocity) *Let $u_0 \in L^\infty(\mathbb{T})$ and $u := [u_1, u_2, u_3] \in L^\infty(\mathbb{T})^3$ satisfy Assumption 40 (a) and define $U \in \mathcal{L}(\widehat{\mathfrak{H}})$ by*

$$U := m[u_0]\sigma_0 + m[u]\sigma. \tag{164}$$

If $\mathrm{e}^{\mathrm{i}tU}\mathrm{dom}(P) \subseteq \mathrm{dom}(P)$ for all $t \in \mathbb{R}$ and if, for all $\Phi \in \mathrm{dom}(P)$, the limit for $t \to \infty$ of $\mathrm{e}^{-\mathrm{i}tU}P\mathrm{e}^{\mathrm{i}tU}\Phi/t$ exists in $\widehat{\mathfrak{H}}$, the operator $V : \mathrm{dom}(P) \to \widehat{\mathfrak{H}}$ defined, for all $\Phi \in \mathrm{dom}(P)$, by

$$V\Phi := \lim_{t\to\infty} \frac{1}{t}\, \mathrm{e}^{-\mathrm{i}tU}P\mathrm{e}^{\mathrm{i}tU}\Phi, \tag{165}$$

is called asymptotic velocity (with respect to U).

Remark 45 Under Assumption 40 *(a)*, the operator U from (164) is bounded on $\widehat{\mathfrak{H}}$ (due to (139)) and symmetric. Hence, $U^* = U$ and the propagator $\mathrm{e}^{\mathrm{i}tU}$ is well-defined for all $t \in \mathbb{R}$.

Under a simple regularity assumption specific to Section 6, we get the natural explicit form of the asymptotic velocity.

Proposition 46 (Asymptotic velocity) *Let $u_0 \in L^\infty(\mathbb{T})$ and $u := [u_1, u_2, u_3] \in L^\infty(\mathbb{T})^3$ satisfy Assumption 40 (a) and (b) and define $U \in \mathcal{L}(\widehat{\mathfrak{H}})$ by $U := m[u_0]\sigma_0 + m[u]\sigma$. Then:*

(a) The asymptotic velocity V with respect to U exists and is a bounded symmetric operator on $\mathrm{dom}(P)$.

(b) The bounded extension $\bar{V} \in \mathcal{L}(\widehat{\mathfrak{H}})$ of V to $\widehat{\mathfrak{H}}$ is selfadjoint and has the form

$$\bar{V} = m[v_0]\sigma_0 + m[v]\sigma, \tag{166}$$

where $v_0 \in L^\infty(\mathbb{T})$ and $v \in L^\infty(\mathbb{T})^3$ are defined by

$$v_0 := u_0', \tag{167}$$

$$v := \begin{cases} (\tilde{u}u')\tilde{u}, & \text{on } \mathcal{Z}_u^c, \\ u', & \text{on } \mathcal{Z}_u. \end{cases} \tag{168}$$

Proof. (a) We first want to show that $\mathrm{e}^{\mathrm{i}tU}\mathrm{dom}(P) \subseteq \mathrm{dom}(P)$ for all $t \in \mathbb{R}$. To this end, we make use of Proposition 86 *(a)* which asserts that, for all $t \in \mathbb{R}$,

$$\mathrm{e}^{\mathrm{i}tU} = m[\exp\circ(\mathrm{i}tu_0)C_t]\sigma_0 + \mathrm{i}t\, m[\exp\circ(\mathrm{i}tu_0)S_t u]\sigma, \tag{169}$$

where the maps $\mathbb{R} \ni t \to C_t \in L^\infty(\mathbb{T})$ and $\mathbb{R} \ni t \to S_t \in L^\infty(\mathbb{T})$ are given, for all $t \in \mathbb{R}$, by

$$C_t := \cos\circ(t|u|), \tag{170}$$

$$S_t := \mathrm{sinc}\circ(t|u|), \tag{171}$$

and $\mathrm{sinc} \in C^\infty(\mathbb{R})$ stands for the usual cardinal sine function. In order to verify the first property in (159) (and (162)), we note that, for all $t \in \mathbb{R}$, the functions C_t and S_t are differentiable with respect to k for all $k \in \mathbb{T}$. Moreover, for all $t \in \mathbb{R}$, the derivatives have the form

$$C_t' = -t^2\, \mathrm{sinc}\circ(t|u|)(uu'), \tag{172}$$

$$S_t' = -\frac{t^2}{2}\big(\mathrm{sinc}\circ(t|u|) + \mathrm{sinc}''\circ(t|u|)\big)(uu'), \tag{173}$$

where, in (173), we used that $x\,\mathrm{sinc}''(x) + 2\,\mathrm{sinc}'(x) + x\,\mathrm{sinc}(x) = 0$ for all $x \in \mathbb{R}$. Due to the first part of Assumption 40 *(b)*, (172) and (173) yield $C_t, S_t \in C^1(\mathbb{T})$ for all $t \in \mathbb{R}$. Hence, since $C^1(\mathbb{T}) \subseteq AC(\mathbb{T})$ and since $AC(\mathbb{T})$ is a $*$-algebra, we get from (169) that $\mathrm{e}^{\mathrm{i}tU}\Phi \in AC(\mathbb{T})^2$

for all $t \in \mathbb{R}$ and all $\Phi \in \operatorname{dom}(P)$. As for the second property in (159), we note that, for all $t \in \mathbb{R}$ and all $\Phi \in \operatorname{dom}(P)$, we have (almost everywhere in $\mathbb{T}$)

$$\big(\mathrm{e}^{\mathrm{i}tU}\Phi\big)' = \big(m[\exp\circ(\mathrm{i}tu_0)(\mathrm{i}tu_0'C_t + C_t')]\sigma_0 + \mathrm{i}t\,m[\exp\circ(\mathrm{i}tu_0)((\mathrm{i}tu_0'S_t + S_t')u + S_tu')]\sigma\big)\Phi + \mathrm{e}^{\mathrm{i}tU}\Phi', \tag{174}$$

where we set $\Phi' := \varphi_1' \oplus \varphi_2'$ if $\Phi = \varphi_1 \oplus \varphi_2$. Hence, since $C(\mathbb{T}) \subseteq L^\infty(\mathbb{T}) \subseteq \hat{\mathfrak{h}}$, the first part of Assumption 40 *(b)* implies that $(\mathrm{e}^{\mathrm{i}tU}\Phi)' \in \widehat{\mathfrak{H}}$ for all $t \in \mathbb{R}$ and all $\Phi \in \operatorname{dom}(P)$. Finally, due to (169) and the second part of Assumption 40 *(b)*, we also get the third property in (159).

Next, let $\Phi \in \operatorname{dom}(P)$ be fixed, let the map $X : \mathbb{R} \to \widehat{\mathfrak{H}}$ be defined, for all $t \in \mathbb{R}$, by

$$X^t := \mathrm{e}^{-\mathrm{i}tU} P \mathrm{e}^{\mathrm{i}tU}\Phi, \tag{175}$$

and let us show that $X \in C^1(\mathbb{R}, \widehat{\mathfrak{H}})$. To this end, let $t \in \mathbb{R}$, let $s \in I := [-1,1] \setminus \{0\}$, and consider the difference quotient

$$\frac{X^{t+s} - X^t}{s} = D_{1,t}^s + D_{2,t}^s, \tag{176}$$

where, for all $i \in \langle 1,2\rangle$ and all $t \in \mathbb{R}$, the maps $D_{i,t} : I \to \widehat{\mathfrak{H}}$ are given, for all $s \in I$, by

$$D_{1,t}^s := \mathrm{e}^{-\mathrm{i}tU}\,\frac{\mathrm{e}^{-\mathrm{i}sU} - 1}{s}\,P\mathrm{e}^{\mathrm{i}tU}\Phi, \tag{177}$$

$$D_{2,t}^s := \mathrm{e}^{-\mathrm{i}tU}\mathrm{e}^{-\mathrm{i}sU} P\,\frac{\mathrm{e}^{\mathrm{i}sU} - 1}{s}\,\mathrm{e}^{\mathrm{i}tU}\Phi. \tag{178}$$

Now, since $U \in \mathcal{L}(\widehat{\mathfrak{H}})$, the limit (in $\widehat{\mathfrak{H}}$) for $s \to 0$ of (177) yields, for all $t \in \mathbb{R}$,

$$\lim_{s\to 0} D_{1,t}^s = -\mathrm{i}\mathrm{e}^{-\mathrm{i}tU} U P \mathrm{e}^{\mathrm{i}tU}\Phi. \tag{179}$$

In order to determine the limit for $s \to 0$ of (178), we make use of (174) and get, for all $s \in I$ and all $\Psi \in \operatorname{dom}(P)$,

$$P\,\frac{\mathrm{e}^{\mathrm{i}sU} - 1}{s}\,\Psi = \left(m\left[\exp\circ(\mathrm{i}su_0)\left(u_0'C_s - \mathrm{i}\frac{C_s'}{s}\right)\right]\sigma_0 + m[\exp\circ(\mathrm{i}su_0)((\mathrm{i}su_0'S_s + S_s')u + S_su')]\sigma\right)\Psi - \mathrm{i}\,\frac{\mathrm{e}^{\mathrm{i}sU} - 1}{s}\,\Psi'. \tag{180}$$

Moreover, since $(U\Psi)' = (m[u_0']\sigma_0 + m[u']\sigma)\Psi + U\Psi'$ for all $\Psi \in \operatorname{dom}(P)$, we get, as above, that $U\Psi \in \operatorname{dom}(P)$ for all $\Psi \in \operatorname{dom}(P)$. Hence, for all $s \in I$ and all $\Psi \in \operatorname{dom}(P)$, the decomposition (180) leads to

$$\left\|P\,\frac{\mathrm{e}^{\mathrm{i}sU} - 1}{s}\,\Psi - \mathrm{i}PU\Psi\right\| \le \sum_{i\in\langle 1,6\rangle} A_i(s), \tag{181}$$

where, for all $i \in \langle 1,6\rangle$, the functions $A_i : I \to \mathbb{R}$ are defined, for all $s \in I$, by

$$A_1(s) := \|m[(\exp\circ(\mathrm{i}su_0)C_s - 1)u_0']\sigma_0\Psi\|, \tag{182}$$

$$A_2(s) := \frac{1}{|s|}\,\|m[C_s']\sigma_0\Psi\|, \tag{183}$$

$$A_3(s) := |s|\|m[u_0'S_s u]\sigma\Psi\|, \tag{184}$$

$$A_4(s) := \|m[S_s'u]\sigma\Psi\|, \tag{185}$$

$$A_5(s) := \|(m[(\exp\circ(\mathrm{i}su_0)S_s - 1)u']\sigma\Psi\|, \tag{186}$$

$$A_6(s) := \left\|\frac{\mathrm{e}^{\mathrm{i}sU}-1}{s}\,\Psi' - \mathrm{i}U\Psi'\right\|, \tag{187}$$

and, in (183)-(185), we used that $|\exp\circ(\mathrm{i}su_0)| = 1$ for all $s \in \mathbb{R}$. In order to estimate (182)-(187), we next write $\Psi = \psi_1 \oplus \psi_2$ for all $\Psi \in \mathrm{dom}(P)$. As for (182)-(183), we have, for all $n \in \langle 1,2\rangle$ and all $s \in I$, that $A_n(s)^2 = \sum_{i\in\langle 1,2\rangle}\|f_{n,i}^s\|^2$, where, for all $n, i \in \langle 1,2\rangle$ and all $s \in I$, we define $f_{n,i}^s \in \hat{\mathfrak{h}}$ by

$$f_{1,i}^s := (\exp\circ(\mathrm{i}su_0)C_s - 1)u_0'\psi_i, \tag{188}$$

$$f_{2,i}^s := \frac{C_s'}{s}\,\psi_i. \tag{189}$$

Using (172) and the bound $|\operatorname{sinc}(x)| \le 1$ for all $x \in \mathbb{R}$ for (189) (which follows from the representation $\operatorname{sinc}(x) = \int_0^1 \mathrm{d}\lambda\, \cos(\lambda x)$ for all $x \in \mathbb{R}$), we get, for all $n, i \in \langle 1,2\rangle$, that $\lim_{s\to 0} f_{n,i}^s(k) = 0$ for all $k \in \mathbb{T}$. Since, in addition, for all $n, i \in \langle 1,2\rangle$, we have $|f_{n,i}^s|^2 \le C_n|\psi_i|^2 \in L^1(\mathbb{T})$ for all $s \in I$, where $C_1 := 4\|u_0'\|_\infty^2$ and $C_2 := 3\sum_{\alpha\in\langle 1,3\rangle}\|u_\alpha\|_\infty^2\|u_\alpha'\|_\infty^2$, Lebesgue's dominated convergence theorem implies that $\lim_{s\to 0} A_n(s) = 0$ for all $n \in \langle 1,2\rangle$. As for (184)-(186), for all $n \in \langle 3,5\rangle$ and all $s \in I$, we can write $A_n(s)^2 \le 3\sum_{i\in\langle 1,2\rangle}\sum_{\alpha\in\langle 1,3\rangle}\|f_{n,i,\alpha}^s\|^2$, where, for all $n \in \langle 3,5\rangle$, all $i \in \langle 1,2\rangle$, all $\alpha \in \langle 1,3\rangle$, and all $s \in I$, we define $f_{n,i,\alpha}^s \in \hat{\mathfrak{h}}$ by

$$f_{3,i,\alpha}^s := su_0'S_s u_\alpha\psi_i, \tag{190}$$

$$f_{4,i,\alpha}^s := S_s'u_\alpha\psi_i, \tag{191}$$

$$f_{5,i,\alpha}^s := (\exp\circ(\mathrm{i}su_0)S_s - 1)u_\alpha'\psi_i. \tag{192}$$

Using (173) and $|\operatorname{sinc}''(x)| \le 1/3$ for all $x \in \mathbb{R}$ for (191), we get, for all $n \in \langle 3,5\rangle$, all $i \in \langle 1,2\rangle$, and all $\alpha \in \langle 1,3\rangle$, that $\lim_{s\to 0} f_{n,i,\alpha}^s(k) = 0$ for all $k \in \mathbb{T}$. Since, in addition, for all $n \in \langle 3,5\rangle$, all $i \in \langle 1,2\rangle$, and all $\alpha \in \langle 1,3\rangle$, we have $|f_{n,i,\alpha}^s|^2 \le C_{n,\alpha}|\psi_i|^2 \in L^1(\mathbb{T})$ for all $s \in I$, where, for all $\alpha \in \langle 1,3\rangle$, we set $C_{3,\alpha} := \|u_0'\|_\infty^2\|u_\alpha\|_\infty^2$, $C_{4,\alpha} := 3(\sum_{\beta\in\langle 1,3\rangle}\|u_\beta\|_\infty^2\|u_\beta'\|_\infty^2)\|u_\alpha\|_\infty^2$, and $C_{5,\alpha} := 4\|u_\alpha'\|_\infty^2$, Lebesgue's dominated convergence theorem again implies that $\lim_{s\to 0} A_n(s) = 0$ for all $n \in \langle 3,5\rangle$. Moreover, we have $\lim_{s\to 0} A_6(s) = 0$ as in (179). Finally, since, for all $t \in \mathbb{R}$ and all $s \in I$, we can write $D_{2,t}^s - \mathrm{i}\mathrm{e}^{-\mathrm{i}tU}PU\mathrm{e}^{\mathrm{i}tU}\Phi = \mathrm{i}\mathrm{e}^{-\mathrm{i}tU}(\mathrm{e}^{-\mathrm{i}sU}-1)PU\mathrm{e}^{\mathrm{i}tU}\Phi + \mathrm{e}^{-\mathrm{i}tU}\mathrm{e}^{-\mathrm{i}sU}(P(\mathrm{e}^{\mathrm{i}sU}-1)\mathrm{e}^{\mathrm{i}tU}\Phi/s - \mathrm{i}PU\mathrm{e}^{\mathrm{i}tU}\Phi)$, we get, for all $t \in \mathbb{R}$ and all $s \in I$,

$$\left\|D_{2,t}^s - \mathrm{i}\mathrm{e}^{-\mathrm{i}tU}PU\mathrm{e}^{\mathrm{i}tU}\Phi\right\| \le \left\|\left(\mathrm{e}^{-\mathrm{i}sU}-1\right)PU\mathrm{e}^{\mathrm{i}tU}\Phi\right\| + \left\|P\,\frac{\mathrm{e}^{\mathrm{i}sU}-1}{s}\,\mathrm{e}^{\mathrm{i}tU}\Phi - \mathrm{i}PU\mathrm{e}^{\mathrm{i}tU}\Phi\right\|, \tag{193}$$

which, using (181) and the strong continuity of the propagator, implies that, for all $t \in \mathbb{R}$,

$$\lim_{s\to 0} D^s_{2,t} = \mathrm{i}\mathrm{e}^{-\mathrm{i}tU} PU \mathrm{e}^{\mathrm{i}tU}\Phi. \tag{194}$$

Therefore, it follows from (176), (179), and (194), that the map X is differentiable in $\widehat{\mathfrak{H}}$ at any point in $\mathbb{R}$ and that its derivative $\dot{X} : \mathbb{R} \to \widehat{\mathfrak{H}}$, defined, for all $t \in \mathbb{R}$, by $\dot{X}^t := \lim_{s\to 0}(X^{t+s} - X^t)/s$, reads, for all $t \in \mathbb{R}$, as

$$\dot{X}^t = \mathrm{e}^{-\mathrm{i}tU} U' \mathrm{e}^{\mathrm{i}tU}\Phi, \tag{195}$$

where the commutator $U' : \mathrm{dom}(P) \to \widehat{\mathfrak{H}}$ is defined by $U'\Phi := -\mathrm{i}(UP\Phi - PU\Phi)$ for all $\Phi \in \mathrm{dom}(P)$. Since, for all $\Phi \in \mathrm{dom}(P)$, we have

$$U'\Phi = (m[u'_0]\sigma_0 + m[u']\sigma)\Phi, \tag{196}$$

(139) implies that $\|U'\Phi\| \le C_{U'}\|\Phi\|$ for all $\Phi \in \mathrm{dom}(P)$ with $C_{U'} := \sum_{\alpha\in\langle 0,3\rangle} \|u'_\alpha\|_\infty$. Moreover, since, as above, $\dot{X}^{t+s} - \dot{X}^t = \mathrm{e}^{-\mathrm{i}tU}(\mathrm{e}^{-\mathrm{i}sU} - 1)U'\mathrm{e}^{\mathrm{i}tU}\Phi + \mathrm{e}^{-\mathrm{i}tU}\mathrm{e}^{-\mathrm{i}sU}U'\mathrm{e}^{\mathrm{i}tU}(\mathrm{e}^{\mathrm{i}sU} - 1)\Phi$ for all $s, t \in \mathbb{R}$, we get, for all $s, t \in \mathbb{R}$,

$$\big\|\dot{X}^{t+s} - \dot{X}^t\big\| \le \big\|\big(\mathrm{e}^{-\mathrm{i}sU} - 1\big)U'\mathrm{e}^{\mathrm{i}tU}\Phi\big\| + C_{U'}\big\|\big(\mathrm{e}^{\mathrm{i}sU} - 1\big)\Phi\big\|. \tag{197}$$

The strong continuity of the propagator and (197) now imply that $\dot{X} \in C(\mathbb{R}, \widehat{\mathfrak{H}})$, i.e., we find that $X \in C^1(\mathbb{R}, \widehat{\mathfrak{H}})$ as desired.

We next want to compute the limit (in $\widehat{\mathfrak{H}}$) for $t \to \infty$ of X^t/t. In order to do so, we note that, due to $\dot{X} \in C(\mathbb{R}, \widehat{\mathfrak{H}})$ and (195), the second fundamental theorem of Banach space-valued Riemann integral calculus yields, for all $t \in \mathbb{R}^+$,

$$\begin{aligned} X^t &= X^0 + \int_0^t \mathrm{d}s\, \dot{X}^s \\ &= P\Phi + \int_0^t \mathrm{d}s\, \mathrm{e}^{-\mathrm{i}sU} U' \mathrm{e}^{\mathrm{i}sU}\Phi. \end{aligned} \tag{198}$$

Using (169), (196), and (7), we compute that $\mathrm{e}^{-\mathrm{i}sU}U'\mathrm{e}^{\mathrm{i}sU}\Phi = (m[u'_0]\sigma_0 + m[a^s]\sigma)\Phi$ for all $s \in \mathbb{R}$, where the map $\mathbb{R} \ni s \mapsto a^s \in L^\infty(\mathbb{T})^3$ has the form $a^s = \sum_{i\in\langle 1,3\rangle} a^s_i$, and, for all $i \in \langle 1, 3\rangle$, the maps $\mathbb{R} \ni s \mapsto a^s_i \in L^\infty(\mathbb{T})^3$ are defined, for all $s \in \mathbb{R}$, by

$$a^s_1 := C_{2s} u', \tag{199}$$

$$a^s_2 := 2sC_sS_s(u \wedge u'), \tag{200}$$

$$a^s_3 := 2s^2 S^2_s (uu')u. \tag{201}$$

As for (199), since for all $i \in \langle 1, 2\rangle$, all $\alpha \in \langle 1, 3\rangle$, and all $t \in \mathbb{R}^+$, the Riemann integral $\int_0^t \mathrm{d}s\, C_{2s} u'_\alpha \varphi_i$ exists in $\hat{\mathfrak{h}}$ due to the fact that $\dot{X} \in C(\mathbb{R}, \widehat{\mathfrak{H}})$, since, for all $i \in \langle 1, 2\rangle$, all $\alpha \in \langle 1, 3\rangle$, all $k \in \mathbb{T}$, and all $t \in \mathbb{R}^+$, the Riemann integral $\int_0^t \mathrm{d}s\, C_{2s}(k) u'_\alpha(k)\varphi_i(k)$ exists in $\mathbb{C}$, and since every sequence which converges in $\hat{\mathfrak{h}}$ to a limit has a subsequence which converges pointwise always everywhere to the same limit, we get, for all $t \in \mathbb{R}^+$,

$$\int_0^t \mathrm{d}s\; (m[a_1^s]\sigma)\Phi = t\,(m[S_{2t}u']\sigma)\Phi. \tag{202}$$

The terms (200) and (201) are treated analogously. We find, for all $t \in \mathbb{R}^+$,

$$\int_0^t \mathrm{d}s\; (m[a_2^s]\sigma)\Phi = t^2(m[S_t^2(u\wedge u')]\sigma)\Phi, \tag{203}$$

$$\int_0^t \mathrm{d}s\; (m[a_3^s]\sigma)\Phi = t\,(m[(1-S_{2t})(\tilde{u}u')\tilde{u}]\sigma)\Phi, \tag{204}$$

where $\tilde{u}$ is given after (152). Hence, using (198) and (202)-(204), we get, for all $t \in \mathbb{R}^+$,

$$\frac{X^t}{t} = \frac{P\Phi}{t} + (m[u_0']\sigma_0)\Phi + (m[S_{2t}u']\sigma)\Phi + t(m[S_t^2(u\wedge u')]\sigma)\Phi + (m[(1-S_{2t})(\tilde{u}u')\tilde{u}]\sigma)\Phi. \tag{205}$$

Since, on $\mathcal{Z}_u$, the fourth and fifth term on the right hand side of (205) satisfy $tS_t^2(u\wedge u') = (1-S_{2t})(\tilde{u}u')\tilde{u} = 0$ whereas, for the third term, we have $S_{2t}u' = u'$ on $\mathcal{Z}_u$, we decompose the latter as $S_{2t}u' = 1_{\mathcal{Z}_u}u' + S_{2t}1_{\mathcal{Z}_u^c}u'$. Hence, we get, for all $t \in \mathbb{R}^+$,

$$\left\|\frac{X^t}{t} - \big((m[u_0']\sigma_0)\Phi + (m[1_{\mathcal{Z}_u}u']\sigma)\Phi + (m[(\tilde{u}u')\tilde{u}]\sigma)\Phi\big)\right\| \le \sum_{i\in\langle 1,4\rangle} B_i(t), \tag{206}$$

where, for all $i \in \langle 1,4\rangle$, we define $B_i : \mathbb{R}^+ \to \mathbb{R}$, for all $t \in \mathbb{R}^+$, by

$$B_1(t) := \frac{1}{t}\|P\Phi\|, \tag{207}$$

$$B_2(t) := \|(m[S_{2t}1_{\mathcal{Z}_u^c}u']\sigma)\Phi\|, \tag{208}$$

$$B_3(t) := t\|(m[S_t^2(u\wedge u')]\sigma)\Phi\|, \tag{209}$$

$$B_4(t) := \|(m[S_{2t}(\tilde{u}u')\tilde{u}]\sigma)\Phi\|. \tag{210}$$

Setting $\Phi = \varphi_1 \oplus \varphi_2$ and proceeding as above, we have, for all $n \in \langle 2,4\rangle$ and all $t \in \mathbb{R}^+$, that $B_n(t)^2 \le 3\sum_{i\in\langle 1,2\rangle}\sum_{\alpha\in\langle 1,3\rangle}\|g_{n,i,\alpha}^t\|^2$, where, for all $n \in \langle 2,4\rangle$, all $i \in \langle 1,2\rangle$, all $\alpha \in \langle 1,3\rangle$, and all $t \in \mathbb{R}^+$, we define $g_{n,i,\alpha}^t \in \hat{\mathfrak{h}}$ by

$$g_{2,i,\alpha}^t := S_{2t}1_{\mathcal{Z}_u^c}u'_\alpha\varphi_i, \tag{211}$$

$$g_{3,i,\alpha}^t := tS_t^2\sum_{\beta,\gamma\in\langle 1,3\rangle}\varepsilon_{\alpha\beta\gamma}u_\beta u'_\gamma\varphi_i, \tag{212}$$

$$g_{4,i,\alpha}^t := S_{2t}(\tilde{u}u')\tilde{u}_\alpha\varphi_i. \tag{213}$$

Since, for all $x \in \mathbb{R} \setminus \{0\}$, we have $\lim_{t\to\infty} \operatorname{sinc}(tx) = 0$ and $\lim_{t\to\infty} t \operatorname{sinc}^2(tx) = 0$, we get, for all $n \in \langle 2,4\rangle$, all $i \in \langle 1,2\rangle$, and all $\alpha \in \langle 1,3\rangle$, that $\lim_{t\to\infty} g^t_{n,i,\alpha}(k) = 0$ for all $k \in \mathbb{T}$. Moreover, for all $n \in \langle 2,4\rangle$, all $i \in \langle 1,2\rangle$, and all $\alpha \in \langle 1,3\rangle$, we have $|g^t_{n,i,\alpha}|^2 \le D_{n,\alpha}|\varphi_i|^2 \in L^1(\mathbb{T})$ for all $t \in \mathbb{R}^+$, where, for all $\alpha \in \langle 1,3\rangle$, we set $D_{2,\alpha} := \|u'_\alpha\|^2_\infty$ and, using $|\tilde u_\alpha| \le 1$ for all $\alpha \in \langle 1,3\rangle$, we also have $D_{3,\alpha} := 27\sum_{\gamma\in\langle 1,3\rangle} \|u'_\gamma\|^2_\infty$ and $D_{4,\alpha} := 3\sum_{\beta\in\langle 1,3\rangle} \|u'_\beta\|^2_\infty$ (independent of α). Hence, Lebesgue's dominated convergence theorem again implies that $\lim_{t\to\infty} B_n(t) = 0$ for all $n \in \langle 2,4\rangle$ and since $\lim_{t\to\infty} B_1(t) = 0$ holds, too, (206) yields the limit in $\widehat{\mathfrak{H}}$ for $t \to \infty$ of X^t/t, i.e., we get, for all $\Phi \in \operatorname{dom}(P)$,

$$\begin{aligned} V\Phi &= \lim_{t\to\infty} \frac{X^t}{t} \\ &= (m[v_0]\sigma_0 + m[v]\sigma)\Phi, \end{aligned} \tag{214}$$

where $v_0 \in L^\infty(\mathbb{T})$ and $v \in L^\infty(\mathbb{T})^3$ are defined by $v_0 := u'_0$ and $v := 1_{\mathcal{Z}_u} u' + 1_{\mathcal{Z}_u^c}(\tilde u u')\tilde u$.

Finally, due to (214) and (139), V is a bounded operator on $\operatorname{dom}(P)$ and, due to Assumption 40 *(a)*, V is also symmetric.

(b) Since V is bounded on the dense domain $\operatorname{dom}(P)$, we know that the unique bounded extension of V to $\widehat{\mathfrak{H}}$ is given by $\bar V := V^{**} \in \mathcal{L}(\widehat{\mathfrak{H}})$. Moreover, since V is symmetric due to part *(a)*, i.e., since $V \subseteq V^*$, we get $\bar V = V^{**} \subseteq V^{***} = \bar V^*$ and, hence, $\bar V^* = \bar V$. Finally, since the right hand side of (214) defines a bounded operator on $\widehat{\mathfrak{H}}$, the uniqueness of the bounded extension implies that the action of $\bar V$ on $\widehat{\mathfrak{H}}$ is also given by (214). □

Remark 47 Using the usual group homomorphism between $\mathrm{SU}(2)$ and $\mathrm{SO}(3)$ which, for all $\theta \in \mathbb{R}$, all $a = [a_1, a_2, a_3] \in \mathbb{R}^3$ with $\sum_{i\in\langle 1,3\rangle} a_i^2 = 1$, and all $x \in \mathbb{R}^3$, is given by

$$\mathrm{e}^{-\mathrm{i}\frac{\theta}{2}(a\sigma)}(x\sigma)\mathrm{e}^{\mathrm{i}\frac{\theta}{2}(a\sigma)} = (R(a,\theta)x)\sigma, \tag{215}$$

where $R(a,\theta)x := (ax)a + \cos(\theta)(x - (ax)a) + \sin(\theta)a \wedge x$ stands for the positive rotation of x by the angle θ around the axis a, we obtain the geometric interpretation of (199)-(201).

The following condition will be used in the sequel.

Assumption 48 (Asymptotic velocity) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (b), let the Pauli coefficient functions $u_0 \in L^\infty(\mathbb{T})$ and $u \in L^\infty(\mathbb{T})^3$ of $\widehat{H}$ satisfy Assumption 40 (b), and let $\bar V \in \mathcal{L}(\widehat{\mathfrak{H}})$ be the bounded extension of the asymptotic velocity with respect to $\widehat{H}$.*

(a) $0 \notin \operatorname{eig}(\bar V)$

In the following, we use the sign function $\operatorname{sign} : \mathbb{R} \to \{-1, 0, 1\}$ which is defined according to the convention that $\operatorname{sign}(x) := -1$ if $x < 0$, $\operatorname{sign}(0) := 0$, and $\operatorname{sign}(x) := 1$ if $x > 0$. Moreover, recall Definition 16 *(b)* for the R/L generator Δ, Definition 41 for $e'_\pm$, and define the mean inverse temperature $\beta \in \mathbb{R}$ and (half) the affinity $\delta \in \mathbb{R}$, driving the heat flux between the reservoirs, by

$$\beta := \frac{\beta_R + \beta_L}{2}, \tag{216}$$

$$\delta := \frac{\beta_R - \beta_L}{2}. \tag{217}$$

The R/L generator has the following form.

Proposition 49 (R/L generator) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (b) and let the Pauli coefficient functions $u_0 \in L^\infty(\mathbb{T})$ and $u \in L^\infty(\mathbb{T})^3$ of $\widehat{H}$ satisfy Assumption 40 (b). Moreover, let the bounded extension $\bar{V} \in \mathcal{L}(\widehat{\mathfrak{H}})$ of the asymptotic velocity with respect to $\widehat{H}$ satisfy Assumption 48 (a) and let $\beta_L, \beta_R \in \mathbb{R}$ be the inverse reservoir temperatures. Then:*

(a) In momentum space, the R/L generator for H and β_L, β_R has the form

$$\widehat{\Delta} = (\beta 1 + \delta \operatorname{sign}(\bar{V})) 1_{ac}(\widehat{H}). \tag{218}$$

(b) The sign function of the asymptotic velocity can be written as

$$\operatorname{sign}(\bar{V}) = m[w_0]\sigma_0 + m[w]\sigma, \tag{219}$$

where $w_0 \in L^\infty(\mathbb{T})$ and $w \in L^\infty(\mathbb{T})^3$ are defined by

$$w_0 := \frac{1}{2}\begin{cases} \operatorname{sign}\circ e_+' + \operatorname{sign}\circ e_-', & \text{on } \mathcal{Z}_u^c, \\ \operatorname{sign}\circ f_+ + \operatorname{sign}\circ f_-, & \text{on } \mathcal{Z}_u, \end{cases} \tag{220}$$

$$w := \frac{1}{2}\begin{cases} (\operatorname{sign}\circ e_+' - \operatorname{sign}\circ e_-')\,\tilde{u}, & \text{on } \mathcal{Z}_u^c, \\ (\operatorname{sign}\circ f_+ - \operatorname{sign}\circ f_-)\,\widetilde{u'}, & \text{on } \mathcal{Z}_u, \end{cases} \tag{221}$$

and $f_\pm \in L^\infty(\mathbb{T})$ is defined by $f_\pm := u_0' \pm |u'|$.

In the following proof, $\mathrm{sr}-\lim$ stands for the convergence in the strong resolvent sense.

Proof. (a) We first note that, due to (42), the R/L generator can be written as

$$\Delta = \beta 1_{ac}(H) + \delta P_{RL}, \tag{222}$$

where $P_{RL} := P_R - P_L \in \mathcal{L}(\mathfrak{H})$. Since $f_0 := (1_R - 1_L) - \operatorname{sign}\restriction_{\mathbb{Z}} \in \ell^0(\mathbb{Z})$, we have $m[f_0] \in \mathcal{L}^0(\mathfrak{h})$ and, hence, using (35)-(36) and (39)-(40), we get

$$\begin{aligned} P_{RL} &= \mathrm{s}-\lim_{t\to\infty} \mathrm{e}^{-\mathrm{i}tH}(m[1_R - 1_L]\sigma_0)\mathrm{e}^{\mathrm{i}tH} 1_{ac}(H) \\ &= \mathrm{s}-\lim_{t\to\infty} \mathrm{e}^{-\mathrm{i}tH}(m[\operatorname{sign}\restriction_{\mathbb{Z}}]\sigma_0)\mathrm{e}^{\mathrm{i}tH} 1_{ac}(H), \end{aligned} \tag{223}$$

where, with (46), we used that $\mathcal{L}^0(\mathfrak{H}) \subseteq \ker(\mu_H)$, i.e., we have $\mu_H(m[f_0]\sigma_0) = 0$. In order to express (223) be means of the position operator in momentum space, we use the uniqueness property of the resolution of the identity stated in Theorem 80 *(a)* and define the map $E^m : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathfrak{H})$ by $E^m(\chi) := m[\chi\restriction_{\mathbb{Z}}]\sigma_0$ for all $\chi \in \mathcal{B}(\mathbb{R})$. In order to obtain $E^m = E_Q$, Theorem 80 *(a)* asserts that it is enough to verify that $\bar{E}^m(\kappa_1) = Q$ since E^m is a resolution of the identity. Using (351)-(352), we have $\mathrm{dom}(\bar{E}^m(\kappa_1)) = \mathrm{ran}\,(E^m(\kappa_{-1})) = \{m[\kappa_{-1}\restriction_{\mathbb{Z}}]f_1 \oplus m[\kappa_{-1}\restriction_{\mathbb{Z}}]f_2 \,|\, f_1, f_2 \in \mathfrak{h}\} = \mathrm{dom}(Q)$ because $\mathrm{ran}\,(m[\kappa_{-1}\restriction_{\mathbb{Z}}]) = \mathrm{dom}(q)$, i.e., for all $F = f_1 \oplus f_2 \in \mathrm{dom}(Q)$, there exists $G = g_1 \oplus g_2 \in \mathfrak{H}$ with $F = E^m(\kappa_{-1})G$, and $\bar{E}^m(\kappa_1)F = \bar{E}^m(\kappa_1)E^m(\kappa_{-1})G = E^m(\kappa_1\kappa_{-1})G = (m[(\kappa_1\kappa_{-1})\restriction_{\mathbb{Z}}]\sigma_0)G = m[\kappa_1\restriction_{\mathbb{Z}}]m[\kappa_{-1}\restriction_{\mathbb{Z}}]g_1 \oplus m[\kappa_1\restriction_{\mathbb{Z}}]m[\kappa_{-1}\restriction_{\mathbb{Z}}]g_2 = qf_1 \oplus qf_2 = QF$. Therefore, since $\mathrm{sign} \in \mathcal{B}(\mathbb{R})$, (223) and Theorem 80 *(a)* imply that

$$P_{RL} = \mathrm{s}-\lim_{t\to\infty} \mathrm{e}^{-\mathrm{i}tH}\mathrm{sign}(Q)\,\mathrm{e}^{\mathrm{i}tH}1_{ac}(H). \tag{224}$$

Note that, here and at various other analogous places, we could have used Theorem 80 *(b)* and Remark 81 instead of Theorem 80 *(a)* (see the proof of Lemma 83 *(c)* for example). Applying Lemma 82 to $\mathcal{H} = \mathfrak{H}$, $\mathcal{K} = \widehat{\mathfrak{H}}$, and $U = \mathfrak{F}$, we get $B = P$ and $\mathfrak{F}E_Q(\chi)\mathfrak{F}^* = E_P(\chi)$ for all $\chi \in \mathcal{B}(\mathbb{R})$ if $A = Q$ and, likewise, $B = \widehat{H}$ and $\mathfrak{F}E_H(\chi)\mathfrak{F}^* = E_{\widehat{H}}(\chi)$ for all $\chi \in \mathcal{B}(\mathbb{R})$ if $A = H$. Hence, since $\mathrm{e}_t \in C_b(\mathbb{R})$ for all $t \in \mathbb{R}$ (where $\mathrm{e}_t(x) := \mathrm{e}^{\mathrm{i}tx}$ for all $x \in \mathbb{R}$ stems from Theorem 80 *(b)*) and using that there exists $M_{ac} \in \mathcal{M}(\mathbb{R})$ such that $1_{ac}(H) = E_H(1_{M_{ac}})$, (224) leads to

$$\widehat{P}_{RL} = \mathrm{s}-\lim_{t\to\infty} \mathrm{e}^{-\mathrm{i}t\widehat{H}}\mathrm{sign}(P)\,\mathrm{e}^{\mathrm{i}t\widehat{H}}1_{ac}(\widehat{H}). \tag{225}$$

Now, recall from the proof of Proposition 46 *(a)* that $\mathrm{e}^{\mathrm{i}t\widehat{H}}\mathrm{dom}(P) \subseteq \mathrm{dom}(P)$ for all $t \in \mathbb{R}$. Hence, for all $t \in \mathbb{R}^+$, we set $\mathrm{dom}(V^t) := \mathrm{dom}(P)$, we define the operator $V^t : \mathrm{dom}(V^t) \to \widehat{\mathfrak{H}}$, for all $\Phi \in \mathrm{dom}(V^t)$, by

$$V^t\Phi := \frac{1}{t}\,\mathrm{e}^{-\mathrm{i}t\widehat{H}}P\mathrm{e}^{\mathrm{i}t\widehat{H}}\Phi, \tag{226}$$

and we note that V^t is unbounded for all $t \in \mathbb{R}^+$ (since, for all $t \in \mathbb{R}^+$ and all $n \in \mathbb{N}$, we have $\|V^t\Phi_n\| \geq \sqrt{2}(n+1)/t$, where $\Phi_n := \mathrm{e}^{-\mathrm{i}t\widehat{H}}\hat{f}_n \oplus \hat{f}_n \in \mathrm{dom}(P)$ and $f_n \in \mathrm{dom}(q)$ is given after (156)). In order to express (225) be means of (226), we again use Lemma 82 for $\mathcal{H} = \mathcal{K} = \widehat{\mathfrak{H}}$, $U = \mathrm{e}^{-\mathrm{i}t\widehat{H}}$ for all $t \in \mathbb{R}^+$, and $A = P$, and obtain $B = tV^t$ and $\mathrm{e}^{-\mathrm{i}t\widehat{H}}E_P(\chi)\mathrm{e}^{\mathrm{i}t\widehat{H}} = E_{tV^t}(\chi)$ for all $t \in \mathbb{R}^+$ and all $\chi \in \mathcal{B}(\mathbb{R})$. Moreover, Remark 85 yields $E_{tV^t}(\chi) = E_{V^t}(\chi_t)$ for all $t \in \mathbb{R}^+$ and all $\chi \in \mathcal{B}(\mathbb{R})$ and, hence, we get

$$\widehat{P}_{RL} = \mathrm{s}-\lim_{t\to\infty} \mathrm{sign}(V^t)1_{ac}(\widehat{H}), \tag{227}$$

where we used that $\mathrm{sign}_t = \mathrm{sign}$ for all $t \in \mathbb{R}^+$. Since $\mathrm{dom}(V^t) = \mathrm{dom}(P)$ for all $t \in \mathbb{R}\setminus\{0\}$, since $\mathrm{dom}(P)$ is a core for $\bar{V}$ because the closure of V is equal to the bounded extension $\bar{V}$ of V, and since $\lim_{t\to\infty} V^t\Phi = \bar{V}\Phi$ for all $\Phi \in \mathrm{dom}(P)$, due to Proposition 46, we have

$$\mathrm{sr}-\lim_{t\to\infty} V^t = \bar{V}. \tag{228}$$

Finally, since $\mathrm{sign} = \kappa_0 - 1_{(-\infty,0]} - 1_{(-\infty,0)}$, where κ_0 is the unity function from (345), we have $\mathrm{sign}(V^t) = E_{V^t}(\mathrm{sign}) = 1 - E_{V^t}(1_{(-\infty,0]}) - E_{V^t}(1_{(-\infty,0)})$. Hence, since we know that, under Assumption 48 *(a)* (which is equivalent to $E_{\bar V}(1_{\{0\}}) = 0$), (228) implies $\mathrm{s}-\lim_{t\to\infty} E_{V^t}(1_{(-\infty,0]}) = E_{\bar V}(1_{(-\infty,0]})$ and $\mathrm{s}-\lim_{t\to\infty} E_{V^t}(1_{(-\infty,0)}) = E_{\bar V}(1_{(-\infty,0)})$, we arrive at

$$\mathrm{s}-\lim_{t\to\infty} \mathrm{sign}(V^t) = \mathrm{sign}(\bar V). \tag{229}$$

(b) Using Proposition 86 *(b)* and the Pauli coefficient functions $v_0 \in L^\infty(\mathbb{T})$ and $v \in L^\infty(\mathbb{T})^3$ of $\bar V$ from (167)-(168), we can write $\mathrm{sign}(\bar V) = m[w_0]\sigma_0 + m[w]\sigma$, where $w_0 \in L^\infty(\mathbb{T})$ and $w \in L^\infty(\mathbb{T})^3$ are given by

$$w_0 := \frac{1}{2}(\mathrm{sign}\circ(v_0 + |v|) + \mathrm{sign}\circ(v_0 - |v|)), \tag{230}$$

$$w := \frac{1}{2}(\mathrm{sign}\circ(v_0 + |v|) - \mathrm{sign}\circ(v_0 - |v|))\tilde v, \tag{231}$$

and we have $v_0 = u_0'$ and

$$|v| = \begin{cases} |\tilde u u'|, & \text{on } \mathcal{Z}_u^c, \\ |u'|, & \text{on } \mathcal{Z}_u. \end{cases} \tag{232}$$

In order to simplify (230)-(231), we make the decomposition $\mathbb{T} = (\mathcal{Z}_v \cap \mathcal{Z}_u^c) \cup (\mathcal{Z}_v \cap \mathcal{Z}_u) \cup (\mathcal{Z}_v^c \cap \mathcal{Z}_u^c) \cup (\mathcal{Z}_v^c \cap \mathcal{Z}_u)$, where we have $\mathcal{Z}_v \cap \mathcal{Z}_u^c = \{k \in \mathcal{Z}_u^c \,|\, (uu')(k) = 0\}$ and $\mathcal{Z}_v \cap \mathcal{Z}_u = \{k \in \mathcal{Z}_u \,|\, |u'|(k) = 0\}$. As for (230), we get $w_0 = \mathrm{sign}\circ u_0'$ on $\mathcal{Z}_v \cap \mathcal{Z}_u^c$ and $\mathcal{Z}_v \cap \mathcal{Z}_u$. Moreover, making the further decomposition $\mathcal{Z}_v^c \cap \mathcal{Z}_u^c = (\mathcal{Z}_v^c \cap \mathcal{Z}_u^c)_+ \cup (\mathcal{Z}_v^c \cap \mathcal{Z}_u^c)_-$ with $(\mathcal{Z}_v^c \cap \mathcal{Z}_u^c)_\pm := \{k \in \mathcal{Z}_v^c \cap \mathcal{Z}_u^c \,|\, \pm(uu')(k) > 0\}$, we can write, on $\mathcal{Z}_v^c \cap \mathcal{Z}_u^c$,

$$\begin{aligned} w_0 &= \frac{1}{2}(\mathrm{sign}\circ(u_0' + |\tilde u u'|) + \mathrm{sign}\circ(u_0' - |\tilde u u'|)) \\ &= \frac{1}{2}\begin{cases} \mathrm{sign}\circ(u_0' + \tilde u u') + \mathrm{sign}\circ(u_0' - \tilde u u'), & \text{on } (\mathcal{Z}_v^c \cap \mathcal{Z}_u^c)_+, \\ \mathrm{sign}\circ(u_0' - \tilde u u') + \mathrm{sign}\circ(u_0' + \tilde u u'), & \text{on } (\mathcal{Z}_v^c \cap \mathcal{Z}_u^c)_- \end{cases} \\ &= \frac{1}{2}(\mathrm{sign}\circ e_+' + \mathrm{sign}\circ e_-'), \end{aligned} \tag{233}$$

where we recall from Definition 41 that $e_\pm' = u_0' \pm \tilde u u'$ on $\mathcal{Z}_u^c$. On the other hand, on $\mathcal{Z}_v^c \cap \mathcal{Z}_u$, we can write $w_0 = (\mathrm{sign}\circ(u_0' + |u'|) + \mathrm{sign}\circ(u_0' - |u'|))/2$. Hence, since $e_\pm' = u_0'$ on $\mathcal{Z}_v \cap \mathcal{Z}_u^c$ and since $f_\pm = u_0' \pm |u'| = u_0'$ on $\mathcal{Z}_v \cap \mathcal{Z}_u$, we arrive at (220). As for (231), we first note that

$$\tilde v = \begin{cases} \mathrm{sign}\circ(\tilde u u')\tilde u, & \text{on } \mathcal{Z}_v^c \cap \mathcal{Z}_u^c, \\ \dfrac{u'}{|u'|}, & \text{on } \mathcal{Z}_v^c \cap \mathcal{Z}_u, \\ 0, & \text{on } \mathcal{Z}_v. \end{cases} \tag{234}$$

Hence, $w=0$ on $\mathcal{Z}_v\cap\mathcal{Z}_u^c$ and $\mathcal{Z}_v\cap\mathcal{Z}_u$ and, on $\mathcal{Z}_v^c\cap\mathcal{Z}_u^c$, we have

$$\begin{aligned} w &= \frac{1}{2}(\operatorname{sign}\circ(u_0'+|\tilde{u}u'|)-\operatorname{sign}\circ(u_0'-|\tilde{u}u'|))\operatorname{sign}\circ(\tilde{u}u')\tilde{u} \\ &= \frac{1}{2}\begin{cases} (\operatorname{sign}\circ(u_0'+\tilde{u}u')-\operatorname{sign}\circ(u_0'-\tilde{u}u'))\tilde{u}, & \text{on } (\mathcal{Z}_v^c\cap\mathcal{Z}_u^c)_+, \\ -(\operatorname{sign}\circ(u_0'-\tilde{u}u')-\operatorname{sign}\circ(u_0'+\tilde{u}u'))\tilde{u}, & \text{on } (\mathcal{Z}_v^c\cap\mathcal{Z}_u^c)_- \end{cases} \\ &= \frac{1}{2}(\operatorname{sign}\circ e_+'-\operatorname{sign}\circ e_-')\tilde{u}. \end{aligned} \tag{235}$$

Moreover, on $\mathcal{Z}_v^c\cap\mathcal{Z}_u$, we have $w=(\operatorname{sign}\circ f_+-\operatorname{sign}\circ f_-)\widetilde{u'}/2$. Therefore, we arrive at (221) as above. □

6 Heat flux

In this section, we determine the expectation value of the macroscopic heat flux observable in general R/L mover states. Moreover, we prove strict positivity of the entropy production in such states and provide examples of physically important models for such systems.

In the following, we make use of the selfdual second quantization b introduced in Definition 1 *(e)*. Moreover, for any separable complex Hilbert space $\mathcal{H}$, we denote by $\operatorname{tr}:\mathcal{L}^1(\mathcal{H})\to\mathbb{C}$ the usual trace on $\mathcal{L}^1(\mathcal{H})$ (as a special case, the same notation will be used on $\mathbb{C}^{n\times n}$ for all $n\in\mathbb{N}$) and, for all $A\in\mathcal{L}(\mathcal{H})$, we set $\operatorname{Re}(A):=(A+A^*)/2$ and $\operatorname{Im}(A):=(A-A^*)/(2\mathrm{i})$.

Definition 50 (R/L mover heat flux) *Let $H\in\mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (a) and (c), and let $T_0\in\mathcal{L}(\mathfrak{H})$ be an initial 2-point operator, $\rho\in\mathcal{B}(\mathbb{R})$ a Fermi function, and $\beta_L,\beta_R\in\mathbb{R}$ the inverse reservoir temperatures. Moreover, let $T\in\mathcal{L}(\mathfrak{H})$ be the R/L mover 2-point operator for H, T_0, ρ, and β_L,β_R, and let $\omega_T\in\mathcal{E}_{\mathfrak{A}}$ be an R/L mover state.*

(a) The 1-particle observable $\Phi\in\mathcal{L}^1(\mathfrak{H})$ describing the heat flux from the left reservoir into the sample is defined by

$$\Phi:=-\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0}\mathrm{e}^{\mathrm{i}tH}H_L\,\mathrm{e}^{-\mathrm{i}tH}. \tag{236}$$

(b) The R/L mover heat flux is defined to be the expectation value of the macroscopic heat flux observable in the R/L mover state ω_T, i.e.,

$$J:=\omega_T(b(\Phi)). \tag{237}$$

Moreover, we set $J_{pp}:=-\operatorname{tr}(T_{pp}\Phi)$ and $J_{ac}:=-\operatorname{tr}(T_{ac}\Phi)$.

(c) The entropy production rate $\sigma\in\mathbb{R}$ in the R/L mover state is defined by

$$\sigma:=(\beta_R-\beta_L)J. \tag{238}$$

Remark 51 Since, for all $s \in \mathbb{R} \setminus \{0\}$, we have $(\mathrm{e}^{\mathrm{i}sH} H_L \mathrm{e}^{-\mathrm{i}sH} - H_L)/s - \mathrm{i}[H, H_L] = ([(\mathrm{e}^{\mathrm{i}sH} - 1)/s - \mathrm{i}H]H_L - H_L[(\mathrm{e}^{\mathrm{i}sH} - 1)/s - \mathrm{i}H])\mathrm{e}^{-\mathrm{i}sH} + \mathrm{i}[H, H_L](\mathrm{e}^{-\mathrm{i}sH} - 1)$ and $\|(\mathrm{e}^{\mathrm{i}sH} - 1)/s - \mathrm{i}H\| \leq \|H\|(\mathrm{e}^{|s|\|H\|} - 1)$, the map $\Psi : \mathbb{R} \to \mathcal{L}(\mathfrak{H})$, defined by $\Psi^t := -\mathrm{e}^{\mathrm{i}tH} H_L \mathrm{e}^{-\mathrm{i}tH}/2$ for all $t \in \mathbb{R}$, has a well-defined derivative with respect to the operator norm at all points $t \in \mathbb{R}$, i.e., due to the fact that $H \in \mathcal{L}(\mathfrak{H})$, the limit defining the derivative in (236) exists with respect to the uniform topology on $\mathcal{L}(\mathfrak{H})$ (note that, since $\mathrm{spec}(H)$ is compact and since the exponential series converges compactly, the estimate of Proposition 76 *(a)* leads to the same conclusion).

Remark 52 Applying Remark 13, the 1-particle heat flux observable reads

$$\Phi = -\frac{\mathrm{i}}{2}[H, H_L] \tag{239}$$

$$= -\mathrm{Im}(H_L(H_{LS} + H_{LR})). \tag{240}$$

Hence, since $H_{LR} \in \mathcal{L}^1(\mathfrak{H})$ by Assumption 14 *(c)*, we get $\Phi \in \mathcal{L}^1(\mathfrak{H})$ as stated in Definition 50 *(a)*. Moreover, (239), and (26) for H and (51), respectively, imply

$$\Phi^* = \Phi, \tag{241}$$

$$\Gamma\Phi\Gamma = -\Phi, \tag{242}$$

i.e., Φ is a selfdual observable. Next, we know (see [2]) that, if $T \in \mathcal{L}(\mathfrak{H})$ is a 2-point operator, $\omega_T \in \mathcal{E}_{\mathfrak{A}}$ a state with 2-point operator T, and $A \in \mathcal{L}^1(\mathfrak{H})$ with $\Gamma A \Gamma = -A^*$, we have

$$\omega_T(b(A)) = -\mathrm{tr}(TA), \tag{243}$$

where $b(A) \in \mathfrak{A}$ is the selfdual second quantization of A from Definition 1 *(e)*. Due to (241)-(242) and the fact that $\dot{\Psi}^0 = \Phi$ and $\dot{\Psi}^t = \mathrm{e}^{\mathrm{i}tH}\Phi\mathrm{e}^{-\mathrm{i}tH}$ for all $t \in \mathbb{R}$, where Ψ stems from Remark 51 (and the dot stands for the derivative with respect to t), we have $\dot{\Psi}^t \in \mathcal{L}^1(\mathfrak{H})$, $(\dot{\Psi}^t)^* = \dot{\Psi}^t$, and $\Gamma\dot{\Psi}^t\Gamma = -\dot{\Psi}^t$ for all $t \in \mathbb{R}$. Hence, (243) yields, for all $t \in \mathbb{R}$,

$$\omega_T(b(\dot{\Psi}^t)) = -\mathrm{tr}(\mathrm{e}^{-\mathrm{i}tH}T\mathrm{e}^{\mathrm{i}tH}\Phi)$$

$$= \omega_T(b(\Phi)), \tag{244}$$

where we used the cyclicity of the trace, $[T, H] = 0$ from Proposition 25 *(b)*, and the first part of the proof of Lemma 83 *(d)*. Therefore, the R/L mover heat flux (237) is independent of the choice $t = 0$ in (236).

Remark 53 Since $\omega_T(A^*) = \overline{\omega_T(A)}$ for all $A \in \mathcal{E}_{\mathfrak{A}}$, (241) and the fact that $b(A)^* = b(A^*)$ for all $A \in \mathcal{L}^1(\mathfrak{H})$ from Remark 3 imply that $J \in \mathbb{R}$.

Remark 54 Let us denote by J_R the expectation value in the R/L mover state of the macroscopic heat flux observable $b(\Phi_R)$ whose 1-particle observable Φ_R describes the heat flux from the right reservoir into the sample, i.e., Φ_R is defined as in (236) but with H_L replaced by H_R. Setting $Q := H - (H_L + H_R)$, we get $Q \in \mathcal{L}^1(\mathfrak{H})$ due to (47) and Assumption 14 *(c)*. Moreover, since $\Phi + \Phi_R = \mathrm{i}[H, Q]/2$, (243) and Proposition 25 *(b)* yield

$$\begin{aligned} J + J_R &= -\frac{\mathrm{i}}{2}\mathrm{tr}(T[H, Q]) \\ &= -\frac{\mathrm{i}}{2}\mathrm{tr}([T, H]Q) \\ &= 0, \end{aligned} \tag{245}$$

i.e., we obtain the first law of thermodynamics in the R/L mover state. Moreover, due to (245), the definition of the entropy production rate from (238) boils down to the usual one, i.e., we have $\sigma = -(\beta_L J + \beta_R J_R)$.

In the following, we make use of Assumption 14 *(d)* which means that there is no direct coupling between the two reservoirs, i.e., that the range of the Hamiltonian is bounded by the finite number n_S of the sites in the configuration space $\mathbb{Z}_S$ of the confined sample. This assumption is physically meaningful since the coupling interaction of a real physical sample to a thermal reservoir usually acts by short-range forces across the boundaries of the sample (for a lattice spacing of the order of $10^{-10}m$ and a sample dimension of the order of $10^{-3}m$ [see [30] for example], we get $n_S \sim 10^7$). Under the additional Assumption 14 *(d)*, the Hamiltonian can be written as follows.

Lemma 55 (Finite range) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (b), (d), and (e) and let $u_0 \in L^\infty(\mathbb{T})$ and $u = [u_1, u_2, u_3] \in L^\infty(\mathbb{T})^3$ be the Pauli coefficient functions of $\widehat{H}$. Then, there existst $\nu \in \langle 1, n_S\rangle$ such that the Pauli coefficients of H read, for all $\alpha \in \langle 0, 3\rangle$,*

$$h_\alpha = \begin{cases} -2\sum_{n\in\langle 1,\nu\rangle} \mathrm{Im}(\check{u}_\alpha(n))\,\mathrm{Im}(\theta^n), & \alpha \in \langle 0, 2\rangle, \\ \mathrm{Re}(\check{u}_3(0))1 + 2\sum_{n\in\langle 1,\nu\rangle} \mathrm{Re}(\check{u}_3(n))\,\mathrm{Re}(\theta^n), & \alpha = 3. \end{cases} \tag{246}$$

The smallest number ν such that (246) *holds is called the range of the Hamiltonian H.*

Proof. Recall that the Pauli coefficients $h_0 \in \mathcal{L}(\mathfrak{h})$ and $h = [h_1, h_2, h_3] \in \mathcal{L}(\mathfrak{h})^3$ of the Hamiltonian $H = h_0\sigma_0 + h\sigma$ satisfy (144)-(145). Therefore, since $Q_\kappa = q_\kappa\sigma_0$ for all $\kappa \in \{L, S, R\}$, Assumption 14 *(d)* is equivalent to the fact that, for all $\alpha \in \langle 0, 3\rangle$,

$$q_L h_\alpha q_R = 0. \tag{247}$$

Using Assumption 14 *(b)*, which is equivalent to the fact that, for all $\alpha \in \langle 0, 3\rangle$,

$$[h_\alpha, \theta] = 0, \tag{248}$$

and using that $\delta_x = \theta^x\delta_0$ and $(\theta^x)^* = \theta^{-x}$ for all $x \in \mathbb{Z}$ (where we set $\theta^0 := 1$ and $\theta^{-x} := (\theta^{-1})^x$ for all $x \in \mathbb{N}$), we can write, for all $x \in \mathbb{Z}_L$, all $y \in \mathbb{Z}_R$, and all $\alpha \in \langle 0, 3\rangle$, that $(\delta_{x-y}, h_\alpha\delta_0) = (\delta_x, h_\alpha\delta_y) = (q_L\delta_x, h_\alpha q_R\delta_y) = (\delta_x, q_L h_\alpha q_R\delta_y) = 0$, and then, with (144), that $(\delta_{y-x}, h_\alpha\delta_0) = 0$, too. Moreover, we have $x - y \geq n_S + 1 \geq 2$ for all $x \in \mathbb{Z}_R$ and all $y \in \mathbb{Z}_L$, and any $z \in \mathbb{Z}$

with $z \geq n_S + 1$ can be written as $z = x - y$ with $x \in \mathbb{Z}_R$ and $y \in \mathbb{Z}_L$ (and analogously if $z \leq -(n_S + 1)$). Hence, since, for all $\alpha \in \langle 0, 3 \rangle$, the function $\check{u}_\alpha \in \mathfrak{h}$ is given, for all $x \in \mathbb{Z}$, by

$$\begin{aligned} \check{u}_\alpha(x) &= (\mathrm{e}_x, m[u_\alpha]\mathrm{e}_0) \\ &= (\delta_x, h_\alpha \delta_0), \end{aligned} \tag{249}$$

we get $\check{u}_\alpha(x) = 0$ for all $\alpha \in \langle 0, 3 \rangle$ and all $x \in \mathbb{Z}$ with $|x| \geq n_S + 1$. Therefore, there exists a smallest number $\nu \in \langle 1, n_S \rangle$ such that, for all $\alpha \in \langle 0, 3 \rangle$ and all $x \in \mathbb{Z}$ with $|x| \geq \nu + 1$,

$$\check{u}_\alpha(x) = 0, \tag{250}$$

and $\nu = 0$ is excluded due to Assumption 14 *(e)*. Hence, (250) implies that, for all $\alpha \in \langle 0, 3 \rangle$ and all $y \in \mathbb{Z}$, we have $h_\alpha \delta_y = \theta^y h_\alpha \delta_0 = \theta^y \sum_{x \in \langle -\nu, \nu \rangle} \check{u}_\alpha(x) \delta_x = \sum_{x \in \langle -\nu, \nu \rangle} \check{u}_\alpha(x) \theta^x \delta_y$, i.e., we get, for all $\alpha \in \langle 0, 3 \rangle$,

$$h_\alpha = \sum_{x \in \langle -\nu, \nu \rangle} \check{u}_\alpha(x) \theta^x \tag{251}$$

$$= \check{u}_\alpha(0) 1 + 2 \sum_{n \in \langle 1, \nu \rangle} \mathrm{Re}(\check{u}_\alpha(n) \theta^n) \tag{252}$$

$$= \begin{cases} -2 \sum_{n \in \langle 1, \nu \rangle} \mathrm{Im}(\check{u}_\alpha(n)) \, \mathrm{Im}(\theta^n), & \alpha \in \langle 0, 2 \rangle, \\ \mathrm{Re}(\check{u}_3(0)) 1 + 2 \sum_{n \in \langle 1, \nu \rangle} \mathrm{Re}(\check{u}_3(n)) \, \mathrm{Re}(\theta^n), & \alpha = 3, \end{cases} \tag{253}$$

where we used (144) for (252) and (145) for (253). □

Remark 56 Let $A \in \mathcal{L}^1(\mathfrak{H})$ with $\Gamma A \Gamma = -A^*$. Then, for all $B \in \mathfrak{A}$, we define the map $f_B : \mathbb{R} \to \mathfrak{A}$ by $f_B^t := \mathrm{e}^{\mathrm{i}tb(A)/2} B \mathrm{e}^{-\mathrm{i}tb(A)/2}$ for all $t \in \mathbb{R}$, where the exponential is defined through its absolutely convergent series with respect to the C^*-norm of $\mathfrak{A}$. Hence, the Cauchy product in $\mathfrak{A}$ yields (as in Remark 51) that, for all $s \in \mathbb{R} \setminus \{0\}$,

$$\begin{aligned} \frac{f_B^{t+s} - f_B^t}{s} - f^t_{\frac{\mathrm{i}}{2}[b(A),B]} &= \mathrm{e}^{\mathrm{i}t\frac{1}{2}b(A)} \left[\frac{\mathrm{e}^{\mathrm{i}s\frac{1}{2}b(A)} - 1}{s} - \frac{\mathrm{i}}{2} b(A), B \right] \mathrm{e}^{-\mathrm{i}(t+s)\frac{1}{2}b(A)} \\ &\quad + \mathrm{e}^{\mathrm{i}t\frac{1}{2}b(A)} \frac{\mathrm{i}}{2} [b(A), B] \big(\mathrm{e}^{-\mathrm{i}s\frac{1}{2}b(A)} - 1 \big) \mathrm{e}^{-\mathrm{i}t\frac{1}{2}b(A)}. \end{aligned} \tag{254}$$

Since, due to (22), we again have $\|(\mathrm{e}^{\mathrm{i}sb(A)/2} - 1)/s - \mathrm{i}b(A)/2\| \leq \|A\|_1 (\mathrm{e}^{|s| \|A\|_1} - 1)$, the map f_B is differentiable everywhere on $\mathbb{R}$ (the dot again stands for the derivative with respect to t) and, for all $t \in \mathbb{R}$, we get

$$\dot{f}_B^t = f^t_{\frac{\mathrm{i}}{2}[b(A),B]}. \tag{255}$$

Hence, f_B is infinitely differentiable on $\mathbb{R}$, and since the n-th derivative of f_B at the point $s \in \mathbb{R}$ is bounded by $\|B\| \mathrm{e}^{|s| \|A\|_1} \|A\|_1^n$ for all $n \in \mathbb{N}$, Taylor's theorem for $\mathfrak{A}$ implies that f_B is real analytic on $\mathbb{R}$. Moreover, since Definition 1 *(d)* and *(e)* imply that $[b(A), B(F)] = 2B(AF)$

for all $F \in \mathfrak{H}$ and all $A \in \mathcal{L}^1(\mathfrak{H})$ with $\Gamma A \Gamma = -A^*$, the Taylor series for $f_{B(F)}$ in $\mathfrak{A}$ and for the map $\mathbb{R} \ni t \mapsto \mathrm{e}^{\mathrm{i}tA} F \in \mathfrak{H}$ yield, for all $t \in \mathbb{R}$, all $F \in \mathfrak{H}$, and all $A \in \mathcal{L}^1(\mathfrak{H})$ with $\Gamma A \Gamma = -A^*$,

$$\mathrm{e}^{\mathrm{i}t\frac{1}{2}b(A)} B(F) \mathrm{e}^{-\mathrm{i}t\frac{1}{2}b(A)} = B(\mathrm{e}^{\mathrm{i}tA} F). \tag{256}$$

Similarly, since $[b(A), b(B)] = 2b([A, B])$ for all $A, B \in \mathcal{L}^1(\mathfrak{H})$ with $\Gamma A \Gamma = -A^*$ and $\Gamma B \Gamma = -B^*$, the Taylor series for $f_{b(B)}$ in $\mathfrak{A}$ and for the map $\mathbb{R} \ni t \mapsto \mathrm{e}^{\mathrm{i}tA} B \mathrm{e}^{-\mathrm{i}tA} \in \mathcal{L}^1(\mathfrak{H})$ yield, for all $t \in \mathbb{R}$ and all $A, B \in \mathcal{L}^1(\mathfrak{H})$ with $\Gamma A \Gamma = -A^*$ and $\Gamma B \Gamma = -B^*$,

$$\mathrm{e}^{\mathrm{i}t\frac{1}{2}b(A)} b(B) \mathrm{e}^{-\mathrm{i}t\frac{1}{2}b(A)} = b(\mathrm{e}^{\mathrm{i}tA} B \mathrm{e}^{-\mathrm{i}tA}). \tag{257}$$

Next, for all $N \in \mathbb{N}$, let us define $q_N := m[1_{\langle -N,N \rangle}]$ and $Q_N := q_N \sigma_0 \in \mathcal{L}^0(\mathfrak{H})$, and set $H_N := Q_N H Q_N$ for all $N \in \mathbb{N}$. Moreover, for all $\kappa, \lambda \in \{L, S, R\}$ and all $N \in \mathbb{N}$, we set $H_{\kappa,N} := Q_N H_\kappa Q_N$ and $H_{\kappa\lambda,N} := Q_N H_{\kappa\lambda} Q_N$. Using (7), we note that all the Pauli coefficients of $H_L H_{LS}$ are linear combinations of operators of the form $q_L h_\alpha q_L h_\beta q_S$, where $\alpha, \beta \in \langle 0, 3 \rangle$ (see also (284)-(285) below). With the help of (251), we can write $q_L h_\alpha q_L h_\beta q_S = \sum_{x,y \in \langle -\nu,\nu \rangle} \check{u}_\alpha(x) \check{u}_\beta(y) q_L(\theta^x q_L) m[1_{\langle x_L+x+y, x_R+x+y \rangle}] \theta^{x+y}$ for all $\alpha, \beta \in \langle 0, 3 \rangle$. Similarly, we get $q_N(q_L h_\alpha q_L) q_N(q_L h_\beta q_S) q_N = \sum_{x,y \in \langle -\nu,\nu \rangle} \check{u}_\alpha(x) \check{u}_\beta(y) q_L(\theta^x q_L) m[1_{N,x,y}] m[1_{\langle x_L+x+y, x_R+x+y \rangle}] \theta^{x+y}$ for all $\alpha, \beta \in \langle 0, 3 \rangle$ and all $N \in \mathbb{N}$, where, for all $N \in \mathbb{N}$ and all $x, y \in \langle -\nu, \nu \rangle$, the function $1_{N,x,y} \in \ell^\infty(\mathbb{Z})$ is defined by $1_{N,x,y} := 1_{\langle -N,N \rangle} 1_{\langle -N+x, N+x \rangle} 1_{\langle -N+x+y, N+x+y \rangle}$. If we assume that

$$N \geq |x_L| + |x_R| + 2\nu, \tag{258}$$

we have $1_{N,x,y} 1_{\langle x_L+x+y, x_R+x+y \rangle} = 1_{\langle x_L+x+y, x_R+x+y \rangle}$ for all $x, y \in \langle -\nu, \nu \rangle$. Therefore, we can write $H_{L,N} H_{LS,N} = H_L H_{LS}$, i.e., using (240), we get, for all $N \in \mathbb{N}$ satisfying (258),

$$\begin{aligned} [H_N, H_{L,N}] &= -2\mathrm{i}\,\mathrm{Im}(H_{L,N} H_{LS,N}) \\ &= -2\mathrm{i}\,\mathrm{Im}(H_L H_{LS}) \\ &= [H, H_L], \end{aligned} \tag{259}$$

where, in the first equality, we used the fact that $[Q_\kappa, Q_N] = 0$ for all $\kappa \in \{L, S, R\}$ and all $N \in \mathbb{N}$ (and Assumption 14 *(d)*). Now, due to (256), we note that the quasifree dynamics generated by the local Hamiltonian $H_N \in \mathcal{L}^0(\mathfrak{H})$ on the 1-particle Hilbert space $\mathfrak{H}$ is induced, macroscopically, by the selfdual second quantization of $H_N/2$ and the local macroscopic Hamiltonian of the left reservoir is given by $b(H_{L,N})/2$. Hence, using (255), the commutator identity after (256), (259), and (239), we get, for all $N \in \mathbb{N}$ satisfying (258),

$$\begin{aligned} -\frac{\mathrm{d}}{\mathrm{d}t}\bigg|_{t=0} \mathrm{e}^{\mathrm{i}t\frac{1}{2}b(H_N)} \frac{1}{2} b(H_{L,N}) \mathrm{e}^{-\mathrm{i}t\frac{1}{2}b(H_N)} &= b\Big(-\frac{\mathrm{i}}{2}[H_N, H_{L,N}]\Big) \\ &= b(\Phi), \end{aligned} \tag{260}$$

i.e., the fact that macroscopic dynamics is generated by the selfdual second quantization of $H_N/2$ explains the existence of the factor $1/2$ in (236).

Remark 57 Let $\omega_T \in \mathcal{E}_{\mathfrak{A}}$ be a gauge-invariant state with 2-point operator $T \in \mathcal{L}(\mathfrak{H})$ and let $H \in \mathcal{L}(\mathfrak{H})$ be a gauge-invariant Hamiltonian. Then, due to Lemma 28 *(b)* (and its proof), there exist $s, h \in \mathcal{L}(\mathfrak{h})$ with $0 \leq s \leq 1$ and $h^* = h$ such that $T = (1-s) \oplus \zeta s \zeta$ and $H = h \oplus (-\zeta h \zeta)$. Hence, the heat flux observable (236) has the form

$$\Phi = \frac{1}{2}\, \varphi \oplus (-\zeta \varphi \zeta), \tag{261}$$

where $\varphi \in \mathcal{L}(\mathfrak{h})$ is given by $\varphi := -\mathrm{i}[h, q_L h q_L]$. Due to Assumption 14 *(d)*, we then have $\varphi = -\mathrm{i}[q_L h q_S + q_S h q_L, q_L h q_L] \in \mathcal{L}^0(\mathfrak{h})$ and, hence, $\Phi \in \mathcal{L}^0(\mathfrak{H})$. Moreover, $\Phi^* = \Phi$ and $\Gamma\Phi\Gamma = -\Phi$ which implies, with (243), that

$$\begin{aligned} \omega_T(b(\Phi)) &= \frac{1}{2}\operatorname{tr}(s\varphi) + \frac{1}{2}\operatorname{tr}(\zeta s \varphi \zeta) - \frac{1}{2}\operatorname{tr}(\varphi) \\ &= \operatorname{tr}(s\varphi), \end{aligned} \tag{262}$$

where we used that $\zeta\delta_x = \delta_x$ for all $x \in \mathbb{Z}$, the commutator form of φ, and the cyclicity of the trace on $\mathfrak{h}$. Note that $\omega_s(\mathrm{d}\Gamma(\varphi)) = \operatorname{tr}(s\varphi)$, where $\omega_s \in \mathcal{E}_{\mathfrak{A}}$ is the state defined in Remark 29 and $\mathrm{d}\Gamma$ is the usual second quantization.

We next clarify the effect of Assumption 14 *(d)* on the assumptions used in the foregoing sections.

Lemma 58 (Assumptions) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (b), (d), and (e). Moreover, let $u_0 \in L^\infty(\mathbb{T})$ and $u = [u_1, u_2, u_3] \in L^\infty(\mathbb{T})^3$ be the Pauli coefficient functions of $\widehat{H}$ and let us define the following mutually exclusive, exhaustive, and non-empty cases:*

$$\textit{Case} \begin{cases} \textit{1}, & u_0 = 0,\ u \neq 0, \textit{ and } uu' = 0 \\ \textit{2}, & u_0 = 0 \textit{ and } uu' \neq 0 \\ \textit{3}, & u_0 \neq 0 \textit{ and } u = 0 \\ \textit{4}, & u_0 \neq 0,\ u \neq 0, \textit{ and } uu' = 0 \\ \textit{5}, & u_0 \neq 0,\ uu' \neq 0, \textit{ and } u_0^2 \neq u^2 \\ \textit{6}, & u_0 \neq 0 \textit{ and } u_0^2 = u^2 \end{cases} \tag{263}$$

Then:

(a) In all cases, Assumptions 14 (c), 40 (a) and (b) are satisfied.

(b) We have

$$[1_{pp}(H), 1_{ac}(H), 1_{sc}(H)] = \begin{cases} [1,0,0], & \textit{Case 1}, \\ [0,1,0], & \textit{Case 2, 3, 4, and 5}, \\ [1_0(H), 1 - 1_0(H), 0], & \textit{Case 6}, \end{cases} \tag{264}$$

where, in Case 6, $\dim(\operatorname{ran}(1_0(H))) = \infty$ but $1_0(H) \neq 1$. In particular, in all cases, Assumption 14 (a) is satisfied.

(c) The bounded extension $\bar V \in \mathcal{L}(\widehat{\mathfrak{H}})$ of the asymptotic velocity with respect to $\widehat{H}$ satisfies

$$\operatorname{eig}(\bar V) \cap \{0\} = \begin{cases} \{0\}, & \textit{Case 1 and 6}, \\ \emptyset, & \textit{Case 2, 3, 4, and 5}. \end{cases} \tag{265}$$

In particular, in Case 2, 3, 4, and 5, Assumption 48 (a) holds.

Remark 59 If Assumption 14 *(e)* does not hold, Remark 15 yields $H = 0$, i.e., we have $u_\alpha = 0$ for all $\alpha \in \langle 0, 3\rangle$. Hence, Assumptions 14 *(c)*, 40 *(a)* and *(b)* are satisfied. Moreover, since $1_{pp}(H) = 1$ and since $\{1_{pp}(H), 1_{ac}(H), 1_{sc}(H)\}$ is a complete orthogonal family of orthogonal projections, Assumption 14 *(a)* is also satisfied. Finally, due to (167)-(168) (or directly from (165)), we have $\bar V = 0$, i.e., Assumption 48 *(a)* does not hold.

Remark 60 Since $u_0 u_0' = u u'$ if $u_0^2 = u^2$, the first and the third condition of *Case 4* imply $u_0^2 \neq u^2$ (see *Case 3* in the proof of Lemma 58 *(b)*). Hence, the six cases are mutually exclusive and exhaust all the possibilities.

In the following, we denote by $TP(\mathbb{T})$ the real trigonometric polynomials on $\mathbb{T}$ (for the structure of this ring, see [25] for example). Note that, due to the fundamental theorem of algebra, we have, for all $v \in TP(\mathbb{T})$,

$$\operatorname{card}(\mathcal{Z}_v) < \infty \text{ if and only if } v \neq 0. \tag{266}$$

Proof. Due to Assumption 14 *(b)*, *(d)*, and *(e)* and Lemma 55, the Pauli coefficients of $\widehat{H}$ have the form $\hat h_\alpha = m[u_\alpha]$ for all $\alpha \in \langle 0, 3\rangle$, where the Pauli coefficient functions $u_0 \in L^\infty(\mathbb{T})$ and $u = [u_1, u_2, u_3] \in L^\infty(\mathbb{T})^3$ are given, for all $\alpha \in \langle 0, 3\rangle$, by

$$u_\alpha = \begin{cases} -2\sum_{n\in\langle 1,\nu\rangle} c_{\alpha,n} \sin(n\,\cdot), & \alpha \in \langle 0, 2\rangle, \\ c_{3,0} + 2\sum_{n\in\langle 1,\nu\rangle} c_{3,n} \cos(n\,\cdot), & \alpha = 3, \end{cases} \tag{267}$$

i.e., we have $u_\alpha \in TP(\mathbb{T})$ for all $\alpha \in \langle 0, 3\rangle$. Here, for all $\alpha \in \langle 0, 2\rangle$ and all $x \in \mathbb{Z}$, we set

$$c_{\alpha,x} := \operatorname{Im}(\check u_\alpha(x)), \tag{268}$$
$$c_{3,x} := \operatorname{Re}(\check u_3(x)), \tag{269}$$

and we note that, due to (142)-(143), we have $\check u_\alpha(x) = \mathrm{i} c_{\alpha,x}$ and $\check u_3(x) = c_{3,x}$ for all $\alpha \in \langle 0, 2\rangle$ and all $x \in \mathbb{Z}$, respectively.

(a) In all cases, Assumption 14 *(d)* implies Assumption 14 *(c)*. Moreover, since $u_\alpha \in TP(\mathbb{T})$ for all $\alpha \in \langle 0, 3\rangle$, Assumptions 40 *(a)* and *(b)* are satisfied.

(b) Using part *(a)*, (385) from Remark 89 yields

$$\operatorname{spec}(\widehat{H}) = \operatorname{ran}(e_+) \cup \operatorname{ran}(e_-). \tag{270}$$

Moreover, for all $\lambda \in \mathbb{R}$, we define $p_\lambda \in TP(\mathbb{T})$ by $p_\lambda := \det([\widehat{H}] - \lambda 1)$, where $[\widehat{H}] \in L^\infty(\mathbb{T}, \mathbb{C}^{2\times 2})$ is the identification specified in Remark 89. Hence, for all $\lambda \in \mathbb{R}$, we have

$$p_\lambda = (u_0 - \lambda)^2 - u^2, \tag{271}$$

and we know that $\lambda \in \mathrm{eig}(\widehat{H})$ if and only if $|\mathcal{Z}_{p_\lambda}| > 0$ (see [17] for example), i.e., with (266),

$$\lambda \in \mathrm{eig}(\widehat{H}) \text{ if and only if } p_\lambda = 0. \tag{272}$$

Furthermore, due to Lemma 90, we can write

$$u^2 = a_0 + 2 \sum_{m \in \langle 1, 2\nu \rangle} a_m \cos(m\,\cdot), \tag{273}$$

where we set $a_n := \sum_{\alpha \in \langle 1,3 \rangle} a_{\alpha,n}$ for all $n \in \langle 0, 2\nu \rangle$ and the coefficients $a_{\alpha,n} \in \mathbb{R}$ for all $\alpha \in \langle 0, 3 \rangle$ and all $n \in \langle 0, 2\nu \rangle$ are given in Lemma 90.

Case 1 Since $uu' = (u^2)'/2$ and since we know that $\{1, 2\sin(n\,\cdot), 2\cos(n\,\cdot)\}_{n \in \mathbb{N}}$ constitutes an orthonormal basis of $\hat{\mathfrak{h}}$, (273) implies that $u^2 = a_0$, and $a_0 > 0$ because $u \neq 0$. Hence, we get $e_\pm = \pm\sqrt{a_0}$ and, due to (270),

$$\mathrm{spec}(\widehat{H}) = \{-\sqrt{a_0}, \sqrt{a_0}\}. \tag{274}$$

Moreover, since the points $\pm\sqrt{a_0}$ are isolated in $\mathrm{spec}(\widehat{H})$, we know that $\pm\sqrt{a_0} \in \mathrm{eig}(\widehat{H})$ (or by directly using (272)) and, hence, we get $\mathrm{spec}(\widehat{H}) = \mathrm{eig}(\widehat{H})$. Therefore, since $E_{\widehat{H}}(1_{\mathrm{eig}(\widehat{H})}) = 1_{pp}(\widehat{H})$, since $E_{\widehat{H}}(1_{\mathrm{spec}(\widehat{H})}) = 1$, and since $\{1_{pp}(\widehat{H}), 1_{ac}(\widehat{H}), 1_{sc}(\widehat{H})\}$ is a complete orthogonal family of orthogonal projections, we get $1_{pp}(\widehat{H}) = 1$ and, hence, $1_{ac}(\widehat{H}) = 1_{sc}(\widehat{H}) = 0$. Since $1_\mu(\widehat{H}) = \mathfrak{F} 1_\mu(H) \mathfrak{F}^*$ for all $\mu \in \{pp, ac, sc\}$ (which follows from Lemma 82), we arrive at $1_{pp}(H) = 1$ and $1_{ac}(H) = 1_{sc}(H) = 0$.

Case 2 Since $u \neq 0$ due to $uu' \neq 0$, (266) and (151) imply $\mathrm{card}(\mathcal{Z}_u) < \infty$. Moreover, since $e'_\pm = \pm uu'/|u|$ on $\mathcal{Z}_u^c$, we get $\mathcal{Z}_\pm = \{k \in \mathcal{Z}_u^c \,|\, (uu')(k) = 0\}$ and, since $uu' \in TP(\mathbb{T})$, (266) leads to $\mathrm{card}(\mathcal{Z}_\pm) < \infty$. Therefore, Assumption 43 *(a)* and *(b)* are satisfied for $M = \mathrm{spec}(\widehat{H}) \in \mathcal{M}(\mathbb{R})$ and Proposition 88 and Remark 89 yield $1_{ac}(\widehat{H}) = 1$. Hence, we get $1_{pp}(\widehat{H}) = 1_{sc}(\widehat{H}) = 0$.

Case 3 We have $\mathcal{Z}_u \cap e_\pm^{-1}(M) = u_0^{-1}(M)$ for all $M \in \mathcal{M}(\mathbb{R})$. Hence, there exists no $M \in \mathcal{M}(\mathbb{R})$ with $\mathrm{spec}(\widehat{H}) = \mathrm{ran}\,(u_0) \subseteq M$ such that Assumption 43 *(a)* holds (compare with Remark 89). But note that $\mathrm{ran}\,(1_{ac}(\widehat{H})) = \mathrm{ran}\,(1_{ac}(m[u_0]) \oplus 1_{ac}(m[u_0]))$ and, hence, $1_{ac}(\widehat{H}) = 1_{ac}(m[u_0]) \oplus 1_{ac}(m[u_0])$. Since $u_0 \in TP(\mathbb{T})$ has the form (267), we also have $u_0' \neq 0$, and (266) yields $\mathrm{card}(\mathcal{Z}_{u_0'}) < \infty$. Hence, for the scalar multiplication operator $m[u_0] \in \mathcal{L}(\hat{\mathfrak{h}})$, we know that $1_{ac}(m[u_0]) = 1$ (we can also readily adapt the proof of Proposition 88 by replacing (388) by $e_\pm^{-1}(A') = u_0^{-1}(A') = (u_0^{-1}(A') \cap \mathcal{Z}_{u_0'}) \cup (u_0^{-1}(A') \cap \mathcal{Z}_{u_0'}^c)$ and by carrying out the further decompositions of $u_0^{-1}(A') \cap \mathcal{Z}_{u_0'}^c$ analogously). Hence, we get $1_{ac}(\widehat{H}) = 1$ and $1_{pp}(\widehat{H}) = 1_{sc}(\widehat{H}) = 0$.

Case 4 Since $u^2 \in TP(\mathbb{T})$ and $u^2 \neq 0$, (266) yields $\mathrm{card}(\mathcal{Z}_u) < \infty$. Moreover, we have $e'_\pm = u'_0$ on $\mathcal{Z}_u^c$ and, as in Case 3, $u'_0 \in TP(\mathbb{T})$ satisfies $u'_0 \neq 0$. Hence, (266) implies $\mathrm{card}(\mathcal{Z}_\pm) < \infty$. Therefore, Assumption 43 *(a)* and *(b)* are satisfied for $M = \mathrm{spec}(\widehat{H}) \in \mathcal{M}(\mathbb{R})$ and Proposition 88 and Remark 89 yield $1_{ac}(\widehat{H}) = 1$. Hence, we get $1_{pp}(\widehat{H}) = 1_{sc}(\widehat{H}) = 0$.

Case 5 As in *Case 4*, we have $\mathrm{card}(\mathcal{Z}_u) < \infty$. We next want to show that $\mathrm{card}(\mathcal{Z}_\pm) < \infty$. To this end, we make the following three steps which require $u_0 \neq 0$ and $u \neq 0$ to hold only. First, since $\mathrm{card}(\mathcal{Z}_u) < \infty$, there exists $N \in \mathbb{N}$ and $\{a_i, b_i\}_{i\in\langle 1,N\rangle} \subseteq \mathbb{R}$ with $a_i < b_i$ for all $i \in \langle 1, N\rangle$ such that $(a_i, b_i) \cap (a_j, b_j) = \emptyset$ for all $i, j \in \langle 1, N\rangle$ with $i \neq j$ and $\mathcal{Z}_u^c = \bigcup_{i\in\langle 1,N\rangle}(a_i, b_i)$ if $u^2(\pi) = 0$ and $\mathcal{Z}_u^c = (\bigcup_{i\in\langle 1,N\rangle}(a_i, b_i)) \cup \{-\pi, \pi\}$ if $u^2(\pi) \neq 0$. Let $a, b \in \mathbb{R}$ with $a < b$, let $I := (a, b) \subseteq (a_i, b_i)$ for some $i \in \langle 1, N\rangle$, and let $\kappa \in \{\pm\}$ be fixed. The function e_κ is differentiable on I and if $e'_\kappa = 0$ on I, there exists $\lambda \in \mathbb{R}$ such that $p_\lambda = 0$ on I (see (271)). Hence, due to (266), we get $p_\lambda = \lambda^2 - 2\lambda u_0 + u_0^2 - u^2 = 0$ on $\mathbb{T}$. Using (142)-(143), we thus find $\lambda u_0 = 0$ on $\mathbb{T}$ which implies $\lambda = 0$ since $u_0 \neq 0$. Hence, we arrive at $p_0 = 0$ (on $\mathbb{T}$). Second, let $p \in TP(\mathbb{T})$ be defined by

$$p := u_0'^2 u^2 - (uu')^2, \tag{275}$$

and let us show that, in general, $p = 0$ if and only if $p_0 = 0$. If $p_0 = 0$, we have $p'_0 = 2(u_0 u'_0 - uu') = 0$ which implies $p = -u_0'^2 p_0 = 0$. Conversely, if $p = 0$, there exists a function $\sigma : \mathcal{Z}_u^c \to \{-1, 1\}$ such that $u'_0 = \sigma uu'/|u|$ on $\mathcal{Z}_u^c$ and, in particular, $u'_0 = \sigma uu'/|u|$ on (a_i, b_i) for all $i \in \langle 1, N\rangle$. Moreover, for all $i \in \langle 1, N\rangle$, there exists $k_i \in (a_i, b_i)$ such that $u'_0(k_i) \neq 0$ (assuming the opposite contradicts $u_0 \neq 0$) and, hence, $(uu')(k_i) \neq 0$. Let $i \in \langle 1, N\rangle$ be fixed and let $u'_0(k_i) > 0$ (the case $u'_0(k_i) < 0$ is completely analogous). Since u'_0 is continuous on (a_i, b_i), there exists $\varepsilon > 0$ such that $(k_i - \varepsilon, k_i + \varepsilon) \subseteq (a_i, b_i)$ and $u'_0(k) > 0$ for all $k \in (k_i - \varepsilon, k_i + \varepsilon)$. Since uu' is continuous on (a_i, b_i), too, if $(uu')(k_i) > 0$, there exists $\varepsilon' > 0$ such that $(k_i - \varepsilon', k_i + \varepsilon') \subseteq (a_i, b_i)$ and $(uu)'(k) > 0$ for all $k \in (k_i - \varepsilon', k_i + \varepsilon')$. Setting $\delta := \min\{\varepsilon, \varepsilon'\}$, we get $\sigma = 1$ on $I_i := (k_i - \delta, k_i + \delta)$ and, hence, $e'_- = 0$ on I_i. Then, the first step yields $p_0 = 0$ (if $(uu')(k_i) < 0$, we get $e'_+ = 0$ on I_i and again $p_0 = 0$ from the first step). Third, let $M \subseteq \mathcal{Z}_u^c$ such that $\mathrm{card}(M) = \infty$ (not finite) and let $\kappa \in \{\pm\}$ be fixed. If $e'_\kappa = 0$ on M, we also have $p = 0$ on M since $p = u^2 e'_+ e'_-$ on $\mathcal{Z}_u^c$. Since $p \in TP(\mathbb{T})$ and since $\mathrm{card}(M) = \infty$, (266) implies that $p = 0$. It then follows from the second step that $p_0 = 0$.

Suppose now that $\mathrm{card}(\mathcal{Z}_\pm) = \infty$. Then, it follows from the third step that $p_0 = 0$ which contradicts $u_0^2 \neq u^2$. Hence, we have $\mathrm{card}(\mathcal{Z}_\pm) < \infty$ and, as in *Case 4*, Assumption 43 *(a)* and *(b)* are satisfied for $M = \mathrm{spec}(\widehat{H}) \in \mathcal{M}(\mathbb{R})$ and Proposition 88 and Remark 89 yield $1_{ac}(\widehat{H}) = 1$ and, thus, $1_{pp}(\widehat{H}) = 1_{sc}(\widehat{H}) = 0$.

Case 6 Since $p_0 = 0$, (272) yields $0 \in \mathrm{eig}(\widehat{H})$. On the other hand, we know from the end of the first step in *Case 5* that $p_\lambda = 0$ implies $\lambda = 0$ if $u_0 \neq 0$, i.e., $\mathrm{eig}(\widehat{H}) \subseteq \{0\}$ due to (272). Hence, we get $\mathrm{eig}(\widehat{H}) = \{0\}$ and $1_{pp}(\widehat{H}) = E_{\widehat{H}}(1_{\mathrm{eig}(\widehat{H})}) = 1_0(\widehat{H})$. Moreover, we know that $\mathrm{ran}\,(1_0(\widehat{H}))$ is infinite dimensional (see [17] for example). But, due to (270), we have $|\mathrm{spec}(\widehat{H})| > 0$ because (142)-(143) and $u_0 \neq 0$ imply that $e_\pm$ are non constant, i.e., we also get $1_0(\widehat{H}) \neq 1$. We next want to apply Proposition 88 for $M = \mathrm{spec}(\widehat{H}) \setminus \{0\} \in \mathcal{M}(\mathbb{R})$. First, as in *Case 4*, we have $\mathrm{card}(\mathcal{Z}_u) < \infty$ and, hence, Assumption 43 *(a)* is satisfied. In order to verify Assumption 43 *(b)*, we write $\mathcal{Z}_\pm \cap e_\pm^{-1}(M) = \{k \in \mathcal{Z}_u^c \,|\, e_\pm(k) \neq 0$ and $e'_\pm(k) = 0\}$. Since $u_0^2 = u^2$ implies $u_0 u_0' = uu'$, we get $e'_\pm = \pm u_0' e_\pm/|u|$ on $\mathcal{Z}_u^c$ and, hence, $\mathcal{Z}_\pm \cap e_\pm^{-1}(M) \subseteq \mathcal{Z}_u^c \cap \mathcal{Z}_{u_0'}$. Since $u_0 \neq 0$, we have, as in *Case 3*, that $\mathrm{card}(\mathcal{Z}_{u_0'}) < \infty$, i.e., Assumption 43 *(b)* is satisfied. Therefore, Proposition 88 yields $\mathrm{ran}\,(1_M(\widehat{H})) \subseteq \mathrm{ran}\,(1_{ac}(\widehat{H}))$, i.e., we have $1_M(\widehat{H}) = 1_{ac}(\widehat{H})1_M(\widehat{H})$. On the other hand, we also have $1 = E_{\widehat{H}}(1_{\mathrm{spec}(\widehat{H})}) = 1_{pp}(\widehat{H}) + 1_M(\widehat{H})$ since $\mathrm{spec}(\widehat{H}) = \{0\} \cup M$. Hence, we get $1_M(\widehat{H}) = 1_{ac}(\widehat{H})(1 - 1_{pp}(\widehat{H})) = 1_{ac}(\widehat{H})$ since $1_{ac}(\widehat{H})1_{pp}(\widehat{H}) = 0$, and we arrive at $1_{sc}(\widehat{H}) = 1 - (1_{pp}(\widehat{H}) + 1_{ac}(\widehat{H})) = 0$.

(c) As above (see (272)), we use that $0 \in \mathrm{eig}(\bar{V})$ if and only if $|\mathcal{Z}_{\varphi_0}| > 0$, where $\varphi_0 \in L^\infty(\mathbb{T})$ is defined by $\varphi_0 := \det([\bar{V}]) = v_0^2 - v^2$ and the Pauli coefficient functions are given by $v_0 = u_0'$ and $v = (\tilde{u}u')\tilde{u}$ on $\mathcal{Z}_u^c$ and $v = u'$ on $\mathcal{Z}_u$. Hence, we can write $\mathcal{Z}_{\varphi_0} = A \cup B$, where $A, B \in \mathcal{M}(\mathbb{R})$ are defined by $A := \{k \in \mathcal{Z}_u^c \,|\, p(k) = 0\}$ and $B := \{k \in \mathcal{Z}_u \,|\, q(k) = 0\}$ and where p stems from (275) and $q \in TP(\mathbb{T})$ is given by

$$q := u_0'^2 - u'^2. \tag{276}$$

Case 1 Since $u^2 = a_0 > 0$ as in *Case 1* of part *(a)*, we have $\mathcal{Z}_u = \emptyset$. Hence, we get $v_0 = 0$, and $v = 0$ on $\mathcal{Z}_u^c = \mathbb{T}$, i.e., $\bar{V} = 0$ and $0 \in \mathrm{eig}(\bar{V})$.

Case 2 Since $p \in TP(\mathbb{T})$ and $p = -(uu')^2 \neq 0$, (266) yields $\mathrm{card}(\mathcal{Z}_p) < \infty$ and, hence, $\mathrm{card}(A) < \infty$. Moreover, since $\mathrm{card}(B) < \infty$ because $u \neq 0$, we get $\mathrm{card}(\mathcal{Z}_{\varphi_0}) < \infty$, i.e., $0 \notin \mathrm{eig}(\bar{V})$.

Case 3 Since $u = 0$, we have $A = \emptyset$ and $q = u_0'^2$. Hence, we get $\mathrm{card}(B) = \mathrm{card}(\mathcal{Z}_q) = \mathrm{card}(\mathcal{Z}_{u_0'})$ and, as in *Case 3* of part *(a)*, we have $\mathrm{card}(\mathcal{Z}_{u_0'}) < \infty$. This implies $0 \notin \mathrm{eig}(\bar{V})$.

Case 4 We have $p = u_0'^2 u^2 \neq 0$ and, hence, $\mathrm{card}(A) \leq \mathrm{card}(\mathcal{Z}_p) < \infty$. Since $\mathrm{card}(B) \leq \mathrm{card}(\mathcal{Z}_u) < \infty$, we get $0 \notin \mathrm{eig}(\bar{V})$.

Case 5 Due to the second step in *Case 5* of part *(a)*, we have $p = 0$ if and only if $p_0 = u_0^2 - u^2 = 0$. Hence, $p \neq 0$ and $\mathrm{card}(A) \leq \mathrm{card}(\mathcal{Z}_p) < \infty$. Since again $\mathrm{card}(B) \leq \mathrm{card}(\mathcal{Z}_u) < \infty$, we get $0 \notin \mathrm{eig}(\bar{V})$.

Case 6 Since $p_0 = 0$, we have $p = 0$ and $|A| = |\mathcal{Z}_u^c| > 0$ since $u \neq 0$, i.e., we get $0 \in \mathrm{eig}(\bar{V})$.

Hence, for the bounded extension $\bar{V} \in \mathcal{L}(\widehat{\mathfrak{H}})$ of the asymptotic velocity with respect to $\widehat{H}$ to satisfy Assumption 48 *(a)* is equivalent for the Pauli coefficient functions $u_0 \in L^\infty(\mathbb{T})$ and $u \in L^\infty(\mathbb{T})^3$ of $\widehat{H}$ to belong to *Case 2, 3, 4 or 5*, i.e., due to part *(b)*, to the absence of eigenvalues of H (compare also directly with (165)). □

For the following, recall from Remark 85 that, for all $\chi \in \mathcal{B}(\mathbb{R})$ and all $r \in \mathbb{R}$, the function $\chi_r \in \mathcal{B}(\mathbb{R})$ is given by $\chi_r(x) = \chi(rx)$ for all $r, x \in \mathbb{R}$.

We now arrive at our main result. It asserts that the R/L mover heat flux has the following properties.

Theorem 61 (R/L mover heat flux) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (b), (d), and (e) and let the bounded extension $\bar{V} \in \mathcal{L}(\widehat{\mathfrak{H}})$ of the asymptotic velocity with respect to $\widehat{H}$ satisfy Assumption 48 (a). Moreover, let $u_0 \in L^\infty(\mathbb{T})$ and $u \in L^\infty(\mathbb{T})^3$ be the*

Pauli coefficient functions of $\widehat{H}$, and let $T \in \mathcal{L}(\mathfrak{H})$ be an R/L mover 2-point operator for H, for an initial 2-point operator $T_0 \in \mathcal{L}(\mathfrak{H})$, for a Fermi function $\rho \in \mathcal{B}(\mathbb{R})$, and for the inverse reservoir temperatures $\beta_L, \beta_R \in \mathbb{R}$. Then, the heat flux in the R/L mover state $\omega_T \in \mathcal{E}_{\mathfrak{A}}$ has the decomposition $J = J_{pp} + J_{ac}$, where:

(a) The pure point contribution satisfies $J_{pp} = 0$.

(b) The absolutely continuous contribution is given by

$$J_{ac} = \frac{1}{2} \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi}\, e(k)|e'(k)|\Delta_{\beta_L,\beta_R}(e(k)), \tag{277}$$

where $\Delta_{\beta_L,\beta_R} \in \mathcal{B}(\mathbb{R})$ reads

$$\Delta_{\beta_L,\beta_R} := \rho_{\beta_R} - \rho_{\beta_L}, \tag{278}$$

and $e, e' \in L^\infty(\mathbb{T})$ are defined by $e := u_0 + |u|$ and $e' := u_0' + \tilde{u}u'$.

Remark 62 If $u \neq 0$, i.e., in *Case 2, 4 and 5* under Assumption 48 *(a)*, we have have $e = e_+$ on $\mathbb{T}$ and $e' = e_+' = u_0' + (uu')/|u|$ on $\mathcal{Z}_u^c$ with $\mathrm{card}(\mathcal{Z}_u) < \infty$ (as discussed in the first step of *Case 5* of the proof of Lemma 58 *(a)*). Moreover, $e_+ \in C(\mathbb{T}) \cap C^\infty(\mathbb{T}\backslash\mathcal{Z}_u)$ and $|e_+'| \leq |u_0'| + |u'|$ on $\mathcal{Z}_u^c$. Therefore, due to Remark 84, the integrand of (277) satisfies $|ee'|\Delta_{\beta_L,\beta_R} \in L^\infty(\mathbb{T})$. In *Case 3*, the only case with $u = 0$ under Assumption 48 *(a)*, we have $e = e_+ = u_0$ and $e' = u_0'$ on $\mathbb{T} = \mathcal{Z}_u$ (see (152)), and the same conclusion holds again.

Remark 63 Since Assumption 48 *(a)* is equivalent with *Case 2, 3, 4, and 5* of Lemma 58, we get, in all these cases, that $1_{ac}(H) = 1$.

Remark 64 With the help of $P := (1\sigma_0 + m[\tilde{u}]\sigma)/2 \in \mathcal{L}(\widehat{\mathfrak{H}})$ (which is an orthogonal projection if $u \neq 0$), we can write $\hat{H}\bar{V}P = (m[ee']\sigma_0 + m[ee'\tilde{u}]\sigma)/2$ and, for all $k \in \mathcal{Z}_u^c$ in *Case 2, 4, and 5* and for all $k \in \mathbb{T}$ in *Case 3*, we get $\mathrm{tr}([\hat{H}^2 P](k)) = e(k)^2$ and

$$\mathrm{tr}([\hat{H}\bar{V}P](k)) = e(k)e'(k), \tag{279}$$

where we used the notation of Remark 89. This expression highlights the dependence of the absolutely continuous contribution J_{ac} on the asymptotic velocity $\bar{V}$.

In the following, we set $E_x := \delta_x \oplus 0$ for all $x \in \mathbb{Z}$. For all $a \in \mathcal{L}(\mathfrak{h})$ and all $b = [b_1, b_2, b_3] \in \mathcal{L}(\mathfrak{h})^3$, we also use the notations $\{a, b\} := [\{a, b_1\}, \{a, b_2\}, \{a, b_3\}] \in \mathcal{L}(\mathfrak{h})^3$ and $b^2 := bb \in \mathcal{L}(\mathfrak{h})$, where the latter is defined after (7). Moreover, recall that, for all $\varphi \in \hat{\mathfrak{h}}$, the function $\check{\varphi} \in \mathfrak{h}$ is given by $\check{\varphi}(x) = (\mathfrak{f}^*\varphi)(x) = (\mathrm{e}_x, \varphi)$. If $\varphi = [\varphi_1, \varphi_2, \varphi_3] \in \hat{\mathfrak{h}}^3$, we set $\check{\varphi}(x) := [\check{\varphi}_1(x), \check{\varphi}_2(x), \check{\varphi}_3(x)] \in \mathbb{C}^3$ for all $x \in \mathbb{Z}$.

Proof. Due to (240) and Assumption 14 *(d)*, the 1-particle heat flux observable reads

$$\Phi = -\operatorname{Im}(H_L H_{LS}), \tag{280}$$

i.e., we have $\Phi \in \mathcal{L}^0(\mathfrak{H})$ since $H_{LS} \in \mathcal{L}^0(\mathfrak{H})$. Moreover, Definiton 50 *(b)* and (241)-(243) imply that $J = J_{pp} + J_{ac}$.

(a) Since we have $1_{ac}(H) = 1$ as discussed in Remark 63, we get $T_{pp} = 0$ and, hence, from Definition 50 *(b)*, $J_{pp} = 0$.

(b) Since $\mathrm{tr}(A\,\mathrm{Im}(B)) = (\mathrm{tr}(AB) - \overline{\mathrm{tr}(A^*B)})/(2\mathrm{i})$ for all $A \in \mathcal{L}(\mathfrak{H})$ and all $B \in \mathcal{L}^1(\mathfrak{H})$ and since $T_{ac}^* = T_{ac}$ due to Proposition 25 *(a)*, Definition 50 *(b)* and (280) yield

$$\begin{aligned} J_{ac} &= -\,\mathrm{tr}(T_{ac}\Phi) \\ &= \mathrm{tr}(T_{ac}\,\mathrm{Im}((Q_L H)^2 Q_S)) \\ &= \mathrm{Im}(\mathrm{tr}(T_{ac}(Q_L H)^2 Q_S)) \\ &= \sum_{\substack{x\in\mathbb{Z}_S \\ \alpha\in\langle 0,1\rangle}} \mathrm{Im}((\Gamma^\alpha E_x, T_{ac}(Q_L H)^2 \Gamma^\alpha E_x)). \end{aligned} \tag{281}$$

Writing $T_{ac} = r_0\sigma_0 + r\sigma$ and $(Q_L H)^2 = s_0\sigma_0 + s\sigma$ with $r_0, s_0 \in \mathcal{L}(\mathfrak{h})$ and $r, s \in \mathcal{L}(\mathfrak{h})^3$, we get

$$J_{ac} = 2\sum_{x\in\mathbb{Z}_S} \mathrm{Im}(j_{ac}(x)), \tag{282}$$

where $j_{ac} : \mathbb{Z}_S \to \mathbb{C}$ is defined, for all $x \in \mathbb{Z}_S$, by

$$j_{ac}(x) := (\delta_x, (r_0 s_0 + rs)\delta_x), \tag{283}$$

and we used that $\sum_{\alpha\in\langle 0,1\rangle}(\Gamma^\alpha E_x, (a_0\sigma_0 + a\sigma)(b_0\sigma_0 + b\sigma)\Gamma^\alpha E_x) = 2(\delta_x, (a_0 b_0 + ab)\delta_x)$ for all $x \in \mathbb{Z}$, all $a_0, b_0 \in \mathcal{L}(\mathfrak{h})$, and all $a, b \in \mathcal{L}(\mathfrak{h})^3$. Next, we want to compute (283). First, since $Q_L H = (q_L h_0)\sigma_0 + (q_L h)\sigma$, we can write

$$s_0 = (q_L h_0)^2 + (q_L h)^2, \tag{284}$$

$$s = \{q_L h_0, q_L h\} + \mathrm{i}(q_L h) \wedge (q_L h). \tag{285}$$

Using (251), for all $\alpha, \beta \in [0, 3]$ and all $x \in \mathbb{Z}_S$, the main ingredient of (284)-(285) reads

$$q_L h_\alpha q_L h_\beta \delta_x = \sum_{y,z\in\langle -\nu,\nu\rangle} 1_L(x+y) 1_L(x+y+z)\, \check{u}_\alpha(z)\, \check{u}_\beta(y)\, \delta_{x+y+z}. \tag{286}$$

As for r_0 and r, since $1_{ac}(H) = 1$ as discussed in Remark 63, (59) yields $T_{ac} = \rho(\Delta H)$. Moreover, due to (218), the R/L mover generator reads $\widehat{\Delta} = \beta 1 + \delta\,\mathrm{sign}(\bar{V})$ and (229) leads to $\mathrm{sign}(\bar{V}) = m[w_0]\sigma_0 + m[w]\sigma$, where $w_0 \in L^\infty(\mathbb{T})$ and $w \in L^\infty(\mathbb{T})^3$ are given by (220) and (221), respectively. We next discuss *Case 2, 4, and 5* and *Case 3* separately.

Case 2, 4, and 5 Since $u \neq 0$ in all these cases, we have $\mathrm{card}(\mathcal{Z}_u) < \infty$. Hence, (220)-(221) yield, on $\mathcal{Z}_u^c$,

$$w_0 = \frac{1}{2}(\mathrm{sign}\circ e'_+ + \mathrm{sign}\circ e'_-), \tag{287}$$

$$w = \frac{1}{2}(\mathrm{sign}\circ e'_+ - \mathrm{sign}\circ e'_-)\tilde{u}. \tag{288}$$

Moreover, since $\widehat{H} = m[u_0]\sigma_0 + m[u]\sigma$, we get $\widehat{\Delta}\widehat{H} = m[b_0]\sigma_0 + m[b]\sigma$, where $b_0 \in L^\infty(\mathbb{T})$ and $b \in L^\infty(\mathbb{T})^3$ have the form $b_0 := \beta u_0 + \delta(w_0 u_0 + wu)$ and $b := \beta u + \delta(w_0 u + u_0 w + \mathrm{i} w \wedge u)$. Using (287)-(288) and noting that the wedge product vanishes, we get, on $\mathcal{Z}_u^c$,

$$b_0 = \beta u_0 + \frac{\delta}{2}((\mathrm{sign}\circ e'_+)e_+ + (\mathrm{sign}\circ e'_-)e_-), \tag{289}$$

$$b = \beta u + \frac{\delta}{2}((\mathrm{sign}\circ e'_+)e_+ - (\mathrm{sign}\circ e'_-)e_-)\tilde{u}. \tag{290}$$

Since $\widehat{T}_{ac} = E_{\widehat{\Delta}\widehat{H}}(\rho)$ (see Lemma 82), Proposition 86 *(b)* yields

$$\widehat{T}_{ac} = m[a_0]\sigma_0 + m[a]\sigma, \tag{291}$$

where $a_0 \in L^\infty(\mathbb{T})$ and $a \in L^\infty(\mathbb{T})^3$ are given by $a_0 := (\rho\circ b_+ + \rho\circ b_-)/2$ and $a = (\rho\circ b_+ - \rho\circ b_-)\tilde{b}/2$, and $b_\pm := b_0 \pm |b|$. Since $b = (\tilde{u}b)\tilde{u}$ due to (290), we get, on $\mathcal{Z}_u^c$,

$$a_0 = \frac{1}{2}(\rho_+ + \rho_-), \tag{292}$$

$$a = \frac{1}{2}(\rho_+ - \rho_-)\tilde{u}, \tag{293}$$

where $\rho_\pm \in L^\infty(\mathbb{T})$ is given by

$$\rho_\pm := \rho\circ((\beta + \delta\,\mathrm{sign}\circ e'_\pm)e_\pm). \tag{294}$$

Now, plugging (286) into (284)-(285), writing the resulting expression for (283) in momentum space, and using that $\hat{r}_\alpha = m[a_\alpha]$ for all $\alpha \in \langle 0, 3\rangle$, we get $j_{ac}(x) = \sum_{y,z\in\langle -\nu,\nu\rangle} 1_L(x+y)1_L(x+y+z)G(y+z,z,y)$ for all $x \in \mathbb{Z}_S$, where $G : \mathbb{Z}^3 \to \mathbb{C}$ is defined, for all $x, y, z \in \mathbb{Z}$, by

$$\begin{aligned} G(x,y,z) := {} & \check{a}_0(-x)(\check{u}_0(y)\check{u}_0(z) + \check{u}(y)\check{u}(z)) \\ & + \check{a}(-x)(\check{u}_0(y)\check{u}(z) + \check{u}_0(z)\check{u}(y) + \mathrm{i}\check{u}(y)\wedge\check{u}(z)), \end{aligned} \tag{295}$$

and we recall that $\check{u}(x)\check{u}(y)$ for all $x, y \in \mathbb{Z}$ stands for the real Euclidean scalar product between $\check{u}(x) \in \mathbb{C}^3$ and $\check{u}(y) \in \mathbb{C}^3$ (see after (7)). Hence, summing over all $x \in \mathbb{Z}_S$, we get

$$\sum_{x\in\mathbb{Z}_S} j_{ac}(x) = \sum_{(y,z)\in X} \chi(y,z)\, G(y+z,z,y), \tag{296}$$

where the staircase type function $\chi : \mathbb{Z}^2 \to \langle 0, n_S\rangle$ is defined by $\chi(y,z) := \sum_{x\in\mathbb{Z}_S} 1_L(x+y)1_L(x+y+z)$ for all $y, z \in \mathbb{Z}$, and the summation on the right hand side of (296) is carried out over the set $X := \bigcup_{n\in\langle 1,n_S\rangle} \chi^{-1}(\{n\})\cap\langle -\nu,\nu\rangle^2$. Next, let us make the decomposition $X = \bigcup_{n\in\langle 1,\nu\rangle}(X_{1,n}\cup X_{2,n})$, where, for all $n \in \langle 1,\nu\rangle$, we define $X_{1,n} := \chi^{-1}(\{n\})\cap(\langle -\nu,\nu\rangle\times\langle 0,\nu\rangle)$ and $X_{2,n} := \chi^{-1}(\{n\})\cap(\langle -\nu,\nu\rangle\times\langle -\nu,-1\rangle)$, see Figure 2.

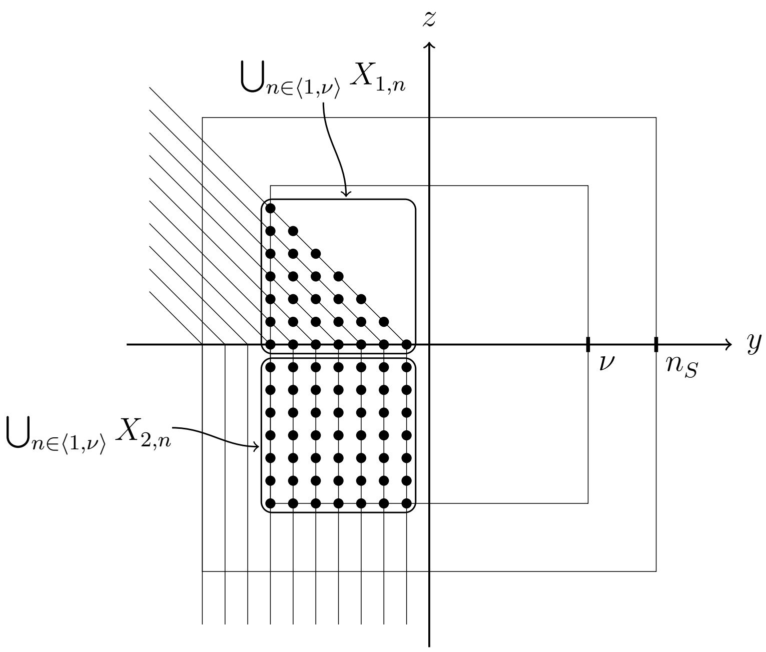


Figure 2: The set $X = \bigcup_{n\in\langle 1,\nu\rangle}(X_{1,n} \cup X_{2,n})$.

Since, for all $n \in \langle 1, \nu\rangle$, we have $y + z = -n$ for all $(y, z) \in X_{1,n}$ and $y = -n$ for all $(y, z) \in X_{2,n}$, (282) becomes

$$J_{ac} = 2 \sum_{n\in\langle 1,\nu\rangle} n \sum_{z\in\langle 0,\nu-n\rangle} \mathrm{Im}(G(-n, z, -n - z)) + 2 \sum_{n\in\langle 1,\nu\rangle} n \sum_{z\in\langle -\nu,-1\rangle} \mathrm{Im}(G(-n + z, z, -n)). \tag{297}$$

In order to determine the imaginary parts on the right hand side of (297), we first note that, due to (141), we have $\zeta\check{u}_\alpha = \xi\check{u}_\alpha$ for all $\alpha \in \langle 0, 3\rangle$ (and the same holds for $\check{a}_\alpha$ for all $\alpha \in \langle 0, 3\rangle$ due to (292)-(293)). Moreover, (142) and (143) yield $\xi\check{u}_\alpha = -\check{u}_\alpha$ for all $\alpha \in \langle 0, 2\rangle$ and $\xi\check{u}_3 = \check{u}_3$, respectively. Hence, we get $\check{u}_\alpha = \mathrm{i}\mathrm{Im}(\check{u}_\alpha)$ for all $\alpha \in \langle 0, 2\rangle$ and $\check{u}_3 = \mathrm{Re}(\check{u}_3)$ which implies, for all $x, y, z \in \mathbb{Z}$,

$$\mathrm{Im}(G(x, y, z)) = \eta_{0,-x}(c_{0,y}c_{0,-z} + c_y c_{-z}) + \eta_{-x}(c_{0,y}c_{-z} + c_{0,-z}(Lc_y) + c_y \wedge (Lc_{-z})), \tag{298}$$

where $c_{\alpha,x} \in \mathbb{R}$ for all $\alpha \in \langle 0, 3\rangle$ and all $x \in \mathbb{Z}$ are given in (268)-(269) and we set $c_x := [c_{1,x}, c_{2,x}, c_{3,x}] \in \mathbb{R}^3$ for all $x \in \mathbb{Z}$. Moreover, the diagonal matrix $L \in \mathbb{C}^{3\times 3}$ is given by $L := \mathrm{diag}[1, 1, -1]$ and, for all $x \in \mathbb{Z}$, we set $\eta_{\alpha,x} := \mathrm{Im}(\check{a}_\alpha(x))$ for all $\alpha \in \langle 0, 2\rangle$, $\eta_{3,x} := \mathrm{Re}(\check{a}_3(x))$, and $\eta_x := [\eta_{1,x}, \eta_{2,x}, \eta_{3,x}] \in \mathbb{R}^3$. Hence, (297) can be written as

$$J_{ac} = -\int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \left(\mu_1(k) + \mu_2(k) + \frac{1}{|u(k)|} \sum_{i\in\langle 3,8\rangle} \mu_i(k)\right)\rho_+(k)$$
$$-\int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} \left(\mu_1(k) + \mu_2(k) - \frac{1}{|u(k)|} \sum_{i\in\langle 3,8\rangle} \mu_i(k)\right)\rho_-(k), \tag{299}$$

where, for all $i \in \langle 1, 8\rangle$, the explicit expressions of the functions $\mu_i \in L^\infty(\mathbb{T})$ are given in Lemma 91. Furthermore, using (267), a direct computation yields

$$\mu_1 + \mu_2 = -\frac{1}{2}(u_0 u_0' + uu'), \tag{300}$$

$$\sum_{i\in\langle 3,8\rangle} \mu_i = -\frac{1}{2}(u_0(uu') + u_0'|u|^2), \tag{301}$$

where, in (408), (410), (412), and (414) of Lemma 91, we used that, for all families $\{f_n\}_{n\in\langle 1,\nu\rangle}$ of functions $f_n : \mathbb{T} \to \mathbb{R}$, we have $\sum_{n\in\langle 1,\nu\rangle, l\in\langle 0,\nu-n\rangle} f_n(k) c_{\alpha_1,l} c_{\alpha_2,n+l} = \sum_{n\in\langle 1,\nu\rangle, m\in\langle 0,n-1\rangle} f_{n-m}(k)$ $c_{\alpha_1,m} c_{\alpha_2,n}$ for all $k \in \mathbb{T}$ and all $\alpha_1, \alpha_2 \in \langle 0, 3\rangle$ (that $c_{\alpha,0} = 0$ for all $\alpha \in \langle 0, 2\rangle$, and that all the contributions in (410)-(415) involving a product of the form $c_{1,n}c_{2,m}c_{3,l}$ add up to zero, where $n, m \in \langle 1, \nu\rangle$ and $l \in \langle 1, \nu\rangle$ or $l = 0$). Moreover, note that, due to (301), the modulus of $\sum_{i\in\langle 3,8\rangle} \mu_i/|u|$ in (299) is bounded from above by $(|u_0||u'| + |u_0'||u|)/2$. Plugging (300)-(301) into (299), using that $e_\pm e_\pm' = u_0 u_0' + uu' \pm (u_0(\tilde{u}u') + u_0'|u|)$ on $\mathcal{Z}_u^c$ and that $\mathrm{card}(\mathcal{Z}_u) < \infty$, (299) becomes

$$J_{ac} = \frac{1}{2}\int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} (e_+(k)e_+'(k)\rho_+(k) + e_-(k)e_-'(k)\rho_-(k)) \tag{302}$$
$$= \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi} e_+(k)e_+'(k)\rho((\beta + \delta\mathrm{sign}(e_+'(k)))e_+(k)), \tag{303}$$

where, in (303), we also used that $\hat{\xi}e_- = -e_+$ and $\hat{\xi}e_-' = e_+'$ on $\mathcal{Z}_u^c$ due to (142)-(143), that (57) holds, and that $e_+e_+' = (e_+^2)'/2$ on $\mathcal{Z}_u^c$. Finally, plugging $e_+e_+' = (1_{\mathcal{Z}_{++}} + 1_{\mathcal{Z}_{+-}} + 1_{\mathcal{Z}_{-+}} + 1_{\mathcal{Z}_{--}})e_+e_+'$ into(303), where $\mathcal{Z}_{\pm\pm} := \{k \in \mathcal{Z}_u^c \,|\, \pm e_+(k) > 0$ and $\pm e_+'(k) > 0\}$ and $\mathcal{Z}_{\pm\mp} := \{k \in \mathcal{Z}_u^c \,|\, \pm e_+(k) > 0$ and $\mp e_+'(k) > 0\}$, the integrand in (303) can be written, on $\mathcal{Z}_u^c$, as

$$e_+e_+'\rho((\beta + \delta\mathrm{sign} \circ e_+')e_+) = \frac{1}{2}|e_+e_+'|(\rho\circ(\beta_R|e_+|) - \rho\circ(\beta_L|e_+|))$$
$$+ \frac{1}{2}e_+e_+'(\rho\circ(\beta_R e_+) + \rho\circ(\beta_L e_+)). \tag{304}$$

Since, due to Definition 18, the restriction of ρ to $[-a, a]$ satisfies $\rho \in L^1([-a, a])$, where $a := (1 + |\beta_L| + |\beta_R|)\sum_{\alpha\in\langle 0,3\rangle} \|u_\alpha\|_\infty/2 > 0$, the first fundamental theorem of calculus yields that the function $\rho_1 : [-a, a] \to \mathbb{R}$, defined by $\rho_1(x) := \int_{-a}^{x} \mathrm{d}t\, \rho(t)$ for all $x \in [-a, a]$, is absolutely continuous and an antiderivative of ρ almost everywhere on $[-a, a]$. Similarly, the function $\rho_2 : [-a, a] \to \mathbb{R}$, defined by $\rho_2(x) := \int_{-a}^{x} \mathrm{d}t\, \rho_1(t)$ for all $x \in [-a, a]$, is an antiderivative of ρ_1 on $[-a, a]$. Hence, for all $\kappa \in \{L, R\}$ for which $\beta_\kappa \neq 0$, using twice partial integration (for absolutely continuous functions), the property $e_+(-\pi) = e_+(\pi)$, and the fact that $e_+ e_+' \rho \circ (\beta_\kappa e_+) = e_+ (\rho_1 \circ (\beta_\kappa e_+))'/\beta_\kappa$ and $e_+' \rho_1 \circ (\beta_\kappa e_+) = (\rho_2 \circ (\beta_\kappa e_+))'/\beta_\kappa$, the integral of each term in the second expression on the right hand side of (304) vanishes (if $\beta_\kappa = 0$ for some $\kappa \in \{L, R\}$, (57) yields $e_+ e_+' \rho \circ (\beta_\kappa e_+) = e_+ e_+'/2 = (e_+^2)'/4$). Therefore, (303) takes the form

$$J_{ac} = \frac{1}{2} \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi}\, |e_+(k) e_+'(k)|\, \Delta_{\beta_L, \beta_R}(|e_+(k)|), \tag{305}$$

where $\Delta_{\beta_L, \beta_R} \in \mathcal{B}(\mathbb{R})$ stems from (278) and, with the help of (57), we arrive at (277).

Case 3 If $u = 0$ (and $u_0 \neq 0$), due to (220)-(221), (287)-(288) become $w_0 = \mathrm{sign} \circ u_0'$ and $w = 0$, respectively. Moreover, we get $b_0 = \beta u_0 + \delta(\mathrm{sign} \circ u_0') u_0$ and $b = 0$, and $a_0 = \rho \circ b_0$ and $a = 0$ instead of (289)-(293). Formula (299) then reads as $J_{ac} = \int_{-\pi}^{\pi} \mathrm{d}k\, u_0(k) u_0'(k) \rho((\beta + \delta \mathrm{sign}(u_0'(k))) u_0(k))/(2\pi)$ and the same arguments apply to its integrand as the ones used for (304). Hence, since we defined $e' = u_0 + \tilde{u} u'$ on $\mathbb{T}$, (277)-(278) also hold for *Case 3*. $\square$

Remark 65 Since, for all $b \in \mathcal{L}(\mathfrak{h})$ and all $A = a_0 \sigma_0 + a \sigma \in \mathcal{L}(\mathfrak{H})$ with $a_0 \in \mathcal{L}(\mathfrak{h})$ and $a = [a_1, a_2, a_3] \in \mathcal{L}(\mathfrak{h})^3$, we have $[A, b\sigma_3] = [a_3, b]\sigma_0 + [\mathrm{i}\{a_2, b\}, -\mathrm{i}\{a_1, b\}, [a_0, b]]\sigma$, we get

$$u_0 = 0 \text{ if and only if } [H, \xi \sigma_3] = 0, \tag{306}$$

where we used (142)-(143) and the fact that $[m[u_\alpha], \hat{\xi}] = 2m[\mathrm{Od}(u_\alpha)]\hat{\xi}$ and $\{m[u_\alpha], \hat{\xi}\} = 2m[\mathrm{Ev}(u_\alpha)]\hat{\xi}$ for all $\alpha \in \langle 0, 3 \rangle$. Hence, in this special case, which occurs frequently in practice, the R/L mover heat flux has the form

$$J = \frac{1}{2} \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi}\, |(uu')(k)|\, \Delta_{\beta_L, \beta_R}(|u|(k)). \tag{307}$$

Remark 66 For all $x, y \in \mathbb{Z}$, we have $p_{x,y}\sigma_0 = (E_x, \cdot)E_y + (\Gamma E_x, \cdot)\Gamma E_y$, $p_{x,y}\sigma_1 = (\Gamma E_x, \cdot)E_y + (E_x, \cdot)\Gamma E_y$, $p_{x,y}\sigma_2 = -\mathrm{i}(\Gamma E_x, \cdot)E_y + \mathrm{i}(E_x, \cdot)\Gamma E_y$, and $p_{x,y}\sigma_3 = (E_x, \cdot)E_y - (\Gamma E_x, \cdot)\Gamma E_y$, where we recall that $p_{x,y} = (\delta_x, \cdot\,)\, \delta_y \in \mathcal{L}^0(\mathfrak{h})$ for all $x, y \in \mathbb{Z}$ and $E_x = \delta_x \oplus 0$ for all $x \in \mathbb{Z}$. Therefore, the selfdual second quantization (15) yields, for all $x, y \in \mathbb{Z}$,

$$b(p_{x,y}\sigma_0) = a_y^* a_x + a_y a_x^*, \tag{308}$$
$$b(p_{x,y}\sigma_1) = a_y^* a_x^* + a_y a_x, \tag{309}$$
$$b(p_{x,y}\sigma_2) = -\mathrm{i}(a_y^* a_x^* - a_y a_x), \tag{310}$$
$$b(p_{x,y}\sigma_3) = a_y^* a_x - a_y a_x^*, \tag{311}$$

where we used the notation of Remark 2. Since, for all $N \in \mathbb{N}$ satisfying (258), we have $q_N \theta^n q_N = \sum_{x \in \langle -N, N-n \rangle} p_{x,x+n}$ for all $n \in \langle 1, \nu \rangle$, where q_N stems from Remark 56, we get for the local zeroth Pauli coefficient of H and for all $N \in \mathbb{N}$ satisfying (258),

$$b((q_N h_0 q_N)\sigma_0) = -2\mathrm{i} \sum_{n \in \langle 1, \nu \rangle} c_{0,n} \sum_{x \in \langle -N, N-n \rangle} (a_x^* a_{x+n} - a_{x+n}^* a_x). \tag{312}$$

Moreover, using the generalized Jordan-Wigner transformation (see again Remark 2), we can write, for all $x \in \mathbb{Z}$ and all $n \in \mathbb{N}$,

$$a_x^* a_{x+n} - a_{x+n}^* a_x = \begin{cases} \frac{\mathrm{i}}{2}\big(\sigma_1^{(x)}\sigma_2^{(x+1)} - \sigma_2^{(x)}\sigma_1^{(x+1)}\big), & n = 1, \\ \frac{\mathrm{i}}{2}\big(\sigma_1^{(x)}\big(\prod_{i\in\langle 1,n-1\rangle}\sigma_3^{(x+i)}\big)\sigma_2^{(x+n)} - \sigma_2^{(x)}\big(\prod_{i\in\langle 1,n-1\rangle}\sigma_3^{(x+i)}\big)\sigma_1^{(x+n)}\big), & n \geq 2, \end{cases} \tag{313}$$

i.e., we get (generalized) Dziyaloshinskii-Moriya type interactions. For the sake of completeness, we display the selfdual second quantization of the local first, second, and third Pauli coefficient of H in the fermionic and the spin picture in Appendix E.

We next illustrate the R/L mover heat flux for two well-known examples. The first example is the prominent XY spin chain (see Remark 2).

Example 67 (XY model) *Let $c_{2,1}, c_{3,0} \in \mathbb{R}$. The XY model with anisotropy $c_{2,1}$ and spatially homogeneous exterior magnetic field $c_{3,0}$ is specified by*

$$h_0 = 0, \tag{314}$$

$$h_1 = 0, \tag{315}$$

$$h_2 = -2c_{2,1}\mathrm{Im}(\theta), \tag{316}$$

$$h_3 = c_{3,0}1 + \mathrm{Re}(\theta). \tag{317}$$

Hence, we have $\nu = 1$ and, for all $c_{2,1}, c_{3,0} \in \mathbb{R}$, Assumptions 14 (b), (d), and (e) are satisfied (note that $c_{3,1} = 1/2$). Moreover, for all $k \in \mathbb{T}$, we get from (314)-(317) *that $u_0 = u_1 = 0$, $u_2(k) = -2c_{2,1}\sin(k)$, and $u_3(k) = c_{3,0} + \cos(k)$. Writing $u^2 = a_0 + 2\sum_{m\in\langle 1,2\nu\rangle} a_m \cos(m\,\cdot)$ as in* (273)*, Lemma 90 (a) yields*

$$a_0 = \frac{1}{2} + 2c_{2,1}^2 + c_{3,0}^2, \tag{318}$$

$$a_1 = c_{3,0}, \tag{319}$$

$$a_2 = \frac{1}{4} - c_{2,1}^2. \tag{320}$$

Therefore, the function $uu' = (u^2)'/2 \in TP(\mathbb{T})$ satisfies $uu' = 0$ (i.e., Case 1 occurs) if and only if $(c_{2,1}, c_{3,0}) \in \{(-1/2, 0), (1/2, 0)\}$ (the Ising model), i.e., due to (265)*, Assumption 48 (a) holds if and only if $(c_{2,1}, c_{3,0}) \in \mathbb{R}^2 \setminus \{(-1/2, 0), (1/2, 0)\}$. In these cases, Theorem 61 is applicable and, for all Fermi functions $\rho \in \mathcal{B}(\mathbb{R})$ and all inverse reservoir temperatures $\beta_L, \beta_R \in \mathbb{R}$, the R/L mover heat flux is given by* (307)*. Moreover, if the Fermi function ρ is the Fermi-Dirac distribution* (74)*, we get*

$$J = \frac{1}{2}\int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi}\, |(uu')(k)|\, \frac{\sinh(\delta|u|(k))}{\cosh(\delta|u|(k)) + \cosh(\beta|u|(k))}, \tag{321}$$

where we used that $1/(1+\mathrm{e}^{-x}) - 1/(1+\mathrm{e}^{-y}) = \sinh((x-y)/2)/(\cosh((x-y)/2) + \cosh((x+y)/2))$ for all $x, y \in \mathbb{R}$. The formula (321) *has been obtained in [11] for $c_{2,1} \in (-1/2, 1/2)$ and $c_{3,0} \in \mathbb{R}$.*

Remark 68 Let the Pauli coefficient functions of $\widehat{H}$ from Theorem 61 satisfy $u_\alpha = 0$ for all $\alpha \in \langle 0, 2\rangle$ and $u_3 = 1$, i.e., we have *Case 1* for which the proof of Lemma 58 *(c)* asserts that $\bar{V} = 0$. Since $\mathrm{spec}(Q) = \mathrm{spec}_{pp}(q) = \mathbb{Z}$ and since $\mathrm{ran}\,(E_q(1_\lambda)) = \mathrm{span}\,\{\delta_\lambda\}$ and $\mathrm{ran}\,(E_Q(1_\lambda)) = \mathrm{span}\,\{E_\lambda, \Gamma E_\lambda\}$ for all $\lambda \in \mathbb{Z}$, we get $\mathrm{spec}(P) = \mathrm{spec}_{pp}(P) = \mathbb{Z}$ and $\mathrm{ran}\,(E_P(1_\lambda)) = \mathrm{span}\,\{\mathrm{e}_\lambda \oplus 0, 0 \oplus \mathrm{e}_\lambda\}$ for all $\lambda \in \mathbb{Z}$ as in the proof of Proposition 49 *(a)*. Moreover, (226) and (205) yield $V^t\Phi = P\Phi/t$ for all $\Phi \in \mathrm{dom}(P)$ and all $t \in \mathbb{R}^+$ and, with the help of Remark 85, we get $E_{V^t}(1_{(-\infty,0)}) = E_P(1_{(-\infty,0)})$ and $E_{V^t}(1_{(-\infty,0]}) = E_P(1_{(-\infty,0]})$ for all $t \in \mathbb{R}^+$. Hence, since $\mathrm{sign} = \kappa_0 - 1_{(-\infty,0]} - 1_{(-\infty,0)}$, we find, for all $t \in \mathbb{R}^+$,

$$E_{V^t}(\mathrm{sign}) = E_P(\mathrm{sign}). \tag{322}$$

Moreover, since, on one hand, $E_P(\mathrm{sign})\mathrm{e}_1 \oplus 0 = E_P(\mathrm{sign})E_P(1_1)\mathrm{e}_1 \oplus 0 = \mathrm{e}_1 \oplus 0$ because $1_1\mathrm{sign} = 1_1$ and, on the other hand, $\mathrm{sign}(\bar{V}) = 0$, we arrive at

$$\mathrm{s}-\lim_{t\to\infty} \mathrm{sign}(V^t) \neq \mathrm{sign}(\bar{V}), \tag{323}$$

i.e., in general, Proposition 49 *(a)* does not hold if Assumption 48 *(a)* is not satisfied (see (229) at the end of the proof of Proposition 49 *(a)*).

The second example, introduced in [31], is a generalized form of the foregoing XY model. The corresponding local Hamiltonians in the fermionic and the spin picture are given in Appendix E.

Example 69 (Suzuki model) *Let $\nu \in \langle 1, n_S\rangle$, let $\{c_{2,n}\}_{n\in\langle 1,\nu\rangle} \subseteq \mathbb{R}$, and let $\{c_{3,n}\}_{n\in\langle 0,\nu\rangle} \subseteq \mathbb{R}$. The Suzuki model (also called generalized XY model or νXY model) is specified by*

$$h_0 = 0, \tag{324}$$

$$h_1 = 0, \tag{325}$$

$$h_2 = -2 \sum_{n\in\langle 1,\nu\rangle} c_{2,n} \mathrm{Im}(\theta^n), \tag{326}$$

$$h_3 = c_{3,0}1 + 2 \sum_{n\in\langle 1,\nu\rangle} c_{3,n} \mathrm{Re}(\theta^n). \tag{327}$$

Hence, Assumptions 14 (b) and (d) are satisfied. If at least one of the coefficients from $\{c_{2,n}\}_{n\in\langle 1,\nu\rangle}$ and $\{c_{3,n}\}_{n\in\langle 0,\nu\rangle}$ is different from zero, Assumptions 14 (e) also holds. Moreover, (324)-(327) *lead to $u_0 = u_1 = 0$, $u_2(k) = -2\sum_{n\in\langle 1,\nu\rangle} c_{2,n}\sin(nk)$, $u_3(k) = c_{3,0} + 2\sum_{n\in\langle 1,\nu\rangle} c_{3,n}\cos(nk)$ for all $k \in \mathbb{T}$, and Lemma 90 (b) yields the coefficients in* (273) *for (n_S sufficiently large and) $\nu = 2$,*

$$a_0 = 2(c_{2,1}^2 + c_{2,2}^2 + c_{3,1}^2 + c_{3,2}^2) + c_{3,0}^2, \tag{328}$$

$$a_1 = 2(c_{2,1}c_{2,2} + c_{3,1}(c_{3,0} + c_{3,2})), \tag{329}$$

$$a_2 = -c_{2,1}^2 + c_{3,1}^2 + 2c_{3,1}(c_{3,0} + c_{3,2}), \tag{330}$$

$$a_3 = -2(c_{2,1}c_{2,2} - c_{3,1}c_{3,2}), \tag{331}$$

$$a_4 = -c_{2,2}^2 + c_{3,2}^2, \tag{332}$$

and, for $\nu \geq 3$, the coefficients $a_0, \ldots, a_{2\nu}$ are given in Lemma 90 (c). Since we have $uu' = -\sum_{m\in\langle 1,2\nu\rangle} ma_m \sin(m\cdot)$, we get $uu' = 0$ (i.e., Case 1 occurs) if and only if $a_m = 0$ for all $m \in \langle 1, 2\nu\rangle$. The solutions of this system of 2ν multivariate homogeneous quadratic equations in $2\nu + 1$ variables specify the Suzuki models for which Assumption 48 (a) is not satisfied (for example, $c_{2,1} = c_{3,1} = 0$, $c_{2,2} = c_{3,2}$, and any $c_{3,0}$ for the $\nu = 2$ system given by (329)-(332)*). In all the other cases, Theorem 61 is applicable and, for all Fermi functions $\rho \in \mathcal{B}(\mathbb{R})$ and all inverse reservoir temperatures $\beta_L, \beta_R \in \mathbb{R}$, the R/L mover heat flux is again given by* (307)*.*

Finally, we want to discuss the following example.

Example 70 (Full range 1 model) *Let $\nu = 1$ and $\{c_{0,1}, c_{1,1}, c_{2,1}, c_{3,0}, c_{3,1}\} \subseteq \mathbb{R}$. The full range 1 model is specified by*

$$h_0 = -2c_{0,1}\mathrm{Im}(\theta), \tag{333}$$
$$h_1 = -2c_{1,1}\mathrm{Im}(\theta), \tag{334}$$
$$h_2 = -2c_{2,1}\mathrm{Im}(\theta), \tag{335}$$
$$h_3 = c_{3,0}1 + 2c_{3,1}\mathrm{Re}(\theta). \tag{336}$$

Hence, Assumptions 14 (b) and (d) are satisfied. If at least one of the coefficients from $\{c_{0,1}, c_{1,1}, c_{2,1}, c_{3,0}, c_{3,1}\}$ is different from zero, Assumptions 14 (e) also holds. Moreover, (333)-(336) *lead to $u_\alpha(k) = -2c_{\alpha,1}\sin(k)$ for all $\alpha \in \langle 0, 2\rangle$ and all $k \in \mathbb{T}$ and $u_3(k) = c_{3,0} + 2c_{3,1}\cos(k)$ for all $k \in \mathbb{T}$. Hence, Lemma 90 (b) yields the coefficients in* (273)*, i.e.,*

$$a_0 = 2(c_{1,1}^2 + c_{2,1}^2 + c_{3,1}^2) + c_{3,0}^2, \tag{337}$$
$$a_1 = 2c_{3,0}c_{3,1}, \tag{338}$$
$$a_2 = -(c_{1,1}^2 + c_{2,1}^2) + c_{3,1}^2. \tag{339}$$

Hence, Case 1 occurs if and only if $c_{3,0} = 0$ and $c_{1,1}^2 + c_{2,1}^2 = c_{3,1}^2 \neq 0$ or $c_{3,0} \neq 0$ and $c_{1,1} = c_{2,1} = c_{3,1} = 0$. Moreover, Case 6 occurs if and only if $c_{3,0} = 0$, $c_{3,1} = 0$, and $c_{1,1}^2 + c_{2,1}^2 = c_{0,1}^2 \neq 0$. In all the other cases, Theorem 61 is applicable and, for all Fermi functions $\rho \in \mathcal{B}(\mathbb{R})$ and all inverse reservoir temperatures $\beta_L, \beta_R \in \mathbb{R}$, the R/L mover heat flux is given by (307) *(in Case 2) and* (277) *(in Case 3, 4, and 5).*

For the following, recall the definitions of e, e', and Δ_{β_L,β_R} from Theorem 61 *(b)*.

Using the additional Assumption 20 *(a)* and *(c)* leads to the strict positivity of the R/L mover heat flux.

Theorem 71 (Nonvanishing heat flux) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (b), (d), and (e) and let the bounded extension $\bar{V} \in \mathcal{L}(\widehat{\mathfrak{H}})$ of the asymptotic velocity with respect to $\widehat{H}$ satisfy Assumption 48 (a). Moreover, let $u_0 \in L^\infty(\mathbb{T})$ and $u \in L^\infty(\mathbb{T})^3$ be the Pauli coefficient functions of $\widehat{H}$, and let $T \in \mathcal{L}(\mathfrak{H})$ be an R/L mover 2-point operator for H, for an initial 2-point operator $T_0 \in \mathcal{L}(\mathfrak{H})$, for a Fermi function $\rho \in \mathcal{B}(\mathbb{R})$, and for the inverse* *reservoir temperatures $\beta_L, \beta_R \in \mathbb{R}$. Moreover, let the Fermi function and the inverse temperatures satisfy Assumption 20 (a) and (c), respectively. Then, the heat flux in the R/L mover state $\omega_T \in \mathcal{E}_{\mathfrak{A}}$ is nonvanishing and the heat is flowing from the left to the right reservoir,*

$$J > 0. \tag{340}$$

Proof. Under Assumption 20 *(a)* and *(c)*, the difference $\Delta_{\beta_L,\beta_R} \circ |e|$ is nonnegative on $\mathbb{T}$ and strictly positive on $\mathcal{Z}_e^c$. Hence, in order for (340) to hold, it is sufficient to show that $\mathrm{card}(\mathcal{Z}_e) < \infty$ and $\mathrm{card}(\mathcal{Z}_{e'}) < \infty$ since, from (305), we have

$$J = \frac{1}{2} \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi}\, |e(k)e'(k)|\, \Delta_{\beta_L,\beta_R}(|e(k)|). \tag{341}$$

In order to do so, we use the same type of arguments as in the proof of Lemma 58.

Case 1 and 6 These cases are excluded due to Assumption 48 *(a)*.

Case 2 Since $e = |u|$ and $e' = \tilde{u}u'$, we have $\mathrm{card}(\mathcal{Z}_e) = \mathrm{card}(\mathcal{Z}_u) < \infty$ and $\mathrm{card}(\mathcal{Z}_{e'}) \leq \mathrm{card}(\mathcal{Z}_u) + \mathrm{card}(\mathcal{Z}_{uu'}) < \infty$ due to $uu' \neq 0$.

Case 3 Since $e = u_0$ and $e' = u_0'$, we have $\mathrm{card}(\mathcal{Z}_e) = \mathrm{card}(\mathcal{Z}_{u_0}) < \infty$ and $\mathrm{card}(\mathcal{Z}_{e'}) = \mathrm{card}(\mathcal{Z}_{u_0'}) < \infty$ because $u_0 = 0$ if and only if $u_0' = 0$.

Case 4 We have $e = u_0 + |u|$ and $e' = u_0'$. Suppose that there exists $M \subseteq \mathcal{Z}_u^c$ with $\mathrm{card}(M) = \infty$ such that $e = 0$ on M. It then follows that $p_0 = 0$ on M (see (271)) and, hence, $p_0 = 0$ (on $\mathbb{T}$). Since $u^2 = a_0 > 0$, we get $u_0^2 = a_0 > 0$ which contradicts $u_0 \neq 0$ (and $u_0' \neq 0$) due to (266). Hence, $\mathrm{card}(\mathcal{Z}_e) < \infty$. Moreover, since $e' = u_0'$ and since $u_0' \neq 0$, we also get $\mathrm{card}(\mathcal{Z}_{e'}) < \infty$.

Case 5 We have $e = u_0 + |u|$ and $e' = u_0' + \tilde{u}u'$. Suppose that there exists $M \subseteq \mathcal{Z}_u^c$ with $\mathrm{card}(M) = \infty$ such that $e = 0$ on M. It then follows, as in *Case 4*, that $p_0 = 0$ which contradicts $u_0^2 \neq u^2$ and, hence, $\mathrm{card}(\mathcal{Z}_e) < \infty$. Moreover, suppose also that there exists $M' \subseteq \mathcal{Z}_u^c$ with $\mathrm{card}(M') = \infty$ such that $e' = 0$ on M'. Hence, the third step of *Case 5* in the proof of Lemma 58 *(b)* implies $p_0 = 0$ and we again get a contradiction. Therefore, $\mathrm{card}(\mathcal{Z}_{e'}) < \infty$ holds, too. □

As an immediate consequence of the Theorem 71, we get the following corollary.

Corollary 72 (Strict positivity of the entropy production rate) *Under the conditions of Theorem 71, the entropy production rate in the R/L mover state is strictly positive,*

$$\sigma > 0. \tag{342}$$

Proof. Plug (341) into (238) and use (340). □

Remark 73 Since $[\widehat{H}](k)[P](k) = e(k)[P](k)$ for all $k \in \mathbb{T}$, where $P \in \mathcal{L}(\widehat{\mathfrak{H}})$ stems from Remark 64, we get $|e(k)| \leq |[\widehat{H}](k)|_0$ for all $k \in \mathbb{T}$, where $|\cdot|_0$ stands for the usual operator norm on $\mathbb{C}^{2\times 2}$ induced by the Euclidean vector norm on $\mathbb{C}^2$. Hence, since we know that $\|H\| = \|\widehat{H}\| = \operatorname{ess\,sup}_{k\in\mathbb{T}}|[\widehat{H}](k)|_0$ (see [13] for example), we have $|e(k)| \leq \|H\|$ for all $k \in \mathbb{T}$. Moreover, due Remark 21 and its consequence for the integral of the derivatives of monotonically increasing functions, ρ' exists almost everywhere in $[0, \beta_R\|H\|]$ and $\rho(\beta_R|e(k)|) - \rho(\beta_L|e(k)|) \geq \int_{\beta_L|e(k)|}^{\beta_R|e(k)|}\mathrm{d}x\,\rho'(x)$ for all $k \in \mathbb{T}$. Hence, under the conditions of Theorem 71 and the additional Assumption 20 *(b)*, (238) and (341) yield the strictly positive lower bound

$$\sigma \geq 2c\delta^2 \int_{-\pi}^{\pi} \frac{\mathrm{d}k}{2\pi}\, e(k)^2|e'(k)|. \tag{343}$$

A Spectral theory

In this appendix, we present a brief summary of the approach to spectral theory based on [18] (see also [19]). The spectral properties used in the foregoing sections are direct consequences of the following presentation or can be derived from it in a simple way. Since this approach is somewhat different from the more standard ones, we precisely state the first three claims without giving proofs (Proposition 76, Proposition 78, and Theorem 80 below). Subsequently, we rather explicitly carry out the implications of these claims in view of their applications to the foregoing sections.

In the following, let $\mathcal{H}$ stand for any separable complex Hilbert space and $\mathcal{L}(\mathcal{H})$ for the C*-algebra of bounded operators on $\mathcal{H}$. Moreover, equipped with the usual pointwise operations and with the norm given, for all $\chi \in \ell^\infty(\mathbb{R})$, by

$$|\chi|_\infty := \sup_{x\in\mathbb{R}} |\chi(x)|, \tag{344}$$

we denote by $\ell^\infty(\mathbb{R})$, $C_b(\mathbb{R})$, and $C_0(\mathbb{R})$ the C*-algebra of bounded complex-valued functions on $\mathbb{R}$, the C*-algebra of continuous bounded complex-valued functions on $\mathbb{R}$, and the (non complete) normed $*$-algebra of continuous complex-valued functions on $\mathbb{R}$ with compact support, respectively.

Definition 74 (Projection-valued measure) *A $*$-algebra homomorphism $E_0 : C_0(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ is called a projection valued measure.*

For the following, let $\kappa_0, \kappa_{-1} \in C_b(\mathbb{R})$ and $\kappa_1 \in C(\mathbb{R})$ be defined, for all $x \in \mathbb{R}$, by

$$\kappa_0(x) := 1, \tag{345}$$

$$\kappa_1(x) := x, \tag{346}$$

$$\kappa_{-1}(x) := \frac{1}{1+|x|}, \tag{347}$$

where $C(\mathbb{R})$ stands for the $*$-algebra of continuous complex-valued functions on $\mathbb{R}$ (equipped with the same pointwise operations as the foregoing functions spaces). Moreover, for some of the following notions, see also [20].

Definition 75 (Borel functions)

(a) *Let $\chi : \mathbb{R} \to \mathbb{C}$ and let $(\chi_n)_{n\in\mathbb{N}}$ be a sequence in $\ell^\infty(\mathbb{R})$. If there exists $C > 0$ such that $|\chi_n|_\infty \leq C$ for all $n \in \mathbb{N}$ and if $\lim_{n\to\infty} \chi_n(x) = \chi(x)$ for all $x \in \mathbb{R}$, we write*

$$\mathcal{B} - \lim_{n\to\infty} \chi_n = \chi, \tag{348}$$

and we say that $(\chi_n)_{n\in\mathbb{N}}$ is Borel convergent to $\chi \in \ell^\infty(\mathbb{R})$.

(b) *Let $\mathcal{F} \subseteq \ell^\infty(\mathbb{R})$ be a family of functions having the following properties:*

(B1) $C_0(\mathbb{R}) \subseteq \mathcal{F}$

(B2) *If $\chi \in \ell^\infty(\mathbb{R})$ and if $(\chi_n)_{n\in\mathbb{N}}$ in $\mathcal{F}$ is such that $\mathcal{B} - \lim_{n\to\infty} \chi_n = \chi$, then $\chi \in \mathcal{F}$.*

The smallest such $\mathcal{F}$, denoted by $\mathcal{B}(\mathbb{R})$, is called the family of bounded Borel functions. It is a normed unital $*$-algebra with unity κ_0, and $C_b(\mathbb{R}) \subseteq \mathcal{B}(\mathbb{R})$.

(c) *A set $M \subseteq \mathbb{R}$ is called a Borel set if $1_M \in \mathcal{B}(\mathbb{R})$. The σ-algebra of all Borel sets is denoted by $\mathcal{M}(\mathbb{R})$.*

Proposition 76 (Extension to Borel functions) *Let E_0 be a projection-valued measure.*

(a) *There exists a unique extension from E_0 to a $*$-algebra homomorphism $E : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ on $\mathcal{B}(\mathbb{R})$. Moreover, for all $\chi \in \mathcal{B}(\mathbb{R})$, we have*

$$\|E(\chi)\| \leq |\chi|_\infty, \tag{349}$$

and $E(\chi) \geq 0$ for all $\chi \in \mathcal{B}(\mathbb{R})$ with $\chi \geq 0$.

(b) *Let $(\chi_n)_{n\in\mathbb{N}}$ in $\mathcal{B}(\mathbb{R})$ be such that $\mathcal{B} - \lim_{n\to\infty} \chi_n = \chi$ for some $\chi \in \ell^\infty(\mathbb{R})$. Then, $\chi \in \mathcal{B}(\mathbb{R})$ and the extended projection-valued measure E from (a) satisfies*

$$\mathrm{s} - \lim_{n\to\infty} E(\chi_n) = E(\chi). \tag{350}$$

Proof. See [18] (and [19]). □

Definition 77 (Resolution of the identity) *A $*$-algebra homomorphism $E : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{H})$ is called a resolution of the identity if $E(\kappa_0) = 1$.*

Proposition 78 (Extension to the identity function) *Let E be a resolution of the identity and let the dense subspace $\mathcal{D}$ of $\mathcal{H}$ be defined by*

$$\mathcal{D} := \mathrm{ran}(E(\kappa_{-1})). \tag{351}$$

(a) *The operator* $\bar{E}(\kappa_1) : \mathcal{D} \to \mathcal{H}$*, defined, for all* $\psi \in \mathcal{H}$*, by*

$$\bar{E}(\kappa_1)E(\kappa_{-1})\psi := E(\kappa_1\kappa_{-1})\psi, \tag{352}$$

and suitably extended to the whole of $\mathcal{D}$*, is selfadjoint.*

(b) *For all* $\chi \in \mathcal{B}(\mathbb{R})$ *with* $\kappa_1\chi \in \mathcal{B}(\mathbb{R})$*, we have*

$$\bar{E}(\kappa_1)E(\chi) = E(\kappa_1\chi). \tag{353}$$

Proof. See [18] (and [19]). □

Remark 79 Since E is a resolution of the identity, the set $\mathcal{C} := \operatorname{span}\{E(\chi)\psi \,|\, \chi \in C_0(\mathbb{R}), \psi \in \mathcal{H}\}$ is dense in $\mathcal{H}$. For all $\eta \in C(\mathbb{R})$, defining the operator $\mathcal{E}(\eta)$ on $\mathcal{C}$ by $\mathcal{E}(\eta)E(\chi)\psi := E(\eta\chi)\psi$ for all $\chi \in C_0(\mathbb{R})$, the map $C(\mathbb{R}) \ni \eta \mapsto \mathcal{E}(\eta)$ satisfies $\mathcal{E}(\eta)\mathcal{C} \subseteq \mathcal{C}$ and, on $\mathcal{C}$, preserves the linear operations and the multiplication. Moreover, we have $\mathcal{E}(\bar{\eta}) \subseteq \mathcal{E}(\eta)^*$ for all $\eta \in C(\mathbb{R})$. Therefore, $\mathcal{E}(\eta)$ is closable for all $\eta \in C(\mathbb{R})$ and the closure of $\mathcal{E}(\eta)$ defines an extension of E to $C(\mathbb{R})$ which preserves the $*$-operation.

In the following, $\mathcal{S}(\mathbb{R})$ stands for the usual Schwartz space of rapidly decreasing functions on $\mathbb{R}$. Note that $\mathcal{S}(\mathbb{R}) \subseteq C_b(\mathbb{R}) \subseteq \mathcal{B}(\mathbb{R})$. Moreover, using the same notation as the one introduced before (137), the Fourier transform of $\chi \in \mathcal{S}(\mathbb{R})$ is denoted by $\hat{\chi} \in \mathcal{S}(\mathbb{R})$ and we use the convention $\hat{\chi}(t) := \int_{\mathbb{R}} \mathrm{d}x\, \chi(x)\mathrm{e}^{-\mathrm{i}tx}/\sqrt{2\pi}$ for all $t \in \mathbb{R}$.

Theorem 80 (Spectral theorem) *Let* A *be a (not necessarily bounded) selfadjoint linear operator on* $\mathcal{H}$*.*

(a) *There exists a unique resolution of the identity* E *such that* $A = \bar{E}(\kappa_1)$*.*

(b) *On* $\mathcal{S}(\mathbb{R})$*, the resolution of the identity* E *from (a) can be expressed as an inverse Fourier transform, i.e., for all* $\chi \in \mathcal{S}(\mathbb{R})$ *and all* $\psi \in \mathcal{H}$*, we have*

$$E(\chi)\psi = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} \mathrm{d}t\, \hat{\chi}\,(t)\mathrm{e}^{\mathrm{i}tA}\psi, \tag{354}$$

where the integral is defined as a Hilbert space-valued improper Riemann integral. Moreover, the strongly continuous unitary 1-parameter group generated by A *(through Stone's theorem) satisfies* $\mathrm{e}^{\mathrm{i}tA} = E(\mathrm{e}_t)$ *for all* $t \in \mathbb{R}$*, where* $\mathrm{e}_t \in C_b(\mathbb{R})$ *is given by* $\mathrm{e}_t(x) := \mathrm{e}^{\mathrm{i}tx}$ *for all* $t, x \in \mathbb{R}$*.*

Proof. See [18] (and [19]). □

In the following, if we need to display the dependence on A, we sometimes use the notation $\chi(A) := E(\chi)$ or $E_A(\chi) := E(\chi)$ for all $\chi \in \mathcal{B}(\mathbb{R})$. Moreover, for all (not necessarily bounded) selfadjoint linear operators A on $\mathcal{H}$, we denote by $\operatorname{dom}(A)$ the domain of A.

Remark 81 Note that $C_0^\infty(\mathbb{R}) \subseteq \mathcal{S}(\mathbb{R})$ and that the resolution of the identity is already uniquely determined by its restriction to $C_0^\infty(\mathbb{R})$ since $C_0^\infty(\mathbb{R})$ is dense in $C_0(\mathbb{R})$ with respect to the norm (344) and since (349) holds.

In the following, if $\mathcal{H}$ and $\mathcal{K}$ are complex Hilbert spaces, $\mathcal{D} \subseteq \mathcal{H}$ and $A : \mathcal{H} \to \mathcal{K}$ a bounded linear operator, we set $A\mathcal{D} := \{A\Psi \,|\, \Psi \in \mathcal{D}\} \subseteq \mathcal{K}$.

A first application of this formalism, used in the foregoing sections, is the following standard property.

Lemma 82 (Identification) *Let $\mathcal{H}$ and $\mathcal{K}$ be separable complex Hilbert spaces, let A a (not necessarily bounded) selfadjoint operator on $\mathcal{H}$, and let $U : \mathcal{H} \to \mathcal{K}$ be unitary. Then:*

(a) The operator $B : \mathrm{dom}(B) \subseteq \mathcal{K} \to \mathcal{K}$, defined by $\mathrm{dom}(B) := U\mathrm{dom}(A)$ and $B\Phi := UAU^*\Phi$ for all $\Phi \in \mathrm{dom}(B)$, is selfadjoint.

(b) The map $E^U : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathcal{K})$, defined by $E^U(\chi) := UE_A(\chi)U^*$ for all $\chi \in \mathcal{B}(\mathbb{R})$, satisfies $E^U = E_B$.

Proof. (a) Since B is densely defined and symmetric, and since, due to the standard criterion for selfadjointness, $\mathrm{ran}\,(B \pm \mathrm{i}1) = U\mathrm{ran}\,(A \pm \mathrm{i}1) = U\mathcal{H} = \mathcal{K}$, the operator B is selfadjoint.

(b) Note that E^U is a resolution of the identity. Moreover, $\mathrm{dom}(\bar{E}^U(\kappa_1)) = \mathrm{ran}\,(E^U(\kappa_{-1})) = U\mathrm{ran}\,(E_A(\kappa_{-1})) = U\mathrm{dom}(A) = \mathrm{dom}(B)$, where we used that $\mathrm{dom}(A) = \mathrm{ran}\,((A - \mathrm{i}1)^{-1}) = \mathrm{ran}\,(E_A(\kappa_{-1}))$. Hence, for all $\Phi \in \mathrm{dom}(B)$, there exists $\Psi \in \mathcal{H}$ such that $\Phi = E^U(\kappa_{-1})\Psi$ and, from (352) and Theorem 80 *(a)*, we get

$$\begin{aligned} \bar{E}^U(\kappa_1)\Phi &= \bar{E}^U(\kappa_1)E^U(\kappa_{-1})\Psi \\ &= E^U(\kappa_1\kappa_{-1})\Psi \\ &= UE_A(\kappa_1\kappa_{-1})U^*\Psi \\ &= U\bar{E}_A(\kappa_1)U^*E^U(\kappa_{-1})\Psi \\ &= B\Phi. \end{aligned} \tag{355}$$

The uniqueness property of the resolution of the identity from Theorem 80 *(a)* then yields the conclusion. □

In the following, we also denote by ζ the operation of complex conjugation from Definition 1 *(b)* when applied to $\chi \in \ell^\infty(\mathbb{R})$. Moreover, let $\ell^\infty(\mathbb{R}, \mathbb{R})$, $C_0(\mathbb{R}, \mathbb{R})$, and $\mathcal{B}(\mathbb{R}, \mathbb{R})$ stand for the bounded real-valued functions on $\mathbb{R}$, the continuous real-valued functions on $\mathbb{R}$ with compact support, and the smallest family of functions satisfying the conditions *(B1')* and *(B2')*, respectively, where *(B1')* and *(B2')* stand for the modified conditions *(B1)* and *(B2)* from Definition 75 *(b)* in which $\ell^\infty(\mathbb{R})$, $C_0(\mathbb{R})$, and $\mathcal{B}(\mathbb{R})$ have been replaced by $\ell^\infty(\mathbb{R}, \mathbb{R})$, $C_0(\mathbb{R}, \mathbb{R})$, and $\mathcal{B}(\mathbb{R}, \mathbb{R})$, respectively.

Lemma 83 (Spectral identities) *Let $A \in \mathcal{L}(\mathfrak{H})$ be selfadjoint and $\chi \in \mathcal{B}(\mathbb{R})$. Then:*

(a) $\Gamma\chi(A)\Gamma = (\zeta\chi)(\Gamma A\Gamma)$

(b) $\chi(\psi(A)) = (\chi \circ \psi)(A)$ *for all* $\psi \in \mathcal{B}(\mathbb{R}, \mathbb{R})$

(c) *For all orthogonal families of orthogonal projections* $\{P, Q\} \subseteq \mathcal{L}(\mathfrak{H})$ *satisfying* $[P, A] = [Q, A] = 0$ *and all* $r, s \in \mathbb{R}$*, we have*

$$\chi(rAP + sAQ)(P + Q) = \chi(rA)P + \chi(sA)Q. \tag{356}$$

(d) *If* $B \in \mathcal{L}(\mathfrak{H})$ *is selfadjoint,* $[A, B] = 0$*, and* $\psi \in \mathcal{B}(\mathbb{R})$*, we have*

$$[\chi(A), \psi(B)] = 0. \tag{357}$$

Remark 84 On the right hand side of the equations in Lemma 83 *(a)* and *(b)*, we used that $\zeta\chi \in \mathcal{B}(\mathbb{R})$ for all $\chi \in \mathcal{B}(\mathbb{R})$ and $\chi \circ \psi \in \mathcal{B}(\mathbb{R})$ for all $\chi \in \mathcal{B}(\mathbb{R})$ and all $\psi \in \mathcal{B}(\mathbb{R}, \mathbb{R})$, respectively. In order to verify these properties, we make use of the following recurrent argument which we detail for the slightly more involved case *(b)* only. So, let $\chi \in C_0(\mathbb{R})$ be fixed and set

$$\mathcal{F}_\chi := \{\psi \in \ell^\infty(\mathbb{R}, \mathbb{R}) \,|\, \chi \circ \psi \in \mathcal{B}(\mathbb{R})\}. \tag{358}$$

Since $\chi \circ \psi \in C_0(\mathbb{R})$ for all $\psi \in C_0(\mathbb{R}, \mathbb{R})$, we have $C_0(\mathbb{R}, \mathbb{R}) \subseteq \mathcal{F}_\chi$, i.e., $\mathcal{F}_\chi$ satisfies *(B1')*. Moreover, let $(\psi_n)_{n\in\mathbb{N}}$ be a sequence in $\mathcal{F}_\chi$ with $\mathcal{B} - \lim_{n\to\infty} \psi_n = \psi$ for some $\psi \in \ell^\infty(\mathbb{R}, \mathbb{R})$. Since $\chi \circ \psi_n \in \mathcal{B}(\mathbb{R})$ for all $n \in \mathbb{N}$ and since $\mathcal{B} - \lim_{n\to\infty} \chi \circ \psi_n = \chi \circ \psi$ because $\chi \in C_0(\mathbb{R})$, we get $\chi \circ \psi \in \mathcal{B}(\mathbb{R})$ (since $\mathcal{B}(\mathbb{R})$ satisfies *(B2)*), i.e., $\mathcal{F}_\chi$ satisfies *(B2')*. Hence, $\mathcal{B}(\mathbb{R}, \mathbb{R}) \subseteq \mathcal{F}_\chi$. Next, let $\psi \in \mathcal{B}(\mathbb{R}, \mathbb{R})$ be fixed and set

$$\mathcal{G}_\psi := \{\chi \in \ell^\infty(\mathbb{R}) \,|\, \chi \circ \psi \in \mathcal{B}(\mathbb{R})\}. \tag{359}$$

Since $\mathcal{B}(\mathbb{R}, \mathbb{R}) \subseteq \mathcal{F}_\chi$ for all $\chi \in C_0(\mathbb{R})$, the family $\mathcal{G}_\psi$ satisfies *(B1)*. Moreover, let $(\chi_n)_{n\in\mathbb{N}}$ be a sequence in $\mathcal{G}_\psi$ with $\mathcal{B} - \lim_{n\to\infty} \chi_n = \chi$ for some $\chi \in \ell^\infty(\mathbb{R})$. Hence, we get $\mathcal{B} - \lim_{n\to\infty} \chi_n \circ \psi = \chi \circ \psi$ and $\chi \circ \psi \in \mathcal{B}(\mathbb{R})$, i.e., $\mathcal{G}_\psi$ satisfies *(B2)*, too. Therefore, we arrive at $\mathcal{B}(\mathbb{R}) \subseteq \mathcal{G}_\psi$ for all $\psi \in \mathcal{B}(\mathbb{R}, \mathbb{R})$.

Remark 85 Due to the fact that $E_A(1_{\mathrm{spec}(A)}) = 1$ for all selfadjoint operators $A \in \mathcal{L}(\mathcal{H})$, where $\mathrm{spec}(A) \in \mathcal{M}(\mathbb{R})$ is a (non-empty) compact subset of $\mathbb{R}$, (353) yields $A = E_A(\kappa_1 1_{\mathrm{spec}(A)})$ because $\kappa_1 1_{\mathrm{spec}(A)} \in \mathcal{B}(\mathbb{R})$ since $1_{\mathrm{spec}(A)} = 1_{[-a,a]} 1_{\mathrm{spec}(A)}$ with $a := \|A\|$ and since $\kappa_1 1_{[-a,a]} \in \mathcal{B}(\mathbb{R})$ (being the limit of a Borel convergent sequence of functions in $C_0(\mathbb{R})$). Since $rA = E_A(\psi)$ with $\psi := r\kappa_1 1_{\mathrm{spec}(A)} \in \mathcal{B}(\mathbb{R})$ for all $r \in \mathbb{R}$, Lemma 83 *(b)* yields

$$\chi(rA) = \chi_r(A), \tag{360}$$

where we define $\chi_r(x) := \chi(rx)$ for all $\chi \in \ell^\infty(\mathbb{R})$ and all $r, x \in \mathbb{R}$, and $\chi_r \in \mathcal{B}(\mathbb{R})$ for all $\chi \in \mathcal{B}(\mathbb{R})$ and all $r \in \mathbb{R}$ (by arguing as in Remark 84). Note that, using (354), a change of variables, Remark 81, and a minimality type argument as in Remark 84 (see also the proof of Lemma 83 *(c)* and *(d)* below), (360) also holds for unbounded selfadjoint operators.

We next turn to the proof of Lemma 83. For illustration, we use the uniqueness type argument (as in the proof of Lemma 82 *(b)*) for *(a)* and *(b)* and the minimality type argument (as in Remark 84) for *(c)* and *(d)*.

Proof. (a) Let us define the map $E^\Gamma : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathfrak{H})$ by $E^\Gamma(\chi) := \Gamma E_A(\zeta\chi)\Gamma$ for all $\chi \in \mathcal{B}(\mathbb{R})$. In order to show that $E^\Gamma = E_{\Gamma A\Gamma}$, we first note that E^Γ is a resolution of the identity because $\Gamma \in \bar{\mathcal{L}}(\mathfrak{H})$ is an antiunitary involution. Moreover, we have $\mathrm{dom}(\bar{E}^\Gamma(\kappa_1)) = \mathrm{ran}\,(E^\Gamma(\kappa_{-1})) = \Gamma\mathrm{ran}\,(E_A(\kappa_{-1})) = \Gamma\mathrm{dom}(A) = \mathfrak{H}$. Hence, for all $F \in \mathfrak{H}$, there exists $G \in \mathfrak{H}$ such that $F = E^\Gamma(\kappa_{-1})G$ and we compute that $\bar{E}^\Gamma(\kappa_1)F = \Gamma A\Gamma F$ as in (355). Theorem 80 *(a)* then implies that $\Gamma E_A(\zeta\chi)\Gamma = E_{\Gamma A\Gamma}(\chi)$ for all $\chi \in \mathcal{B}(\mathbb{R})$.

(b) Let $\psi \in \mathcal{B}(\mathbb{R},\mathbb{R})$ and define the map $E^\psi : \mathcal{B}(\mathbb{R}) \to \mathcal{L}(\mathfrak{H})$ by $E^\psi(\chi) := E_A(\chi \circ \psi)$ for all $\chi \in \mathcal{B}(\mathbb{R})$. It then follows that E^ψ is a resolution of the identity and that $\mathrm{dom}(\bar{E}^\psi(\kappa_1)) = \mathrm{ran}\,(E^\psi(\kappa_{-1})) = \mathrm{ran}\,(E_A(\kappa_{-1} \circ \psi))$. Moreover, since $\mathfrak{H} = \mathrm{dom}(A) = \mathrm{ran}\,((A - \mathrm{i}1)^{-1})$ and since $\mathrm{ran}\,((A-\mathrm{i}1)^{-1}) \subseteq \mathrm{ran}\,(E_A(\kappa_{-1} \circ \psi))$ due to the fact that $(A-\mathrm{i}1)^{-1} = E_A((\kappa_1 - \mathrm{i})^{-1}) = E_A((\kappa_{-1}\circ\psi)(\kappa_1-\mathrm{i})^{-1}(\kappa_{-1}\circ\psi)^{-1})$ and $(\kappa_1-\mathrm{i})^{-1}(\kappa_{-1}\circ\psi)^{-1} \in \mathcal{B}(\mathbb{R})$, we get $\mathrm{dom}(\bar{E}^\psi(\kappa_1)) = \mathfrak{H}$. Hence, for all $F \in \mathfrak{H}$, there exists $G \in \mathfrak{H}$ such that $F = E^\psi(\kappa_{-1})G$ and we compute that $\bar{E}^\psi(\kappa_1)F = \psi(A)F$.

(c) Let $r, s \in \mathbb{R}$ be fixed and note that $rAP + sAQ \in \mathcal{L}(\mathfrak{H})$ is selfadjoint. Moreover, since $[AP, AQ] = 0$, we have $\mathrm{e}^{\mathrm{i}t(rAP+sAQ)} = \mathrm{e}^{\mathrm{i}trAP}\mathrm{e}^{\mathrm{i}tsAQ} = \mathrm{e}^{\mathrm{i}trA}P + \mathrm{e}^{\mathrm{i}tsA}Q + 1 - (P+Q)$ for all $t \in \mathbb{R}$, where we used the (in $\mathcal{L}(\mathfrak{H})$ converging) exponential series for the propagators. Hence, for all $\chi \in \mathcal{S}(\mathbb{R})$, (354) leads to

$$E_{rAP+sAQ}(\chi) = E_{rA}(\chi)P + E_{sA}(\chi)Q + \chi(0)(1 - (P+Q)). \tag{361}$$

Next, let $\chi \in C_0(\mathbb{R})$ and let $(\chi_n)_{n\in\mathbb{N}}$ be a sequence in $C_0^\infty(\mathbb{R}) \subseteq \mathcal{S}(\mathbb{R})$ which converges to χ with respect to the norm (344) (such a sequence exists due to Remark 81). Since $E_{rAP+sAQ}(\chi) - (E_{rA}(\chi)P + E_{sA}(\chi)Q + \chi(0)(1-(P+Q))) = E_{rAP+sAQ}(\chi - \chi_n) + E_{rA}(\chi_n - \chi)P + E_{sA}(\chi_n - \chi)Q + (\chi_n(0) - \chi(0))(1-(P+Q))$, (349) yields the estimate $\|E_{rAP+sAQ}(\chi) - (E_{rA}(\chi)P + E_{sA}(\chi)P + \chi(0)(1-(P+Q)))\| \le 2(1 + \|P\| + \|Q\|)|\chi - \chi_n|_\infty$. Hence, (361) also holds for all $\chi \in C_0(\mathbb{R})$. In order to show that (361) holds for all $\chi \in \mathcal{B}(\mathbb{R})$, too, we set

$$\mathcal{F} := \{\chi \in \mathcal{B}(\mathbb{R}) \,|\, E_{rAP+sAQ}(\chi) = E_{rA}(\chi)P + E_{sA}(\chi)Q + \chi(0)(1-(P+Q))\}, \tag{362}$$

and $\mathcal{F}$ satisfies *(B1)* from Defintion 75 *(b)*. Next, let $(\chi_n)_{n\in\mathbb{N}}$ be a sequence in $\mathcal{F}$ with $\mathcal{B}-\lim_{n\to\infty}\chi_n = \chi$ for some $\chi \in \ell^\infty(\mathbb{R})$. Since $\chi_n \in \mathcal{B}(\mathbb{R})$ for all $n \in \mathbb{N}$ and since $\mathcal{B}(\mathbb{R})$ satisfies *(B2)*, we have $\chi \in \mathcal{B}(\mathbb{R})$. Moreover, (350) yields $\mathrm{s}-\lim_{n\to\infty} E_{rAP+sAQ}(\chi_n) = E_{rAP+sAQ}(\chi)$, the analogous properties hold for $E_{rA}(\chi_n)P$ and $E_{sA}(\chi_n)Q$, and $\lim_{n\to\infty}\chi_n(0)(1-(P+Q))F = \chi(0)(1-(P+Q))F$ for all $F \in \mathfrak{H}$ since $(\chi_n)_{n\in\mathbb{N}}$ is pointwise convergent. Hence, $\mathcal{F}$ also satisfies *(B2)*. Therefore, we get $\mathcal{B}(\mathbb{R}) \subseteq \mathcal{F}$, i.e., (361) holds for all $\chi \in \mathcal{B}(\mathbb{R})$. Multiplying (361) from the right by $P + Q$ yields (356).

(d) For all $\chi \in \mathcal{S}(\mathbb{R})$, (354) yields

$$[E_A(\chi), B] = 0. \tag{363}$$

Now, let $\chi \in C_0(\mathbb{R})$ and let $(\chi_n)_{n\in\mathbb{N}}$ be a sequence in $C_0^\infty(\mathbb{R})$ which converges to χ with respect to the norm (344). Hence, since $[E_A(\chi), B] = [E_A(\chi - \chi_n), B]$ for all $n \in \mathbb{N}$, (349) yields $\|[E_A(\chi), B]\| \leq 2\|B\||\chi - \chi_n|_\infty$, i.e., (363) also holds for all $\chi \in C_0(\mathbb{R})$. In order to show that (363) holds for all $\chi \in \mathcal{B}(\mathbb{R})$, too, we set

$$\mathcal{F} := \{\chi \in \mathcal{B}(\mathbb{R}) \,|\, [E_A(\chi), B] = 0\}, \tag{364}$$

and $\mathcal{F}$ satisfies *(B1)*. In order to verify *(B2)*, let $(\chi_n)_{n\in\mathbb{N}}$ be a sequence in $\mathcal{F}$ with $\mathcal{B} - \lim_{n\to\infty} \chi_n = \chi$ for some $\chi \in \ell^\infty(\mathbb{R})$. Hence, $\chi \in \mathcal{B}(\mathbb{R})$ and, writing again $[E_A(\chi), B] = [E_A(\chi - \chi_n), B]$ for all $n \in \mathbb{N}$, we get $\|[E_A(\chi), B]F\| \leq \|E_A(\chi - \chi_n)BF\| + \|B\|\|E_A(\chi - \chi_n)F\|$ for all $F \in \mathfrak{H}$ and all $n \in \mathbb{N}$. Therefore, due to (350), we get $\chi \in \mathcal{F}$, i.e., $\mathcal{F}$ also satisfies *(B2)* which implies $\mathcal{B}(\mathbb{R}) \subseteq \mathcal{F}$ (note that we did not use the selfadjointness of B yet). In order to show (357), we get, as for (363), for fixed $\chi \in \mathcal{B}(\mathbb{R})$ and all $\psi \in \mathcal{S}(\mathbb{R})$,

$$[E_A(\chi), E_B(\psi)] = 0. \tag{365}$$

Then, proceeding as before, (365) holds for all $\psi \in C_0(\mathbb{R})$. Finally, setting $\mathcal{G} := \{\psi \in \mathcal{B}(\mathbb{R}) \,|\, [E_A(\chi), E_B(\psi)] = 0\}$, we verify that $\mathcal{G}$ satisfies *(B1)* and *(B2)* and get $\mathcal{B}(\mathbb{R}) \subseteq \mathcal{G}$. □

B Matrix multiplication operators

In this appendix, we derive the properties of matrix multiplication operators in momentum space used in the foregoing sections.

In the following, we make use of the notation introduced after Assumption 40 and of the spectral theory from Appendix A. Moreover, $\operatorname{sinc} \in C^\infty(\mathbb{R})$ (the infinitely differentiable complex valued functions on $\mathbb{R}$) stands for the usual cardinal sine function defined by $\operatorname{sinc}(x) := \sin(x)/x$ for all $x \in \mathbb{R} \setminus \{0\}$ and $\operatorname{sinc}(0) := 1$.

Proposition 86 (Functional calculus) *Let $u_0 \in L^\infty(\mathbb{T})$ and $u := [u_1, u_2, u_3] \in L^\infty(\mathbb{T})^3$ satisfy Assumption 40 (a) and define $U \in \mathcal{L}(\widehat{\mathfrak{H}})$ by $U := m[u_0]\sigma_0 + m[u]\sigma$. Then:*

(a) For all $t \in \mathbb{R}$, we have

$$\mathrm{e}^{\mathrm{i}tU} = m[p_0^t]\sigma_0 + m[p^t]\sigma, \tag{366}$$

where, for all $t \in \mathbb{R}$, we define $p_0^t \in L^\infty(\mathbb{T})$ and $p^t \in L^\infty(\mathbb{T})^3$ by

$$p_0^t := \exp\circ(\mathrm{i}tu_0)\cos\circ(t|u|), \tag{367}$$

$$p^t := \mathrm{i}t\exp\circ(\mathrm{i}tu_0)\operatorname{sinc}\circ(t|u|)u. \tag{368}$$

(b) For all $\chi \in \mathcal{B}(\mathbb{R})$, we have

$$\chi(U) = m[v_0]\sigma_0 + m[v]\sigma, \tag{369}$$

where $v_0 \in L^\infty(\mathbb{T})$ *and* $v \in L^\infty(\mathbb{T})^3$ *are given by*

$$v_0 := \frac{1}{2}\left(\chi \circ e_+ + \chi \circ e_-\right), \tag{370}$$

$$v := \frac{1}{2}\left(\chi \circ e_+ - \chi \circ e_-\right)\tilde{u}, \tag{371}$$

and we recall that $e_\pm = u_0 \pm |u| \in L^\infty(\mathbb{T})$*.*

Proof. (a) We first note that, due to Assumption 40 *(a)* and Remark 45, we have $U^* = U$. For the following, let $t \in \mathbb{R}$ be fixed. Since $m[u_0]\sigma_0, m[u]\sigma \in \mathcal{L}(\widehat{\mathfrak{H}})$ and since $[m[u_0]\sigma_0, m[u_\alpha]\sigma_\alpha] = 0$ for all $\alpha \in \langle 1, 3\rangle$, we have $\mathrm{e}^{\mathrm{i}tU} = \mathrm{e}^{\mathrm{i}tm[u_0]\sigma_0}\mathrm{e}^{\mathrm{i}tm[u]\sigma}$ and $\mathrm{e}^{\mathrm{i}tm[u]\sigma} = \lim_{N\to\infty} P_N$, where, for all $N \in \mathbb{N}$, we set $P_N := \sum_{n\in\langle 0,N\rangle} (\mathrm{i}t)^n/(n!)(m[u]\sigma)^n \in \mathcal{L}(\widehat{\mathfrak{H}})$ and the limit exists with respect to the uniform topology on $\mathcal{L}(\widehat{\mathfrak{H}})$. Moreover, since, due to (7), we have $(m[u]\sigma)^{2n} = m[|u|^{2n}]\sigma_0$ and $(m[u]\sigma)^{2n+1} = m[|u|^{2n}u]\sigma$ for all $n \in \mathbb{N}$, we can write $P_N = C_N + S_N$, where $C_N, S_N \in \mathcal{L}(\widehat{\mathfrak{H}})$ are defined by $C_N := \sum_{n\in\langle 0,N\rangle}(-1)^n t^{2n}/((2n)!)(m[|u|^{2n}]\sigma_0)$ and $S_N := \mathrm{i}\sum_{n\in\langle 0,N\rangle}(-1)^n t^{2n+1}/((2n+1)!)(m[|u|^{2n}u]\sigma)$ for all $N \in \mathbb{N}$. Since, for all $\Phi = \varphi_1 \oplus \varphi_2 \in \widehat{\mathfrak{H}}$ and all $N \in \mathbb{N}$, we have $\|m[\cos\circ(t|u|)]\sigma_0\Phi - C_N\Phi\|^2 = \sum_{i\in\langle 1,2\rangle}\int_{-\pi}^{\pi}\mathrm{d}k/(2\pi)|f_i^N(k)|^2$, where, for all $i \in \langle 1, 2\rangle$ and all $N \in \mathbb{N}$, the function $f_i^N \in \hat{\mathfrak{h}}$ is defined by

$$f_i^N := \cos\circ(t|u|)\varphi_i - \sum_{n\in\langle 0,N\rangle}\frac{(-1)^n t^{2n}}{(2n)!}|u|^{2n}\varphi_i, \tag{372}$$

and since, for all $i \in \langle 1, 2\rangle$ and almost all $k \in \mathbb{T}$, we have that $\lim_{N\to\infty} f_i^N(k) = 0$ and $|f_i^N|^2 \le \cosh^2(|t|\||u|\|_\infty)|\varphi_i|^2 \in L^1(\mathbb{T})$, Lebesgue's dominated convergence theorem implies $\mathrm{s}-\lim_{N\to\infty} C_N = m[\cos\circ(t|u|)]\sigma_0$. Moreover, since $(C_N)_{N\in\mathbb{N}}$ is a Cauchy sequence with respect to the uniform topology on $\mathcal{L}(\widehat{\mathfrak{H}})$, we get $\lim_{N\to\infty} C_N = m[\cos\circ(t|u|)]\sigma_0$ in $\mathcal{L}(\widehat{\mathfrak{H}})$. Finally, for all $\Phi = \varphi_1 \oplus \varphi_2 \in \widehat{\mathfrak{H}}$ and all $N \in \mathbb{N}$, we have $\|m[\mathrm{i}t\,\mathrm{sinc}\circ(t|u|)u]\sigma\Phi - S_N\Phi\|^2 \le 3\sum_{i\in\langle 1,2\rangle}\sum_{\alpha\in\langle 1,3\rangle}\int_{-\pi}^{\pi}\mathrm{d}k/(2\pi)|g_{i,\alpha}^N(k)|^2$, where, for all $i \in \langle 1, 2\rangle$, all $\alpha \in \langle 1, 3\rangle$, and all $N \in \mathbb{N}$, the function $g_{i,\alpha}^N \in \hat{\mathfrak{h}}$ is defined by $g_{i,\alpha}^N := \mathrm{i}t\,\mathrm{sinc}\circ(t|u|)u_\alpha\varphi_i - \mathrm{i}\sum_{n\in\langle 0,N\rangle}(-1)^n t^{2n+1}/((2n+1)!)|u|^{2n}u_\alpha\varphi_i$. Hence, the contribution S_N can be treated analogously to C_N.

(b) Let $\chi \in \mathcal{S}(\mathbb{R})$ and plug (366)-(368) into (354). Then, for all $\Phi = \varphi_1 \oplus \varphi_2 \in \widehat{\mathfrak{H}}$, we get

$$E_U(\chi)\Phi = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\mathrm{d}t\, f_1^t \oplus f_2^t + \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}}\mathrm{d}t\,(g_{1,3}^t + g_{2,1}^t - \mathrm{i}g_{2,2}^t) \oplus (g_{1,1}^t + \mathrm{i}g_{1,2}^t - g_{2,3}^t), \tag{373}$$

where, for all $i \in \langle 1, 2\rangle$ and all $\alpha \in \langle 1, 3\rangle$, the maps $f_i : \mathbb{R} \to \hat{\mathfrak{h}}$ and $g_{i,\alpha} : \mathbb{R} \to \hat{\mathfrak{h}}$ are defined, for all $t \in \mathbb{R}$, by

$$f_i^t := \hat{\chi}(t)\exp\circ(\mathrm{i}tu_0)\cos\circ(t|u|)\varphi_i, \tag{374}$$

$$g_{i,\alpha}^t := \mathrm{i}t\hat{\chi}(t)\exp\circ(\mathrm{i}tu_0)\,\mathrm{sinc}\circ(t|u|)u_\alpha\varphi_i, \tag{375}$$

and we note that $f_i, g_{i,\alpha} \in C(\mathbb{R}, \hat{\mathfrak{h}})$ for all $i \in \langle 1,2\rangle$ and all $\alpha \in \langle 1,3\rangle$. Using the analogous arguments as the ones which lead to (202) in the proof of Proposition 46 *(a)*, we get

$$\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \mathrm{d}t\, f_i^t = \frac{1}{2}\,(\chi\circ(u_0+|u|)+\chi\circ(u_0-|u|))\varphi_i, \tag{376}$$

$$\begin{aligned}\frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} \mathrm{d}t\, g_{i,\alpha}^t &= \begin{cases}\frac{1}{2}\,(\chi\circ(u_0+|u|)-\chi\circ(u_0-|u|))\frac{u_\alpha}{|u|}\varphi_i, & \text{on } \mathcal{Z}_u^c,\\ 0, & \text{on } \mathcal{Z}_u,\end{cases}\\ &= \frac{1}{2}\,(\chi\circ(u_0+|u|)-\chi\circ(u_0-|u|))\tilde{u}_\alpha\varphi_i,\end{aligned} \tag{377}$$

where we used Euler's formula, the fact that Fourier transform is a bijection on $\mathcal{S}(\mathbb{R})$, and the notation (152). Hence, (369)-(371) holds for all $\chi \in \mathcal{S}(\mathbb{R})$. We next proceed by using the minimality type argument (as in Remark 84). To this end, let $\chi \in C_0(\mathbb{R})$ and let $(\chi_n)_{n\in\mathbb{N}}$ be a sequence in $C_0^\infty(\mathbb{R})$ which converges to χ with respect to the norm (344). Hence, we can write, for all $\Phi \in \widehat{\mathfrak{H}}$ and all $n \in \mathbb{N}$,

$$E_U(\chi)\Phi - (m[v_0]\sigma_0 + m[v]\sigma)\Phi = E_U(\chi-\chi_n)\Phi + (m[v_0(\chi_n-\chi)]\sigma_0 + m[v(\chi_n-\chi)]\sigma)\Phi, \tag{378}$$

where, for all $\chi \in \mathcal{B}(\mathbb{R})$, we denote (370) and (371) by $v_0(\chi)$ and $v(\chi)$, respectively. Due to (349), the first term on the right hand side of (378) is bounded by $\|E_U(\chi-\chi_n)\Phi\| \le |\chi-\chi_n|_\infty\|\Phi\|$ for all $\Phi \in \widehat{\mathfrak{H}}$ and all $n \in \mathbb{N}$. In order to estimate the second and third term in (378), we note that $\|v_0(\chi_n-\chi)\|_\infty \le (\|(\chi_n-\chi)\circ(u_0+|u|)\|_\infty + \|(\chi_n-\chi)\circ(u_0-|u|)\|_\infty)/2 \le |\chi-\chi_n|_\infty$ for all $n \in \mathbb{N}$. Similarly, for all $\alpha \in \langle 1,3\rangle$ and all $n \in \mathbb{N}$, we have $\|v_\alpha(\chi_n-\chi)\|_\infty \le |\chi-\chi_n|_\infty$ since $\|\tilde{u}_\alpha\|_\infty \le 1$ for all $\alpha \in \langle 1,3\rangle$. Applying (139), we get, for all $\Phi \in \widehat{\mathfrak{H}}$ and all $n \in \mathbb{N}$,

$$\begin{aligned}\|(m[v_0(\chi_n-\chi)]\sigma_0 + m[v(\chi_n-\chi)]\sigma)\Phi\| &\le \sum_{\alpha\in\langle 0,3\rangle} \|v_\alpha(\chi_n-\chi)\|_\infty\|\Phi\|\\ &\le 4|\chi-\chi_n|_\infty\|\Phi\|.\end{aligned} \tag{379}$$

Hence, (369)-(371) also holds for all $\chi \in C_0(\mathbb{R})$ (see Remark 84 for the composition of Borel functions). In order to show that (369)-(371) also holds for all $\chi \in \mathcal{B}(\mathbb{R})$, we again use the minimality type argument (as in Remark 84). To this end, we set

$$\mathcal{F} := \{\chi \in \mathcal{B}(\mathbb{R}) \,|\, E_U(\chi) = m[v_0]\sigma_0 + m[v]\sigma \text{ with (370) and (371)}\}, \tag{380}$$

and $\mathcal{F}$ satisfies *(B1)*. Next, let $(\chi_n)_{n\in\mathbb{N}}$ be a sequence in $\mathcal{F}$ with $\mathcal{B}-\lim_{n\to\infty}\chi_n = \chi$ for some $\chi \in \ell^\infty(\mathbb{R})$ and, hence, $\chi \in \mathcal{B}(\mathbb{R})$. Making again the decomposition (378), (350) applied to the first term on the right hand side of (378) yields $\mathrm{s}-\lim_{n\to\infty} E_U(\chi-\chi_n) = 0$. As for the second term in (378), we have, for all $\Phi = \varphi_1 \oplus \varphi_2 \in \widehat{\mathfrak{H}}$ and all $n \in \mathbb{N}$, that $\|m[v_0(\chi_n-\chi)]\sigma_0\Phi\|^2 \le \sum_{i\in\langle 1,2\rangle}\sum_{\sigma\in\{\pm1\}}\int_{-\pi}^{\pi}\mathrm{d}k/(2\pi)|f_{i,\sigma}^n(k)|^2/2$, where, for all $i \in \langle 1,2\rangle$, all $\sigma \in \{\pm1\}$, and all $n \in \mathbb{N}$, the function $f_{i,\sigma}^n \in \hat{\mathfrak{h}}$ is given by

$$f_{i,\sigma}^n := ((\chi_n-\chi)\circ(u_0+\sigma|u|))\varphi_i. \tag{381}$$

Since the sequence $(\chi_n)_{n\in\mathbb{N}}$ is Borel convergent to χ, we get, for all $i\in\langle 1,2\rangle$, all $\sigma\in\{\pm 1\}$, all $n\in\mathbb{N}$, and almost all $k\in\mathbb{T}$, that $\lim_{n\to\infty} f^n_{i,\sigma}(k)=0$ and $|f^n_{i,\sigma}|^2\le 4C^2|\varphi_i|^2\in L^1(\mathbb{T})$, where the constant $C>0$ stems from Definition 75 *(a)*. Hence, Lebesgue's dominated convergence theorem implies that $\mathrm{s}-\lim_{n\to\infty} m[v_0(\chi_n-\chi)]\sigma_0=0$. Similarly, as for the third term on the right hand side of (378), we have, for all $\Phi=\varphi_1\oplus\varphi_2\in\widehat{\mathfrak{H}}$ and all $n\in\mathbb{N}$, that $\|m[v(\chi_n-\chi)]\sigma\Phi\|^2\le(3/2)\sum_{i\in\langle 1,2\rangle}\sum_{\alpha\in\langle 1,3\rangle}\sum_{\sigma\in\{\pm 1\}}\int_{-\pi}^{\pi}\mathrm{d}k/(2\pi)|g^n_{i,\alpha,\sigma}(k)|^2$, where, for all $i\in\langle 1,2\rangle$, all $\alpha\in\langle 1,3\rangle$, all $\sigma\in\{\pm 1\}$, and all $n\in\mathbb{N}$, the function $g^n_{i,\alpha,\sigma}\in\hat{\mathfrak{h}}$ is given by $g^n_{i,\alpha,\sigma}:=[(\chi_n-\chi)\circ(u_0+\sigma|u|)]\tilde{u}_\alpha\varphi_i$. We again get, for all $i\in\langle 1,2\rangle$, all $\alpha\in\langle 1,3\rangle$, all $\sigma\in\{\pm 1\}$, all $n\in\mathbb{N}$, and almost all $k\in\mathbb{T}$, that $\lim_{n\to\infty} g^n_{i,\alpha,\sigma}(k)=0$ and $|g^n_{i,\alpha,\sigma}|^2\le 4C^2|\varphi_i|^2\in L^1(\mathbb{T})$, where we used that $\|\tilde{u}_\alpha\|_\infty\le 1$ for all $\alpha\in\langle 1,3\rangle$. Hence, Lebesgue's dominated convergence theorem also implies that $\mathrm{s}-\lim_{n\to\infty} m[v(\chi_n-\chi)]\sigma=0$. Therefore, (369)-(371) holds for χ, i.e., $\mathcal{F}$ also satisfies *(B2)*, and we get $\mathcal{B}(\mathbb{R})\subseteq\mathcal{F}$. □

Remark 87 Instead of applying the explicit form of the propagator (366)-(368), we can also diagonalize U with the help of its eigenvalue functions $e_\pm\in L^\infty(\mathbb{T})$ and its (not yet normalized) eigenvector functions $\Phi_\pm\in\widehat{\mathfrak{H}}$ given by

$$\Phi_\pm := (u_3\pm|u|)\oplus(u_1+\mathrm{i}u_2), \tag{382}$$

$$e_\pm = u_0\pm|u|, \tag{383}$$

i.e., we have $U\Phi_\pm=m[e_\pm]\sigma_0\Phi_\pm$.

In the following, we denote by $L^2(\mathbb{T},\mathbb{C}^2)$ the space of vector-valued functions $\mathbb{T}\to\mathbb{C}^2$ whose entry functions belong to $L^2(\mathbb{T})$. Analogously, $L^\infty(\mathbb{T},\mathbb{C}^{2\times 2})$ stands for the space of matrix-valued functions $\mathbb{T}\to\mathbb{C}^{2\times 2}$ whose entry functions belong to $L^\infty(\mathbb{T})$. Moreover, if $f:D\to\mathbb{C}$ is a function defined on $D\subseteq\mathbb{R}$, we use the notation $f(M):=\{f(x)\,|\,x\in M\}$ for all $M\subseteq D$ and, for all $Y\subseteq\mathbb{C}$, the preimage of Y under f is denoted by $f^{-1}(Y):=\{x\in D\,|\,f(x)\in Y\}$.

The following proposition provides us with a useful sufficient condition for a matrix multiplication operator to be absolutely continuous on some spectral domain.

Proposition 88 (Absolute continuity) *Let $u_0\in L^\infty(\mathbb{T})$ and $u=[u_1,u_2,u_3]\in L^\infty(\mathbb{T})^3$ satisfy Assumption 40 (a) and (b) and define $U\in\mathcal{L}(\widehat{\mathfrak{H}})$ by $U:=m[u_0]\sigma_0+m[u]\sigma$. Moreover, let $M\in\mathcal{M}(\mathbb{R})$ and let Assumption 43 (a) and (b) hold. Then,*

$$\mathrm{ran}\,(1_M(U))\subseteq\mathrm{ran}\,(1_{ac}(U)). \tag{384}$$

Remark 89 Since we know (see [17] for example) that, under the assumptions of Proposition 88, the property $\mathrm{spec}(U)=\bigcup_{k\in\mathbb{T}}\mathrm{spec}([U](k))$ holds, where $[U]\in L^\infty(\mathbb{T},\mathbb{C}^{2\times 2})$ is given by $KUK^*=m[[U]]$, where the unitary natural identification operator $K\in\mathcal{L}(\widehat{\mathfrak{H}},L^2(\mathbb{T},\mathbb{C}^2))$ reads as $(K\Phi)(k):=[\varphi_1(k),\varphi_2(k)]\in\mathbb{C}^2$ for all $\Phi=\varphi_1\oplus\varphi_2\in\widehat{\mathfrak{H}}$ and almost all $k\in\mathbb{T}$, and where, for all $A \in L^\infty(\mathbb{T}, \mathbb{C}^{2\times 2})$, the multiplication operator $m[A] \in \mathcal{L}(L^2(\mathbb{T}, \mathbb{C}^2))$ is given by $(m[A][\varphi_1, \varphi_2])(k) := A(k)[\varphi_1(k), \varphi_2(k)]$ for all $[\varphi_1, \varphi_2] \in L^2(\mathbb{T}, \mathbb{C}^2)$ and almost all $k \in \mathbb{T}$, we get

$$\begin{aligned} \mathrm{spec}(U) &= \bigcup_{k\in\mathbb{T}} \{e_+(k), e_-(k)\} \\ &= \mathrm{ran}\,(e_+) \cup \mathrm{ran}\,(e_-). \end{aligned} \tag{385}$$

Hence, if the set $M \in \mathcal{M}(\mathbb{R})$ from Proposition 88 has the property $\mathrm{spec}(U) \subseteq M$, we get $e_\kappa^{-1}(M) = \mathbb{T}$ for all $\kappa \in \{\pm\}$. Moreover, $\mathrm{ran}\,(1_M(U)) = \widehat{\mathfrak{H}}$ since $E_U(1_{\mathrm{spec}(U)}) = 1$ (see Remark 85). Therefore, if Assumption 43 *(a)* and *(b)* hold, Proposition 88 yields that U is absolutely continuous, i.e., that $1_{ac}(U) = 1$.

For the following, recall the definitions (150)-(154).

Proof. Since $U^* = U \in \mathcal{L}(\widehat{\mathfrak{H}})$ and since we know that

$$\mathrm{ran}\,(1_{ac}(U)) = \{\Phi \in \widehat{\mathfrak{H}} \,|\, E_U(1_A)\Phi = 0 \text{ for all } A \in \mathcal{M}(\mathbb{R}) \text{ with } |A| = 0\}, \tag{386}$$

we want to show that $E_U(1_A)E_U(1_M)\Psi = E_U(1_{A\cap M})\Psi = 0$ for all $A \in \mathcal{M}(\mathbb{R})$ with $|A| = 0$ and all $\Psi \in \widehat{\mathfrak{H}}$. To this end, using Proposition 86 *(b)*, we write that, for all $\Psi = \psi_1 \oplus \psi_2 \in \widehat{\mathfrak{H}}$ and all $A \in \mathcal{M}(\mathbb{R})$,

$$\begin{aligned} \|E_U(1_{A\cap M})\Psi\|^2 &= (\Psi, E_U(1_{A\cap M})\Psi) \\ &\le \frac{1}{2} \sum_{\kappa\in\{\pm\}} \sum_{i\in\langle 1,2\rangle} \int_{e_\kappa^{-1}(A\cap M)} \frac{\mathrm{d}k}{2\pi}\; |\psi_i(k)|^2 \\ &\quad + \frac{1}{2} \sum_{\kappa\in\{\pm\}} \sum_{\alpha\in\langle 1,2\rangle} \sum_{\substack{i,j\in\langle 1,2\rangle \\ i\neq j}} \int_{e_\kappa^{-1}(A\cap M)} \frac{\mathrm{d}k}{2\pi}\; |\tilde{u}_\alpha(k)||\psi_i(k)||\psi_j(k)| \\ &\quad + \frac{1}{2} \sum_{\kappa\in\{\pm\}} \sum_{i\in\langle 1,2\rangle} \int_{e_\kappa^{-1}(A\cap M)} \frac{\mathrm{d}k}{2\pi}\; |\tilde{u}_3(k)||\psi_i(k)|^2, \end{aligned} \tag{387}$$

where, due to Assumption 40 *(b)*, we have $e_\pm \in C(\mathbb{T})$ and, hence, $e_\pm^{-1}(A \cap M) \in \mathcal{M}(\mathbb{T})$ for all $A \in \mathcal{M}(\mathbb{R})$. Moreover, all the integrals on the right hand side of (387) exist since $\varphi_i \in \hat{\mathfrak{h}}$ for all $i \in \langle 1, 2\rangle$ and $|\tilde{u}_\alpha|_\infty \le 1$ for all $\alpha \in \langle 1, 3\rangle$. In order to make the left hand side of (387) vanish for all $A \in \mathcal{M}(\mathbb{R})$ with $|A| = 0$ and all $\Psi \in \widehat{\mathfrak{H}}$, it is sufficient to show that $|e_\pm^{-1}(A \cap M)| = 0$ for all $A \in \mathcal{M}(\mathbb{R})$ with $|A| = 0$. In order to do so, let us stick to the case of e_+ in the following (the case of e_- being completely analogous). Let us start off by making the decompositions $\mathbb{T} = \mathcal{Z}_u \cup \mathcal{Z}_u^c$ and $\mathcal{Z}_u^c = \mathcal{Z}_+ \cup (\mathcal{Z}_u^c \setminus \mathcal{Z}_+)$ (recall that $\mathcal{Z}_+ \subseteq \mathcal{Z}_u^c$). Hence, writing $A' := A \cap M$ and $e_+^{-1}(A') = e_+^{-1}(A') \cap \mathbb{T}$, we get

$$e_+^{-1}(A') = (e_+^{-1}(A') \cap \mathcal{Z}_u) \cup (e_+^{-1}(A') \cap \mathcal{Z}_+) \cup (e_+^{-1}(A') \cap (\mathcal{Z}_u^c \setminus \mathcal{Z}_+)). \tag{388}$$

Moreover, since $\mathcal{Z}_u^c = (\mathcal{Z}_u^c \cap \{-\pi\}) \cup (\mathcal{Z}_u^c \cap \{\pi\}) \cup (\mathcal{Z}_u^c \cap \mathring{\mathbb{T}})$, where $\mathring{\mathbb{T}} := (-\pi, \pi)$, the last term on the right hand side of (388) has the form

$$\begin{aligned} e_+^{-1}(A') \cap (\mathcal{Z}_u^c \setminus \mathcal{Z}_+) = (e_+^{-1}(A') \cap ((\mathcal{Z}_u^c \cap \{-\pi\}) \setminus \mathcal{Z}_+)) \cup (e_+^{-1}(A') \cap ((\mathcal{Z}_u^c \cap \{\pi\}) \setminus \mathcal{Z}_+)) \\ \cup (e_+^{-1}(A') \cap B), \end{aligned} \tag{389}$$

where we set $B := (\mathcal{Z}_u^c \cap \mathring{\mathbb{T}}) \setminus \mathcal{Z}_+$. Denoting the restriction of e_+ to $\mathcal{Z}_u^c \cap \mathring{\mathbb{T}}$ by f, we have

$$B = \{k \in \mathcal{Z}_u^c \cap \mathring{\mathbb{T}} \,|\, f'(k) \neq 0\}, \tag{390}$$

and B is open (in $\mathbb{R}$) since B is open relative to $\mathcal{Z}_u^c \cap \mathring{\mathbb{T}}$ and since $\mathcal{Z}_u^c \cap \mathring{\mathbb{T}}$ is open. Since we know that there exists a countable family of compact intervals $\{I_n\}_{n\in\mathbb{N}}$ in $\mathbb{R}$ satisfying $\mathring{I}_n \cap \mathring{I}_{n'} = \emptyset$ for all $n, n' \in \mathbb{N}$ with $n \neq n'$ and $B = \bigcup_{n\in\mathbb{N}} I_n$, the last term in (389) reads

$$e_+^{-1}(A') \cap B = \bigcup_{n\in\mathbb{N}} (e_+^{-1}(A') \cap I_n). \tag{391}$$

Denoting by $g \in C^1(B)$ the restriction of e_+ to B, we have $g'(k) \neq 0$ for all $k \in B$. Hence, for all $k \in B$, the inverse function theorem guarantees the existence of an open set $U_k \subseteq B$ with $k \in U_k$ and of an open set $V_{g(k)} \subseteq \mathbb{R}$ with $g(k) \in V_{g(k)}$ such that the restriction of g to U_k, denoted by g_k, is a bijection between U_k and $V_{g(k)}$. Moreover, since, for all $n \in \mathbb{N}$, we have $I_n \subseteq \bigcup_{k\in I_n} U_k$ and since I_n is compact, there exists $N_n \in \mathbb{N}$ and $\{k_{n,1}, \ldots, k_{n,N_n}\} \subseteq I_n$ such that $I_n \subseteq \bigcup_{m\in\langle 1,N_n\rangle} U_{k_{n,m}}$ which implies

$$e_+^{-1}(A') \cap B \subseteq \bigcup_{n\in\mathbb{N}} \bigcup_{m\in\langle 1,N_n\rangle} (e_+^{-1}(A') \cap U_{k_{n,m}}). \tag{392}$$

Since, for all $n \in \mathbb{N}$ and all $m \in \langle 1, N_n\rangle$, it holds that

$$\begin{aligned} e_+^{-1}(A') \cap U_{k_{n,m}} &= \{k \in U_{k_{n,m}} \,|\, g_{k_{n,m}}(k) \in A' \cap V_{g(k_{n,m})}\} \\ &= g_{k_{n,m}}^{-1}(A' \cap V_{g(k_{n,m})}), \end{aligned} \tag{393}$$

the properties (388)-(389) and (392)-(393) yield $e_+^{-1}(A') \subseteq \bigcup_{i\in\langle 1,5\rangle} M_i$, where, for all $i \in \langle 1, 5\rangle$, the sets $K_i \in \mathcal{M}(\mathbb{T})$ are defined by

$$K_1 := e_+^{-1}(A') \cap \mathcal{Z}_u, \tag{394}$$

$$K_2 := e_+^{-1}(A') \cap \mathcal{Z}_+, \tag{395}$$

$$K_3 := e_+^{-1}(A') \cap ((\mathcal{Z}_u^c \cap \{-\pi\}) \setminus \mathcal{Z}_+), \tag{396}$$

$$K_4 := e_+^{-1}(A') \cap ((\mathcal{Z}_u^c \cap \{\pi\}) \setminus \mathcal{Z}_+), \tag{397}$$

$$K_5 := \bigcup_{n\in\mathbb{N}} \bigcup_{m\in\langle 1,N_n\rangle} g_{k_{n,m}}^{-1}(A' \cap V_{g(k_{n,m})}). \tag{398}$$

Using Assumption 43 *(a)* and *(b)*, we get $|K_1| = |e_+^{-1}(A) \cap (\mathcal{Z}_u \cap e_+^{-1}(M))| \leq |\mathcal{Z}_u \cap e_+^{-1}(M)| = 0$ and $|K_2| \leq |\mathcal{Z}_+ \cap e_+^{-1}(M)| = 0$, respectively. Moreover, we have $\mathrm{card}(K_i) \in \{0, 1\}$ for all

$i \in \langle 3, 4 \rangle$. Hence, it remains to estimate (398). We first note that, since, for all $n \in \mathbb{N}$ and all $m \in \langle 1, N_n \rangle$, the set $V_{g(k_{n,m})}$ is open, there exists again a countable family of compact intervals $\{J_{n,m,p}\}_{p\in\mathbb{N}}$ in $\mathbb{R}$ satisfying $\mathring{J}_{n,m,p} \cap \mathring{J}_{n,m,p'} = \emptyset$ for all $p, p' \in \mathbb{N}$ with $p \neq p'$ and $V_{g(k_{n,m})} = \bigcup_{p\in\mathbb{N}} J_{n,m,p}$. Furthermore, since $A' \in \mathcal{M}(\mathbb{R})$ has the property $|A'| \leq |A| = 0$, we know that, for all $\varepsilon > 0$, there exists a countable family of compact intervals $\{L_q\}_{q\in\mathbb{N}}$ in $\mathbb{R}$ such that $A' \subseteq \bigcup_{q\in\mathbb{N}} L_q$ and $\sum_{q\in\mathbb{N}} |L_q| < \varepsilon$. Hence, for all $n \in \mathbb{N}$ and all $m \in \langle 1, N_n \rangle$, we get

$$g_{k_{n,m}}^{-1}(A' \cap V_{g(k_{n,m})}) \subseteq \bigcup_{p,q\in\mathbb{N}} g_{k_{n,m}}^{-1}(J_{n,m,p} \cap L_q). \tag{399}$$

Furthermore, the inverse function theorem also guarantees that, for all $n \in \mathbb{N}$ and all $m \in \langle 1, N_n \rangle$, the inverse of $g_{k_{n,m}}$, denoted by $h_{k_{n,m}}$, satisfies $h_{k_{n,m}} \in C^1(V_{g(k_{n,m})})$ and, hence, $h_{k_{n,m}}$ is Lipschitz continuous on the compact interval $J_{n,m,p}$ with a Lipschitz constant $C_{n,m,p} > 0$. Therefore, for all $n \in \mathbb{N}$, all $m \in \langle 1, N_n \rangle$, and all $p, q \in \mathbb{N}$, we get

$$\sup_{x,y\in J_{n,m,p}\cap L_q} |h_{k_{n,m}}(x) - h_{k_{h,m}}(y)| \leq C_{n,m,p}|L_q|, \tag{400}$$

and the set $g_{k_{n,m}}^{-1}(J_{n,m,p} \cap L_q) = h_{k_{n,m}}(J_{n,m,p} \cap L_q) \in \mathcal{M}(\mathbb{T})$ is contained in a compact interval of length $C_{n,m,p}|L_q|$ (and $C_{n,m,p}$ is independent of ε). Since $\sum_{q\in\mathbb{N}} |L_q| < \varepsilon$, we get $|g_{k_{n,m}}^{-1}(J_{n,m,p} \cap L_q)| = 0$ for all $n \in \mathbb{N}$, all $m \in \langle 1, N_n \rangle$, and all $p, q \in \mathbb{N}$. Hence, using (398)-(399), we arrive at $|K_5| = 0$. □

C Real trigonometric polynomials

In this appendix, we carry out the computations of the squares in $TP(\mathbb{T})$ used in the foregoing sections (for more information on the structure of this ring, see [25] for example). To this end, let $\nu \in \mathbb{N}$ and, for all $\alpha \in \langle 0, 3 \rangle$, let $u_\alpha \in L^\infty(\mathbb{T})$ be given by

$$u_\alpha = \begin{cases} -2\sum_{n\in\langle 1,\nu\rangle} c_{\alpha,n} \sin(n\,\cdot), & \alpha \in \langle 0, 2 \rangle, \\ c_{3,0} + 2\sum_{n\in\langle 1,\nu\rangle} c_{3,n} \cos(n\,\cdot), & \alpha = 3, \end{cases} \tag{401}$$

where $c_{\alpha,n} \in \mathbb{R}$ for all $\alpha \in \langle 0, 2 \rangle$ and all $n \in \langle 1, \nu \rangle$ and $c_{3,n} \in \mathbb{R}$ for all $n \in \langle 0, \nu \rangle$ (recall that in (267), we have $\nu \in \langle 1, n_S \rangle$).

Lemma 90 (Squares) *For all $\alpha \in \langle 0, 3 \rangle$, the squares of $u_\alpha \in L^\infty(\mathbb{T})$ from* (401) *read as*

$$u_\alpha^2 = a_{\alpha,0} + 2\sum_{m\in\langle 1,2\nu\rangle} a_{\alpha,m} \cos(m\,\cdot), \tag{402}$$

where $a_{\alpha,m} \in \mathbb{R}$ for all $\alpha \in \langle 0, 3 \rangle$ and all $m \in \langle 0, 2\nu \rangle$. Moreover, setting $b_{\alpha,m} := [a_{\alpha,m}, a_{3,m}] \in \mathbb{R}^2$ for all $\alpha \in \langle 0, 2 \rangle$ and all $m \in \langle 0, 2\nu \rangle$, we have:

(a) *For* $\nu = 1$*, for all* $\alpha \in \langle 0, 2\rangle$ *and all* $m \in \langle 0, 2\rangle$*,*

$$b_{\alpha,m} = \begin{cases} [2c_{\alpha,1}^2, c_{3,0}^2 + 2c_{3,1}^2], & m = 0, \\ [0, 2c_{3,0}c_{3,1}], & m = 1, \\ [-c_{\alpha,1}^2, c_{3,1}^2], & m = 2. \end{cases} \tag{403}$$

(b) *For* $\nu = 2$*, for all* $\alpha \in \langle 0, 2\rangle$ *and all* $m \in \langle 0, 4\rangle$*,*

$$b_{\alpha,m} = \begin{cases} [2(c_{\alpha,1}^2 + c_{\alpha,2}^2), c_{3,0}^2 + 2(c_{3,1}^2 + c_{3,2}^2)], & m = 0, \\ [2c_{\alpha,1}c_{\alpha,2}, 2(c_{3,0}c_{3,1} + c_{3,1}c_{3,2})], & m = 1, \\ [-c_{\alpha,1}^2, 2c_{3,0}c_{3,2} + c_{3,1}^2], & m = 2, \\ [-2c_{\alpha,1}c_{\alpha,2}, 2c_{3,1}c_{3,2}], & m = 3, \\ [-c_{\alpha,2}^2, c_{3,2}^2], & m = 4. \end{cases} \tag{404}$$

(c) *For all* $\nu \geq 3$*, all* $\alpha \in \langle 0, 2\rangle$ *and all* $m \in \langle 0, 2\nu\rangle$*,*

$$b_{\alpha,m} = \begin{cases} [2\sum_{n\in\langle 1,\nu\rangle} c_{\alpha,n}^2, c_{3,0}^2 + 2\sum_{n\in\langle 1,\nu\rangle} c_{3,n}^2], & m = 0, \\ [2\sum_{n\in\langle 1,\nu-1\rangle} c_{\alpha,n}c_{\alpha,n+1}, 2(c_{3,0}c_{3,1} + \sum_{n\in\langle 1,\nu-1\rangle} c_{3,n}c_{3,n+1})], & m = 1, \\ [2\sum_{n\in\langle 1,\nu-m\rangle} c_{\alpha,n}c_{\alpha,m+n} - \sum_{n\in\langle 1,m-1\rangle} c_{\alpha,n}c_{\alpha,m-n}, & \\ 2(c_{3,0}c_{3,m} + \sum_{n\in\langle 1,\nu-m\rangle} c_{3,n}c_{3,m+n}) + \sum_{n\in\langle 1,m-1\rangle} c_{3,n}c_{3,m-n}], & m \in \{2, \nu-1\}, \\ [-\sum_{n\in\langle 1,\nu-1\rangle} c_{\alpha,n}c_{\alpha,\nu-n}, 2c_{3,0}c_{3,\nu} + \sum_{n\in\langle 1,\nu-1\rangle} c_{3,n}c_{3,\nu-n}], & m = \nu, \\ [-\sum_{n\in\langle m-\nu,\nu\rangle} c_{\alpha,n}c_{\alpha,m-n}, \sum_{n\in\langle m-\nu,\nu\rangle} c_{3,n}c_{3,m-n}], & m \in \{\nu+1, 2\nu\}. \end{cases} \tag{405}$$

Proof. Note that $2\sin(x)\sin(y) = \cos(x-y) - \cos(x+y)$ and $2\cos(x)\cos(y) = \cos(x-y) + \cos(x+y)$ for all $x, y \in \mathbb{R}$ and that, for all $\nu \geq 2$ and all $\{b_{i,j}\}_{i,j\in\langle 1,\nu\rangle} \subseteq \mathbb{R}$, we have

$$\sum_{i,j\in\langle 1,\nu\rangle} b_{i,j} = \sum_{\substack{m\in\langle 0,\nu-1\rangle\\ i\in\langle m+1,\nu\rangle}} b_{i,i-m} + \sum_{\substack{m\in\langle -\nu+1,-1\rangle\\ i\in\langle 1,\nu+m\rangle}} b_{i,i-m}, \tag{406}$$

$$= \sum_{\substack{m\in\langle 2,\nu+1\rangle\\ i\in\langle 1,m-1\rangle}} b_{i,m-i} + \sum_{\substack{m\in\langle \nu+2,2\nu\rangle\\ i\in\langle m-\nu,\nu\rangle}} b_{i,m-i}. \tag{407}$$

Squaring (401) and applying (406)-(407) to the terms in the foregoing trigonometric expressions whose arguments are differences ($i - (i - m) = m$) and sums ($i + (m - i) = m$), respectively, we arrive at (403)-(405). □

D Heat flux contributions

In this appendix, we collect the explicit expressions for the contributions to J_{ac} appearing in the proof of Theorem 61 *(b)*.

Lemma 91 (Expansion) *Let the assumptions of Theorem 61 hold. Then, for all* $i \in \langle 1, 8\rangle$*, the functions* $\mu_i \in L^\infty(\mathbb{T})$ *appearing in* (299) *are given by*

$$\mu_1 := \sum_{\substack{n\in\langle 1,\nu\rangle\\ l\in\langle 0,\nu-n\rangle}} n\sin(n\,\cdot)\,(c_{0,l}c_{0,n+l} + c_{1,l}c_{1,n+l} + c_{2,l}c_{2,n+l} + c_{3,l}c_{3,n+l}), \tag{408}$$

$$\mu_2 := -\sum_{n,m\in\langle 1,\nu\rangle} n\sin((n+m)\,\cdot)\,(c_{0,n}c_{0,m} + c_{1,n}c_{1,m} + c_{2,n}c_{2,m} - c_{3,n}c_{3,m}), \tag{409}$$

$$\mu_3 := -2\sum_{\substack{n,m\in\langle 1,\nu\rangle\\ l\in\langle 0,\nu-n\rangle}} n\sin(n\,\cdot)\sin(m\,\cdot)\,c_{1,m}(c_{0,l}c_{1,n+l} + c_{0,n+l}c_{1,l} - c_{2,l}c_{3,n+l} - c_{2,n+l}c_{3,l}), \tag{410}$$

$$\mu_4 := 2\sum_{n,m,l\in\langle 1,\nu\rangle} n\sin((n+l)\,\cdot)\sin(m\,\cdot)\,c_{1,m}(c_{0,n}c_{1,l} + c_{0,l}c_{1,n} + c_{2,n}c_{3,l} - c_{2,l}c_{3,n}), \tag{411}$$

$$\mu_5 := -2\sum_{\substack{n,m\in\langle 1,\nu\rangle\\ l\in\langle 0,\nu-n\rangle}} n\sin(n\,\cdot)\sin(m\,\cdot)\,c_{2,m}(c_{0,l}c_{2,n+l} + c_{0,n+l}c_{2,l} + c_{1,l}c_{3,n+l} + c_{1,n+l}c_{3,l}), \tag{412}$$

$$\mu_6 := 2\sum_{n,m,l\in\langle 1,\nu\rangle} n\sin((n+l)\,\cdot)\sin(m\,\cdot)\,c_{2,m}(c_{0,n}c_{2,l} + c_{0,l}c_{2,n} - c_{1,n}c_{3,l} + c_{1,l}c_{3,n}), \tag{413}$$

$$\begin{aligned}\mu_7 := &-\sum_{\substack{n\in\langle 1,\nu\rangle\\ l\in\langle 0,\nu-n\rangle}} n\cos(n\,\cdot)\,c_{3,0}(c_{0,l}c_{3,n+l} - c_{0,n+l}c_{3,l} + c_{1,l}c_{2,n+l} - c_{1,n+l}c_{2,l})\\ &-2\sum_{\substack{n,m\in\langle 1,\nu\rangle\\ l\in\langle 0,\nu-n\rangle}} n\cos(n\,\cdot)\cos(m\,\cdot)\,c_{3,m}(c_{0,l}c_{3,n+l} - c_{0,n+l}c_{3,l} + c_{1,l}c_{2,n+l} - c_{1,n+l}c_{2,l}),\end{aligned} \tag{414}$$

$$\begin{aligned}\mu_8 := &\sum_{n,m\in\langle 1,\nu\rangle} n\cos((n+m)\,\cdot)\,c_{3,0}(c_{0,n}c_{3,m} + c_{0,m}c_{3,n} - c_{1,n}c_{2,m} + c_{1,m}c_{2,n})\\ &+2\sum_{n,m,l\in\langle 1,\nu\rangle} n\cos((n+l)\,\cdot)\cos(m\,\cdot)\,c_{3,m}(c_{0,n}c_{3,l} + c_{0,l}c_{3,n} - c_{1,n}c_{2,l} + c_{1,l}c_{2,n}).\end{aligned} \tag{415}$$

Proof. Noting that, for all $x \in \mathbb{Z}$ and all $\alpha \in \langle 1, 2\rangle$,

$$\eta_{0,x} = -\frac{1}{2}\int_{-\pi}^{\pi}\frac{\mathrm{d}k}{2\pi}\,\sin(kx)(\rho_+(k) + \rho_-(k)), \tag{416}$$

$$\eta_{\alpha,x} = -\frac{1}{2}\int_{-\pi}^{\pi}\frac{\mathrm{d}k}{2\pi}\,\sin(kx)\tilde{u}_\alpha(k)(\rho_+(k) - \rho_-(k)), \tag{417}$$

$$\eta_{3,x} = \frac{1}{2}\int_{-\pi}^{\pi}\frac{\mathrm{d}k}{2\pi}\,\cos(kx)\tilde{u}_3(k)(\rho_+(k) - \rho_-(k)), \tag{418}$$

plugging (298) for $G(-n,z,-n-z)$ and $G(-n+z,z,-n)$ into (297), using (267), and separating the terms with respect to ρ_+ and ρ_-, we arrive at (408)-(415). □

E Hamiltonian densities

In this appendix, we display the selfdual second quantization of the local first, second and third Pauli coefficient of H in the fermionic and the spin picture (the selfdual second quantization of the zeroth Pauli coefficient of H is given in Remark 66).

For the following, recall that $q_N = m[1_{\langle -N,N\rangle}] \in \mathcal{L}^0(\mathfrak{h})$ for all $N \in \mathbb{N}$ as defined after (257).

Lemma 92 (Hamiltonian densities) *Let $H \in \mathcal{L}(\mathfrak{H})$ be a Hamiltonian satisfying Assumption 14 (b), (d), and (e). Then:*

(a) The selfdual second quantizations of the local first, second and third Pauli coefficient of H in the fermionic picture are given, for all $N \in \mathbb{N}$ satifying (258)*, by*

$$b((q_N h_1 q_N)\sigma_1) = -2\mathrm{i} \sum_{n\in\langle 1,\nu\rangle} c_{1,n} \sum_{x\in\langle -N,N-n\rangle} (a_x^* a_{x+n}^* - a_{x+n} a_x), \tag{419}$$

$$b((q_N h_2 q_N)\sigma_2) = -2 \sum_{n\in\langle 1,\nu\rangle} c_{2,n} \sum_{x\in\langle -N,N-n\rangle} (a_x^* a_{x+n}^* + a_{x+n} a_x), \tag{420}$$

$$b((q_N h_3 q_N)\sigma_3) = c_{3,0} \sum_{x\in\langle -N,N\rangle} (2a_x^* a_x - 1) + 2 \sum_{n\in\langle 1,\nu\rangle} c_{3,n} \sum_{x\in\langle -N,N-n\rangle} (a_x^* a_{x+n} + a_{x+n}^* a_x). \tag{421}$$

(b) In the spin picture we have, for all $x \in \mathbb{Z}$ and all $n \in \mathbb{N}$,

$$a_x^* a_{x+n}^* - a_{x+n} a_x = \begin{cases} -\frac{\mathrm{i}}{2}\big(\sigma_1^{(x)}\sigma_2^{(x+1)} + \sigma_2^{(x)}\sigma_1^{(x+1)}\big), & n=1,\\ -\frac{\mathrm{i}}{2}\big(\sigma_1^{(x)}\big(\prod_{i\in\langle 1,n-1\rangle}\sigma_3^{(x+i)}\big)\sigma_2^{(x+n)} + \sigma_2^{(x)}\big(\prod_{i\in\langle 1,n-1\rangle}\sigma_3^{(x+i)}\big)\sigma_1^{(x+n)}\big), & n\geq 2,\end{cases} \tag{422}$$

$$a_x^* a_{x+n}^* + a_{x+n} a_x = \begin{cases} -\frac{1}{2}\big(\sigma_1^{(x)}\sigma_1^{(x+1)} - \sigma_2^{(x)}\sigma_2^{(x+1)}\big), & n=1,\\ -\frac{1}{2}\big(\sigma_1^{(x)}\big(\prod_{i\in\langle 1,n-1\rangle}\sigma_3^{(x+i)}\big)\sigma_1^{(x+n)} - \sigma_2^{(x)}\big(\prod_{i\in\langle 1,n-1\rangle}\sigma_3^{(x+i)}\big)\sigma_2^{(x+n)}\big), & n\geq 2,\end{cases} \tag{423}$$

$$a_x^* a_{x+n} + a_{x+n}^* a_x = \begin{cases} -\frac{1}{2}\big(\sigma_1^{(x)}\sigma_1^{(x+1)} + \sigma_2^{(x)}\sigma_2^{(x+1)}\big), & n=1,\\ -\frac{1}{2}\big(\sigma_1^{(x)}\big(\prod_{i\in\langle 1,n-1\rangle}\sigma_3^{(x+i)}\big)\sigma_1^{(x+n)} + \sigma_2^{(x)}\big(\prod_{i\in\langle 1,n-1\rangle}\sigma_3^{(x+i)}\big)\sigma_2^{(x+n)}\big), & n\geq 2.\end{cases} \tag{424}$$

Moreover, we have $2a_x^* a_x - 1 = \sigma_3^{(x)}$ for all $x \in \mathbb{Z}$.

Proof. See Remark 66 and, for example, [11]. □

References

[1] Araki H 1968 *On the diagonalization of a bilinear Hamiltonian by a Bogoliubov transformation* Publ. RIMS Kyoto Univ. Ser. A 4 387-412

[2] Araki H 1971 *On quasifree states of CAR and Bogoliubov automorphisms* Publ. RIMS Kyoto Univ. 6 385-442

[3] Araki H 1984 *On the XY-model on two-sided infinite chain* Publ. RIMS Kyoto Univ. 20 277-296

[4] Araki H 1987 *Bogoliubov automorphisms and Fock representations of canonical anticommutation relations* Contemp. Math. 62 23-141

[5] Araki H and Ho T G 2000 *Asymptotic time evolution of a partitioned infinite two-sided isotropic XY-chain* Proc. Steklov Inst. Math. 228 191-204

[6] Araki H and Matsui T 1985 *Ground states of the XY model* Commun. Math. Phys. 101 213-245

[7] Aschbacher W H 2011 *Broken translation invariance in quasifree fermionic correlations out of equilibrium* J. Funct. Anal. 260 3429-3456

[8] Aschbacher W H 2016 *On a quantum phase transition in a steady state out of equilibrium* J. Phys. A: Math. Theor. 49 415201 1-21

[9] Aschbacher W H 2019 *A rigorous scattering approach to quasifree fermionic systems out of equilibrium* J. Non-Equilib. Thermodyn. 44 (3) 261-275

[10] Aschbacher W H, Jakšić V, Pautrat Y, and Pillet C A 2007 *Transport properties of quasi-free fermions* J. Math. Phys. 48 032101 1-28

[11] Aschbacher W H and Pillet C-A 2003 *Non-equilibrium steady states of the XY chain* J. Stat. Phys. 112 1153-1175

[12] Baumgärtel H and Wollenberg M 1983 *Mathematical scattering theory* (Birkhäuser)

[13] Böttcher A and Silbermann B 2006 *Analysis of Toeplitz operators* (Springer)

[14] Bratteli O and Robinson D W 1987/1997 *Operator algebras and quantum statistical mechanics 1/2* (Springer)

[15] Culvahouse J W, Schinke D P, and Pfortmiller L G 1969 *Spin-spin interaction constants from the hyperfine structure of coupled ions* Phys. Rev. 177 454-464

[16] Emch G G 1972 *Algebraic methods in statistical mechanics and quantum field theory* (Reprint, Dover, 2009)

[17] Hardt V and Wagenführer E 1996 *Spectral properties of a multiplication operator* Math. Nachr. 178 135-156

[18] Hunziker W (n.d.) Lecture notes, ETH Zurich

[19] Jost R 1973 *Quantenmechanik II* (Verlag der Fachvereine an der ETH Zürich)

[20] Kechris A S 1995 *Classical descriptive set theory* (Springer)

[21] Lieb E, Schultz T, and Mattis D 1961 *Two soluble models of an antiferromagnetic chain* Ann. Physics 16 407-466

[22] Matsui T and Ogata Y 2003 *Variational principle for non-equilibrium steady states of the XX model* Rev. Math. Phys. 15 905-923

[23] Mikeska H-J and Kolezhuk A K 2004 *One-dimensional magnetism* in Schollwöck U, Richter J, Farnell D J J, and Bishop R F (Ed.) *Quantum Magnetism* Lect. Notes Phys. 645 1-83 (Springer)

[24] Nambu Y 1950 *A note on the eigenvalue problem in crystal statistics* Progr. Theor. Phys. 5 1 1-13

[25] Picavet G and Picavet-L'Hermite M 2003 *Trigonometric polynomial rings* Lecture notes Pure Appl. Math. (Marcel Dekker) 231 419-433.

[26] Primas H 1983 *Chemistry, quantum mechanics, and reductionism* (Springer)

[27] Ruelle D 2001 *Entropy production in quantum spin systems* Commun. Math. Phys. 224 3-16

[28] Sewell G 1986 *Quantum theory of collective phenomena* (Reprint, Dover, 2014)

[29] Simon B 1977 *Notes on infinite determinants of Hilbert space operators* Adv. Math. 24 244-273

[30] Sologubenko A V, Giannò K, Ott H R, Vietkine A, and Revcolevschi A 2001 *Heat transport by lattice and spin excitations in the spin-chain compounds* $\mathrm{SrCuO_2}$ *and* $\mathrm{Sr_2CuO_3}$ Phys. Rev. B 64 054412 1-11

[31] Suzuki M 1971 *Relationship among exactly soluble models of critical phenomena, I* Prog. Theor. Phys. 46 (5) 1337-1359