Exact solution of Markovian master equations for quadratic Fermi systems: thermal baths, open XY spin chains and non-equilibrium phase transition

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Abstract. We generalize the method of third quantization to a unified exact treatment of Redfield and Lindblad master equations for open quadratic systems of \( n \) fermions in terms of diagonalization of a \( 4n \times 4n \) matrix. Non-equilibrium thermal driving in terms of the Redfield equation is analyzed in detail. We explain how one can compute all the physically relevant quantities, such as non-equilibrium expectation values of local observables, various entropies or information measures, or time evolution and properties of relaxation. We also discuss how to exactly treat explicitly time-dependent problems. The general formalism is then applied to study a thermally driven open XY spin 1/2 chain. We find that the recently proposed non-equilibrium quantum phase transition in the open XY chain survives the thermal driving within the Redfield model. In particular, the phase of long-range magnetic correlations can be characterized by hypersensitivity of the non-equilibrium steady state to external (bath or bulk) parameters. Studying the heat transport, we find negative differential thermal conductance for sufficiently strong thermal driving as well as non-monotonic dependence of the heat current on the strength of the bath coupling.
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1. Introduction

One of the main challenges of many-body theory and non-equilibrium statistical mechanics is to understand the properties of relaxation of large interacting quantum systems. There are two common approaches to these types of problems. One important direction is to try to define dynamics in the thermodynamic limit and to investigate its properties with rigorous mathematical methods of operator algebras [1]–[3]. However, in this context explicit results that go beyond existence proofs are quite limited. A second approach is to split a large system into a tensor product of a smaller system of interest, and the rest (environment), and trying to eliminate all the degrees of freedom of the large, macroscopic environment (see e.g. [4, 5]). This approach, although involving a series of approximations, is usually more fruitful for explicit calculations and quantitative analyses. We may be interested in relaxation to either equilibrium or non-equilibrium steady states (NESSs), depending on the equal or non-equal values of thermodynamic potentials assigned to possibly several pieces of environment—which we shall call the baths. Such calculations of the quantitative properties of steady states may be very useful, for example, in the realm of transport theory [6], and may complement the linear response calculations and suggest nonlinear responses or far-from-equilibrium effects.

However, to date we have had very few explicit calculations of the non-equilibrium properties of open many-body quantum systems, and mainly they had to focus on small systems with a single or a pair of degrees of freedom (such as spins or bosons); see for example [7, 8]. The reason is that there has been no theoretical technique to deal with open many-body problems except for the Keldysh formalism of non-equilibrium Green’s functions, which however can easily get too involved for explicit calculations. Recently, two new directions have been proposed, both in the direction of numerical simulation and theoretical analysis. Namely, in the context of numerical simulations of open many-body systems, time-dependent density matrix renormalization group techniques [9] have been demonstrated to efficiently simulate relaxation to steady states with the Lindblad master equation [10]. On the other hand, it has been shown [11] that the Lindblad equation for general quadratic fermionic systems, for example, for
XY-like quantum spin chains that are mappable to quadratic fermionic systems, can be solved explicitly with the technique of canonical quantization in the Fock space of operators—third quantization for short.

In this paper, we shall show how the third quantization can be generalized to treat quadratic systems with arbitrary Markovian master equations, which are not necessarily of the Lindblad form. In particular, we shall focus on the Redfield dissipator in terms of which we can simulate simple thermal reservoirs, and thermal driving of the system under non-equilibrium conditions. After giving a short account on mathematical formulation of Markovian master equations and the basic physical assumptions and approximations involved in the derivation (in section 2), we shall in section 3 present a short but self-contained generalization of the theory [11]. In addition, we shall outline the calculation of dynamical correlation functions in Liouvillean dynamics, and formulate an exact treatment of explicitly time-dependent quantum Liouville problems. In section 4, we shall apply our technique to treat an open XY spin chain in the non-equilibrium Redfield model. We shall outline several intriguing exact numerical results on large spin chains. In particular, we show that the recently announced quantum phase transition in the open XY chain in the local Lindblad bath model generalizes also to the non-equilibrium thermal Redfield model with qualitatively identical characteristics. The transition is characterized by the spontaneous emergence of long-range magnetic correlations, and hypersensitivity of the steady state to the external system’s parameters, when the transverse magnetic field drops below the critical value $|\hbar| < h_c = |1 - \gamma|^2$, where $\gamma$ is the anisotropy parameter. Furthermore, we analyze in some detail the heat transport in the XY chain, and find regions of negative differential heat conductance for strong thermal driving, namely non-monotonic dependence of the heat current on the temperature difference between the baths.

2. Markovian master equations in non-equilibrium quantum physics

Decomposing the Hilbert space of the universe into a tensor product $\mathcal{H} = \mathcal{H}_s \otimes \mathcal{H}_b$ of the central system $\mathcal{H}_s$ and the bath (or a set of baths) $\mathcal{H}_b$ (environment), one writes the total Hamiltonian as

$$H = H_s \otimes \mathbb{1}_b + \mathbb{1}_s \otimes H_b + \lambda \sum_{\mu} X_\mu \otimes Y_\mu,$$

where $X_\mu$ are linear operators over $\mathcal{H}_s$, and $Y_\mu$ are linear operators over $\mathcal{H}_b$. Note that $X_\mu, Y_\mu$ can always be chosen to be Hermitian, so this shall be assumed throughout this paper. The Markovian quantum master equation for the time evolution of the central system’s density matrix $\rho(t)$ is derived [4] using three main assumptions: (i) weak coupling (assuming $\lambda$ to be small), (ii) factorizability of the initial density matrix $\rho_s(0) \otimes \rho_b(0)$ and (iii) Born–Markov approximation, which rests upon the assumption that the bath-correlation functions

$$\Gamma_{\mu, \nu}^\beta(t) := \lambda^2 \text{tr} (\tilde{Y}_\mu(t) Y_\nu e^{-\beta H_b}) / \text{tr} e^{-\beta H_b}, \quad \tilde{Y}_\mu(t) := e^{itH_b} Y_\mu e^{-itH_b}$$

decay on much shorter timescales than the central system’s dynamics $\tilde{X}_\mu(t) := e^{itH_s} X_\mu e^{-itH_s}$. We use units in which Planck’s constant $\hbar = 1$, and may use different inverse temperatures $\beta$ for different pieces of the environment (for different baths). The resulting master equation is referred to as the Redfield equation

$$\frac{d}{dt} \rho(t) = -i[H_s, \rho(t)] + \hat{D}\rho(t),$$

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where the dissipator map has a memoryless kernel with the following general form:

$$\dot{D}\rho = \sum_{\mu,\nu} \int_0^\infty d\tau \Gamma_{\tau}^{\beta}(\mu)(-\tau) \rho, X_\nu + h.c. \tag{4}$$

If one additionally assumes the so-called rotating wave-approximation, one arrives at the dynamical semi-group that manifestly preserves the positivity of the density matrix at all times and can be generally described by the dissipator in the Lindblad form

$$\dot{D}'\rho = \sum_{\mu,\nu} \gamma_{\tau}(\mu)(-\tau) \rho, X_\nu + h.c., \tag{5}$$

where the only condition is that $$\gamma$$ is a Hermitian $$\gamma_{\mu,\nu} = \gamma_{\nu,\mu}^*$$ and a positive definite matrix. The standard Lindblad form is obtained by diagonalizing the matrix $$\gamma$$ whose eigenvectors yield the usual Lindblad operators. The important property of the bath-correlation functions (2) (which constitute all that we need to know about the baths) is the Kubo–Martin–Schwinger (KMS) condition

$$\Gamma_{\tau}^{\beta}(\mu)(-t) = \Gamma_{\tau}^{\beta}(\tau), \tag{6}$$

which is needed to prove that the thermal state $$\rho_{\text{gibbs}} = e^{-\beta H} / \text{tr} e^{-\beta H}$$ is a steady state of the master equation (3), provided that all baths are thermalized to the same inverse temperature.

However, in the case of several thermal baths with possibly different temperatures we may expect that $$\rho(t)$$ relaxes to a physically very interesting NESS.

3. Diagonalization of quantum Liouvilleans for quadratic Fermi systems

In this section we give a short account on the general technique of canonical quantization in Liouville space (‘third quantization’) and complete diagonalization of Markovian master equations (3), with (4) or (5), for quadratic fermionic problems. We treat a finite problem with n fermionic degrees of freedom, described by $$2n$$ anti-commuting Hermitian operators $$w_j, j = 1, 2, \ldots, 2n$$, in which the Hamiltonian $$H$$ may take a general quadratic form and the coupling operators may be general linear forms:

$$H_k = \sum_{j,k=1}^{2n} w_j H_{j,k} w_k = w \cdot H w, \tag{7}$$

$$X_\mu = \sum_{j=1}^{2n} x_{\mu,j} w_j = x_\mu \cdot w. \tag{8}$$

Thus, $$2n \times 2n$$ matrix $$H$$ can be chosen to be antisymmetric $$H^T = -H$$. Throughout this paper $$x = (x_1, x_2, \ldots)^T$$ will designate a vector (column) of appropriate scalar-valued or operator-valued symbols $$x_k$$. This formalism is immediately applicable for describing either (i) physical fermions $$c_m, m = 1, 2, \ldots, n$$, where $$w_{2m-1} = c_m + c_m^\dagger, w_{2m} = i(c_m - c_m^\dagger),$$ or

1 This is not the case for equations (3) and (4) which allow for possible breaking of positivity at an initial short time interval, the so-called sleeapage time.

2 With an additional technical condition of neglecting the Cauchy principal value contribution to the time integral (4), see the discussion at the end of section 3.2.
(ii) XY-like systems of spins 1/2 with canonical Pauli operators $\vec{\sigma}_m$, $m = 1, 2, \ldots, n$, where the fermionic operators are represented by the famous Jordan–Wigner transformation

$$w_{2m-1} = \sigma_m^x \prod_{m'<m} \sigma_{m'}^z, \quad w_{2m} = \sigma_m^y \prod_{m'<m} \sigma_{m'}^z.$$

(9)

3.1. Fock space of operators

The fundamental concept for our analysis is a Fock space structure over the $4^n$-dimensional Liouville space of operators $\mathcal{K}$, which density matrix $\rho(t)$ is also a member of. From here on, we shall adopt Dirac bra-ket notation for the operator space $\mathcal{K}$, which is fixed by the following definition of the inner product:

$$\langle x | y \rangle = \text{tr} x^\dagger y, \quad x, y \in \mathcal{K}. \quad (10)$$

We note that $2^{2n}$ operator-products $|P_\alpha\rangle$, labeled with a binary multi-index $\alpha$,

$$P_{\alpha_1, \alpha_2, \ldots, \alpha_{2n}} := 2^{-n/2} w_1^{\alpha_1} w_2^{\alpha_2} \ldots w_{2n}^{\alpha_{2n}}, \quad \alpha_j \in \{0, 1\},$$

(11)

constitute a complete orthonormal basis of $\mathcal{K}$ with respect to an inner product.

In fact it is easy to show that $|P_\alpha\rangle$ is a fermionic Fock basis, and powers 1 in the product (11) can be considered like a sort of fermionic excitation, if we define the following set of linear annihilation maps $\hat{c}_j$ over $\mathcal{K}$,

$$\hat{c}_j |P_\alpha\rangle = \alpha_j w_j P_\alpha,$$

(12)

and derive the actions of their Hermitian adjoints—the creation linear maps $\hat{c}_j^\dagger$,

$$\hat{c}_j^\dagger |P_\alpha\rangle = (1 - \alpha_j) w_j P_\alpha,$$

(13)

which satisfy canonical anticommutation relations

$$\{\hat{c}_j, \hat{c}_k\} = 0, \quad \{\hat{c}_j, \hat{c}_k^\dagger\} = \delta_{j,k}, \quad j, k = 1, 2, \ldots, 2n.$$

(14)

3.2. Bilinear form of the Liouvillean

The aim is now to show that the generator of the master equation (3)

$$\hat{L} := -i \text{ad} H + \hat{D},$$

(15)

is in general a quadratic form in these adjoint fermionic maps $\hat{c}_j, \hat{c}_j^\dagger$. In order to see that clearly, let us define the left and right multiplication maps over $\mathcal{K}$:

$$\hat{w}_j^L |x\rangle := |w_j x\rangle, \quad \hat{w}_j^R |x\rangle := |x w_j\rangle.$$

(16)

Inspecting the actions of $\hat{w}_j^L, \hat{w}_j^R$ on the Fock basis $|P_\alpha\rangle$, one arrives at the following useful identities

$$\hat{w}_j^L = \hat{c}_j + \hat{c}_j^\dagger,$$

(17)

$$\hat{w}_j^R = \hat{P} (\hat{c}_j - \hat{c}_j^\dagger) = - (\hat{c}_j - \hat{c}_j^\dagger) \hat{P},$$

(18)

3. We shall use notation where linear maps over the operator space (in physics literature sometimes referred to as ‘super-operators’) are designated by $\hat{\cdot}$. 

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are a parity map and a number map, respectively, which count the parity and number of adjoint fermionic excitations (number of factors in (11)). Note that \( \hat{P} \) anticommutes with all \( \hat{c}_j, \hat{c}_j^\dagger \), hence the second equality of (18), and \( \hat{P}^2 = \hat{1} \).

The unitary part of the Liouvillean (15) now trivially reads

\[
-\mathrm{i} \mathrm{ad} \, H_s = -\mathrm{i} \hat{w}_0^L \cdot \hat{H}_s \hat{L}^\dagger + \mathrm{i} \hat{H}_s \hat{L}^R \cdot \hat{w}_0 = -4\mathrm{i} \hat{c}_j^\dagger \cdot \hat{H}_s. \tag{20}
\]

The dissipator (4) can be represented as a map over \( K \) as

\[
\hat{D} = \sum_{\mu, \nu} \sum_{j,k=1}^{2n} x_{\nu, k} \int_0^\infty \mathrm{d}\tau f_{\mu, j}(-\tau) \left( \Gamma_{\nu, \mu}^\beta(\tau) \hat{L}_j' + \Gamma_{\nu, \mu}^\beta(\tau) \hat{L}_j' \right), \tag{21}
\]

where \( f_{\mu, j}(t) \) is a (real-valued) propagator of Heisenberg dynamics in the closed system

\[
\hat{X}_\mu(t) = x_{\mu, \nu} \cdot \exp(-\mathrm{i} \mathrm{ad} \, H_s t) \hat{w} =: f_{\mu, j}(t) \cdot \hat{w}, \tag{22}
\]

which—due to (20)—can be explicitly solved for a quadratic Hamiltonian (7), giving

\[
f_{\mu, j}(t) = \exp(4\mathrm{i} \hat{H}_s t) x_{\mu, \nu}, \tag{23}
\]

and

\[
\hat{L}_j' x := [x, x_j], \quad \hat{L}_j'' x := [x, x_j] \tag{24}
\]

are fundamental basis dissipators which, using (17) and (18) evaluate to

\[
\hat{L}_j' = \hat{w}_j^L \cdot \hat{w}_j^R - \hat{w}_j^L \cdot \hat{w}_j^R = (\hat{1} + \hat{P})(\hat{c}_j^\dagger \hat{c}_k^\dagger \hat{c}_j \hat{c}_k) + (\hat{1} - \hat{P})(\hat{c}_j \hat{c}_k - \hat{c}_k \hat{c}_j), \tag{25}
\]

\[
\hat{L}_j'' = \hat{w}_j^L \cdot \hat{w}_j^R - \hat{w}_j^L \cdot \hat{w}_j^R = (\hat{1} - \hat{P})(\hat{c}_j^\dagger \hat{c}_k^\dagger \hat{c}_j \hat{c}_k) + (\hat{1} - \hat{P})(\hat{c}_j \hat{c}_k - \hat{c}_k \hat{c}_j). \tag{26}
\]

It will prove useful if we express the internal dynamics (23) explicitly in terms of eigenvalues and eigenvectors of the Hamiltonian matrix \( H \). Since a \( 2n \times 2n \) matrix is anti-symmetric and Hermitian, its real eigenvalues come in pairs \( \epsilon_m, -\epsilon_m, m = 1, \ldots, n \), with the corresponding eigenvectors \( u_m, u_m^\ast \), namely \( H u_m = \epsilon_m u_m \) and \( H u_m^\ast = -\epsilon_m u_m^\ast \) since \( H^\ast = -H \). The eigenvectors may and should always be chosen orthonormal (even in the case of degeneracies), meaning

\[
u_j \cdot u_m = 0, \quad \nu_j \cdot u_m^\ast = \delta_{j, m}. \tag{27}
\]

Then the spectral decomposition of the Heisenberg dynamics reads

\[
f_{\mu, j}(t) = \sum_{m=1}^n \left( e^{-4\mathrm{i} \epsilon_m t} (\nu_{\mu, j} \cdot u_m) u_m^\ast + e^{4\mathrm{i} \epsilon_m t} (\nu_{\mu, j} \cdot u_m^\ast) u_m \right). \tag{28}
\]

Note that \( \hat{P}_\pm = (\hat{1} \pm \hat{P})/2 \) are orthogonal projectors that commute with all the terms (20), (25) and (26) that constitute the Liouvillean (15), \( [\hat{P}_{\pm}, \hat{L}] = 0 \), and hence the dynamics (3) does not mix the operator subspaces \( K^\pm = \hat{P}_{\pm} K \) composed of an even/odd number of fermionic operators. Since we are mainly interested in the expectation values of even observables, such as
currents and densities, we shall in the present paper focus on the dynamics in subspace $K^+$ only, and consider the corresponding Liouvillean $\hat{\mathcal{L}}_{|K^+}$:

$$\hat{\mathcal{L}}_+ = \hat{\mathcal{P}}_r \hat{\mathcal{L}} \hat{\mathcal{P}}_r.$$  \hfill (29)

The extension to the odd parity subspace is straightforward. Collecting the results (20), (21), (25) and (26), it is now obvious that $\hat{\mathcal{L}}_+$ is a bilinear form in $\hat{c}_j$ and $\hat{\bar{c}}_j$. For convenience, we define $4n$ Hermitian Majorana maps $\hat{a}_r$, $r = 1, \ldots, 4n$,

$$\hat{a}_j = \frac{1}{\sqrt{2}} (\hat{c}_j + \hat{\bar{c}}_j), \quad \hat{a}_j^\dagger = \frac{i}{\sqrt{2}} (\hat{c}_j - \hat{\bar{c}}_j),$$  \hfill (30)

and express the Liouvillean as

$$\hat{\mathcal{L}}_+ = \hat{\mathcal{A}} \cdot \hat{\mathcal{A}}^\dagger - A_0 \hat{c},$$  \hfill (31)

where the $4n \times 4n$ complex antisymmetric matrix $\mathcal{A}$, later referred to as a structure matrix, and a scalar $A_0$, can be expressed as

$$A_{2j-1,2k-1} = -2i H_{j,k} - M_{j,k} + M_{k,j},$$
$$A_{2j-1,2k} = i M_{j,k} + i M_{j,k}^*,$$
$$A_{2j,2k-1} = -i M_{j,k} - i M_{k,j}^*,$$
$$A_{2j,2k} = -2i H_{j,k} - M_{j,k}^* + M_{k,j}^*,$$
$$A_0 = \text{tr} (\mathcal{M}^* + \mathcal{M})$$

where $\mathcal{M}$ is a $2n \times 2n$ bath matrix that can be compactly written as

$$\mathcal{M} := \sum_v \mathcal{z}_v \otimes \mathcal{z}_v,$$  \hfill (33)

$$\mathcal{z}_v := \sum_\mu \int_0^\infty \text{d}\tau \Gamma^\beta_{\mu,v} (\tau) \mathcal{f}_{\mu}(-\tau).$$  \hfill (34)

Defining the bath-spectral functions $\Gamma^\beta_{\mu,v}(\omega) := \frac{1}{2\pi} \int_{-\infty}^\infty \text{d}\tau \Gamma^\beta_{\mu,v} (\tau)e^{-i \omega \tau}$ for which the KMS condition reads

$$\tilde{\Gamma}^\beta_{\mu,v}(-\omega) = e^{i \omega \mu} \tilde{\Gamma}^\beta_{\mu,v}(\omega),$$  \hfill (35)

and extending the range of integration in (34) to $[-\infty, \infty]$, or better still, neglecting the Cauchy principal value parts in the integrals—which exactly amounts to neglecting the Lamb-shift Hamiltonian term [4] in the master equation—we obtain a very simple expression (involving only finite sums) for the bath vectors:

$$\mathcal{z}_v = \pi \sum_\mu \sum_m^n \tilde{\Gamma}^\beta_{\mu,v} (4\epsilon_m) \left( (x_\mu \cdot u_m^*) u_m + e^{4\epsilon_\mu} (x_\mu \cdot u_m) u_m^* \right).$$  \hfill (36)

At this point a remark on neglecting the Lamb-shift term is in order. As the Redfield model already involves a series of physical assumptions and approximations, it is somewhat difficult to argue under what conditions these terms can be dropped on the same level of approximations. However, one can straightforwardly show, using the KMS condition (6) and hermiticity $(\Gamma^\beta_{\mu,v}(\tau))^* = \Gamma^\beta_{\nu,\mu}(\tau)$, that only if the Cauchy principal value terms are dropped (i.e. if the range of integration in (4) is extended to $[-\infty, \infty]$) the Redfield dissipator annihilates
the Gibbs state $\hat{D}|e^{-\beta H_s}\rangle = 0$, and hence the Gibbs state is the steady state of the equilibrium thermal Redfield model.

Note again that the inverse temperature in (36) could, in principle, be a function of the bath index $\beta = \beta_\nu$ in case one would be interested in the non-equilibrium situation with couplings to several different temperatures. But we should stress that different temperatures only make sense among uncorrelated baths labelled by $\mu, \nu$, for which $\Gamma^\beta_{\mu,\nu} \equiv 0$ for any $\beta$.

We note also that the present formalism uniformly covers both the Redfield and the Lindblad master equations, as the Lindblad dissipator (5) is obtained from (4) by simply taking the limit $\Gamma^\beta_{\mu,\nu}(t) = \gamma_{\mu,\nu}\delta(t + 0)$, and then the bath matrix reduces to a Hermitian form $M = \sum_{\nu,\mu} \gamma_{\nu,\mu} x_\nu \otimes x_\mu = M^\dagger$, which is equivalent to the one used in [11].

### 3.3. Static Liouvillean: normal modes, NESS and decay spectrum

Having the compact form of the Liouvillean (31)—and assuming for the time being that the structure matrix $A$ is static, i.e. there is no explicit time dependence in the matrix $H$ or coupling vectors $x_\mu$—we follow [11] and explicitly construct its normal form, the NESS, which is exactly the right-vacuum state of (31) $\hat{L}_s|\text{NESS}\rangle = 0$, the spectral gap, and the full spectrum of Liouvillean decay modes, all in terms of spectral decomposition of $4n \times 4n$ matrix $A$. We state the main results here in a compact form.

Assuming the structure matrix is diagonalizable, its eigenvalues can be paired as $\beta_j, -\beta_j, j = 1, \ldots, 2n$, assuming $\text{Re}\beta_j \geq 0$, and its eigenvectors $v_{2j-1}$ (corresponding to $\beta_j$) and $v_{2j}$ (corresponding to $-\beta_j$) can always be normalized—irrespective of possible degeneracies among $\beta_j$, which shall be called rapidities—such that

$$V V^T = J, \quad J := \sigma^x \otimes 1_{2n},$$

(37)

where $V$ is a $4n \times 4n$ matrix whose $r$th row is given by $v_r$, $V_{r,s} := v_{r,s}$. Thus the structure matrix allows the following decomposition,

$$A = V^T \text{diag}\{\beta_1, -\beta_1, \ldots, \beta_{2n}, -\beta_{2n}\} V J,$$

(38)

which after plugging into the Liouvillean (31) immediately brings it to a normal form

$$\hat{L}_s = -2 \sum_{j=1}^{2n} \beta_j \hat{b}_j \hat{b}_j^\dagger,$$

(39)

where

$$\hat{b}_j := v_{2j-1} \cdot \hat{a}, \quad \hat{b}_j^\dagger := v_{2j} \cdot \hat{a},$$

(40)

are the normal-master-mode (NMM) maps, satisfying almost canonical anti-commutation relations

$$\{\hat{b}_j, \hat{b}_k\} = 0, \quad \{\hat{b}_j, \hat{b}_k^\dagger\} = \delta_{j,k}, \quad \{\hat{b}_j^\dagger, \hat{b}_k^\dagger\} = 0.$$

(41)

The map $\hat{b}_j$ could be interpreted as an annihilation map and $\hat{b}_j^\dagger$ as a creation map of the $j$th NMM, but we should note that $\hat{b}_j^\dagger$ is in general not the Hermitian adjoint of $\hat{b}_j$. The right vacuum

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is now essentially defined by \( \hat{b}_j |\text{NESS}\rangle = 0 \), whereas the left vacuum is trivial \( \langle 1 | \hat{L}^+ = 0 \) and satisfies \( \langle 1 | \hat{b}_j^\dagger = 0 \). Note that the left vacuum simply corresponds to the identity operator \( 1 \in \mathcal{K} \), i.e. an empty state \( 2^{n/2} p_{0,0,\ldots,0} \) with respect to a-fermions \( \hat{c}_j \).

Assuming that the whole rapidity spectrum is strictly away from the imaginary line \( \text{Re} \beta_j > 0 \), we state the following exact results:

1. \( |\text{NESS}\rangle \) is unique.
2. Almost any initial density matrix relaxes to \( \text{NESS} \) with an exponential rate \( \Delta = 2 \min \text{Re} \beta_j \) (the spectral gap of the Liouvillian). The complete spectrum of \( 4^n \) eigenvalues of \( \hat{L}^+ \) is obtained by all possible binary linear combinations \( \lambda_\nu = -2\nu \cdot \beta, \nu_j \in \{0, 1\} \).
3. The expectation value of any quadratic observable \( w_j w_k \) in a (unique) \( \text{NESS} \) can be explicitly computed as

\[
\langle w_j w_k \rangle_{\text{NESS}} := \text{tr} w_j w_k \rho_{\text{NESS}} = 2 \langle 1 | \hat{a}_j \hat{a}_k |\text{NESS}\rangle
\]

\[
= 2 \sum_{m=1}^{2n} v_{2m,j-1} v_{2m-1,k-1}
\]

\[
= -\frac{1}{\pi} \int_{-\infty}^{\infty} d\omega \ G_{2j-1,2k-1}(\omega),
\]

where

\[
G(\omega) := (A - i\omega I)^{-1}
\]

is a matrix of the non-equilibrium Green’s function. The first equality is proven in [11] whereas the last equality requires a simple contour integration on the spectral decomposition of the resolvent (45).

4. The Wick theorem may be used for the calculation of expectation values of arbitrary higher order (even!) observables by the sums of all possible pairwise contractions of the form (42).

Note that as soon as some of the rapidities condense to the imaginary axis, or vanish, \( \text{NESS} \) typically becomes non-unique (see [13] for a detailed discussion of Liouvillian degeneracies).

### 3.4. Static Liouvillian: time-dependent correlation functions

The complete Liouvillian propagator can be written explicitly as

\[
\exp(t \hat{L}^+) = \sum_{\nu \in \{0,1\}^{2n}} \exp(-2t \nu \cdot \beta) (\hat{b}_1^\dagger)^{\nu_1} \ldots (\hat{b}_n^\dagger)^{\nu_{2n}} |\text{NESS}\rangle \langle 1 | (\hat{b}_n)^{\nu_{2n}} \ldots (\hat{b}_1)^{\nu_1}.
\]

It may be of some physical interest to evaluate dynamical response after perturbing the \( \text{NESS} \) by multiplying it with some local observable. In order to avoid discussion of negative parity dynamics \( \hat{L}^- \), we take a pair of simplest even-order, quadratic observables, and define

\[
\text{Small simplification has been made with respect to the statement of theorem 3 of [11] which has been pointed out by Pižorn [12].}
\]
the corresponding non-equilibrium time-dependent correlation function—or non-equilibrium response function—as

\[ C_{(j,k),l,m}(t) := \langle w_j(t) w_k(t) w_l(0) w_m(0) \rangle_{\text{NESS}} \]

\[ = 4 \langle 1 | \hat{a}_{2j-1} \hat{a}_{2k-1} \exp(t \hat{L}_+ \hat{a}_{2l-1} \hat{a}_{2m-1}) | \text{NESS} \rangle. \] (47)

Expressing the multiplication maps \( \hat{a}_{2j-1} = \sum_{r=1}^{2n} (V_{2r, 2j-1} \hat{b}_r + V_{2r-1, 2j-1} \hat{b}'_r) \) and plugging in the propagator (46), while noting that only the terms with 0 or 2 Liouvillean excitations contribute, we obtain a simple expression

\[ C_{(j,k),l,m}(t) = 4 \left( \sum_{r=1}^{2n} v_{2r, 2j-1} v_{2r-1, 2k-1} \right) \left( \sum_{r'=1}^{2n} v_{2r', 2l-1} v_{2r'-1, 2m-1} \right) \]

\[ - 4 \sum_{1 \leq r < r' \leq 2n} e^{-2t(\beta_r + \beta_{r'})} \left( v_{2r', 2j-1} v_{2r, 2k-1} - v_{2r, 2r'-1} v_{2r'-1, 2k-1} \right) \]

\[ \times \left( v_{2r'-1, 2j-1} v_{2r-1, 2m-1} - v_{2r-1, 2r'-1} v_{2r'-1, 2m-1} \right). \] (48)

### 3.5. Time-dependent Liouvilleans

In this section, we indicate how to efficiently treat explicitly time-dependent master equations, written in third quantized form as

\[ \frac{d}{dt} |\rho(t)\rangle = \hat{L}_+(t)|\rho(t)\rangle, \quad \hat{L}_+(t) = \hat{a} \cdot \mathbf{A}(t) \hat{a} - A_0(t) \hat{a}, \] (49)

where explicit time-dependence of the structure matrix \( \mathbf{A}(t) \) may physically arise due to driving by means of an external time-dependent force (time-dependent matrix \( \mathbf{H}(t) \)) or time-dependent coupling operators (time-dependent vectors \( x_{\mu}(t) \)). In this situation NESS cannot exist, but we shall show that one may still efficiently evaluate the propagator

\[ |\rho(t)\rangle = \hat{U} |\rho(0)\rangle, \quad \hat{U} := \hat{T} \exp \left( \int_0^t d\tau \hat{L}_+(\tau) \right), \] (50)

where \( \hat{T} \) indicates a time-ordered product.

The procedure is the following. Note that the space of all anti-symmetric complex structure matrices forms a Lie algebra \( \mathfrak{so}(4n, \mathbb{C}) \). The following straightforward identity

\[ \left[ \frac{1}{2} \hat{\mathbf{A}} \cdot \hat{\mathbf{A}}, \frac{1}{2} \hat{\mathbf{B}} \cdot \hat{\mathbf{B}} \right] = \frac{1}{2} \hat{\mathbf{A}} \cdot [\mathbf{A}, \mathbf{B}] \hat{\mathbf{A}}, \] (51)

holding for any pair of complex \( 4n \times 4n \) matrices \( \mathbf{A}, \mathbf{B} \), indicates that Liouvilleans (31) and (49) generate a \( 4^n \)-dimensional representation of \( \mathfrak{so}(4n, \mathbb{C}) \). Thus, the time-ordered product (50) can be evaluated within a Lie group \( \text{SO}(4n, \mathbb{C}) \) of \( 4n \times 4n \) matrices,

\[ \hat{U} = \hat{T} \exp \left( 2 \int_0^t d\tau \mathbf{A}(\tau) \right), \] (52)

and then the full Liouvillean propagator is written as

\[ \hat{U} = \exp(\hat{\mathbf{A}} \cdot \mathbf{C} \hat{\mathbf{A}} - C_0 \hat{\mathbf{A}}), \quad \mathbf{C} = \frac{1}{2} \ln \mathbf{U}, \quad C_0 = \int_0^t d\tau A_0(\tau). \] (53)

\textsuperscript{5} Even if this has to be done numerically, using Trotter–Suzuki decomposition schemes, the computational complexity is only polynomial in \( n \).
The logarithm of $\hat{U}$ can now be considered as a ‘static’ Liouvillean, so we can diagonalize it by the methods of section 3.3, leading to spectral decomposition of the form (46).

4. XY spin chains

The theory of the previous sections shall now be applied to investigate a homogeneous, finite XY chain of $n$ spins, described by Pauli matrices $\sigma^x_j, \sigma^y_j, \sigma^z_j, j = 1, \ldots, n$, with the Hamiltonian

$$H = \sum_{j=1}^{n-1} \left( \frac{1 + \gamma}{2} \sigma^x_j \sigma^x_{j+1} + \frac{1 - \gamma}{2} \sigma^y_j \sigma^y_{j+1} \right) + \sum_{j=1}^{n} \hbar \sigma^z_j,$$

(54)

which is described by two real parameters, anisotropy $\gamma$ and transverse magnetic field $h$. Without loss of generality we may assume that $\gamma, h \in [0, \infty)$. We decide to couple the XY chain thermally only at its ends, so we consider the most general four coupling operators that allow for an explicit solution,

$$X_1 = \kappa_1(\sigma^x_1 \cos \theta_1 + \sigma^y_1 \sin \theta_1), \quad X_2 = \kappa_2(\sigma^x_1 \cos \theta_2 + \sigma^y_1 \sin \theta_2),$$

(55)

$$X_3 = \kappa_3(\sigma^x_N \cos \theta_3 + \sigma^y_N \sin \theta_3), \quad X_4 = \kappa_4(\sigma^x_N \cos \theta_4 + \sigma^y_N \sin \theta_4),$$

and fully decorrelated baths $\Gamma^\beta_{\mu,\nu} = \delta_{\mu,\nu} \Gamma^\beta_{\mu}$. We take standard baths of harmonic oscillators at two ends with possibly different inverse temperatures, and Ohmic spectral functions

$$\tilde{\Gamma}^\beta_{\mu,\nu}(\omega) = \lambda^2 \delta_{\mu,\nu} \frac{\omega}{\exp(\omega \beta_{\mu}) - 1}, \quad \beta_{1,2} \equiv \beta_L, \quad \beta_{3,4} \equiv \beta_R.$$

(56)

Note that the frequency cutoff in the spectral function is irrelevant as we neglect the Lamb-shift term in the master equation.

The entire problem can be fermionized by means of Jordan–Wigner transformation (9), namely the Hamiltonian and the coupling operators transform to

$$H = -i \sum_{j=1}^{n-1} \left( \frac{1 - \gamma}{2} w_{2j} w_{2j+1} - \frac{1 + \gamma}{2} w_{2j-1} w_{2j+2} \right) - i \sum_{j=1}^{n} \hbar w_{2j-1} w_{2j},$$

$$X_1 = \kappa_1(w_1 \cos \theta_1 + w_2 \sin \theta_1), \quad X_3 = W \kappa_3(w_{2n} \cos \theta_3 - w_{2n-1} \sin \theta_3),$$

(57)

$$X_2 = \kappa_2(w_1 \cos \theta_2 + w_2 \sin \theta_2), \quad X_4 = W \kappa_4(w_{2n} \cos \theta_4 - w_{2n-1} \sin \theta_4),$$

where $W = (-i)^{n-1} w_1 w_2 \ldots w_{2n}$ is an operator that commutes with all the elements of $K^+$ (or anti-commutes with all the elements of $K^-$) and satisfies $WW^\dagger = W^\dagger W = 1$, hence it has no effect on the dissipator (4) in $\hat{L}$. We note, however, that the commutation of $W$ through $\rho$ in (4) for the dynamics in $K^-$ produces a minus sign in all the bath terms, i.e. it changes the sign of $\hat{D}_- \hat{D}_\rho \hat{D}_-$, with respect to a pure fermionic problem.

The $4n \times 4n$ structure matrix now has a specific block-tridiagonal + block-bordered form,

$$A = A' + B,$$

(58)
\[ A' = \begin{pmatrix}
  a & b & 0 & 0 & \cdots & 0 \\
  c & a & b & 0 & \cdots & 0 \\
  0 & c & a & b & \cdots & 0 \\
  \vdots & \ddots & \ddots & \ddots & \ddots & \ddots \\
  0 & 0 & \ldots & c & a & b \\
  0 & 0 & \ldots & 0 & c & a
\end{pmatrix}, \quad B = \begin{pmatrix}
  l_1 & l_2 & \cdots & l_{n-1} & l_n \\
  l'_2 & 0 & \cdots & 0 & r'_2 \\
  \vdots & \vdots & \ddots & \ddots & \ddots \\
  l'_{n-1} & 0 & \cdots & 0 & r'_{n-1} \\
  r_1 & r_2 & \cdots & r_{n-1} & r_n
\end{pmatrix}, \quad (59) \]

where \( a, b, c \) are 4 \times 4 matrices:
\[ a = -ih \mathbb{1}_2 \otimes \sigma^y, \quad b = \frac{1}{2} \mathbb{1}_2 \otimes (i\sigma^y - \gamma \sigma^x), \quad c = -b^T. \quad (60) \]

The sequences of 4 \times 4 matrices \( l_j, l'_j, r_j, r'_j \), which form the block-bordered part \( B \), can be straightforwardly computed (see (32)) from the form of the coupling vectors \( \Delta_{1,2} = (\kappa_{1,2} \cos \theta_{1,2}, \kappa_{1,2} \sin \theta_{1,2}, 0, \ldots, 0)^T \), \( \Delta_{3,4} = (0, \ldots, 0, -\kappa_{3,4} \sin \theta_{3,4}, \kappa_{3,4} \cos \theta_{3,4})^T \), and their bath-transformations (36) with (56). Although we are unable to give closed-form general expressions, we can make an asymptotic estimate—for large \( n \)—on the decay of these matrices with distance from the diagonal
\[ ||l_j|| \sim ||l'_j|| \sim ||r_{n+1-j}|| \sim ||r'_{n+1-j}|| \propto \exp(-Kj). \quad (61) \]

The coefficient \( K > 0 \) in general depends only on \( \gamma, h \) and \( \beta_L \) (for \( l_j \)) or \( \beta_R \) (for \( r_j \)). Note that for the special case of \textit{local Lindblad coupling} (5) with the same local coupling operators (57), the only non-vanishing blocks that remain are the diagonal ones \( l_1 \) and \( r_n \), given explicitly in (11).

Below we shall present some intriguing numerical results of the non-equilibrium thermal Redfield equation (3) and (4) for the open XY chain given by (54)–(56), in comparison with the local non-equilibrium Lindblad model (5) where a suitable set of coupling operators of the form (55) and 4 \times 4 coupling matrix \( \gamma_{l,v} \) can be chosen to parametrize the Lindblad operators
\[ L_{1,2} = \sqrt{\Gamma_{1,2}^L \sigma_1^\pm}, \quad L_{3,4} = \sqrt{\Gamma_{1,2}^R \sigma_\rho^\pm}, \quad \text{parametrized in exactly the same way as in} [11, 14]. \]

For all the numerical results reported for the thermal Redfield model, we consider the bath parameter values \( \kappa_1 = \kappa_3 = 1, \kappa_2 = \kappa_4 = 0, \theta_1 = \theta_3 = \pi/6, \) and \( \beta_L = 0.3, \beta_R = 5.2 \) unless \( \beta \)s are varying, and \( \lambda = 0.1 \) unless \( \lambda \) varying, whereas for the Lindblad model we always take the bath parameters \( \Gamma_{1,1}^L = 0.5, \Gamma_{1,2}^L = 0.3, \Gamma_{1,1}^R = 0.5, \Gamma_{1,2}^R = 0.1 \).

\[ 4.1. \text{Non-equilibrium phase transition} \]

In [14] an intriguing suggestion of a quantum phase transition far from equilibrium in the steady state of an open boundary driven XY spin chain has been put forward. Numerical and heuristic theoretical evidence has been given for the spontaneous emergence of long-range magnetic order in \textit{NESS} as soon as the magnetic field drops below the critical value \( |h| < h_c \),
\[ h_c = |1 - \gamma^2|. \quad (62) \]

However, that study was done with local Lindblad reservoirs, so the question remained whether the effect persists in the presence of local thermal reservoirs satisfying KMS conditions for non-vanishing temperatures. It is an easy task now to follow the recipes of section 3.3 and numerically evaluate the spin–spin correlator (note the use of the Wick theorem as the spin–spin correlator is of fourth order in \( w_j \)):
\[ C_{1,m} = \text{tr} (\sigma^j_1 \sigma^m_1 \rho_{\text{NESS}}) - \text{tr} (\sigma^j_1 \rho_{\text{NESS}}) \text{tr} (\sigma^m_1 \rho_{\text{NESS}}) \]
\[ = \langle w_{2l-1} w_{2m-1} \rangle_{\text{NESS}} \langle w_{2l} w_{2m} \rangle_{\text{NESS}} - \langle w_{2l-1} w_{2m} \rangle_{\text{NESS}} \langle w_{2l} w_{2m-1} \rangle_{\text{NESS}}. \quad (63) \]
First, we use efficient prescription (43) to compute correlation matrices at non-equilibrium conditions $\beta_L = 0.3 \neq \beta_R = 5.2$ and plot them for two different system sizes and five different values of $h$ around $h_c$ in figure 1. The results look qualitatively identical to those for Lindblad driving, even for other quantities that were investigated numerically in detail in [14].

For example, in figure 2, we plot the phase diagram of the residual correlator $C_{\text{res}} = \sum_{l,m} |l-m|>n/2 |C_{l,m}| / \sum_{l,m} |l-m|>n/2 1$, which also reveals possible criticality in the region of a large anisotropy $\gamma > 1$ previously not discussed. We note that the size dependence of the residual magnetic correlator $C_{\text{res}}$ shows very characteristic behavior: namely

\begin{align}
C_{\text{res}} \propto \exp(-\eta n) & \quad \text{with } \eta > 0 \quad \text{for } |h| > h_c \text{ or } h = 0, \quad (64) \\
C_{\text{res}} \propto 1/n & \quad \text{for } 0 < |h| < h_c. \quad (65)
\end{align}

Thus we shall refer to the regime with $0 < |h| < h_c$ as long-range magnetic correlation (LRMC) phase\(^6\), the regime with $|h| > h_c$, or $h = 0$, as non-LRMC phase, and the regime with $|h| = h_c$ as critical. Scaling (64) and (65) is illustrated in figure 3. Exponential decay of the $C_{\text{res}}(n)$ in non-LRMC phase (64) is consistent with the exponential decay of a two-point correlator with the distance between sites $C(r) = \sum_{j-i=r} C_{i,j} / \sum_{j-i=r} 1 \sim \exp(-\xi r)$, as can be qualitatively noted already in figure 1. However, we demonstrate in figure 4 that the exponent $\xi$ could, in principle, be very different between the Redfield and local Lindblad models. Furthermore, as for the Lindblad model the exponents $\xi$ and $\eta$ (of (64)) appear to be equal, for the Redfield

\(^6\) Note, interestingly, that unlike for the local Lindblad driving [14] the XX line $\gamma = 0, 0 < |h| < 1$, also exhibits long-range magnetic correlations for the thermal Redfield driving.
Figure 2. Phase diagram for the non-equilibrium thermal Redfield model of an open XY chain. We plot the residual correlator $C_{\text{res}}$ against the bulk parameters $\gamma, h$. The dashed curve indicates the critical line $h_c(\gamma)$ (62). The system size is fixed to $n = 100$ and bath parameters are specified in the text.

Figure 3. Residual correlator $C_{\text{res}}$ as a function of system size $n$ for the LRMC phase ($\gamma = 0.5, h = 0.2$, left plot) and the non-LRMC phase ($\gamma = 0.5, h = 0.9$, right plot), where we compare the non-equilibrium thermal Redfield model (red squares) and the non-equilibrium Lindblad model (blue circles) with bath parameters as specified in the text. The thin lines indicate the suggested behavior $1/n$ (on the left) and $\exp(-\eta n)$ (on the right) (with the numerical best fit $\eta = 1.192$ for the Redfield model and $\eta = 0.937$ for the Lindblad model).

model they do not seem to be simply related. Analytical estimation of these exponents presents a challenge for future theoretical work.

However, we note that with the thermal driving with Redfield dissipators, the long-range magnetic order disappears when the temperatures of the baths become equal, $\beta_L = \beta_R$, and there we recover, consistently, all the properties of the thermal state [15] that are most easily numerically reproduced by the method of [16], i.e. fast decay of correlations for any $h$ and absence of long-range order. For example, it is interesting to note how the residual correlator $C_{\text{res}}$
Figure 4. Comparison of the decay of the two-point spin–spin correlator $C(r) = \sum_{j-i=r} C_{i,j} / \sum_{j-i=r} 1 \sim \exp(-\xi r)$ between the non-equilibrium thermal Redfield model (red squares) and the non-equilibrium Lindblad model (blue circles) for the same values of bulk parameters in the non-LRMC phase ($h = 1.05$, $\gamma = 0.2$, $n = 200$) and bath parameters specified in the text. The thin lines indicate suggested exponential decays $\propto \exp(-\xi r)$ with the exponents $\xi = 1.635$ (fitting the Redfield model) and $\xi = 0.937$ (fitting the Lindblad model).

Figure 5. Residual correlation $C_{\text{res}}$ versus (inverse) temperature drop $\Delta \beta$ between the left and the right bath, $\beta_L = 2 - \Delta \beta / 2$, $\beta_R = 2 + \Delta \beta / 2$, for the non-equilibrium thermal Redfield model of an open XY chain in LRMC phase ($\gamma = 0.5$, $h = 0.3$), system size $n = 100$, and the bath parameters specified in the text. The thin line indicates suggested $|\Delta \beta|^2$ behavior.

(for large $n$ in the LRMC phase) decreases as a function of the difference of inverse temperatures $\Delta \beta = \beta_R - \beta_L$, namely the numerics of figure 5 suggests clearly that $C_{\text{res}} \propto (\Delta \beta)^2$.

The heuristic explanation of this non-equilibrium phase transition is rather straightforward [14], however, its exact proof and also the quantitative dependence of the decay exponent $\eta(\gamma, h)$ are still lacking. We note that the transition point $h = h_c$ is characterized by a simple
Figure 6. Liouvillean spectral gap $\Delta$ for the non-equilibrium thermal Redfield model of an open XY chain. We plot three different cases with: $\gamma = 0.5$, $h = 0.8 > h_c$ (non-LRMC phase, light blue circles), $\gamma = 0.5$, $h = 0.75 = h_c$ (critical regime, dark blue squares), $\gamma = 0.5$, $h = 0.3 < h_c$ (LRMC phase, black diamonds), whereas bath parameters are specified in the text. Suggested power law decays $n^{-3}$ and $n^{-5}$ are indicated with thin lines.

property of the XY spin chain quasi-particle dispersion relation

$$\omega(q) = \sqrt{(\cos q - h)^2 + \gamma^2 \sin^2 q},$$

where $\epsilon_j = \omega(2\pi j/n)$ would be exactly the (positive) eigenvalues of matrix $H$ if periodic boundary conditions were imposed on the closed system. Namely, in non-LRMC phase $|h| > h_c$ there exists only a single pair of trivial stationary points $q^* = 0, \pi$, whereas in LRMC phase $|h| < h_c$ there exists another pair of non-trivial stationary points $\pm q^* \neq 0, \pi$, $d\omega/dq\big|_{q=q^*} = 0$, which introduces a new non-trivial length scale $1/q^*$ that determines typical sizes of correlated regions in the matrix $C_{l,m}$ (see figure 1). Therefore, this simple non-equilibrium quasi-particle picture predicts mean-field critical exponent $1/q^* \sim |h_c - h|^{-1/2}$ as $h \uparrow h_c$ (confirmed in [14]).

The non-equilibrium quantum phase transition can also be characterized by the scaling of the Liouvillean spectral gap $\Delta(n)$, namely in the critical regime one expects a qualitative increase in the relaxation time $1/\Delta$ to NESS. Numerical results (see figure 6) suggest that the spectral gap of the Liouvillean remains like in the local Lindblad case [11],

$$\Delta \propto n^{-3} \quad \text{for } h \neq h_c, \quad \Delta \propto n^{-5} \quad \text{for } h = h_c,$$

although we are at the moment unable to prove this conjecture. Also note the slight fluctuations of $\Delta(n)$ in the LRMC phase as opposed to a smooth power law in the non-LRMC phase.

Long-range correlations for $|h| < h_c$ naturally imply sensitivity of NESS to tiny variations in the system’s parameters. For example, one may also expect that local observables in NESS will then be sensitive functions of the bath-driving or even bulk parameters, such as the magnetic field $h$. In figure 7, we plot local magnetization in the center of the chain $s_z = \langle \sigma_{n/2}^z \rangle_{\text{NESS}}$ versus field strength $h$. Indeed, we notice that for $|h| > h_c$, $s_z(h)$ is a smooth function whereas for $|h| < h_c$, $s_z(h)$ becomes a rapidly oscillating or, better still, fluctuating function. Even though the amplitude of these oscillations decreases with $n$, the scale of $h$ on which $s_z(h)$ fluctuates decreases with $n$ even faster, so we predict that in the thermodynamic limit $n \to \infty$, in the
Figure 7. Hypersensitivity of NESS to magnetic field strength \( h \). We plot local magnetization \( s_z(h) = \langle \sigma_z^n \rangle_{\text{NESS}} \) for the non-equilibrium thermal Redfield model of an open XY chain with \( \gamma = 0.5 \) and bath parameters as written in the text. Big blue (small red) circles represent data for \( n = 50 \) (\( n = 100 \)), whereas the vertical line denotes the critical value \( h = h_c \).

LRMC phase the local susceptibility \( ds_z/dh \) would be ill defined. In summary, the LRMC phase can be characterized by hypersensitivity of NESS to external parameters.

4.2. Heat transport and entropies

An important non-equilibrium physical effect that one can investigate more deeply in an open XY chain is heat transport, which has recently been intensively studied in quantum spin chains, see e.g. \([17]–[21]\) or \([22]\) for a recent review on the topic.

Writing the Hamiltonian (54) in the bulk as a sum \( H = \sum_m H_m \) with a two-body energy density operator

\[
H_m = -\frac{1 + \gamma}{2} w_{2m} w_{2m+1} + \frac{1 - \gamma}{2} w_{2m-1} w_{2m+2} - \frac{h_m}{2} w_{2m-1} w_{2m} - \frac{h_{m+1}}{2} w_{2m+1} w_{2m+2},
\]

one can derive the local energy current

\[
Q_m = i[H_m, H_{m+1}]
\]

\[
= i(1 - \gamma^2)(w_{2m-1} w_{2m+3} + w_{2m} w_{2m+4}) - 2i\hbar (1 - \gamma)(w_{2m-1} w_{2m+1} + w_{2m+2} w_{2m+4})
\]

\[
-2i\hbar (1 + \gamma)(w_{2m} w_{2m+2} + w_{2m+1} w_{2m+3}),
\]

which, by construction, satisfies the continuity equation

\[
(d/dt)\langle H_m \rangle = \langle i[H, H_m] \rangle + \text{tr } H_m \hat{D}\rho(t) = -\langle Q_m \rangle + \langle Q_{m-1} \rangle.
\]

The two terms between the two equality signs above correspond to the unitary and dissipative term in the master equation (3). The unitary term has already been transformed to a simple expectation value using cyclicity of the trace \( \text{tr } x[y, z] = \text{tr } y[z, x] \), while the dissipative term can be further shown to vanish in the bulk \( 2 \leq m \leq n-2 \) by exercising the cyclicity of the trace again and transforming the integrand of (4) to terms of the form \( \text{tr } \hat{X}_\mu(-\tau) \rho[X, H_m] \equiv 0 \).

The rhs expression of equation (70) then follows from the nearest-neighbor locality of the

\[
\text{New Journal of Physics 12 (2010) 025016 (http://www.njp.org/)}
\]
Figure 8. NESS expectation value of heat current \(\langle Q_m \rangle_{\text{NESS}}\) versus two inverse temperatures \(\beta_L\) and \(\beta_R\) for the non-equilibrium thermal Redfield model of an open XY chain with \(\gamma = 0.5, h = 0.9\), system size \(n = 53\), and bath parameters given in the text. Note that the ‘shoulders’ of maxima, around \(\beta_L \approx 0.05, \beta_R > 1\), and with L and R exchanged, could be interpreted as negative differential heat conductance.

Hamiltonian. Therefore, in NESS the expectation value of the current \(\langle Q_m \rangle_{\text{NESS}}\) should be independent of the position \(m\). By looking at the dependence of the steady-state current on system size we clearly find ballistic transport, namely \(\langle Q_m \rangle_{\text{NESS}} = \mathcal{O}(n^0)\), irrespective of the temperature differences between the baths and bulk parameters of the model (i.e. whether in the LRMC phase, non-LRMC phase, or critical). However, we find a very interesting dependence of heat current on temperature driving, i.e. on the two temperatures of the thermal baths. In figure 8, we plot \(\langle Q_m \rangle_{\text{NESS}}\) versus \(\beta_L\) and \(\beta_R\) and find a maximum of the current for intermediate driving, namely when one of the temperatures is less than \(1/\beta_L < 1\) and the other temperature is about \(1/\beta_R \approx 20\). This is a clear signature of negative differential heat conductance, which could perhaps be related to similar far-from-equilibrium effects recently observed in spin and charge transport [23].

This behavior can be nicely characterized by computing the Gibbs entropy of NESS. Since NESS is completely characterized by quadratic correlations \(\langle w_j w_k \rangle_{\text{NESS}}\) and the Wick theorem, one can adopt the recipe that has been proposed in [24] for computing block entropies (or entanglement entropies) applied to the entire lattice. In fact, taking an arbitrary block region \(A \subseteq \{1, \ldots, n\}\), one can compute Von Neumann entropy \(S_A(\rho) = -\text{tr}_A \rho_A \log_2 \rho_A\) (in base 2), where \(\rho_A = \text{tr}_A \rho\) is a reduced density matrix and \(\bar{A}\) denotes the complement of \(A\), as

\[
S_A = \sum_{j=1}^{\#(A)} H_2((1 + v_j)/2) \quad \text{with} \quad H_2(x) := -x \log_2 x - (1 - x) \log_2 x,
\]

and \(\pm iv_j\) are the eigenvalues of the \(2\#(A) \times 2\#(A)\) part of the correlation matrix \(B_{j,k}\) defined by \(\langle w_j w_k \rangle_{\text{NESS}} = \delta_{j,k} + iB_{j,k}\), restricted to Majorana operators \(w_j, w_k\) corresponding to spins from block \(A\). The same general procedure has been applied to thermal (Gibbs) states in [16]. When taking the maximal block \(A = \{1, \ldots, n\}\), we obtain exactly the standard Gibbs entropy.
of NESS. In figure 9, we plot the Gibbs entropy $S_{[1,...,n]}$ as a function of two bath temperatures and show that, quite remarkably, the regions of large (maximal) heat current correspond to regions of large (locally maximal) Gibbs entropy. This is not unexpected as the product of the heat current and the inverse temperature difference $\Delta \beta$ may be understood as the entropy production rate.

Calculation of Gibbs entropy of NESS also provides a nice way of controlling the positivity of NESS as a density matrix, since this is by no means guaranteed by the Redfield master equation. Indeed we find that for very small temperatures (large $\beta$s), or for very strong bath coupling $\lambda$, the positivity of NESS might be slightly violated (red region in figure 9), namely some of the correlation matrix eigenvalues $\nu_j$ become slightly larger than 1 (but in our numerical experience never by more than $10^{-7}$ or so).

We can use the concept of block entropy of NESS to further characterize the non-equilibrium phase transition. For example, we may compute the total (quantum plus classical) correlations between two halves of the spin chain in NESS as given by quantum mutual information (QMI) $I(n) = S_{[1,...,n/2]} + S_{[n/2+1,...,n]} - S_{[1,...,n]}$.

Interestingly, we find (see figure 10) that QMI saturates $I(n) = \mathcal{O}(n^0)$ in the non-LRMC phase (for $|h| > h_c$), whereas in the LRMC phase (for $0 < |h| < h_c$) QMI becomes extensive $I(n) = \mathcal{O}(n)$, indicating a drastic enhancement of correlations in NESS. This is again very similar to the behavior of operator space entanglement entropy (OSEE) (analyzed for the Lindblad model in [14]), so one may extend the relationship between QMI and OSEE which has been conjectured for thermal states in [16] to NESS.

In the context of energy transport, it is interesting to look at the energy density profiles in NESS. In figure 11, we plot the relative spatial fluctuation of the energy density $f(m) = |\langle H_m \rangle_{\text{NESS}} - \bar{H}|/|\bar{H}|$, where $\bar{H} = (n - 3)^{-1} \sum_{m=2}^{n-2} \langle H_m \rangle_{\text{NESS}}$ is the averaged energy density. Quite strikingly, we observe a big variation of $f(m)$ from site to site for the LRMC phase and...
Figure 10. Another manifestation of the non-equilibrium phase transition: QMI of NESS for the non-equilibrium thermal Redfield model of an open XY spin chain. The bulk parameters are $\gamma = 0.5$ and $h = 0.9 > h_c = 0.75$ (lightest blue, saturated curve), $h = 0.7$, $h = 0.5$ and $h = 0.3$ (from lighter to darker blue curves). Thin red lines indicate the linear growth of QMI for $h < h_c$.

Figure 11. Another manifestation of non-equilibrium phase transition: positional fluctuations in energy density in NESS of the non-equilibrium thermal Redfield model of an open XY chain. We plot the relative fluctuation $f(m) = |\langle H_m \rangle_{\text{NESS}} - \bar{H}|/|\bar{H}|$, where $\bar{H}$ is the bulk average of energy density $\langle H_m \rangle_{\text{NESS}}$. Three curves correspond to $\gamma = 0.5$ and $h = 0.7 < h_c$ (black curve), $h = 0.75 = h_c$ (dark blue curve) and $h = 0.8 > h_c$ (light blue curve), while the system size is $n = 253$.

very smooth (non fluctuating) behavior for the non-LRMC phase, which is characterized with a bulk-constant $f(m)$ that is exponentially small in $n$. This behavior can again be considered as a manifestation of hypersensitivity of NESS and LRMC.

Finally, we check the dependence of the heat current $\langle Q_m \rangle_{\text{NESS}}$ on the system–bath coupling strength $\lambda$. It was recently reported by Karevski and Platini [25] that the spin current $J_m$ in the local Lindblad model of an open isotropic XX chain $\gamma = 0$ has non-monotonic dependence on $\lambda$ which can be universally described by a formula $\langle J_m \rangle_{\text{NESS}} = a' \lambda^2/(b' + \lambda^4)$, where $a'$, $b'$ are...
some constants. For the anisotropic XY model and general non-equilibrium thermal Redfield driving, we are unable to derive an exact analytic result; however, our numerical simulations suggest very similar behavior for the heat current

$$\langle Q_m \rangle_{\text{NESS}} \approx \frac{a \lambda^2}{b + \lambda^4},$$

(72)

where $a$ and $b$ are again some constants that may depend on all system parameters except $\lambda$. This is particularly interesting because in the anisotropic XY model the spin current is not even well defined as there is no corresponding conservation law. This behavior is demonstrated in figure 12, where one may also notice small but detectable deviations between numerics and the best fit to (72). We note that the error of the fit does not decrease but is roughly constant when we increase the system size $n$.

5. Discussion

The purpose of the present paper was three-fold. Firstly, we have outlined a general method for the exact treatment of quadratic many-body Markovian master equations. Our formalism, which rests upon treating density operators as elements of a suitable operator Fock space (or Liouville–Fock space), is quite flexible and allows for explicit solution of static and time-dependent quantum many-body Liouvillean problems, for example, computation of arbitrary physical observables in the non-equilibrium steady state, decay rates of approach to the steady state, or even time evolution of the density matrix of externally forced systems described by explicitly time-dependent Liouvillians, all with polynomial computation complexity in number of particles (fermionic degrees of freedom).

Secondly, we have analyzed in detail the Redfield model of thermal baths within our framework. In spite of the fact that the Redfield model does not define a proper dynamical semigroup,
namely it is not guaranteed to preserve positivity of the density operator, we have confirmed that steady states typically correspond to proper (positive) density operators. Tiny deviations from positivity have only been observed in some test cases for very small temperatures or very large couplings to the baths (which anyway violate the weak coupling assumption). Furthermore, we have shown that coupling the central system with several thermal baths of the Redfield type at different temperatures produces physically interesting NESSs, for example, such states that carry non-vanishing heat current. We wish to stress this physically obvious but mathematically delicate point with particular care, as we have found qualitatively different results for Lindblad–Davies dissipators which generate proper dynamical semigroups and satisfy the detailed balance condition with respect to Gibbs states [5, 26]. Namely, when we constructed a Lindblad–Davies dissipator with respect to two baths with two different temperatures coupled to two ends of the system (spin chain), we found that the resulting steady state (fixed point of Liouvillean dynamics) is simply some convex combination of two Gibbs states corresponding to the bath temperatures, and as such has always zero heat current and cannot represent the physical steady state. This implies that the secular approximation (sometimes called the rotating wave approximation), which is the one-step from the Redfield to the Lindblad–Davies bath model, prohibits the emergence of the physical out-of-equilibrium steady states with currents; therefore, the seemingly harmless rapidly oscillating terms in the Redfield dissipator may be absolutely essential for non-equilibrium physics. Thus we conjecture that the thermal Redfield model is somehow a minimal mathematical model that can describe non-equilibrium thermal driving of a non-self-thermalizing (e.g. integrable) open quantum system.

Thirdly, we have applied our theory to analyze non-equilibrium quantum phase transition and heat transport in an open XY spin 1/2 chain. We have carefully compared numerical results for the non-equilibrium thermal Redfield model and the local Lindblad model, which has been discussed before [11, 14]. We have found that the phase diagram of the non-equilibrium XY model is insensitive to the theory with which we describe the baths, and the differences were only quantitative. In particular, we wish to stress that thermally driven heat current in the XY chains exhibits non-monotonic dependence on the temperature difference, which may be interpreted as negative differential heat conductance. We believe that our numerical results on a non-equilibrium open XY chain provide a strong motivation for further analytical work. In particular, we believe that the block-tridiagonal plus block-bordered structure of the Liouvillean structure matrix (58) and (59) could be explored in combination with the non-equilibrium Green function formula for the observables (44) and (45) to yield explicit asymptotic results for large $n$.

Note added: formally quite a similar approach to non-equilibrium quasi-particles has recently been developed independently by Kosov [27].

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