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Railway switch transport model

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We propose a simple model of coupled heat and particle transport based on zero-dimensional classical deterministic dynamics, which is reminiscent of a railway switch whose action is a function only of the particle's energy. It is shown that already in the minimal three-terminal model, where the second terminal is considered as a probe with zero net particle and heat currents, one can find extremely asymmetric Onsager matrices as a consequence of time-reversal symmetry breaking of the model. This minimalistic transport model provides a better understanding of thermoelectric heat engines in the presence of time-reversal symmetry breaking.

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Introduction. Minimalistic mathematical models often provide key paradigms in theoretical physics. In the theory of coherent quantum transport [1] of noninteracting electron systems, the conductances can be elegantly formulated solely in terms of transmission and reflection amplitudes [2]. Very similar expressions for conductances can be written also in the realm of classical physics, if the particle's dynamics inside the system is deterministic and conservative (Hamiltonian) (see, for example, [3]). In multiterminal transport theory, probe terminals [4] are conveniently used as minimalistic models of inelastic scattering. A probe is a terminal whose temperature and chemical potential is chosen self-consistently so that there is no average flux of particles and energy between the probe itself and the system under examination. The advantage of such approach lies in its simplicity and independence of microscopic details of inelastic processes. Probe terminals have been widely used in the literature and proved to be useful to unveil nontrivial aspects of phase-breaking processes [1], heat transport and rectification [5–11], and thermoelectric transport [12–18].

In this Brief Report, we propose and study a simple multiterminal classical transport model, where the wires connected to the system are one dimensional (i.e., they have just one momentum state per each value of the energy) and where the *deterministic* dynamics of the system, at fixed energy, is simply a permutation (rewiring) among the terminals. In particular, we focus on three-terminal models, depicted in Fig. 1, where the second terminal is considered as a probe. We discuss the coupled heat and particle deterministic transport between the remaining wires within the linear response limit. In this limit the transport between the first and the third wires is described by the reduced Onsager matrix. As our energy-dependent rewiring is in general not self-inverse, we are particularly interested in the precise conditions for the reduced Onsager matrix to be asymmetric and we discuss how to maximize the asymmetry.

Classical coupled transport formalism. Let us consider a generic N-terminal, noninteracting classical transport model. Each wire labeled by i is connected to a thermochemical bath at reciprocal temperature $\beta_i = \beta + \delta\beta_i$ and chemical potential $\mu_i = \mu + \delta\mu_i$ ($i = 1,\ldots,N$), where β and μ are reference reciprocal temperature and chemical potential, respectively. The $\delta\beta_i$ and $\delta\mu_i$ are considered as gradient fields with regard to reference values. Such gradients in the linear response regime are small in magnitude. The particles are effused from the wires into the junction, with the injections rates

$$\gamma_i = \gamma \frac{\beta}{\beta_i} e^{\beta_i\mu_i - \beta\mu}, \tag{1}$$

where γ denotes the injection rate at the reference values β and μ. Without loss of generality, we set $\gamma = \beta = 1$ and $\mu = 0$. At inverse temperature β, the particles' energies are distributed according to Boltzmann's formula $p(E) = \beta e^{-\beta E}$. In the stationary, linear-response regime, we have in the ith wire a particle current $j_{\rho,i}$ and a heat current $j_{q,i}$ proportional to gradients $\delta\beta_j$ and $-\beta\delta\mu_j = -\delta\mu_j$ [19]. To state this more precisely, we introduce the 2 vector of currents $J_i = (j_{q,i}, j_{\rho,i})$ in the ith terminal, the 2 vector of gradient fields $X_j = (\delta\beta_j, -\delta\mu_j)$ in the jth terminal, and 2×2 blocks of the Onsager matrix

$$L_{i,j} = \begin{bmatrix} K_{i,j} & Q_{i,j} \\ Q_{i,j} & T_{i,j} \end{bmatrix}, \tag{2}$$

connecting the two of them:

$$J_i = \sum_{j=1}^{N} L_{i,j} X_j. \tag{3}$$

The matrix elements of $L_{i,j}$ are defined by

$$(T_{i,j}, Q_{i,j}, K_{i,j}) = \int_{\mathbb{R}_+} dE\, e^{-E}\, \tilde{\tau}_{i,j}(E)(1, E, E^2), \tag{4}$$

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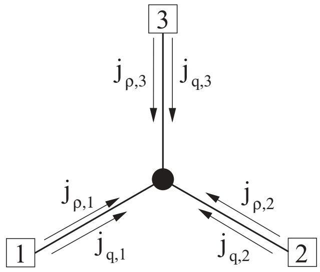


FIG. 1. Schematic drawing of the three-terminal transport model, with $j_{\rho,i}$ and $j_{q,i}$ denoting the particle and heat currents from terminal i.

with $\tilde{\tau}_{i,j} \equiv \delta_{i,j} - \tau_{i\leftarrow j}$, and the *on-shell transmission functions* $\tau_{i\leftarrow j}$ satisfying the probability conservation $\sum_i \tau_{i\leftarrow j}(E) = 1$ and the sum rule $\sum_i \tau_{i\leftarrow j}(E) = \sum_j \tau_{i\leftarrow j}(E)$, ensuring that the currents vanish when all the potentials and temperatures are equal. The conservation of the net currents translates to a 2-vector condition $\sum_{i=1}^{N} J_i = 0$. We note that due to the conservative and noninteracting nature of our model, the Onsager matrix is always, as explicitly written in Eq. (2), block symmetric. This property is a consequence of conservation of total probability and would translate also in any quantum extension of our model, being in that case a consequence of the unitarity of the S matrix [2].

The railway switch model. We consider a *deterministic* transport model in which the outgoing wire for a particle is uniquely determined by the incoming wire and the particle's energy. Such model is not bound to be symmetric with respect to time reversal and therefore allows us to systematically study the effects of time-reversal symmetry breaking. The model is fully specified by transmission functions $\tau_{i\leftarrow j}(E)$ for which only the values zero and one are allowed: $\tau_{i\leftarrow j}(E) = 1$ if particles injected from terminal j with energy E go to terminal i and $\tau_{i\leftarrow j}(E) = 0$ if such particles go to a terminal other than i. The above deterministic on-shell transmission functions can be described using permutation matrices P_k for $k \in I \equiv \{1,\ldots,N!\}$ corresponding to the permutation group $\mathcal{S}_N$ as

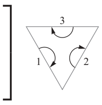
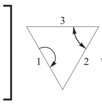
$$\tau_{i\leftarrow j}(E) = [P_{\psi(E)}]_{i,j} \quad i,j = 1,\ldots,N, \tag{5}$$

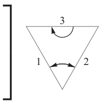
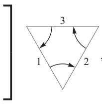
where $\psi(E): \mathbb{R} \to I$ is a piecewise constant function controlling the (energy-dependent) switching between the permutations. The function $\psi(E)$ for n permutation switches is completely specified in terms of a sequence of $n+1$ integers $\pi = (p_0, p_1, \ldots, p_n)$, $p_i \in I$, and a sequence of n threshold energies $\epsilon = (E_1,\ldots,E_n)$, at which the switches occur:

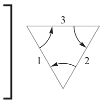
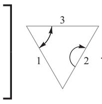
$$\psi(E) = p_i \in I \quad \text{for} \quad E \in [E_i, E_{i+1}], \tag{6}$$

with $i = 0,\ldots,n$, $E_0 \equiv 0$, and $E_{n+1} \equiv \infty$. That is to say, at energy E_i $(i = 1,\ldots,n)$ we switch from permutation $P_{p_{i-1}}$ to P_{p_i}. A *realization* of the model is defined by a pair (π,ϵ).

From now on we focus on the $(N = 3)$-terminal case (Fig. 1), so that the permutation matrices $P_k \in \{0,1\}^{3\times 3}$ read

$$P_1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$ , $$P_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$ .

$$P_3 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$$ , $$P_4 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$ .

$$P_5 = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$$ , $$P_6 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$ .

To the right of each permutation we show the rewiring described by the matrix. Following the figures we see that each permutation has a very simple interpretation, for example, P_1 represents the reflection of the incoming particles to the original terminals, and in P_2 particles from terminal 1 are reflected, particles from terminal 2 go to terminal 3, and particles from terminal 3 go to terminal 2, etc.

Our model has interesting symmetries. By introducing the superoperator of time inversion $\hat{\mathcal{T}}X = X^T$ (with X^T the transpose of X), we can see that

$$\hat{\mathcal{T}}P_k = P_k \quad \text{for} \quad k \in \{1,2,3,6\} \quad \text{and} \quad \hat{\mathcal{T}}P_4 = P_5. \tag{7}$$

This implies that P_4 and P_5 are the only time-asymmetric permutations, with $P_4 = P_5^{-1}$ and $P_5 = P_4^{-1}$, while for all other cases we have $P_k = P_k^{-1}$. When the second terminal acts as a probe, the model is invariant on swapping the first and third terminals. These operations can be performed by the swap superoperator $\hat{\mathcal{S}}X = P_6 X P_6$ acting as

$$\hat{\mathcal{S}}P_1 = P_1, \quad \hat{\mathcal{S}}P_2 = P_3, \quad \hat{\mathcal{S}}P_4 = P_5, \quad \hat{\mathcal{S}}P_6 = P_6. \tag{8}$$

Thermoelectric transport with a probe terminal. To illustrate the railway switch model in a concrete example, we discuss thermoelectric (or thermochemical) transport, when the second terminal acts as a probe, that is, $J_2 = 0$. We choose to measure gradients with regard to the third wire by setting $X_3 = 0$. We end up relating the remaining gradient fields

$$X_2 = -L_{22}^{-1} L_{21} X_1 \tag{9}$$

and connecting the currents between the first and the third wire,

$$J_1 = L_{\text{red}} X_1, \tag{10}$$

in terms of a *reduced Onsager matrix* L_{red}, defined as

$$L_{\text{red}} = L_{11} - L_{12} L_{22}^{-1} L_{21} = \begin{bmatrix} l_{11} & l_{12} \\ l_{21} & l_{22} \end{bmatrix}. \tag{11}$$

The reduced Onsager matrix admits a nice analytic description of matrix element $l_{i,j}$. Let us first introduce the determinant $D = \det L_{22}$ of the Onsager matrix L_{22} for the transmission from the probe, written as

$$D = \frac{1}{2} \int_{\mathbb{R}_+ \times \mathbb{R}_+} \left[\prod_{i=1}^{2} e^{-E_i} \tilde{\tau}_{22}(E_i) dE_i \right] (E_1 - E_2)^2 \tag{12}$$

and define the integration measure

$$d\mu = \left[\prod_{i=1}^{3} e^{-E_i} dE_i \right] \tilde{\tau}_{21}(E_1) \tilde{\tau}_{12}(E_2) \tilde{\tau}_{22}(E_3) \tag{13}$$

over the domain $(E_1,E_2,E_3) \in \mathcal{D} = R_+^3$. [To simplify notation we omit the arguments (E_1,E_2,E_3) in the measure $d\mu$.] Then we can write the matrix elements of $L_{\rm red}$:

$$l_{11} = K_{11} - \frac{1}{D}\int_{\mathcal{D}} d\mu\, E_1E_2(E_1-E_3)(E_2-E_3), \qquad (14)$$

$$l_{22} = T_{11} - \frac{1}{D}\int_{\mathcal{D}} d\mu\,(E_1-E_3)(E_2-E_3), \qquad (15)$$

$$l_{12} = Q_{11} - \frac{1}{D}\int_{\mathcal{D}} d\mu\, f(E_1,E_2,E_3), \qquad (16)$$

$$l_{21} = Q_{11} - \frac{1}{D}\int_{\mathcal{D}} d\mu\, f(E_2,E_1,E_3), \qquad (17)$$

with $f(E_1,E_2,E_3) \equiv E_2E_3^2 + E_1E_2^2 - (E_1+E_2)E_2E_3$. It is convenient to introduce the quantities

$$\begin{aligned} 2\overline{f} &:= f(E_1,E_2,E_3) + f(E_2,E_1,E_3) \\ &= (E_1+E_2)(E_1-E_3)(E_2-E_3), \end{aligned} \qquad (18)$$

$$\begin{aligned} 2\Delta f &:= f(E_1,E_2,E_3) - f(E_2,E_1,E_3) \\ &= \sum_{i,j,k} \epsilon_{i,j,k} E_j E_k^2, \end{aligned} \qquad (19)$$

with $\epsilon_{i,j,k}$ being the Levi-Civita totally asymmetric tensor. Note that $L_{\rm red}$ can be decomposed into the sum of L_{11} and a matrix defining the communication between the wires.

In this work we are mainly interested in the asymmetry measure x of the reduced Onsager matrix, defined as

$$x = \frac{l_{21}}{l_{12}}. \qquad (20)$$

This parameter has been discussed for quantum dots with broken time-reversal symmetry [15,21]. If the transport is time-reversal symmetric, then $\int d\mu \Delta f = 0$ and consequently $x = 1$. Large asymmetries are desirable since they could in principle lead to high thermoelectric efficiencies. Indeed, by considering the reduced system as a heat engine with steady-state power generation $P = -j_{\rho,1}\delta\mu_1$, dissipated heat current $Q = j_{q,1}$, and efficiency $\eta = P/Q$, the maximum efficiency reads [22]

$$\eta_{\max} = \eta_{\rm C}\, x \frac{\sqrt{1+y}-1}{\sqrt{1+y}+1}, \qquad (21)$$

where $\eta_{\rm C} = |\delta\beta_1|$ (for $\beta = 1$) is the Carnot efficiency and $y = \frac{l_{12}l_{21}}{\det L_{\rm red}}$ is the figure of merit. Note that x acts as a multiplier to the efficiency and so its maximization (at fixed y) is desirable for increasing the efficiency. The thermodynamic bounds on x, y, and η are discussed in Ref. [22].

In the following we discuss the asymmetry measure x and the figure of merit y of the reduced Onsager matrix in different realizations of the railway switch model model. At fixed threshold energies ϵ, by considering the sequence of inverted permutations we obtain the same figure of merit and reciprocal measure of asymmetry [23]:

$$y(\hat{\mathcal{T}}\pi) = y(\pi), \quad x(\hat{\mathcal{T}}\pi) = x(\pi)^{-1}, \qquad (22)$$

while exchanging the first and the third wire does not affect the two quantities:

$$y(\hat{\mathcal{S}}\pi) = y(\pi), \quad x(\hat{\mathcal{S}}\pi) = x(\pi). \qquad (23)$$

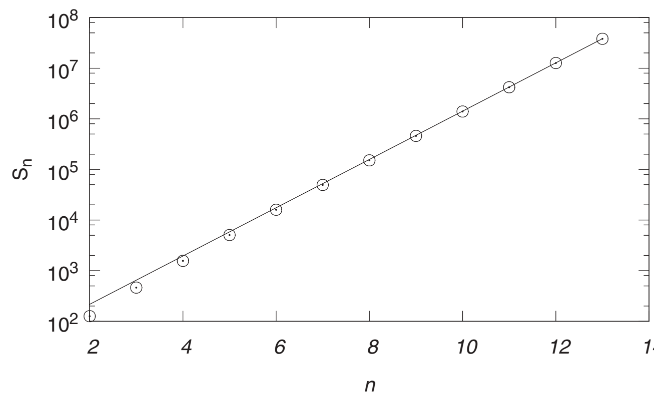


FIG. 2. The number of cases S_n with symmetric Onsager matrix as a function of the number n of switches and best-fitted asymptotic dependence 24×3^n.

If a realization is symmetric with regard to $\pi \to \hat{\mathcal{T}}\pi$, then is has a symmetric Onsager matrix and so $x = 1$. We observed numerically that the Onsager matrix of our model has all elements positive, $l_{i,j} > 0$, so that the asymmetry measure x is always non-negative, $x \geqslant 0$.

The number of all n-switch cases is $N_n = 6 \cdot 5^n$. Let S_n denote the number of cases for which we have $x = 1$. As shown in Fig. 2,

$$S_n \sim C\,\alpha^n \quad \text{as} \quad n \to \infty, \qquad (24)$$

with $\alpha \approx 3$ and $C \approx 24$. We see that S_n is asymptotically approximately six times larger than the number of cases composed of only symmetric permutations, equal to $\tilde{S}_n = 4 \times 3^n$. The number of cases $A_n = N_n - S_n$ with an asymmetric Onsager matrix increases exponentially, as $\mathcal{O}(5^n)$. Hence, most of the cases lead to $x \neq 1$.

In the following, we discuss the properties of our model for different numbers n of switches, thus increasing with n the complexity of the model in a controllable manner. All one-switch ($n = 1$) cases have $x = 1$. The asymmetry $x \neq 1$ is possible only in the cases with two or more switches. In the two-switch ($n = 2$) cases only nonrepeated combinations of permutations P_k with indices in $k \in \{2,3,4,5\}$ produce asymmetry, but the asymmetry parameter x is always limited to a finite interval, namely it is always strictly larger than zero and finite. In the three-switch ($n = 3$) cases the asymmetry parameter can, for specific sequences of permutations, become arbitrarily large. This fact is possible for the following sequences of permutations:

$$\begin{aligned} V = \{&(2,3,1,4), (3,2,1,5), (4,2,1,3), \\ &(4,2,1,5), (5,3,1,2), (5,3,1,4)\}. \end{aligned} \qquad (25)$$

The obtained set is invariant with regard to $\hat{\mathcal{S}}$, swapping the first and the third channels. Therefore we can limit ourselves to consider a desymmetrized set

$$\widetilde{V} = \{(2,3,1,4), (4,2,1,5), (4,2,1,3)\}. \qquad (26)$$

Equally interesting are the cases in which x limits to 0, which are obtained by time-inverting ($\pi \to \hat{\mathcal{T}}\pi$) the cases in V. In all these cases we can tend to the maximal asymmetry, provided the switch energy thresholds are chosen with certain asymptotic scalings. By expressing the threshold energies

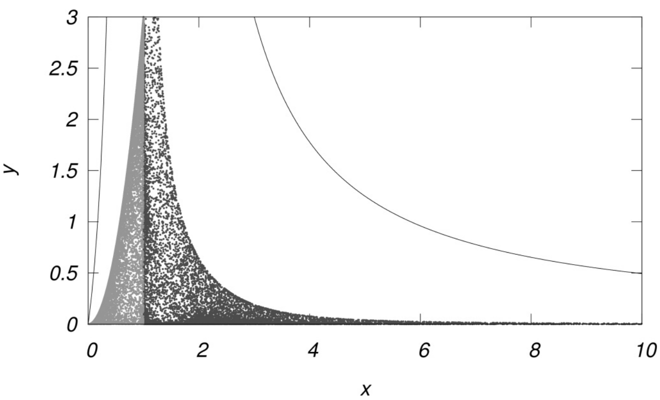


FIG. 3. The relation between x and y for random choices of threshold energies in the case (2,3,1,4) (dark gray dots) and in the time-inverted case (4,2,1,3), that is, in the case (5,2,1,3) (light gray dots). The black curve gives the analytic boundary $y = 4x/(x-1)^2$.

$E_{i+1} = E_i + \Delta E_i$ in terms of the gaps $\Delta E_i > 0$, for the cases of V, a local maximum $x_{\max}$ of x at fixed ΔE_2 follows a curve scaling in the limit $\Delta E_2 \to \infty$ as

$$E_0 \asymp e^{-\alpha \Delta E_2}, \quad \Delta E_1 \asymp e^{-\beta \Delta E_2}, \tag{27}$$

and asymmetry x diverges along this curve according to

$$x_{\max} \asymp e^{(\alpha - \beta)\Delta E_2}. \tag{28}$$

For the first two cases in $\widetilde{V}$ we find $(\alpha,\beta) = (0.488,0.316)$, and for the last one $(\alpha,\beta) \doteq (0.842,0.536)$. We note that three-switch cases of V are obtained from two-switch asymmetric cases by inserting permutation P_1 into the third position. We maximize the asymmetry by increasing the energy interval controlled by P_1 permutation and decrease all other intervals.

In Fig. 3 we show how the figure of merit y is related to the asymmetry measure x in two examples, one from $\pi \in \widetilde{V}$ and the other corresponding to its time inversion $\pi \to \hat{\mathcal{T}}\pi$. We see that increasing the asymmetry x results on average in decreasing the figure of merit y, in such a way that we do not improve the efficiency η. Note that, for $x \geqslant 1$, we are far from the Carnot efficiency, which is achieved on the curve $h(x) = 4x/(x-1)^2$ [22] (black curve in Fig. 3). By further increasing the number of switches, the diversity of cases increases beyond the scope of a detailed case-by-case study. It remains an open problem whether with our model and for a large number of switches one could approach the Carnot efficiency at asymmetries $x \gg 1$.

Generalizations. By replacing permutation matrices $P_i \in \mathcal{S}_3$ with matrices corresponding to the permutation group of arbitrary degree N, our model describes deterministic transport in an N-terminal junction of one-dimensional wires. Seeking optimized transport in our model therefore corresponds to discrete optimization problems on permutation groups. As a principal but completely impractical generalization we note that we can phrase any deterministic scattering dynamics in terms of our switch model. Finally, our model could be easily extended to investigate nonlinear regimes where breaking of time reversibility has nontrivial effects on the transport [24] and reformulated in a quantum mechanical context.

Conclusions. We have presented a minimalistic classical finite-state deterministic transport model which allows us to systematically study the questions of coupled particle and heat transport and thermoelectric and thermochemical efficiency. We have analyzed in particular the three-terminal model, where one terminal serves as the probe, and analyzed in detail the conditions under which one can maximize the asymmetry of the reduced Onsager matrix in relation to time-reversal breaking in the model. We expect that our model may serve as a simple benchmark for mesoscopic coupled transport studies.

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[21] An alternative measure of asymmetry can be defined as

$$z = \frac{l_{21} - l_{12}}{l_{12} + l_{21}} = \frac{\int d\mu \Delta f}{Q_{11} D - \int d\mu \overline{f}}, \tag{29}$$

which is related to x (20) via $x = (1+z)/(1-z)$. In the time-reversal symmetric case $l_{12} = l_{21}$ and therefore $z = 0$. In this

Brief Report we prefer to focus on parameter x rather than z, as it directly appears in formula (21) for maximum thermoelectric efficiency.

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[23] Symmetries (22) imply that, if the realization (π,ϵ) of the railway switch model leads to large asymmetry x and large thermoelectric efficiency, then $(\hat{\mathcal{T}}\pi,\epsilon)$ corresponds to small asymmetry $1/x$ and large refrigeration efficiency [15,22]

$$\eta_{\max}^{(r)} = \eta_C \frac{1}{x} \frac{\sqrt{1+y}-1}{\sqrt{1+y}+1}. \qquad (30)$$

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