# Symmetry properties of the heat current in non-ballistic asymmetric junctions: A case study

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**Abstract**

We consider quantum heat flow in two-terminal junctions and inquire on the connection between the transport mechanism and the junction functionality. Using simple models, we demonstrate that the violation of the Landauer behavior in asymmetric junctions does not necessarily imply the onset of thermal rectification. We also demonstrate through a simple example that a spatial inhomogeneity of the energy spectra is not a necessary condition for thermal rectification.

*Key words:* Heat conduction, Energy transfer, Nonelectronic thermal conduction, Low-dimensional structures

## 1. Introduction

Nonlinear effects in classical [1] and quantum [2, 3] heat conduction open the door for energy management at the nanoscale [4, 5]. In two-terminal junctions, where two thermal reservoirs are connected by a nanoscale link, one of the effects that has recently attracted considerable interest is a diode-like (thermal rectifying) behavior [6, 7, 8, 9, 10, 11, 12], or formally, the onset of *even* terms in the expansion

$$J = \sum_{k=1,2,3..} \beta_k(T_a)\Delta T^k, \tag{1}$$

leading to the inequality $|J(\Delta T)| \neq |J(-\Delta T)|$. Here $J$ is the heat current, $T_a = T_L + T_R$, and $\Delta T = T_L - T_R$; The indices $L, R$ refer to the left and right solids, maintained at fixed temperatures $T_L$ and $T_R$. While thermal rectification (TR) has been exemplified in multitude systems, general rules for its applicability are still limited [11]. Specifically, it is of interest to link the onset of this effect to the intrinsic transport mechanisms. In what follows we ask the following question: Given a conduction mechanism, can we conclude whether rectification takes place in the system, assuming that some spatial asymmetry is presented?

Two limiting heat-conduction mechanisms, extensively discussed and employed in the literature, are the Landauer (ballistic) motion [13, 14] and the Fourier's (diffusional) law [15]. Recent experiments probed their validity in various molecular systems including hydrocarbons [16, 17], proteins [18], and carbon nanotubes [19, 20]. It is established that the onset of the Fourier's dynamics is not a necessary, neither a sufficient condition, for diode-like behavior; Various asymmetric nonlinear systems, which do not follow the Fourier's law, rectify heat. In particular, the Fermi-Pasta-Ulam model was proved to have anomalous conductivity [21], while its mass-graded version gives rise to rectification [10]. From the other direction, it has been recently exemplified that an (asymmetric) system obeying the Fourier's law, does not necessarily rectify heat [22].

In this work we turn our attention to the connection between the breakdown of ballistic dynamics and thermal rectification. In the Landauer formula heat flows ballistically, and equilibration takes place only at the contacts. Therefore, the current passing through the system is given by the net flux of two independent processes: right-moving carriers (of temperature $T_L$ until they reach the right contact), and left-moving carriers (at $T_R$). The Landauer expression for energy transport is [13, 14]

$$J = \int \omega \mathcal{T}(\omega) \left[ f\left(\frac{\omega}{T_L}\right) - f\left(\frac{\omega}{T_R}\right) \right] d\omega, \tag{2}$$

where $\mathcal{T}(\omega)$ is the transmission coefficient, independent of the temperature, and $f(\omega/T_\nu)$ is the particle distribution function at the $\nu = L, R$ contact, $\hbar \equiv 1$. For example, for phononic systems, this expression holds in the absence of nonlinear interactions [2, 23], with $f(\omega/T) = [e^{\omega/T} - 1]^{-1}$ as the Bose-Einstein distribution function. Note that in the weak system-bath coupling limit, the only frequency terms that contribute to the integral are those in resonance with the modes of the central conductor (referred to as the subsystem/link/bridge). For example, for a single-mode bridge of frequency $\omega_0$, $J \propto \omega_0 \left[ f\left(\frac{\omega_0}{T_L}\right) - f\left(\frac{\omega_0}{T_R}\right) \right]$. Going back to the general expression (2), taking $T_L = (T_a + \Delta T)/2$, $T_R = (T_a - \Delta T)/2$, we expand the distribution function to second order in $\omega$ and obtain the net heat current

$$J = -4\frac{\alpha(T_a)}{T_a} \sum_{k=1,3,5...} \frac{\Delta T^k}{T_a^k}, \tag{3}$$

where $\alpha(T_a) = \int \omega^2 \mathcal{T}(\omega) \frac{\partial f(2\omega/T_a)}{\partial(2\omega/T_a)} d\omega$. Notice that only odd $\Delta T$ terms survive. It is obvious that systems following (2) do not rectify heat, since $J(\Delta T) = -J(-\Delta T)$. The answer to the reversed question is not as obvious: Given a system that violates the Landauer dynamics, does it necessarily lead to thermal rectification, given that some asymmetry is presented? In

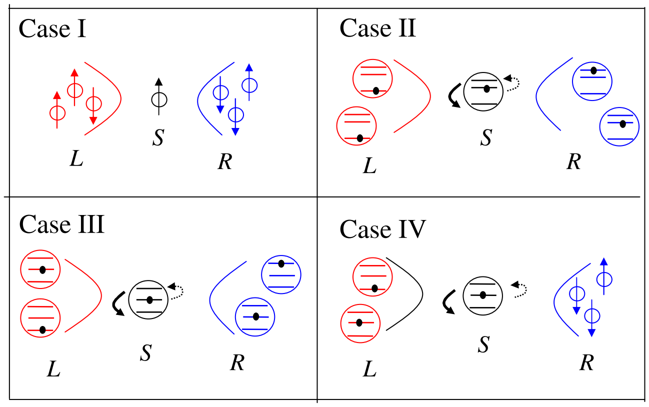


Figure 1: Four models whose transport characteristics are studied in this paper. I. A spin subsystem coupled to two spin baths. II. A 3LS subsystem coupled to 3LS reservoirs, with uneven local energy spacings. III. A 3LS subsystem coupled to 3LS reservoirs, with even onsite energy spacings. IV. A 3LS subsystem coupled to a spin bath and a 3LS reservoir. The arrows represent possible relaxation/excitation processes, induced by the reservoirs. $L$ and $R$ refer to the reservoirs, $S$ denotes the subsystem.

what follows we show that this is not the case, and exemplify that an asymmetric system, violating the Landauer relation, may still lead to a symmetric (non-rectifying) conduction. The second objective of this project is to shed light on the necessary/sufficient conditions for TR. We have recently proved that in order to attain TR, it is *sufficient* to employ reservoirs with distinct density of states [11]. Is it further *necessary* to employ such reservoirs for showing TR? The answer is negative. We demonstrate here that an asymmetric structure with homogeneous energy spectra brings in a "weak", though finite, TR behavior.

## 2. Model and Dynamics

we present next our toy model, useful for studying the fundamentals of heat conduction in bridged two-terminal junctions. The model designed includes an $M$-level subsystem (link/bridge) $H_S$, interacting with two reservoirs (contacts/terminals) $H_\nu^0$ of temperature $T_\nu$, via the coupling terms $V_\nu$. The reservoirs include a collection of noninteracting distinguishable $K$-level system (KLS) particles. The total Hamiltonian is $H = H_S + H_L^0 + H_R^0 + V_L + V_R$. The subsystem Hamiltonian assumes a diagonal form, and we also consider separable couplings,

$$\begin{aligned} H_S &= \sum_{m=1..M} E_m |m\rangle\langle m|, \\ V_\nu &= \lambda_\nu S B_\nu; \quad S = \sum_{m,n} S_{m,n} |m\rangle\langle n|. \end{aligned} \tag{4}$$

Here $S$ is a subsystem operator, $B_\nu$ is a $\nu$-bath operator, and $\lambda$ is the coupling strength. For simplicity we will assume that $S_{m,n}$ and $\lambda$ are real numbers. For the reservoirs, we assume that both the $L$ and $R$ baths include sets of independent $(p = 1, 2, .., P)$ particles,

$$H_\nu^0 = \sum_p h_{\nu,p}^0; \quad B_\nu = \sum_p b_{\nu,p}. \tag{5}$$

Here $b_{\nu,p}$ and $h_{\nu,p}^0$ are (unspecified) operators in terms of the $\nu$ reservoir degrees of freedom. This generic Hamiltonian can be used for modeling the thermal conduction properties of either harmonic or anharmonic molecules connecting two dielectrics [24]. We present next equations of motion for the subsystem degrees of freedom, and an expression for the heat current. These expressions can be derived under a standard set of approximations, including the assumption of weak system-bath coupling and the markovian approximation. The subsystem level populations follow the markovian master equation [11, 25]

$$\begin{aligned} \dot{P}_n(t) &= \sum_{\nu,m} |S_{m,n}|^2 P_m(t) k_{m\to n}^\nu(T_\nu) \\ &- P_n(t) \sum_{\nu,m} |S_{m,n}|^2 k_{n\to m}^\nu(T_\nu), \end{aligned} \tag{6}$$

with the Fermi golden-rule transition rates

$$k_{n\to m}^\nu(T_\nu) = \lambda_\nu^2 \int_{-\infty}^{\infty} d\tau e^{iE_{n,m}\tau} \langle B_\nu(\tau) B_\nu(0)\rangle_{T_\nu}. \tag{7}$$

Here $E_{n,m} = E_n - E_m$ are the subsystem energy spacing, $B(t) = e^{i(H_L^0+H_R^0)t} B e^{-i(H_L^0+H_R^0)t}$ in the interaction representation, and $\langle B_\nu(\tau)B_\nu(0)\rangle_{T_\nu} = \mathrm{Tr}_\nu[\rho_\nu(T_\nu) B_\nu(\tau) B_\nu(0)]$ is the correlation function of the $\nu$ environment, with the reservoirs assumed to be maintained in thermal equilibrium, $\rho_\nu(T_\nu) = e^{-H_\nu^0/T_\nu}/\mathrm{Tr}_\nu[e^{-H_\nu^0/T_\nu}]$. Note that excitation and decay rates are related through the detailed-balance condition, $k_{n\to m}(T_\nu) = k_{m\to n}(T_\nu) e^{\beta_\nu E_{n,m}}$; $\beta_\nu = 1/T_\nu$ with the Boltzmann constant $k_B \equiv 1$. In steady-state $\dot{P}_n = 0$, and we normalize the population to unity $\sum_n P_n = 1$. It can be further shown that the heat current across the system, defined positive when flowing $L$ to $R$, obeys

$$J = \frac{1}{2} \sum_{n,m} E_{m,n} \left|S_{m,n}\right|^2 P_n \times [k_{n\to m}^L(T_L) - k_{n\to m}^R(T_R)], \tag{8}$$

with the population obtained by solving (6) in the long time limit. For details we refer the reader to [11]. Employing Eqs. (4) and (5), we obtain the transition rates between subsystem states,

$$\begin{aligned} k_{n\to m}^\nu(T_\nu) &= 2\pi\lambda_\nu^2 \sum_p \sum_{i,j} \left|\langle i|_p\, b_{\nu,p}\, |j\rangle_p\right|^2 \\ &\times \delta(\epsilon_p(i) - \epsilon_p(j) + E_{n,m}) \frac{e^{-\beta_\nu \epsilon_p(i)}}{Z_p(\beta_\nu)}. \end{aligned} \tag{9}$$

The reservoirs are (each) characterized by the $p$-particle eigenstates $|i\rangle_p$ and eigenvalues $\epsilon_p(i)$; $Z_p(\beta_\nu) = \sum_i e^{-\beta_\nu \epsilon_p(i)}$ is the $p$-particle partition function.

The discussion to this point is general, as we have not yet specified neither the subsystem, nor the bath and its interaction form with the subsystem. We consider next three types of reservoirs: A spin bath, and a three-level system (3LS) bath of even and uneven spacings. While the later two cases are somehow artificial, they are utilized here as a toy model for exploring the fundamentals of quantum heat flow. For a bath of noninteracting spins, states $|0\rangle_p$ and $|1\rangle_p$ with $\epsilon_p(1) > \epsilon_p(0)$, we get

$$k^{\nu}_{n\to m}(T_\nu) = \Gamma^{\nu}_2(E_{n,m}) n^{\nu}_2(-E_{n,m}), \tag{10}$$

with the spin occupation factor $n^{\nu}_2(\omega) = \left[e^{\beta_\nu \omega} + 1\right]^{-1}$, and the temperature independent coefficient

$$\Gamma^{\nu}_2(\omega) = 2\pi\lambda^2_\nu \sum_p |\langle 0|_p\, b_{\nu,p}\, |1\rangle_p|^2 \delta(\omega + \epsilon_p(0) - \epsilon_p(1)). \tag{11}$$

To simplify the presentation, we assume that the $\nu$ reservoir's particles are of the same type, thus we henceforth omit the $p$ index from the reservoirs energies $\epsilon(i)$. Similarly, we can calculate the transition rate between subsystem levels induced by a bath incorporating 3LS particles with states $|i\rangle_p$; $i = 0, 1, 2$. We allow transitions between neighboring states only, $\langle 0|_p b_{\nu,p}|2\rangle_p$=0. The decay rate (9) is then given by

$$\begin{aligned} & k^{\nu}_{n\to m}(T_\nu) = 2\pi\lambda^2_\nu \times \\ & \Bigg[\sum_p |\langle 0|_p b_{\nu,p}|1\rangle_p|^2 \delta(E_{n,m} + \epsilon(0) - \epsilon(1)) \frac{e^{-\beta_\nu \epsilon(0)}}{Z_p(\beta_\nu)} \\ & + \sum_p |\langle 1|_p b_{\nu,p}|2\rangle_p|^2 \delta(E_{n,m} + \epsilon(1) - \epsilon(2)) \frac{e^{-\beta_\nu \epsilon(1)}}{Z_p(\beta_\nu)}\Bigg], \end{aligned} \tag{12}$$

with $Z_p(\beta_\nu) = \sum_{i=0,1,2} e^{-\beta_\nu \epsilon(i)}$. For a 3LS bath with even spacing, $\epsilon(2) - \epsilon(1) = \epsilon(1) - \epsilon(0)$, the relaxation rate reduces to the compact expression

$$k^{\nu}_{n\to m}(T_\nu) = \begin{cases} \Gamma^{\nu}_3(E_{n,m}) \frac{e^{-\beta_\nu \epsilon(0)} + e^{-\beta_\nu \epsilon(1)}}{Z_p(\beta_\nu)}; & E_{n,m} = \epsilon(2) - \epsilon(1) \\ 0; \quad \text{else}, \end{cases} \tag{13}$$

assuming that the interaction matrix elements are independent of the level index, $|\langle 0|_p b_{\nu,p}|1\rangle_p|^2$= $|\langle 1|_p b_{\nu,p}|2\rangle_p|^2$. When the spacings are uneven, we obtain

$$k^{\nu}_{n\to m}(T_\nu) = \begin{cases} \Gamma^{\nu}_3(E_{n,m}) \frac{e^{-\beta_\nu \epsilon(0)}}{Z_p(\beta_\nu)}; & E_{n,m} = \epsilon(1) - \epsilon(0) \\ \Gamma^{\nu}_3(E_{n,m}) \frac{e^{-\beta_\nu \epsilon(1)}}{Z_p(\beta_\nu)}; & E_{n,m} = \epsilon(2) - \epsilon(1) \\ 0; \quad \text{else}. \end{cases} \tag{14}$$

The $\Gamma^{\nu}_3$ coefficients absorb the temperature independent factors in (12). We have now assembled the ingredients for calculating the heat current in various junctions. Given an $M$-level subsystem and two reservoirs, with the left (right) reservoir made of particles with $K_L$ ($K_R$) states, one should first solve (6) in steady-state, then calculate the current with (8), using the rate constants dictated by (9). While in general the matrix elements $S_{m,n}$ depend on the respective levels indices, we will assume below for simplicity that $S_{m,n} = 1$, for all subsystem states. In what follows we will construct four distinct junctions, see Fig 1, and demonstrate that the violation of the Landauer formula in an *asymmetric* structure does not guarantee the onset of TR.

## 3. Results

**Case I.** Our first example is a spin subsystem ($M = 2$) coupled to spin reservoirs ($K_L = K_R = 2$). Using (10) it can be easily shown that

$$J = \omega_0 \frac{\Gamma^L_2 \Gamma^R_2}{\Gamma^L_2 + \Gamma^R_2} [n^L_2(\omega_0) - n^R_2(\omega_0)], \tag{15}$$

with $\omega_0 = E_{1,0}$ the spin spacing, and $\Gamma^{\nu}_2$ evaluated at $\omega_0$. It is interesting to note that this expression is in the form of the Landauer formula (2), with independent carriers flowing in opposite directions. In the present case, however, the only contribution to the energy current comes from the (subsystem) $\omega_0$ frequency term, as a result of the weak system-bath coupling approximation employed. Since $J(\Delta T) = -J(-\Delta T)$, TR is absent here.

**Case II.** Consider next a 3LS subsystem ($M = 3$) coupled to 3LS reservoirs ($K_L = K_R = 3$). We assume that the subsystem and reservoirs consist elements of the same energy structure, $\omega_0 \equiv \epsilon(1) - \epsilon(0) = E_{1,0}$; $\omega_1 \equiv \epsilon(2) - \epsilon(1) = E_{2,1}$, but the spacings in each subunit are taken uneven, i.e. $\omega_0 \neq \omega_1$, see Fig. 1. Utilizing (8), we obtain the current

$$\begin{aligned} J &= \frac{\omega_0}{D_0} k^L_{1\to 0} k^R_{1\to 0} (e^{-\beta_L \omega_0} - e^{-\beta_R \omega_0}) \\ &+ \frac{\omega_1}{D_1} k^L_{2\to 1} k^R_{2\to 1} (e^{-\beta_L \omega_1} - e^{-\beta_R \omega_1}), \end{aligned} \tag{16}$$

where

$$\begin{aligned} D_0 &= k_{0\to 1} k_{1\to 2}/k_{2\to 1} + k_{0\to 1} + k_{1\to 0}; \\ D_1 &= k_{2\to 1} k_{1\to 0}/k_{0\to 1} + k_{2\to 1} + k_{1\to 2}, \end{aligned} \tag{17}$$

and $k_{i\to j} = k^L_{i\to j} + k^R_{i\to j}$, incorporating the microscopic rates defined in (14). Simplifying this expression, it exactly reduces to

$$\begin{aligned} J &= \frac{\mathcal{T}_3}{F(T_L)F(T_R)} \Big[\omega_0 \left(e^{-\omega_0/T_L} - e^{-\omega_0/T_R}\right) \\ &+ \omega_1 \left(e^{-\omega_1/T_L} - e^{-\omega_1/T_R}\right) e^{-\omega_0/T_R} e^{-\omega_0/T_L}\Big], \end{aligned} \tag{18}$$

where $F(T_\nu) = 1 + e^{-\omega_0/T_\nu} + e^{-(\omega_1+\omega_0)/T_\nu}$ and $\mathcal{T}_3 = \frac{\Gamma^L_3 \Gamma^R_3}{\Gamma^L_3 + \Gamma^R_3}$. Inspecting (18), it is clear that the current cannot be separated into independent right-moving (of temperature $T_L$) and left-moving (of temperature $T_R$) terms. Only when $\omega_1 \gg T_\nu$, the second terms dies out, and the expression reduces to (15). Thus, the Landauer picture (2) *does not hold* here. However, it is trivial to note that TR does not take place in this system, even under some asymmetry, $\Gamma^L_3 \neq \Gamma^R_3$, since the current is the same (with opposite sign) with respect to exchanging $T_L$ by $T_R$. We therefore conclude that a three-level unit with *uneven* energy spacings, *asymmetrically* bridging two reservoirs made of collections of 3LS particles, does not obey the ballistic Landauer dynamics (18), *yet it does not lead to thermal rectification.* Thus, the breakdown of the Landauer picture, is not a sufficient condition for TR.

**Case III.** We repeat the previous analysis, adopting identical 3LS subsystem and 3LS reservoirs. However, in the present case we take the local energies to be evenly spaced, $\omega = \omega_0 = \omega_1$, i.e., $\omega = E_{1,0} = E_{2,1}$= $\epsilon(1) - \epsilon(0)$= $\epsilon(2) - \epsilon(1)$. We can exactly calculate the steady-state heat current, in the form of (16) using the rates (13). Expanding it in terms of $\omega$, the first two terms reduce to

$$J = A_1(T_L, T_R)\omega^2 + A_2(T_L, T_R)\omega^4 + O(\omega^6), \tag{19}$$

with the coefficients

$$
\begin{aligned}
A_1 &= \frac{4}{9}\mathcal{T}_3\frac{T_L - T_R}{T_L T_R};\\
A_2 &= -\frac{1}{27}\mathcal{T}_3\frac{1}{(\Gamma_3^L+\Gamma_3^R)^2}\frac{T_L - T_R}{T_R^3 T_L^3}\\
&\times \Big\{(2T_L^2 + 2T_R^2 + T_L T_R)[(\Gamma_3^L)^2 + (\Gamma_3^R)^2]\\
&+ \Gamma_3^R\Gamma_3^R(3T_L^2 + 3T_R^2 + 4T_L T_R)\Big\}. \qquad (20)
\end{aligned}
$$

As before, $\mathcal{T}_3 = \frac{\Gamma_3^L\Gamma_3^R}{\Gamma_3^L+\Gamma_3^R}$, with all constants calculated at the subsystem characteristic frequency $\omega$. Since these terms are rather complicated, we also present the results assuming the subsystem is symmetrically connected to the two ends, $\Gamma \equiv \Gamma^\nu$,

$$
\begin{aligned}
A_1 &= \frac{2\Gamma}{9}\left(\frac{1}{T_R} - \frac{1}{T_L}\right);\\
A_2 &= \frac{7\Gamma}{216}\left(\frac{1}{T_L^3} - \frac{1}{T_R^3}\right) + \frac{\Gamma}{216}\frac{1}{T_L T_R}\left(\frac{1}{T_R} - \frac{1}{T_L}\right). \qquad (21)
\end{aligned}
$$

We note that $A_1$ and the first term in $A_2$ contribute separate $L$ and $R$ contributions. In contrast, the second term in $A_2$ is mixing the temperatures of both reservoirs, indicating that the transport cannot be fully separated into a right-moving and a left-moving components. Thus, similarly to the previous case, the Landauer picture (2) *does not hold* here.

We proceed and manifest the *presence* of TR in this junction by rewriting (19) in terms of $\Delta T$ and $T_a$ (adding the $\omega^6$ order),

$$
\begin{aligned}
J &= \frac{16}{9}\frac{\omega^2}{T_a}\mathcal{T}_3\sum_{k=1,3,5..}\frac{\Delta T^k}{T_a^k} - \frac{\omega^4}{T_a^3}\mathcal{T}_3\sum_{k=1,3,5..}\alpha_k\frac{\Delta T^k}{T_a^k}\\
&+ \frac{\omega^6}{T_a^5}\mathcal{T}_3\left[\sum_{k=1,3,5..}\gamma_k\frac{\Delta T^k}{T_a^k} + \gamma_4\frac{\Delta T^4}{T_a^4} + ...\right] + O(\omega^8). \qquad (22)
\end{aligned}
$$

Here $\alpha_k$ and $\gamma_{k=2n}$ ($n$ is an integer) are symmetric functions with respect to the exchange of $\Gamma_3^L$ with $\Gamma_3^R$. For example, $\alpha_1 = -80/27$, $\alpha_3 = -32/27[9 - 2\mathcal{T}_3/(\Gamma_3^L + \Gamma_3^R)]$. In contrast, $\gamma_4 \propto \Gamma_3^L - \Gamma_3^R$. The last *even* term in this expansion indeed indicates on the *breakdown* of TR, resulting in the inequality $|J(\Delta T)| \neq |J(-\Delta T)|$. Since the effect appears as a high order $\omega$ term, we refer to this behavior as a "weak" TR. Numerical examples (Figs. 2 and 3) are presented below. At this point we would like to emphasize that while Eq. (16) is general, valid for describing transport using 3LS particles of even/uneven spacings, one cannot simply take the limit $\omega_1 = \omega_0$ in Eq. (18), and expect to obtain the heat current (19) for the equally-spaced 3LS model. The reason is that in case III the reservoirs particles have energy spectra which is uniform as well, reflected by the transition rates (13), which should be also adjusted when recalculating (16).

**Case IV.** We proceed and analyze another variant of this model, a 3LS central unit ($M = 3$), connecting a 3LS reservoir ($K_L = 3$), and a 2LS reservoir ($K_R = 2$). All energy spacing are taken to be the same ($\omega$), see Fig. 1. Since $\langle H_L^0\rangle_T \neq \langle H_R^0\rangle_T$, this structure fulfills the sufficient condition for providing TR [11].

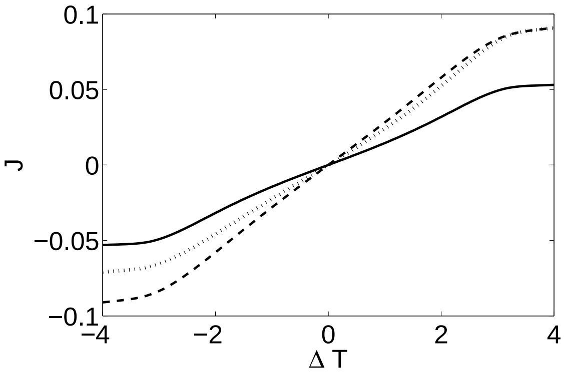


Figure 2: Conduction properties of several junctions. Model II with $\omega_0 = 2$, $\omega_1 = 1$ (full); model III (dashed) and model IV (dotted) with $\omega_2 = \omega_0 = 2$. $T_a = 4$, $\Gamma^L = 1$, $\Gamma^R = 0.1$.

As we show next, this model indeed generates a "strong" TR. Utilizing Eqs. (6)-(9), we again observe a violation of the the Landauer relation

$$
\begin{aligned}
J &\propto \omega^2\left(\frac{1}{T_R} - \frac{1}{T_L}\right)\\
&+ \omega^4\frac{\Delta T}{T_L^3 T_R^3}\left[aT_R^2 + bT_L^2 + cT_L T_R\right] + O(\omega^6), \qquad (23)
\end{aligned}
$$

where $a \neq c \neq b \neq 0$, depend on the system-bath coupling elements. (The explicit expressions were omitted, since they were too cumbersome to be included). In terms of $\Delta T$ and $T_a$, this expression reduces to

$$
\begin{aligned}
J &= \frac{16}{3}\frac{\omega^2}{T_a}\frac{\Gamma_3^L\Gamma_2^R}{4\Gamma_3^L + 3\Gamma_2^R}\sum_{k=1,3,..}\frac{\Delta T^k}{T_a^k}\\
&+ \frac{\omega^4}{T_a^3}\sum_{k=1,2,3...}\alpha_k\frac{\Delta T^k}{T_a^k} + O(\omega^6), \qquad (24)
\end{aligned}
$$

with $\alpha_k \neq 0$ for finite (though arbitrary) $\Gamma^L$ and $\Gamma^R$ coefficients, for example, $\alpha_2 = 128(\Gamma_3^L)^2\Gamma_2^R/(9\Gamma_2^R + 12\Gamma_3^L)^2$. Since even terms survive, we conclude that TR takes place, in agreement with [11]. We refer to this type of behavior as a "strong" TR in comparison to (22), since the effect here is more substantial.

We exemplify this behavior in Figs. 2 and 3, plotting the heat current and the rectification ratio $R \equiv |J(\Delta T)|/|J(-\Delta T)|$ in models II (full), III (dashed), and IV (dotted), using $\Gamma^L \neq \Gamma^R$. We find that case II leads to a symmetric conduction with $R = 1$ (full line). In contrast, model III produces a "weak" TR with a minor deviation from unity $R \sim 0.995$ at $\Delta T = 4$ (dashed line), while model IV yields a "strong" TR with $R \sim 1.3$ at that temperature range (dotted line). It is of interest to emphasize on the sensitivity of the effect. Comparing cases II and III, we note that both junctions are homogeneous, with system and reservoirs made of the same 3LS particles. The only difference between the two models is that in case II the local spacings were taken uneven, while in III the energy spacings were equal, leading to TR. This demonstrates that the conditions for TR discussed in [11] are indeed only *sufficient*, and asymmetric

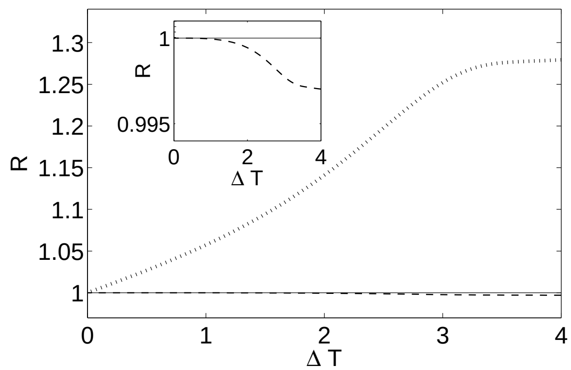


Figure 3: Rectification ratio in several models, parameters are the same as in Fig. 2. Model II with $\omega_0 = 2$, $\omega_1 = 1$ (full); model III (dashed) and model IV (dotted) with $\omega_2 = \omega_0 = 2$. Inset: Same data as in the main plot, zooming near $R = 1$.

systems with uniform energy spectra may still show rectifying behavior.

Before concluding, we would like to emphasize the relation of the examples discussed here and the harmonic model examined, e.g., in [13, 23]. One should note that the harmonic limit is reached when two conditions are simultaneously fulfilled: (i) The subsystem $H_S$ (4) and the reservoirs Hamiltonian (5) acquire a harmonic spectrum, and (ii) system-bath interaction operators $V_\nu$ are bilinear in position, i.e., $V_\nu$ is given by the product of $B_\nu \propto x_\nu$ and $S \propto q$, where $x_\nu$ and $q$ are the $\nu$-bath and subsystem coordinates, respectively. In particular, one should note that the matrix elements of the system operator $S$ have a special structure in the harmonic case: The factors $|S_{m,n}|^2$ are nonzero and proportional to the site index only for $m = n \pm 1$, leading to the dynamical equations (6) with nearest neighbors transitions only. Thus, simply by extending the $n$-level model to infinity, one should not expect to obtain the harmonic result (2).

Finally, It is of interest to contrast thermal rectification with charge rectification. It is well justified that an electric current asymmetry is related to many-body interactions in the system, rather than to simple structural asymmetry [26, 27]. This observation is valid in the thermal case as well. Pure harmonic systems cannot bring in rectification regardless of any structural asymmetry [24]. However some anharmonic-asymmetric systems, disobeying the Landauer-ballistic formula, still do not show thermal rectification, as demonstrated here by case II.

## 4. Summary

We have described here a simple model for probing the fundamentals of quantum heat flow in nonlinear hybrid junctions. Essentially, we were concerned with the possible connection between the inherent transport mechanism and the junction functionality, or the emergence of nonlinear current-temperature bias terms.

Our first (I) spin junction follows the ballistic-Landauer dynamics. We have then presented three examples violating the Landauer picture. In models II and III the subsystem and reservoirs were all equivalent, with the internal level spacings taken either uneven (II) or the same (III). Asymmetry was introduced by unequally connecting the central-subsystem unit to the two terminals. In the fourth model (IV) the energy spectra was made inhomogeneous, adopting distinct reservoirs. We have found that only in case II the current was symmetric around $\Delta T = 0$, obeying $J(\Delta T) = -J(-\Delta T)$.

Based on these observations, the following conclusions can be made: (i) The breakdown of the Landauer-ballistic mechanism is not a sufficient condition for the onset of TR in an asymmetric junction, indicating that non-integrable models with some built in asymmetry may still produce a symmetric conduction. (ii) The inhomogeneity of the energy spectra across the junction is not a necessary condition for the onset of TR.

Derivation of general *necessary* conditions for showing TR is a formidable- unsolved challenge. The case study presented here is a first step in that direction. It is of interest to further explore the connection between transport mechanisms and the system functionality, e.g., the relationship between the onset of negative differential thermal resistance and the microscopic mechanisms [28].

**Acknowledgment**

This work was supported by NSERC and by the University of Toronto Start-up Funds. L. A. Wu has been supported by the Ikerbasque foundation.

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