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On Steady-State Entropy Production of A One-Dimensional Lattice Conductor

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I. INTRODUCTION

The understanding of irreversible phenomena including nonequilibrium steady states is a longstanding problem of statistical mechanics. Since general features of irreversible phenomena are not well understood, rigorous approaches are important.

In their purely dynamical study on nonequilibrium steady states for a classical infinite harmonic chain, Spohn and Lebowitz [1] used semiinfinite left and right segments as reservoirs. They showed that any initial state, where the left and right reservoirs are in equilibrium with different temperatures, evolves towards a steady state with nonvanishing energy current. Recently, following the same line of thoughts as Spohn and Lebowitz, and applying the method of C*-algebra, Ho and Araki [2] proved the approach to nonequilibrium steady states for an isotropic XY-chain.

As the works by Spohn-Lebowitz [1] and Ho-Araki [2], we studied nonequilibrium steady states for a one-dimensional conductor with the aid of the C*-algebra [3]. Left and right semiinfinite segments of the lattice are assigned for electron reservoirs. Initially the two reservoirs are set to be in equilibrium at different temperatures and/or different chemical potentials. The evolution of the initial states for $t \to \pm\infty$ was investigated and two different quasi-free steady states $\omega_{\pm\infty}$ were obtained. Transports and current fluctuations were investigated.

The steady state $\omega_{+\infty}$ carries nonvanishing electric and energy currents, which agree with the nonlinear generalization of the Landauer conductivity and which are consistent with the second law of thermodynamics [3]. The state $\omega_{+\infty}$ is equivalent to the nonequilibrium steady state proposed by MacLennan [4] and Zubarev [5]. The other steady state $\omega_{-\infty}$ carries anti-thermodynamical currents and is the time-reversed state of $\omega_{+\infty}$. Roughly speaking, in "a space of states", the state $\omega_{+\infty}$ behaves as an "attractor" and $\omega_{-\infty}$ as a "repeller". And initial states evolve unidirectionally from the "repeller" to the "attractor" in a way consistent with dynamical reversibility.

Now it is desirable to introduce and study entropy production as its positivity is the very definition of irreversible processes. However, definition of nonequilibrium entropy and its production is still controversial. And the related works are classified into two. On the one hand, an appropriate entropy is introduced and its derivative is calculated. For example, Ojima, Hasegawa and Ichiyanagi [6] defined entropy production for driven systems as the time-derivative of relative entropy with respect to the initial state (see also Ichiyanagi [7] and Ojima [8]). For other examples, see e.g., Ref. [9]. On the other hand, an entropy production is directly introduced based on thermodynamic considerations. Along this line of thought, Spohn and Lebowitz [10] investigated an entropy production of systems weakly coupled with reservoirs in the scaling limit and found that it can be characterized as a time-derivative of a relative entropy. Recently, Ruelle [11] investigated entropy production of nonequilibrium steady states of spin systems within the framework of C^*-algebra and showed its positivity.

In this article, as in the work of Ruelle [11], we study the entropy production of the steady state $\omega_{+\infty}$ and show that it has properties fully consistent with nonequilibrium thermodynamics. Sec. II is devoted to the summary of the previous results [3]. In Sec. III, we generally discuss the possible expressions of entropy productions. In Sec. IV, we calculate the entropy production of the steady state $\omega_{+\infty}$ and show that it is non-negaive and vanishes only when two reservoirs are in equilibrium with each other, and that it has a known quadratic form in the linear response regime. All those features are fully consistent with nonequilibrium thermodynamics. Sec. V is devoted to the summary and concluding remarks, where the relation between entropy production and relative entropy is discussed.

II. MODEL AND NONEQUILIBRIUM STEADY STATES

The system in question consists of electrons on an infinitely extended chain interacting with a localized potential and is defined on a C*-algebra as follows.

The basic dynamical variables are creation and annihilation operators, $c^*_{j,\sigma}$ and $c_{j,\sigma}$ respectively, of an electron at site $j(\in \mathbf{Z})$ with spin $\sigma(=\pm)$. They satisfy the canonical anticommutation realtions (CAR):

$$[c_{j,\sigma}, c_{k,\tau}]_+ = [c^*_{j,\sigma}, c^*_{k,\tau}]_+ = \mathbf{0} \ , \qquad [c_{j,\sigma}, c^*_{k,\tau}]_+ = \delta_{jk}\delta_{\sigma\tau}\mathbf{1} \ , \tag{1}$$

where $[A, B]_+ = AB + BA$ is the anticommutator, $\mathbf{0}$ the null element and $\mathbf{1}$ the unit. The C*-algebra $\mathcal{A}$ of dynamical variables is the CAR algebra [12], i.e., a Banach $*$-algebra with C* norm generated by

$$B(f, g) \equiv \sum_{\sigma=\pm} \sum_{j=-\infty}^{+\infty} \{f_{j,\sigma}c_{j,\sigma} + g_{j,\sigma}c^*_{j,\sigma}\} \ , \tag{2}$$

where the sequences $\{f_{j,\sigma}\}$ and $\{g_{j,\sigma}\}$ are square summable.

The physical states are defined as positive and normalized linear functionals ω over the algebra $\mathcal{A}$, i.e., linear functionals satisfying (i) $\omega(B^*B) \geq 0$ for any $B \in \mathcal{A}$ and (ii) $\omega(\mathbf{1}) = 1$ with $\mathbf{1}$ the unit of $\mathcal{A}$.

The Hamiltonian H of the system is given by

$$H = -\hbar\gamma \sum_{\sigma=\pm} \sum_{j=-\infty}^{+\infty} \left\{c^*_{j,\sigma}c_{j+1,\sigma} + c^*_{j+1,\sigma}c_{j,\sigma}\right\} + \sum_{\sigma=\pm} \sum_{j=1}^{L} \hbar\epsilon_j \ c^*_{j,\sigma}c_{j,\sigma} \ , \tag{3}$$

where $\hbar$ is the Planck constant divided by 2π, $\gamma(> 0)$ is the strength of the electron transfer and ϵ_j stands for the localized potential. The corresponding "first quantized" Schrödinger operator is assumed to admit a complete set of outgoing scattering states and have no bound state. The outgoing state $\psi_q(j)$ $(-\pi \leq q \leq \pi)$ is the solution of the eigenvalue equation corresponding to an eigenvalue $E_q = -2\hbar\gamma \cos q$:

$$-\hbar\gamma \left\{\psi_q(j+1) + \psi_q(j-1)\right\} + \hbar\epsilon_j\psi_q(j) = E_q\psi_q(j) \ , \tag{4}$$

with the outgoing boundary condition:

$$\psi_q(j) \to \frac{1}{\sqrt{2\pi}}\left\{e^{iqj} + R_q e^{-iqj}\right\} \ , \quad \text{when } j \to -\infty(+\infty) \text{ for } q > 0(< 0) \ , \tag{5}$$

where R_q is the reflection amplitude. The time-evolution automorphism $\alpha_t : \mathcal{A} \to \mathcal{A}$ is generated via a truncated Hamiltonian in a standard way [12].

Initial states are prepared in the following way: Firstly, the chain is divided into three: $(-\infty, -M-1]$, $[-M, N]$ and $[N+1, +\infty)$ with $M > 0$ and $N > L$. The two semiinfinite segments serve as reservoirs and the finite one as an embedded system. Corresponding to this division, the algebra $\mathcal{A}$ is decomposed into a tensor product of the three subalgebras $\mathcal{A}_L$, $\mathcal{A}_S$ and $\mathcal{A}_R$: $\mathcal{A} = \mathcal{A}_L \otimes \mathcal{A}_S \otimes \mathcal{A}_R$. Now the Hamiltonian H is represented as a sum of a left-reservoir part H_L, a right-reservoir part H_R, an embedded-system part H_S and a reservoir-system interaction V_{int}: $H = H_L + H_R + H_S + V_{int}$. There is a similar decomposition of the number operator: $N = N_L + N_R + N_S$. Next we introduce an equilibrium state ω_L over the algebra $\mathcal{A}_L$ of the left reservoir variables with inverse temperature β_L and chemical potential μ_L corresponding to the Hamiltonian H_L and the number operator N_L. Similarly, let ω_R be an equilibrium right-reservoir state over $\mathcal{A}_R$ with inverse temperature β_R and chemical potential μ_R corresponding to the Hamiltonian H_R and the number operator N_R. Then, for each embedded-system state ω_S over $\mathcal{A}_S$, an initial state ω_{in} is given by a tensor product

$$\omega_{in} = \omega_L \otimes \omega_S \otimes \omega_R \ . \tag{6}$$

We showed [3] that, for $t \to \pm\infty$, the initial state ω_{in} weakly evolves towards unique quasifree states $\omega_{\pm\infty}$, i.e., for any $B \in \mathcal{A}$, $\lim_{t\to\pm\infty} \omega_{in}(\alpha_t(B)) = \omega_{\pm\infty}(B)$, irrespective to the choice of the separating points M, N and the initial system state ω_S. As the state $\omega_{\pm\infty}$ are quasifree, they are fully characterized by the two-point functions. For example,

$$\omega_{+\infty}(c^*_{j\sigma} c_{j'\sigma'}) = \delta_{\sigma\sigma'} \int_0^\pi dq \left\{F_L(E_q)\psi_q(j)^*\psi_q(j') + F_R(E_q)\psi_{-q}(j)^*\psi_{-q}(j')\right\} \ , \tag{7}$$

where $F_L(E) = 1/\{e^{\beta_L(E-\mu_L)} + 1\}$ and $F_R(E) = 1/\{e^{\beta_R(E-\mu_R)} + 1\}$ are Fermi distribution functions for the left and right reservoirs, respectively.

Eq. (7) gives two-probe Landauer-type formula for the particle flow and the energy flow:

$$\langle J^N_{j-1|j}\rangle_{+\infty} \equiv \omega_{+\infty}\left(J^N_{j-1|j}\right) = \frac{1}{\pi\hbar}\int_{-2\hbar\gamma}^{2\hbar\gamma} dE|T_{q(E)}|^2\left\{F_L(E)-F_R(E)\right\} \tag{8}$$

$$\langle J^E_{j-1|j}\rangle_{+\infty} \equiv \omega_{+\infty}\left(J^E_{j-1|j}\right) = \frac{1}{\pi\hbar}\int_{-2\hbar\gamma}^{2\hbar\gamma} EdE|T_{q(E)}|^2\left\{F_L(E)-F_R(E)\right\}\ , \tag{9}$$

where $\langle\cdots\rangle_{+\infty}$ stands for the average with respect to $\omega_{+\infty}$, $q(E)\equiv\cos^{-1}\{-E/(2\hbar\gamma)\}$, $|T_q|^2\equiv 1-|R_q|^2$ the transmission coefficient, and $J^N_{j-1|j}$ and $J^E_{j-1|j}$ stand, respectively, for the particle-flow and energy-flow operators from the $(j-1)$th to the jth sites:

$$J^N_{j-1|j} = i\gamma\sum_{\sigma=\pm}\left\{c^*_{j,\sigma}c_{j-1,\sigma}-c^*_{j-1,\sigma}c_{j,\sigma}\right\}\ , \tag{10}$$

$$J^E_{j-1|j} = -\hbar\left[\frac{i\gamma^2}{2}\sum_{\sigma=\pm}\left\{c^*_{j,\sigma}c_{j-2,\sigma}+c^*_{j+1,\sigma}c_{j-1,\sigma}-(h.c.)\right\}-\frac{\epsilon_{j-1}+\epsilon_j}{2}J^N_{j-1|j}\right]\ . \tag{11}$$

III. ENTROPY PRODUCTION

- thermodynamic considerations -

Entropy production may be calculated as a time-derivative of an appropriate entropy. However, to avoid an arbitrariness in the definition of entropy, we follow the thermodynamic arguments to introduce an entropy production as in the works of Ruelle [11] and of Spohn and Lebowitz [10].

We consider a system consisting of a finite conductor placed between two infinitely extended electron reservoirs and begin with simple assumptions:

1) Entropy of the finite part exists and is finite.

2) Reservoirs remain to be in equilibrium.

3) Any change in the reservoir state can be regarded as a quasi-static process.

Let S, S_L and S_R be entropies of the finite part, right reservoir and left reservoir, respectively, then the total entropy change per time σ is obviously given by

$$\sigma = \dot{S}+\dot{S}_L+\dot{S}_R \tag{12}$$

In a steady state, all terms in the right-hand side are constant in time. Thus,

$$S = S(0) + \dot{S}t \ , \tag{13}$$

which should be finite because of the assumption 2) for all $t > 0$. And one has $\dot{S} = 0$ at steady states.

The entropy changes of the reservoirs are calculated via assumptions 2) and 3). Let J^E and J^N be energy and particle flows, respectively, from the left to the right reservoirs, then the heat flows J^q_R and J^q_L to the right and left reservoirs are given by

$$J^q_R = J^E - \mu_R J^N \ , \tag{14}$$

$$J^q_L = -J^E + \mu_L J^N \ , \tag{15}$$

where μ_R and μ_L are chemical potentials of the right and left reservoirs, respectively. And, assumptions 2) and 3) lead to

$$\dot{S}_R = \frac{J^q_R}{T_R} = \frac{J^E - \mu_R J^N}{T_R} \ , \tag{16}$$

$$\dot{S}_L = \frac{J^q_L}{T_L} = -\frac{J^E - \mu_L J^N}{T_L} \ , \tag{17}$$

where $T_R = 1/(k_B\beta_R)$ and $T_L = 1/(k_B\beta_L)$ are temperatures of the right and left reservoirs with k_B the Boltzmann constant. Eqs.(12), (16), (17) and $\dot{S} = 0$ give

$$\sigma = \left(\frac{1}{T_R} - \frac{1}{T_L}\right) J^E - \left(\frac{\mu_R}{T_R} - \frac{\mu_L}{T_L}\right) J^N \ , \tag{18}$$

which is the entropy production at a steady state.

IV. POSITIVITY OF THE ENTROPY PRODUCTION

Now we return to the one-dimensional conductor discussed in Sec.II. From eqs.(8), (9) and (18) as well as $J^E = \langle J^E_{j-1|j}\rangle_{+\infty}$ and $J^N = \langle J^N_{j-1|j}\rangle_{+\infty}$, we find

$$\sigma = -\frac{k_B}{\pi\hbar}\int_{-2\hbar\gamma}^{2\hbar\gamma} dE |T_{q(E)}|^2 \left\{\beta_L(E-\mu_L) - \beta_R(E-\mu_R)\right\}\left\{F_L(E) - F_R(E)\right\} \ . \tag{19}$$

As a result of an inequality

$$-(x-y)\left\{\frac{1}{e^x+1} - \frac{1}{e^y+1}\right\} \geq 0 \ ,$$

where the equality holds only when $x = y$, the entropy production is non-negative:

$$\sigma \geq 0 , \tag{20}$$

and vanishes only if $\beta_L = \beta_R$ and $\mu_L = \mu_R$, or both reservoirs are in equilibrium.

Note that the definitions of heat flows (14) and (15) lead to

$$J_R^q + J_L^q = V \langle J_{j-1|j} \rangle_{+\infty} \tag{21}$$

where $V = (\mu_R - \mu_L)/e$ is the voltage difference between the two reservoirs and $J_{j-1|j} = -e \; J_{j-1|j}^N$ is the electric current operator. This implies that the total heat flow from the finite system is the Joule heat.

The relation with thermodynamics is more transparent in the linear transport regime. Let T_0 be the mean temperature of the reservoirs, ΔT the temperature difference, μ_0 the mean chemical potential and V the potential difference:

$$T_R = T_0 - \frac{\Delta T}{2} , \qquad T_L = T_0 + \frac{\Delta T}{2} , \qquad \mu_R = \mu_0 + \frac{eV}{2} , \qquad \mu_L = \mu_0 - \frac{eV}{2} .$$

Then, when $|\Delta T| \ll T_0$ and $e|V| \ll \mu_0$, we have

$$\langle J_{j-1|j} \rangle_{+\infty} = GV + L_1 \frac{\Delta T}{T_0} , \qquad \langle J_{j-1|j}^q \rangle_{+\infty} = L_1 V + L_2 \frac{\Delta T}{T_0} , \tag{22}$$

where the heat flow $J_{j-1|j}^q = J_{j-1|j}^E - \mu_0 J_{j-1|j}^N$ was introduced and the coefficients are [3]

$$G = \frac{e^2}{\pi \hbar} \int_{-2\hbar\gamma}^{2\hbar\gamma} dE \; |T_{q(E)}|^2 \left(- \frac{\partial F_0(E)}{\partial E} \right) , \tag{23}$$

$$L_1 = - \frac{e}{\pi \hbar} \int_{-2\hbar\gamma}^{2\hbar\gamma} dE \; (E - \mu_0) \; |T_{q(E)}|^2 \left(- \frac{\partial F_0(E)}{\partial E} \right) , \tag{24}$$

$$L_2 = \frac{1}{\pi \hbar} \int_{-2\hbar\gamma}^{2\hbar\gamma} dE \; (E - \mu_0)^2 \; |T_{q(E)}|^2 \left(- \frac{\partial F_0(E)}{\partial E} \right) . \tag{25}$$

In the above, $F_0(E) = 1/\{e^{\beta_0 (E - \mu_0)} + 1\}$ with $\beta_0 = 1/(k_B T_0)$.

In this case, the entropy production is given by

$$\sigma = \frac{\Delta T}{T_0^2} \langle J_{j-1|j}^q \rangle_{+\infty} + \frac{V}{T_0} \langle J_{j-1|j} \rangle_{+\infty} = \frac{1}{T_0} \left[GV^2 + 2 L_1 V \frac{\Delta T}{T_0} + L_2 \left(\frac{\Delta T}{T_0} \right)^2 \right] . \tag{26}$$

This agrees with the expression of the entropy production known in the linear non-equilibrium thermodynamics [13].

All those features are fully consistent with nonequilibrium thermodynamics.

V. CONCLUSIONS

We have shown that a nonequilibrium entropy production previously introduced for spin systems by Ruelle [11] can be extended to one-dimensional conductors and that it is fully consistent with nonequilibrium thermodynamics.

Now we explore physical implications of the results. For this purpose, we assume all the states are described by density matrices. First we observe, because of the conservation of energy and particle number, the average energy flow $\langle J^E_{j-1|j}\rangle_{+\infty}$ and the average particle flow $\langle J^N_{j-1|j}\rangle_{+\infty}$ are given in terms of reservoir energies H_L, H_R and particle numbers N_L, N_R:

$$\langle J^E_{j-1|j}\rangle_{+\infty} = -\langle \dot{H}_L\rangle_{+\infty} = \langle \dot{H}_R\rangle_{+\infty} \ , \tag{27}$$

$$\langle J^N_{j-1|j}\rangle_{+\infty} = -\langle \dot{N}_L\rangle_{+\infty} = \langle \dot{N}_R\rangle_{+\infty} \ , \tag{28}$$

where $\dot{H}_L = \frac{d}{dt}\alpha_t(H_L)\Big|_{t=0}$. Furthermore, if an observable A admits a finite average $\langle A\rangle_{+\infty}$, $\langle \dot{A}\rangle_{+\infty} = 0$ because of the invariance of the state $\omega_{+\infty}$.

Then, (27) and (28) give

$$\sigma = k_B\langle \beta_L(\dot{H}_L - \mu_L\dot{N}_L)\rangle_{+\infty} + k_B\langle \beta_R(\dot{H}_R - \mu_R\dot{N}_R)\rangle_{+\infty} \ . \tag{29}$$

Now let $\bar{H}_R \equiv H - H_L$, then the difference $\bar{H}_R - H_R$ admits finite average with respect to $\omega_{+\infty}$ and $\langle \{\dot{\bar{H}}_R - \dot{H}_R\}\rangle_{+\infty} = 0$. This, a similar equation for N_R and (29) lead to

$$\begin{aligned}\sigma &= k_B\langle \beta_L(\dot{H}_L - \mu_L\dot{N}_L)\rangle_{+\infty} + k_B\langle \beta_R(\dot{\bar{H}}_R - \mu_R\dot{\bar{N}}_R)\rangle_{+\infty} \\ &= -k_B\frac{d}{dt}\mathrm{Tr}(\rho(t)\ln\rho_{\mathrm{Loc}})\Big|_{\rho(t)\to\rho_{+\infty}}\end{aligned} \tag{30}$$

where Tr stands for the trace, $\rho(t)$ and $\rho_{+\infty}$ are density matrices for the state at time t and the steady state $\omega_{+\infty}$. The density matrix ρ_{Loc} corresponds to the local equilibrium state:

$$\rho_{\mathrm{Loc}} = \frac{1}{Z_{\mathrm{Loc}}}\exp\{-\beta_L(H_L - \mu_L N_L) - \beta_R(\bar{H}_R - \mu_R\bar{N}_R)\} \ , \tag{31}$$

with Z_{Loc} the normalization constant. The expression (30) suggests that a nonequilibrium entropy is given by $S = -k_B\mathrm{Tr}(\rho\ln\rho_{\mathrm{Loc}})$, which is nothing but Zubarev's definition of nonequilibrium entropy [5].

Since von Neumann entropy $\mathrm{Tr}(\rho(t)\ln\rho(t))$ is constant in time, one also has

$$\sigma = -k_B \frac{d}{dt} S\left(\rho(t)|\rho_{\mathrm{Loc}}\right)\Big|_{\rho(t)\to\rho_{+\infty}} \tag{32}$$

where $S\left(\rho(t)|\rho_{\mathrm{Loc}}\right)$ is the relative entropy [14,15,12]

$$S\left(\rho(t)|\rho_{\mathrm{Loc}}\right) = -\mathrm{Tr}\left(\rho(t)\{\ln\rho(t) - \ln\rho_{\mathrm{Loc}}\}\right) \ . \tag{33}$$

A similar formula to (32) was derived by Spohn and Lebowitz [10] for systems weakly coupled with reservoirs in the scaling limit, where the local equilibrium state is replaced by an equilibrium state.

The entropy production σ can be represented in a different way. By noting that the logarithm of the initial density matrix of the embedded system:$\ln\rho_S(0)$ admits a finite steady-state average, one has

$$\sigma = -k_B \frac{d}{dt} S\left(\rho(t)|\rho(0)\right)\Big|_{\rho(t)\to\rho_{+\infty}} , \tag{34}$$

where $\rho(0)$ stands for the initial state of the whole system. For driven systems, Ojima, Hasegawa and Ichiyanagi [6] introduced entropy production as time-derivative of the relative entropy with respect to the initial state $S\left(\rho(t)|\rho(0)\right)$ (see also Ichiyanagi [7] and Ojima [8]). Eq.(34) suggests that the same formula holds for internally disturbed systems.

We emphasize again that the above arguments are formal and rigorous discussions will be presented elsewhere.

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