Heat rectification on the XX chain

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In order to better understand the minimal ingredients for thermal rectification, we perform a detailed investigation of a simple spin chain, namely, the open XX model with a Lindblad dynamics involving global dissipators. We use a Jordan-Wigner transformation to derive a mathematical formalism to compute the heat currents and other properties of the steady state. We have rigorous results to prove the occurrence of thermal rectification even for slightly asymmetrical chains. Interestingly, we describe cases where the rectification does not decay to zero as we increase the system size, that is, the rectification remains finite in the thermodynamic limit. We also describe some numerical results for more asymmetrical chains. The presence of thermal rectification in this simple model indicates that the phenomenon is of general occurrence in quantum spin systems.

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I. INTRODUCTION

One of the fundamental issues of nonequilibrium statistical physics is the derivation of transport laws from the underlying microscopic dynamics. In particular, a theme of general interest is the investigation of energy transport, which involves two main mechanisms, the conduction by electricity and by heat, issues, however, with quite different status in the literature. On the one hand, the success of modern electronics since the invention of the transistor is well known, with huge impact in our daily lives. On the other hand, we have seen a slow progress of phononics, the counterpart of electronics dedicated to the study and manipulation of heat current. Heat analogs of electronic devices, such as transistors and gates, have already been proposed [1], but the absence of a feasible and efficient thermal diode, the basic ingredient of these devices, makes considerable advancement difficult. A thermal diode or thermal rectifier is a device in which heat has a preferable direction to flow; more precisely, the magnitude of the heat current changes as we invert the device between two thermal baths. Thus, the first obvious ingredient for the occurrence of rectification is the existence of an asymmetry in the system.

The most usual models for the study of heat conduction in insulating solids have been given, since Debye [2] and Peierls [3], by chains of classical harmonic or anharmonic oscillators. Unfortunately, in the more treatable harmonic version there is no thermal rectification. Even for the harmonic classical system with inner self-consistent stochastic reservoirs [4], the absence of thermal rectification has been proved [5]. It is interesting to recall that such a system obeys the Fourier law, which does not hold in purely harmonic chains [6], showing that the inner reservoirs indeed represent some vestiges of anharmonicity, which, however, are not enough for the occurrence of thermal rectification.

The search for the minimal ingredients sufficient to guarantee rectification is a fundamental and difficult problem in transport theory. In this direction we recall the study of simple models, avoiding intricate details which may hide the ingredients. For example, we recall the establishment of rectification in Ref. [7], a toy model of alternating graded bars and bullets. There it was shown that the existence of a local temperature-dependent thermal conductivity together with the graded structure ensures rectification.

Besides this recurrent study of classical oscillators and related models, it is important to stress the currently increasing interest in the study of energy transport at the quantum scale, motivated, e.g., by the emerging field of quantum thermodynamics and advances allowing the manipulation of quantum systems. In particular, there are recurrent investigations of quantum spin models, which involve problems in connection with different areas: condensed matter, cold atoms, quantum information, etc.

In this direction, rectification in the boundary driven XXZ spin-$\frac{1}{2}$ model (with polarization at the edges) is shown in Ref. [8] for the spin current in the case of a homogeneous chain with asymmetrical external magnetic field, and it is shown in Ref. [9] for the energy current in a graded chain. We recall that the XXZ chains are archetypal models for open quantum spin systems. Interestingly, Ref. [8] showed the absence of spin rectification in a system with a zero anisotropy parameter Δ (coefficient of $\sigma_j^z\sigma_{j+1}^z$). For $\Delta \neq 0$, rectification was observed. As the XXZ model can be mapped onto a problem of bosons with creation and annihilation operators, with quadratic terms and a quartic one proportional to Δ (the Tonks-Girardeau model), the vanishing of rectification in the absence of the quartic term is compared to the case of classical

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oscillators, where there is no rectification in the absence of anharmonicity (given by terms of order 4 or higher in the potential).

Anyway, heat rectification has been described in some quadratic models with proper arrangements. For example, the quantum Ising model is shown to rectify [10] if the intersite interaction is long enough to link the first site (connected to the left bath) to the last one (connected to the right bath). Otherwise, there is no rectification in such a model.

In the present work, searching for simple quantum models showing rectification, that is, aiming to shed some light on the question of minimal ingredients necessary for the occurrence of heat rectification, we perform an analytical detailed investigation of the XX spin-$\frac{1}{2}$ model with some specific dissipators and nearest-neighbor interactions only. Even for a slight asymmetric chain, we prove the occurrence of thermal rectification by performing analytical computations. Interestingly, we describe cases of heat rectification which does not decay to zero as the system size increases, that is, it remains finite in the thermodynamic limit. We still show the rectification for more asymmetrical chains by using numerical techniques. The presence of heat rectification in this simple quadratic quantum spin model, i.e., in a simple system without intricate interactions, indicates that it is a ubiquitous phenomenon in the quantum context: For the occurrence of thermal rectification, it seems that we need only asymmetry in the system and a thermal conductivity (or inner parameters) depending on temperature and so parameters which change as we invert the baths leading to rectification.

The rest of the paper is organized as follows. In Sec. II we introduce the model, the Jordan-Wigner transformation, and some initial results. In Sec. III we describe the currents and some properties. In Sec. IV analytical results for the heat rectification are shown. Section V presents some numerical results. We summarize in Sec. VI.

II. MODEL AND PRELIMINARY DETAILS

Here we consider a one-dimensional quantum XX spin chain with N sites, described by the Hamiltonian

$$H = \sum_{j=1}^{N} \frac{h_j}{2}\sigma_j^z + \frac{1}{2}\sum_{j=1}^{N-1} \alpha_j\left(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y\right), \tag{1}$$

where the σ_j^i are the usual Pauli matrices, h_j is the external magnetic field acting on site j, and α_j is the exchange interaction between spins j and $j+1$. The rectification will be directly associated with the asymmetry of the coefficients h_j and α_j with respect to the left-right reflection of the chain.

These spin chains are coupled on the first and last sites to thermal reservoirs and kept at temperatures T_L and T_R, respectively. They are modeled by an infinite number of bosonic degrees of freedom given by the Hamiltonian

$$H_B^i = \sum_l \Omega_{i,l} a_{i,l}^\dagger a_{i,l}, \tag{2}$$

where $a_{i,l}$ is a set of independent bosonic operators and $\Omega_{i,l}$ are the corresponding frequencies, which we assume to take on a quasicontinuum of values in the interval $[0,\infty)$. Moreover, the interactions with the first and last sites are assumed to take the form

$$\begin{aligned} H_I^L &= \sigma_1^x \sum_i g_i(a_{L,i}^\dagger + a_{L,i}),\\ H_I^R &= \sigma_N^x \sum_i g_i(a_{R,i}^\dagger + a_{R,i}). \end{aligned} \tag{3}$$

In order to proceed with the study, we recast the problem as a Lindblad master equation in the weak-coupling regime [11], describing the time evolution of the system's density matrix ρ by

$$\frac{d\rho}{dt} = -i[H,\rho] + \mathcal{D}_L + \mathcal{D}_R, \tag{4}$$

where $\mathcal{D}_L$ and $\mathcal{D}_R$ are the Lindblad dissipators associated with the baths. It is possible to derive them from Eq. (3) using the method of eigenoperators [11].

Consider first only a single system-bath interaction, with Hamiltonian $H_I = A\otimes B$, where A and B are Hamiltonian operators of the system and the bath, respectively. We define

$$\begin{aligned} \Gamma(\omega) &= \int_{-\infty}^{\infty} e^{i\omega t}\langle B(t)B(0)\rangle dt\\ &= \int_{-\infty}^{\infty} e^{i\omega t}\,\mathrm{tr}\left\{e^{iH_B t}Be^{-iH_B t}B\frac{e^{-H_B/T}}{Z}\right\}dt, \end{aligned} \tag{5}$$

that is, the Fourier transform of the bath correlations, evaluated for a bath thermal state, with temperature T and partition function $Z = \mathrm{tr}(e^{-H_B/T})$.

Let us define ϵ to be the eigenenergies of H and Π_ϵ the corresponding projection operators onto the subspace corresponding to ϵ. From the *weak-coupling-limit* derivation [11] we define the eigenoperator corresponding to the bath coupling A as

$$A(\omega) = \sum_{\epsilon,\epsilon'} \Pi_\epsilon A \Pi_{\epsilon'}\delta_{\epsilon-\epsilon',\omega} \tag{6}$$

and they satisfy

$$[H, A(\omega)] = -\omega A(\omega), \quad A^\dagger(\omega) = A(-\omega). \tag{7}$$

In terms of these eigenoperators, it can be shown [11] that the Lindblad dissipator associated with the microscopic interaction $H_I = A\otimes B$ will be, in the rotation-wave approximation,

$$\mathcal{D}(\rho) = \sum_\omega \Gamma(\omega)[A(\omega)\rho A^\dagger(\omega) - \frac{1}{2}\{A^\dagger(\omega)A(\omega),\rho\}]. \tag{8}$$

This method therefore allows us to write down the corresponding dissipator. All it requires is sufficient knowledge of the eigenstates of H in order to compute the $A(\omega)$.

Let us now evaluate $\Gamma(\omega)$ in Eq. (5) for the case of a typical bath-interaction operator $B = \sum_l g_l(a_l^\dagger + a_l)$, which appear in Eq. (3). Using the fact that $\langle a_l^\dagger a_{l'}\rangle = \delta_{l,l'}n(\Omega_l)$, where $n(\alpha) = (e^{\alpha/T} - 1)^{-1}$ is the Bose-Einstein distribution, and carrying out the Fourier transform in (5), we obtain

$$\begin{aligned} \Gamma(\omega) &= 2\pi\sum_l g_l^2\{[1+n(\Omega_l)]\delta(\omega-\Omega_l) + n(\Omega_l)\delta(\omega+\Omega_l)\}\\ &= \int_0^\infty d\Omega\, G(\Omega)\{[1+n(\Omega_l)]\delta(\omega-\Omega_l)\\ &\quad + n(\Omega_l)\delta(\omega+\Omega_l)\}. \end{aligned}$$

In the last line of this equation, the sum was transformed into an integral, assuming that the bath frequencies Ω_l take on a continuum of values. The function $G(\Omega)$ corresponds to $2\pi g_l^2$ times any additional factors that come from the transition from a sum to an integral over Ω_l (which do not depend on T). To simplify, we henceforth assume that $G(\Omega) = \gamma$, where γ is a constant. We have then

$$\Gamma(\omega) = \begin{cases} \gamma[1 + n(\omega)] & \text{for } \omega > 0 \\ \gamma n(-\omega) & \text{for } \omega < 0. \end{cases} \tag{9}$$

A comment is pertinent here. There are other possible spectral densities, for example, the Ohmic case $G(\Omega) = \Omega$. A different density will change the forthcoming computation, but the main result, i.e., the occurrence of rectification, will remain, since, as we will see later, it is essentially due to the existence of asymmetry and temperature-dependent parameters in the system (which change as we invert the baths).

This result is so far general and valid for any type of bath-coupling operator $A(\omega)$. Now we must specialize it for the case $A = \sigma_1^x$ and $A = \sigma_N^x$, which are the coupling operators appearing in Eq. (3). This means that we must find the operator A and to do so we need to know the spectral decomposition of H.

Now, to diagonalize H, we use a fermionic representation through the Jordan-Wigner transformation [12,13] given by

$$\eta_l = Q_l \sigma_l^-, \tag{10}$$

where the operators Q_l are defined by $Q_l = \prod_{j=1}^{l-1}(-\sigma_j^z)$. These operators satisfy the fermionic algebra

$$\{\eta_l^\dagger, \eta_{l'}\} = \delta_{l,l'}, \quad \{\eta_l, \eta_{l'}\} = 0. \tag{11}$$

We first transform the Hamiltonian in terms of σ_l^+ and σ_l^- operators given by

$$\begin{aligned} \sigma_l^+ &= \tfrac{1}{2}(\sigma_l^x + i\sigma_l^y), \\ \sigma_l^- &= \tfrac{1}{2}(\sigma_l^x - i\sigma_l^y). \end{aligned} \tag{12}$$

The Hamiltonian in (1) becomes then

$$H = \sum_{j=1}^{N} \frac{h_j}{2}\left(\sigma_j^+\sigma_j^- - \frac{1}{2}\right) + \frac{1}{2}\sum_{j=1}^{N-1}\alpha_j(\sigma_j^+\sigma_{j+1}^- + \sigma_j^-\sigma_{j+1}^+). \tag{13}$$

Using the Jordan-Wigner transformation (10), we can rewrite (13) in a quadratic form

$$\begin{aligned} H &= \sum_{j=1}^{N} h_j\eta_j^\dagger\eta_j + \sum_{j=1}^{N-1}\alpha_j(\eta_j^\dagger\eta_{j+1} + \eta_{j+1}^\dagger\eta_j) \\ &= \sum_{n,m} W_{n,m}\eta_n^\dagger\eta_m, \end{aligned} \tag{14}$$

where $W_{n,m}$ is a matrix with entries $W_{j,j} = h_j$ and $W_{j,j+1} = W_{j+1,j} = \alpha_j$.

In order to put H in diagonal form, we first diagonalize the matrix W. Since it is symmetric, it may be diagonalized by an orthogonal transformation $S_{n,k}(S^\dagger S = 1)$ as

$$W_{n,m} = \sum_{k=1}^{N} \epsilon_k S_{n,k} S_{m,k}. \tag{15}$$

The actual form of the eigenvalues and eigenvectors will often be complicated, as they depend on the specific choices of h_j and α_j in (1), which are nonuniform. The eigenvector matrices $S_{n,k}$ will turn out to play an important role as effective coupling constants in the global master equation [see, e.g., Eq. (33)].

Here we define a new set of fermionic operators

$$\tilde{\eta}_j = \sum_{k=1}^{N} S_{j,k}\eta_k, \tag{16}$$

in terms of which Eq. (14) becomes

$$H = \sum_{k=1}^{N} \epsilon_k \tilde{\eta}_k^\dagger \tilde{\eta}_k. \tag{17}$$

Now that we know the diagonal structure of the Hamiltonian, we have to find the operator in the dissipator (8) in terms of the fermionic operators $A(\omega)$. We start with the left bath, so $A = \sigma_1^x$. It is easy to see that using (10) and (16) we have

$$\sigma_1^x = \sum_{k=1}^{N} S_{1,k}^{-1}(\tilde{\eta}_k^\dagger + \tilde{\eta}_k). \tag{18}$$

We note that due to the diagonal structure in Eq. (17), it follows that $[H, \tilde{\eta}_k] = -\epsilon_k\tilde{\eta}_k$. Thus, $\tilde{\eta}_k$ and $\tilde{\eta}_k^\dagger$ are eigenoperators of H with allowed transition frequencies $\omega = \epsilon_k$ and $\omega = -\epsilon_k$, respectively. In this way, we can write the eigenoperator $A(\omega)$ as

$$A(\omega) = \sum_{k=1}^{N} \left[S_{1,k}^{-1}(\tilde{\eta}_k\delta_{\epsilon_k,\omega} + \tilde{\eta}_k^\dagger\delta_{-\epsilon_k,\omega})\right]. \tag{19}$$

The dissipator $\mathcal{D}_L(\rho)$, of the left site, is then found from Eq. (8),

$$\begin{aligned} \mathcal{D}_L(\rho) = \sum_{k=1}^{N}\Bigg[&\Gamma(\epsilon_k)\left(S_{1,k}^{-1}\right)^2\left(\tilde{\eta}_k\rho\tilde{\eta}_k^\dagger - \frac{1}{2}\{\tilde{\eta}_k^\dagger\tilde{\eta}_k, \rho\}\right) \\ &+ \Gamma(-\epsilon_k)\left(S_{1,k}^{-1}\right)^2\left(\tilde{\eta}_k^\dagger\rho\tilde{\eta}_k - \frac{1}{2}\{\tilde{\eta}_k\tilde{\eta}_k^\dagger, \rho\}\right)\Bigg]. \end{aligned} \tag{20}$$

Finally, we substitute the expression for Γ using Eq. (9). In order to do so, we must differentiate the cases where $\epsilon_k > 0$ and $\epsilon_k < 0$. We therefore write

$$\begin{aligned} \mathcal{D}_L(\rho) = \sum_{\epsilon_k>0}\gamma\left(S_{1,k}^{-1}\right)^2\Bigg\{&[1 + n_L(\epsilon_k)]\left[\tilde{\eta}_k\rho\tilde{\eta}_k^\dagger - \frac{1}{2}\{\tilde{\eta}_k^\dagger\tilde{\eta}_k, \rho\}\right] \\ &+ n_L(\epsilon_k)\left[\tilde{\eta}_k^\dagger\rho\tilde{\eta}_k - \frac{1}{2}\{\tilde{\eta}_k\tilde{\eta}_k^\dagger, \rho\}\right]\Bigg\} \\ + \sum_{\epsilon_k<0}\gamma\left(S_{1,k}^{-1}\right)^2\Bigg\{&n_L(-\epsilon_k)\left[\tilde{\eta}_k\rho\tilde{\eta}_k^\dagger - \frac{1}{2}\{\tilde{\eta}_k^\dagger\tilde{\eta}_k, \rho\}\right] \\ &+ [1 + n_L(-\epsilon_k)]\left[\tilde{\eta}_k^\dagger\rho\tilde{\eta}_k - \frac{1}{2}\{\tilde{\eta}_k\tilde{\eta}_k^\dagger, \rho\}\right]\Bigg\}, \end{aligned} \tag{21}$$

where n_i is the Bose-Einstein occupation, previously defined.

In Eq. (21) we see that the separation between positive and negative energies is not good to work with. Instead, we may write the terms in a unified way by defining the Fermi-Dirac occupation

$$f_{i,k} = \frac{1}{e^{\epsilon_k}/T_i + 1} \tag{22}$$

and the auxiliary function

$$\chi_{i,k} = 2n(|\epsilon_k|) + 1 = \coth\left(\frac{|\epsilon_k|}{2T_i}\right), \tag{23}$$

which we note is always positive. Then the dissipator finally becomes

$$\mathcal{D}_L(\rho) = \sum_{k=1}^{N} \gamma (S_{1,k}^{-1})^2 \chi_{L,k} \left\{ [1 - f_{L,k}] \left[\tilde{\eta}_k \rho \tilde{\eta}_k^\dagger - \frac{1}{2}\{\tilde{\eta}_k^\dagger \tilde{\eta}_k, \rho\} \right] + f_{L,k} \left[\tilde{\eta}_k^\dagger \rho \tilde{\eta}_k - \frac{1}{2}\{\tilde{\eta}_k \tilde{\eta}_k^\dagger, \rho\} \right] \right\}. \tag{24}$$

Now we turn to the bath coupled to the last site N. Here the relevant operator is $A = \sigma_N^x$. In this case, using the Jordan-Wigner transformation and the fact that $\eta_j^\dagger \eta_j = \sigma_j^+ \sigma_j^-$, we find

$$\sigma_N^x = Q_N(\eta_N^\dagger + \eta_N), \tag{25}$$

where $Q_N = \prod_{j=1}^{N-1}(-\sigma_j^z)$.

Now we define a new operator that counts the total number of fermions

$$\mathcal{N} = \sum_{i=1}^{N} \eta_i^\dagger \eta_i = \sum_{i=1}^{N} \sigma_i^+ \sigma_i^- = \sum_{i=1}^{N} \tilde{\eta}_i^\dagger \tilde{\eta}_i. \tag{26}$$

Here we recall that the number of fermions in the system is proportional to the magnetization in the spin representation. The expression for σ_N^x can be written as

$$\sigma_N^x = e^{i\pi\mathcal{N}} e^{-i\pi \eta_N^\dagger \eta_N} (\eta_N^\dagger + \eta_N). \tag{27}$$

This expression can be simplified to

$$\sigma_N^x = e^{i\pi\mathcal{N}} (\eta_N - \eta_N^\dagger). \tag{28}$$

As before, using the expression (16), we have

$$\sigma_N^x = \sum_{k=1}^{N} S_{N,k}^{-1} e^{-i\pi\mathcal{N}} (\tilde{\eta}_k - \tilde{\eta}_k^\dagger). \tag{29}$$

Since $[H, \mathcal{N}] = 0$, it follows that $S_{N,k}^{-1} e^{i\pi\mathcal{N}} \tilde{\eta}_k$ is also an eigenoperator with transition frequency $\omega = \epsilon_k$, whereas $S_{N,k}^{-1} \tilde{\eta}_k^\dagger e^{i\pi\mathcal{N}}$ is an eigenoperator with frequency $\omega = -\epsilon_k$. Thus we can write the expression for $A = \sigma_N^x$ as

$$A(\omega) = \sum_{k=1}^{N} S_{N,k}^{-1} [e^{i\pi\mathcal{N}} \tilde{\eta}_k \delta_{\epsilon_k,\omega} + \tilde{\eta}_k^\dagger e^{i\pi\mathcal{N}} \delta_{-\epsilon_k,\omega}]. \tag{30}$$

Following the same previous steps, we can write the dissipator $\mathcal{D}_R(\rho)$ as

$$\mathcal{D}_R(\rho) = \sum_{k=1}^{N} \gamma \left(S_{N,k}^{-1}\right)^2 \chi_{R,k} \left\{ [1 - f_{R,k}] \times \left[\tilde{\eta}_k e^{i\pi\mathcal{N}} \rho e^{i\pi\mathcal{N}} \tilde{\eta}_k^\dagger - \frac{1}{2}\{\tilde{\eta}_k^\dagger \tilde{\eta}_k, \rho\} \right] + f_{R,k} \left[\tilde{\eta}_k^\dagger e^{i\pi\mathcal{N}} \rho e^{i\pi\mathcal{N}} \tilde{\eta}_k - \frac{1}{2}\{\tilde{\eta}_k \tilde{\eta}_k^\dagger, \rho\} \right] \right\}. \tag{31}$$

The presence of the global operator $e^{-i\pi\mathcal{N}}$ seems, at a first glance, to complicate matters. However, for all the quantities we consider here, due to the fact that $e^{-2i\pi\mathcal{N}} = 1$, that operator will be irrelevant. Henceforth, we define the values

$$g_{L,k} = S_{1,k}^{-1}, \quad g_{R,k} = S_{N,k}^{-1} \tag{32}$$

to simplify the notation.

III. PROPERTIES OF THE STEADY STATE

A. Occupation numbers

With Eq. (4), we may now study the behavior of observables such as $\langle \tilde{\eta}_k^\dagger \tilde{\eta}_{k'} \rangle$. For the off-diagonal elements ($k \neq k'$) we find

$$\frac{d}{dt}\langle \tilde{\eta}_k^\dagger \tilde{\eta}_{k'} \rangle = -\frac{\gamma}{2}(\mathcal{A}_{L,k} + \mathcal{A}_{L,k'} + \mathcal{A}_{R,k} + \mathcal{A}_{R,k'})\langle \tilde{\eta}_k^\dagger \tilde{\eta}_{k'} \rangle,$$

where $\mathcal{A}_{L(R),k(k')} = g_{L(R),k(k')}\chi_{L(R),k(k')}$. Here we see that the term inside parentheses is always positive; consequently, we conclude that $\langle \tilde{\eta}_k^\dagger \tilde{\eta}_{k'} \rangle$ will relax exponentially toward zero and therefore vanish at the steady state. Now for the diagonal elements, again using Eq. (4), we find

$$\frac{d}{dt}\langle \tilde{\eta}_k^\dagger \tilde{\eta}_k \rangle = \gamma g_{L,k}\chi_{L,k}(f_{L,k} - \langle \tilde{\eta}_k^\dagger \tilde{\eta}_k \rangle) + \gamma g_{R,k}\chi_{R,k}(f_{R,k} - \langle \tilde{\eta}_k^\dagger \tilde{\eta}_k \rangle). \tag{33}$$

With Eq. (33) we can see that, in the steady state, the occupations will converge to

$$\langle \tilde{\eta}_k^\dagger \tilde{\eta}_k \rangle = \frac{g_{L,k}\chi_{L,k} f_{L,k} + g_{R,k}\chi_{R,k} f_{R,k}}{g_{L,k}\chi_{L,k} + g_{R,k}\chi_{R,k}}. \tag{34}$$

When $T_L = T_R$ this reduces to $\langle \tilde{\eta}_k^\dagger \tilde{\eta}_k \rangle = f_k$, as expected. Now let us see what happens if the chain is subjected to a small difference of temperature, given by $T_L = T + \delta T/2$ and $T_R = T - \delta T/2$. Equation (34) reduces to

$$\langle \tilde{\eta}_k^\dagger \tilde{\eta}_k \rangle \simeq f_k + \frac{\delta T}{2}\left(\frac{g_{L,k} - g_{R,k}}{g_{L,k} + g_{R,k}}\right)\frac{\partial f_k}{\partial T} + O(\delta T)^2. \tag{35}$$

If the chain is homogeneous then by symmetry $g_{L,k} = g_{R,k}$ and the first correction will be of order δT^2. This is expected since, for a homogeneous chain, the perturbation should not depend on the sign of δT. However, we see that, in general, when we have an inhomogeneous chain, reversing the order of the baths will change the occupation numbers.

With Eq. (23) we can analyze the behavior of the occupations numbers. We can see that the relaxation in Eq. (33) will occur with typical rates proportional to $\chi_{i,k}$. We note that this function diverges when the energy approaches zero. Thus, the present model predicts that different modes of the Hamiltonian will relax with different rates, the relaxation being faster the smaller the energy of the fermionic mode. This fact is actually quite reasonable from a physical standpoint. The energy ϵ_k of a fermionic mode represents the energy gap that needs to be overcome in a thermal transition. Modes with a small gap should experience a larger number of transitions while they relax to equilibrium and therefore should relax more quickly.

B. Particle and energy current

Using Eq. (4) we can derive some expressions for the energy and particle currents. In the fermionic representation, the temperature unbalance between the two baths will lead to a flow of particles along the chain. In the spin representation, this is mapped into a flow of magnetization.

To evaluate the current of particles or magnetization, we start with a conservation law for the time evolution of $\langle\mathcal{N}\rangle$. Since $[H, \mathcal{N}] = 0$, it follows from Eq. (4) that

$$\frac{d}{dt}\langle\mathcal{N}\rangle = \mathrm{tr}\{\mathcal{N}\mathcal{D}_L(\rho)\} + \mathrm{tr}\{\mathcal{N}\mathcal{D}_R(\rho)\}. \tag{36}$$

The two terms on the right-hand side may be readily identified as the flow of particles from the system to each of the reservoirs. In the steady state we have $d\langle\mathcal{N}\rangle/dt = 0$ and both fluxes will coincide. We then define

$$J_{\mathcal{N}} = \mathrm{tr}\{\mathcal{N}\mathcal{D}_L(\rho)\} = -\mathrm{tr}\{\mathcal{N}\mathcal{D}_R(\rho)\}, \tag{37}$$

which is, we stress, a relation valid in the steady state.

Using Eq. (24) for the dissipator, we find that

$$J_{\mathcal{N}} = \sum_{k=1}^{N} \gamma g_{L,k}\chi_{L,k}[f_{L,k} - \langle\tilde{\eta}_k^\dagger\tilde{\eta}_{k'}\rangle]. \tag{38}$$

Substituting the occupation for the steady state, we have

$$J_{\mathcal{N}} = \sum_{k=1}^{N} \gamma \frac{g_{L,k}\chi_{L,k}g_{R,k}\chi_{R,k}}{g_{L,k}\chi_{L,k} + g_{R,k}\chi_{R,k}}(f_{L,k} - f_{R,k}). \tag{39}$$

We see that the current is essentially a sum of all occupation unbalance, weighted by certain functions. It is important to note that these weights are temperature dependent. Precisely, we see that the current is nothing but a sum of currents associated with each eigenmode of the system.

Now we can define the energy current doing the same steps in terms of the conservation of $\langle H\rangle$. Its form will be analogous to Eqs. (38) and (39), but each term now will be multiplied by ϵ_k:

$$J_E = \sum_{k=1}^{N} \gamma\epsilon_k \frac{g_{L,k}\chi_{L,k}g_{R,k}\chi_{R,k}}{g_{L,k}\chi_{L,k} + g_{R,k}\chi_{R,k}}(f_{L,k} - f_{R,k}). \tag{40}$$

With the expression for the energy current, we can analyze the occurrence of rectification in the system. First let us analyze the expression for the particle current given by Eq. (39). For a small temperature gradient it becomes

$$\begin{aligned} J_{\mathcal{N}} \simeq{}& \gamma\delta T \sum_{k=1}^{N} \frac{g_{L,k}g_{R,k}}{g_{L,k} + g_{R,k}}\chi_k \frac{\partial f_k}{\partial T} \\ &+ \gamma\delta T^2 \sum_{k=1}^{N} \frac{g_{L,k}g_{R,k}(g_{R,k} - g_{L,k})}{(g_{L,k} + g_{R,k})^2}\frac{\partial\chi_k}{\partial T}\frac{\partial f_k}{\partial T}. \end{aligned} \tag{41}$$

When a system does not present rectification, the current will be an odd function of δT. Here we see the presence of a term proportional to δT^2, which will be the lowest-order contribution to the rectification. Note that it will be nonzero when $g_{L,k} \neq g_{R,k}$.

We can write down these results more explicitly, using (22) and (23). Finally, we define

$$J_{\mathcal{N}} = \gamma\delta T J_1 + \gamma\delta T^2 J_2 + \cdots, \tag{42}$$

where

$$J_1 = \sum_{k=1}^{N} \frac{g_{L,k}g_{R,k}}{g_{L,k} + g_{R,k}}\frac{|\epsilon_k|}{2T^2}\mathrm{csch}\left(\frac{\epsilon_k}{T}\right) \tag{43}$$

and

$$J_2 = \sum_{k=1}^{N} \frac{g_{L,k}g_{R,k}(g_{R,k} - g_{L,k})}{(g_{L,k} + g_{R,k})^2}\frac{\epsilon_k|\epsilon_k|}{2T^4}\mathrm{csch}^2\left(\frac{\epsilon_k}{T}\right). \tag{44}$$

Here we note that J_2 is the remaining term of $O(\Delta T)$ for the occurrence of thermal rectification. As we have an inhomogeneous chain, $g_{L,k} - g_{R,k} \neq 0$.

IV. HEAT RECTIFICATION

With the expressions for the energy current, we can investigate the occurrence of thermal rectification in the XX chain. We know from the first law of thermodynamics that the energy current is given by the power current and the heat current

$$\dot{E} = \dot{W} + \sum_r \dot{Q}_r, \tag{45}$$

where $r = L, R$ represents the index of the baths. From the microscopic derivation for the Lindblad equation we can calculate these quantities:

$$\begin{aligned} \dot{W}(t) &= \mathrm{Tr}\{\dot{H}_S(t)\rho_S\}, \\ \dot{Q}_r(t) &= \mathrm{Tr}\{H_S(t)\mathcal{D}_r(\rho_S)\}. \end{aligned} \tag{46}$$

We can see that our Hamiltonian is independent of time, so no work can be done on the system and the energy current is given by the heat current

$$\dot{E} = \sum_r \dot{Q}_r \equiv \dot{Q}. \tag{47}$$

These definitions are justified, for example, in [14].

According to Eq. (40), we have to calculate the eigenvalues and eigenvectors of the matrix associated with the Hamiltonian to compute the heat current. That is, we have to diagonalize an inhomogeneous tridiagonal matrix. The need to introduce more complex asymmetries and interactions makes any analytical treatment for this problem much more difficult.

In order to simplify the interaction matrix and to find an analytical solution, we consider a system subject to a perturbation on the external magnetic field at the first and last sites. The matrix W describing the interaction is given by

$$W = \begin{pmatrix} h-\alpha & \alpha & 0 & \cdots & 0 & \cdots & 0 \\ \alpha & h & \alpha & \ddots & 0 & \cdots & 0 \\ 0 & \alpha & h & \alpha & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & \alpha & h & \alpha & 0 \\ \vdots & \vdots & \vdots & \ddots & \alpha & \ddots & \alpha \\ 0 & 0 & 0 & \cdots & 0 & \alpha & h+\alpha \end{pmatrix}. \tag{48}$$

To be clear, the external magnetic field is given by h for the internal sites $i \in [2, N-1]$. Here α represents the interaction between the neighbors that we assume to be constant and at the first and last sites has a perturbation given by α, the same value of the interaction between the sites. For this specific matrix we have an analytical solution for the eigenvalues and eigenvectors

$$\begin{aligned} \epsilon_k &= h + 2\alpha \cos\left[\frac{(2k-1)\pi}{2N}\right], \\ v_j^k &= \sin\left[\frac{(2j-1)(2k-1)\pi}{4N}\right], \end{aligned} \tag{49}$$

where $k, j = 1, 2, \ldots, N$. All the details and the process of diagonalization can be found in [15].

To proceed with the calculation, we need to normalize the eigenvector. By using the geometric sum we obtain

$$v_j^k = \sqrt{\frac{2}{N}} \sin\left[\frac{(2j-1)(2k-1)\pi}{4N}\right]. \tag{50}$$

Thus, the matrix S that diagonalizes the matrix W [Eq. (15)] is given by

$$S_{j,k} = \sqrt{\frac{2}{N}} \sin\left[\frac{(2j-1)(2k-1)\pi}{4N}\right]. \tag{51}$$

Since S is orthogonal, we can calculate the quantities given by (32). After several manipulations we have

$$\begin{aligned} g_{L,k} &= \frac{2}{N}\sin^2\left[\frac{(2k-1)\pi}{4N}\right], \\ g_{R,k} &= \frac{2}{N}\cos^2\left[\frac{(2k-1)\pi}{4N}\right]. \end{aligned} \tag{52}$$

Substituting (50) and (52) in the expression for the heat flux (40), we arrive at

$$\begin{aligned} J = \frac{2\gamma}{N}\sum_{k=1}^{N}\left[\frac{\sin^2(\delta_k)\cos^2(\delta_k)\chi_{L,k}\chi_{R,k}}{\cos^2(\delta_k)\chi_{L,k} + \sin^2(\delta_k)\chi_{R,k}}\right] \\ \times [h + 2\alpha\cos(2\delta_k)](f_{L,k} - f_{R,k}), \end{aligned} \tag{53}$$

where $\delta_k = \frac{(2k-1)\pi}{4N}$ and $J_E \equiv J$.

To investigate the occurrence of rectification we have to compute the heat flux in the reversed bias. To compute these values, we change the baths. This represents the exchange of the temperatures $T_L' = T_R$ and $T_R' = T_L$. According to (40) and (53), the heat flow in the opposite direction is

$$\begin{aligned} J_r = -\frac{2\gamma}{N}\sum_{k=1}^{N}\left[\frac{\sin^2(\delta_k)\cos^2(\delta_k)\chi_{L,k}\chi_{R,k}}{\cos^2(\delta_k)\chi_{R,k} + \sin^2(\delta_k)\chi_{L,k}}\right] \\ \times [h + 2\alpha\cos(2\delta_k)](f_{L,k} - f_{R,k}), \end{aligned} \tag{54}$$

where the index r means the reversed flow.

As we can see, the expressions (53) and (54) have a complex dependence on the temperature, given by $\chi_{L(R),k}$, and the analytical treatment from these expressions is a complicated task. In order to simplify the analytical calculations, we make some additional assumptions.

As we can see in the expression (49) for the eigenvalues, we can have a spectrum that is entirely positive by taking $h > 0$, $\alpha > 0$, and $h > 2\alpha$. Also, regarding the baths, we take our system subjected to a large temperature gradient. Namely, we consider the limits $T_L \to \infty$ and $T_R \to 0$.

From these assumptions, we have to analyze the behavior of (22) and (23) to calculate the heat flux. According to the Fermi-Dirac occupation, we can see that, when $T_L \to \infty$ and $T_R \to 0$,

$$\begin{aligned} f_{L,k} &\to \tfrac{1}{2}, \\ f_{R,k} &\to 0. \end{aligned} \tag{55}$$

Carrying out the same analysis for $\chi_{L,k}$ and $\chi_{R,k}$ given by (23), we have

$$\begin{aligned} \chi_{L,k} &\to \infty, \\ \chi_{R,k} &\to 1. \end{aligned} \tag{56}$$

Replacing these results in the expression for the heat flow (53) and the reversed heat flow (54), we obtain

$$\begin{aligned} J &= \frac{\gamma}{N}\sum_{k=1}^{N}\left(h + 2\alpha\cos\left[\frac{(2k-1)\pi}{2N}\right]\right)\cos^2\left[\frac{(2k-1)\pi}{4N}\right], \\ J_r &= -\frac{\gamma}{N}\sum_{k=1}^{N}\left(h + 2\alpha\cos\left[\frac{(2k-1)\pi}{2N}\right]\right)\sin^2\left[\frac{(2k-1)\pi}{4N}\right]. \end{aligned} \tag{57}$$

These fluxes can be calculated by using the geometric sum. After some algebraic manipulations we find

$$\begin{aligned} J &= \frac{\gamma(h+\alpha)}{2}, \\ J_r &= -\frac{\gamma(h-\alpha)}{2}, \end{aligned} \tag{58}$$

with $\alpha \neq 0$ [15].[1]

As the values are different ($J \neq J_r$), we have the existence of thermal rectification. By (58) we can see that we have a ballistic transport, that is, the heat flow does not depend on the size of the chain. It is interesting to note that, in such a regime, the difference between the magnitude of the flows depends only on α. Consequently, we note an important result: The rectification factor remains finite when $N \to \infty$.

We can perform the same analysis for a negative spectrum. Now we consider $h < 0$, $\alpha > 0$, and $|h| > 2\alpha$. The procedure is the same as we previously described,

$$\begin{aligned} J &= -\frac{\gamma}{N}\sum_{k=1}^{N}\left(h+2\alpha\cos\left[\frac{(2k-1)\pi}{2N}\right]\right)\left(\cos^2\left[\frac{(2k-1)\pi}{4N}\right]\right), \\ J_r &= \frac{\gamma}{N}\sum_{k=1}^{N}\left(h + 2\alpha\cos\left[\frac{(2k-1)\pi}{2N}\right]\right)\left(\sin^2\left[\frac{(2k-1)\pi}{4N}\right]\right). \end{aligned} \tag{59}$$

[1] As stressed, we cannot take $\alpha = 0$ in the expressions for the rectification (derived for nonzero α). In the case of $\alpha = 0$, we have a homogeneous magnetic field and no interactions between the sites, and so we need to go back to Eq. (40) for the energy flux. For this case, the eigenvectors of the matrix interaction W are equal to the canonical eigenvectors, and so $g_{L,k}$ and $g_{R,k}$ are equal to 0 or 1, depending on k. Analyzing Eq. (39), with this behavior in k, we find $J_E = 0$, as expected.

The heat flows are given by

$$J = \frac{\gamma(|h| - \alpha)}{2}, \qquad J_r = -\frac{\gamma(|h| + \alpha)}{2}. \tag{60}$$

As expected, we have thermal rectification. In more asymmetric systems we expect the improvement of the rectification.

Now we analyze the regime of strong interaction between the sites. If we take α large enough, we split the energy spectrum into positive and negative values. More specifically, for N even, if we assume

$$\alpha > \frac{h}{2}\left|\sec\left[\frac{(N+1)\pi}{2N}\right]\right|,$$

the spectrum is divided into $N/2$ positive values and $N/2$ negative ones. In the regime of a large temperature gradient in (55) and (56), we have the expression for the heat current

$$J = \frac{\gamma}{2}\left[\sum_{k=1}^{N/2}\epsilon_k g_{R,k} - \sum_{k=N/2+1}^{N}\epsilon_k g_{R,k}\right], \tag{61}$$

where $g_{R,k}$ is given by (52). Carrying out the manipulations, we find the heat current

$$J = \frac{\gamma}{N}\csc\left(\frac{\pi}{2N}\right)\left[\alpha + \frac{h}{2}\right]. \tag{62}$$

For the heat current in the reversed bias, we have the expression

$$J_r = -\frac{\gamma}{2}\left[\sum_{k=1}^{N/2}\epsilon_k g_{L,k} - \sum_{k=N/2+1}^{N}\epsilon_k g_{L,k}\right]. \tag{63}$$

Performing the algebraic manipulations, we find

$$J_r = -\frac{\gamma}{N}\csc\left(\frac{\pi}{2N}\right)\left[\alpha - \frac{h}{2}\right]. \tag{64}$$

Again, we have thermal rectification, and comparing with the result obtained in (58), we see that, for strong interaction α, the difference between the magnitude of the flows depends now on the magnetic field h. Moreover, note that, again, we have ballistic transport of heat, since as $N \to \infty$ the currents converge to nonzero values $[\frac{\gamma}{N}\csc(\frac{\pi}{2N}) \to \frac{2\gamma}{\pi}]$, and again we have a finite rectification factor in the thermodynamic limit.

If we define the rectification factor

$$\mathcal{R} = \frac{J + J_r}{\min(J, |J_r|)}, \tag{65}$$

we can write, for (58),

$$\mathcal{R} = \frac{2\alpha}{h - \alpha}$$

and for (62) with (64),

$$\mathcal{R} = \frac{h}{\alpha - h/2}.$$

In the next section we perform some numerical analysis to investigate the behavior of rectification in some interesting and more intricate cases using (65) for the rectification factor.

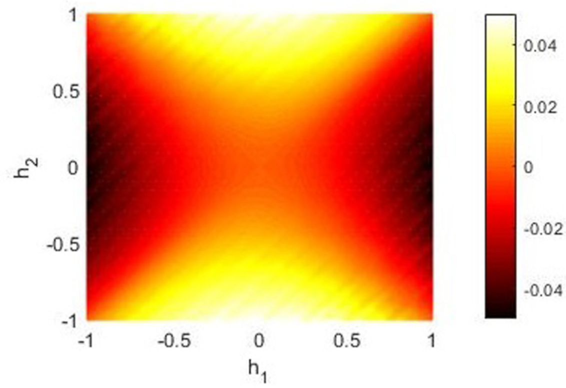

FIG. 1. Rectification profile for a junction of external magnetic fields (66) composed of 50 sites. The difference in temperature is given by $\Delta T = T_L - T_R = 5$ and the interaction is $\alpha_i = 1$.

V. NUMERICAL ANALYSIS

In this section we perform some numerical analysis using the expressions for the heat flow given by (40). We compute the exact eigenvalues and the eigenvectors for an inhomogeneous matrix that represents the interaction of our system (14). We investigate different systems, for example, models given by the sequential coupling of parts with different interactions as the usual proposal of thermal diodes [1,16,17] or graded systems [7,9], which are other recurrent models in this field.

We perform the first analysis by varying the external magnetic field and keeping fixed the interaction between the sites of the chain ($\alpha_i = 1$). We consider a system subjected to two different external magnetic fields

$$h_i = h_1, \quad i \in [1, \dots, N/2], \qquad h_i = h_2, \quad i \in [N/2+1, \dots, N]. \tag{66}$$

The rectification profile for a system of 50 sites is depicted in Fig. 1. If we make the interaction between the sites more intense, we see more nuances in the rectification profile and also a decrease in rectification intensity, as presented in Fig. 2.

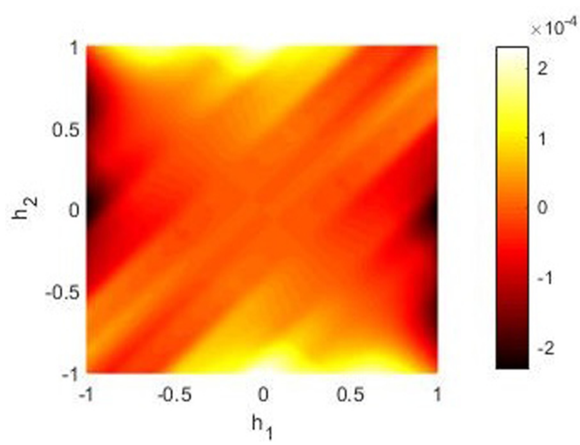

FIG. 2. Rectification profile for a junction of external magnetic fields (66) composed of 50 sites. The difference in temperature is given by $\Delta T = T_L - T_R = 5$ and the interaction is $\alpha_i = 5$.

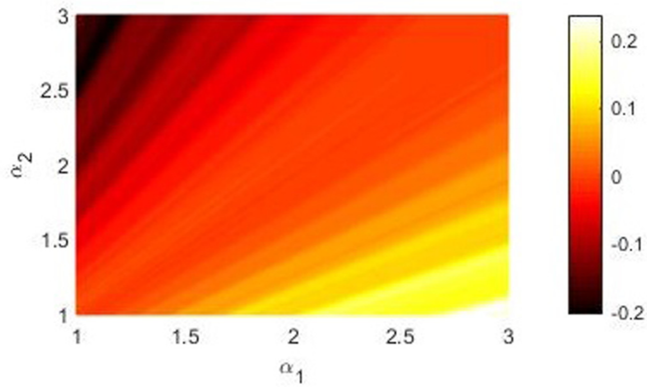

FIG. 3. Rectification profile for a junction of two interactions (67). The system is composed of 50 sites and the difference in temperature is given by $\Delta T = T_L - T_R = 5$, without a magnetic field.

We also study the behavior of the rectification with the interaction between the sites α_i. First, we investigate the existence of rectification without an external magnetic field, $h_i = 0$. We consider a system composed of 50 sites subjected to a difference in temperature $\Delta T = T_L - T_R = 5$.

Here we consider a system composed of two different values of interactions

$$\begin{aligned} \alpha_i &= \alpha_1, \quad i \in [1, \dots, N/2], \\ \alpha_i &= \alpha_2, \quad i \in [N/2 + 1, \dots, N]. \end{aligned} \tag{67}$$

The result for the system in Eq. (67) is given by Fig. 3. As we can see in Fig. 3, we have rectification in a system only changing the interaction α_i, i.e., the existence of an external magnetic field is not essential for the occurrence of thermal rectification.

Now we investigate the behavior with an external magnetic field. We perform the same calculations with a constant external magnetic field, fixed at $h_i = 5$. The result is presented in Fig. 4. We see that the rectification is more sensitive to changes in the external magnetic field compared to changes in the interaction between neighbor sites. We can observe in these rectification profiles that we have a reversal of rectification, that is, there are values of h_i and α_i such that the rectification value changes sign. This phenomenon is discussed in Refs. [18,19].

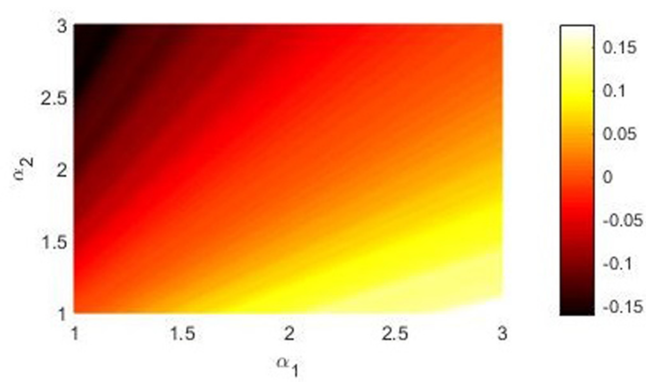

FIG. 4. Rectification profile for a junction of two interactions (67). The system is composed of 50 sites and the difference in temperature is given by $\Delta T = T_L - T_R = 5$. The magnetic field is fixed at $h_i = 5$.

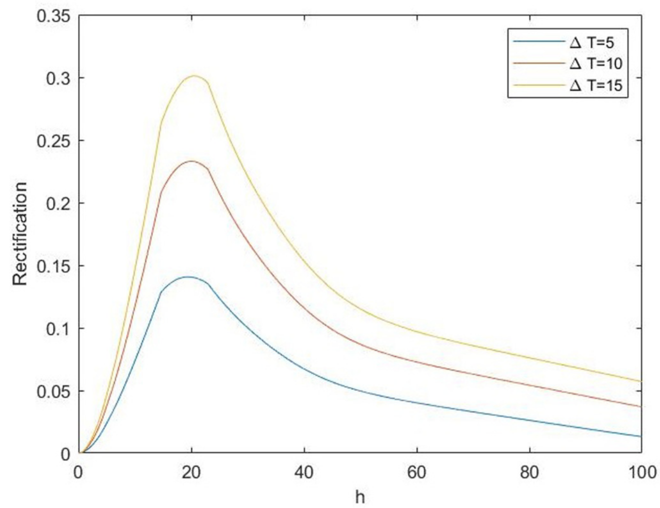

FIG. 5. Rectification profile for a linear graded external magnetic field. The system is composed fo ten sites and the difference in temperature is given by $\Delta T = 5$, 10, and 15. The intersite interaction is fixed at $\alpha_i = 1$. The external graded magnetic field is given by $h_i \propto ih$.

Another common way to construct a thermal diode is the use of graded materials. These materials are abundant in nature and can be manufactured. Hence, we investigate the behavior of thermal rectification in chains with graded structure, i.e., a system in which its internal parameters gradually vary in space. For a graded external magnetic field, we have the pattern for a system composed of ten sites as presented in Fig. 5. The rectification profile for a graded intersite interaction is depicted in Fig. 6. Now, if we make a graded external magnetic field and graded intersite interaction, we find the profile depicted in Fig. 7. In conclusion, we see that the rectification is more significant if we make the temperature

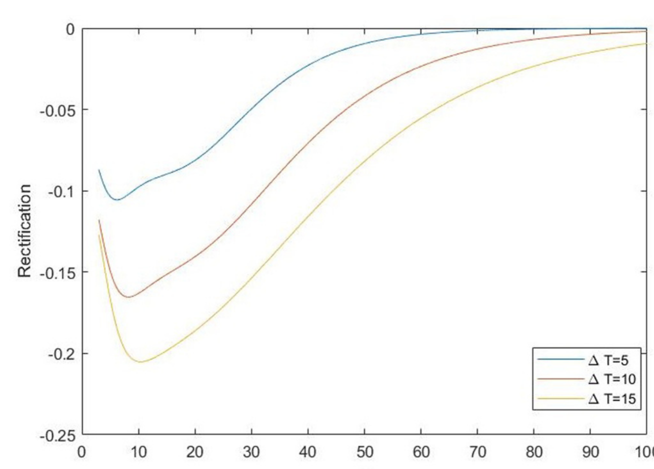

FIG. 6. Rectification profile for a linear graded interaction. The system is composed of ten sites and the difference in temperature is given by $\Delta T = 5$, 10, and 15. The external magnetic field is fixed at $h_i = 5$ and the intersite interaction is given by $\alpha_i \propto i\alpha$.

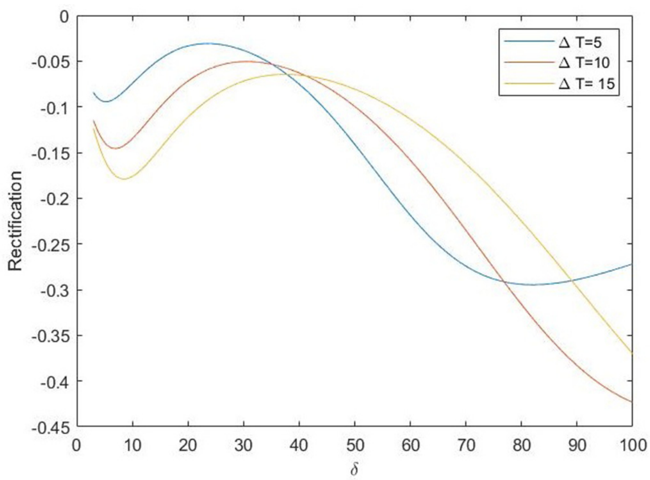

FIG. 7. Rectification profile for a linear graded chain. The external magnetic field and the intersite interaction are linear on δ, more specifically, $h_i \propto i\delta$ and $\alpha_i \propto i\delta$. The system is composed of ten sites and the difference in temperature is given by $\Delta T = 5$, 10, and 15.

gradient more intense (Figs. 5 and 6). In Fig. 7 we see that a graded structure changes the entire pattern of rectification as well as its intensity, compared to Figs. 5 and 6.

VI. CONCLUSION

In the present paper, aiming to understand the mechanism of thermal rectification in quantum systems, we investigated in detail the heat current in the XX chain with nearest-neighbor interactions and global dissipators, a simple quadratic spin model. We showed the existence of thermal rectification even for a simple case of a slightly asymmetrical chain. Interestingly, we gave examples of rectification that remains finite as the system length increases, i.e., it does not vanish in the limit $N \to \infty$.

In relation to the possible experimental realization of such models, we recalled the possibility to engineer XXZ chains with different configurations, i.e., with different values for the coefficients $\sigma_j^x \sigma_{j+1}^x$, $\sigma_j^y \sigma_{j+1}^y$, and $\sigma_j^z \sigma_{j+1}^z$ [20,21]. We also recalled the simulation of these Heisenberg models by means of cold atoms in optical lattices [22] or trapped ions [23]. Experiments with Rydberg atoms in optical traps involving these spin models were presented in Refs. [24–26].

A further comment is pertinent. For other types of dissipators, e.g., for those local dissipators that target polarization at the boundaries of the chain, the energy current is not only heat as it is here, but it consists of heat and work (power). Such a distinction is crucial for thermodynamic consistency. A detailed discussion was presented in Refs. [14,27,28].

To conclude, the results presented here provide insight into the problem of quantum thermal diode proposals: The occurrence of a robust thermal rectification in this simple model shows that rectification in quantum spin systems is a ubiquitous phenomenon.

ACKNOWLEDGMENT

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