Entropy production in systems with spontaneously broken time-reversal*

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Abstract

We study the entropy production in non-equilibrium quantum systems without dissipation, which is generated exclusively by the spontaneous breaking of time-reversal invariance. Systems which preserve the total energy and particle number and are in contact with two heat reservoirs are analysed. Focusing on point-like interactions, we derive the probability distribution induced by the entropy production operator. We show that all its moments are positive in the zero frequency limit. The analysis covers both Fermi and Bose statistics.

1. Introduction

We investigate below non-equilibrium quantum systems with infinite degrees of freedom, where the time reversal symmetry T is spontaneously broken. In particular, we explore the impact of the spontaneous T-breaking on the entropy production, which represents the key indicator for the departure from equilibrium. The presentation summarises our previous results [1, 2] and pursues further our study of the entropy production in systems with the structure shown in Fig. 1. One has two heat reservoirs R_i with (inverse) temperatures $\beta_i \geq 0$ and chemical potentials μ_i , which communicate via the gates G_i with the interaction domain \mathbb{D} . Particles are emitted and absorbed by the reservoirs R_i trough the gates G_i and propagate along the leads L_i to the interaction domain \mathbb{D} . The interaction in \mathbb{D} drives the

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Figure 1: System connected to two heat reservoirs.

system away from equilibrium. The capacity of R_i is assumed large enough so that the particle emission and absorption processes do not change their parameters.

Systems of this type in one space dimension are widely investigated. They are successfully applied for studying the transport properties of quantum wire junctions [3]-[8], quantum Hall edges [9] and recently are also engineered in laboratory by ultracold Bose gases [10]-[12]. The remarkable precision reached in such experiments allows to explore fundamental aspects of non-equilibrium many-body quantum physics.

In the next section we establish some general universal features of non-equilibrium systems, which communicate with two heat reservoirs. Afterwards, in section 3 we provide a microscopic picture for the entropy production in such systems and propose a quantum field theory framework for the derivation of the probability distribution generated by the entropy production operator. In section 4 we illustrate this approach at work exploring two examples - the fermionic and bosonic Schrödinger junctions with point-like interaction. The last section is devoted to the conclusions.

2. Spontaneous breaking of time-reversal invariance

Quantum systems in contact with two heat reservoirs exhibit in general a complex behaviour. In order to simplify the picture, we assume in what follows the conservation of the particle number and the total energy

$$N = \int_{G_1}^{G_2} dx \, j_t(t, x) \,, \quad H = \int_{G_1}^{G_2} dx \, \vartheta_t(t, x) \,, \tag{1}$$

 j_t and ϑ_t being the particle and energy densities. In other words there is no particle and energy dissipation. Let j_x and ϑ_x be the associated local conserved currents which obey the continuity equations

$$\partial_t j_t(t, x) - \partial_x j_x(t, x) = 0, \qquad (2)$$

$$\partial_t \vartheta_t(t, x) - \partial_x \vartheta_x(t, x) = 0. (3)$$

Combining (1) with (2,3) and taking into account the orientation of the leads L_i one finds

$$\dot{N} = 0 \quad \Rightarrow \quad j_x(t, G_1) + j_x(t, G_2) = 0,$$
 (4)

$$\dot{H} = 0 \quad \Rightarrow \quad \vartheta_x(t, G_1) + \vartheta_x(t, G_2) = 0,$$
 (5)

the dot indicating the time derivative. Therefore the particle and energy inflows are equal to the outflows as expected.

Let us consider now the operation of time-reversal. It is well known that this operation is implemented by an anti-unitary operator T, acting in the state space \mathcal{H} of the system. We recall [13] that

$$T j_x(t, x) T^{-1} = -j_x(-t, x)$$
(6)

and assume that the dynamics preserves time-reversal invariance, namely

$$T H T^{-1} = H$$
. (7)

Now, let $\Omega \in \mathcal{H}$ be any time-translation invariant state of the system with non-vanishing particle flow between the two reservoirs

$$\langle j_x(t,x)\rangle_{\Omega} \equiv (\Omega, j_x(t,x)\Omega) \neq 0,$$
 (8)

where (\cdot, \cdot) is the scalar product in \mathcal{H} . Taking the expectation value of (6) one has

$$\langle T j_x(t,x) T^{-1} \rangle_{\Omega} = -\langle j_x(-t,x) \rangle_{\Omega},$$
 (9)

which, combined with the fact that $\langle j_x(t,x)\rangle_{\Omega}$ is actually t-independent due to the time-translation invariance of Ω , implies that

$$T\Omega \neq \Omega$$
. (10)

We conclude that time-reversal is broken in the state $\Omega \in \mathcal{H}$ in spite of the fact that the dynamics is time-reversal invariant (7). This result can be compactly formulated as follows.

Proposition: Any state, which is invariant under time translations and generates a non-vanishing expectation value for the particle current, breaks time-reversal symmetry.

This is a genuine quantum field theory phenomenon of spontaneous breaking of a discrete symmetry, whose order parameter is $\langle j_x(t,x)\rangle_{\Omega}$.

The state Ω has another remarkable feature. Let $q_x(t, G_i)$ be the heat current flowing through the gate G_i . Since the value of the chemical potential in G_i is μ_i , one has [14]

$$q_x(t,G_i) = \vartheta_x(t,G_i) - \mu_i j_x(t,G_i). \tag{11}$$

Notice that we adopt here only the value of the heat current in the gates G_i . The point is that the heat current in the interaction domain \mathbb{D} is not known, because the temperature and the chemical potential are not defined in this region. In order to introduce the concept of local parameters $\beta(x)$ and $\mu(x)$ for $x \in \mathbb{D}$ one needs further model dependent assumptions, which are not relevant and not needed for our construction.

From (11) it follows that for $\mu_1 \neq \mu_2$ the heat flow through G_1 differs from that through G_2 . In fact,

$$\dot{Q} \equiv -q_x(t, G_2) - q_x(t, G_1) = (\mu_2 - \mu_1)j_x(t, G_1) \neq 0.$$
 (12)

Now we recall that the total energy H of the system has two different components - heat and chemical energies. Since H is conserved, (12) implies that these components are not separately conserved and can be converted one into the other. This process, discovered in [15], depends on the state Ω and more precisely on the expectation value

$$\langle \dot{Q} \rangle_{\Omega} = (\Omega \,,\, \dot{Q}\Omega) \,.$$
 (13)

Chemical energy is converted to heat energy if $\langle \dot{Q} \rangle_{\Omega} > 0$. The opposite process takes place for $\langle \dot{Q} \rangle_{\Omega} < 0$ and energy transmutation is absent only if $\langle \dot{Q} \rangle_{\Omega} = 0$. It is worth stressing that there is no dissipation during the energy conversion.

Summarising, the physical consequences of particle and energy conservation in any state Ω , satisfying (8), are:

- (i) spontaneous breaking of time-reversal;
- (ii) conversion of heat to chemical energy or vice versa.

It is worth stressing that these deeply related features follow exclusively from symmetry considerations and do *not* depend on the interaction taking place in \mathbb{D} . In this sense they are *universal* and hold for all systems of the type shown in Fig. 1.

3. Entropy production

The properties (i)-(ii), established in the previous section, have relevant physical implications. Among others, they provide a simple and remarkable mechanism for non-vanishing entropy production \dot{S} in absence of dissipation. Our main goal in what follows will be to study this aspect in detail. According to the second law of classical thermodynamics $\dot{S} \geq 0$. In the quantum case \dot{S} is an operator, which has the following form [14]

$$\dot{S} = -\beta_1 \, q_x(t, G_1) - \beta_2 \, q_x(t, G_2) \tag{14}$$

in terms of the heat currents flowing through the gates G_i . In order to investigate the properties of this operator, one needs a microscopic approach [1, 2] to the particle transport in the system. It is based on the observation that (due to particle number conservation), there are three fundamental elementary processes which take place:

- (a) emission and reabsorption of any number of particles from the same reservoir;
- (b) emission of n particles from the "hot" reservoir R_2 and their absorption by the "cold" one R_1 ;

(c) emission of n particles from the "cold" reservoir R_1 and their absorption by the "hot" one R_2 .

Let us denote by p_0 , p_n and p_{-n} with n = 1, 2, ... the probabilities of the events (a), (b) and (c) respectively. A substantial difference with respect to the classical case is that in the quantum world the processes of the type (c) have a priori non-vanishing probabilities. At this stage it is useful to introduce the sequences

$$P = \{p_n : n = 0, \pm 1, \pm 2, ...\}, \qquad \Sigma = \{\sigma_n : n = 0, \pm 1, \pm 2, ...\},$$
 (15)

where σ_n is the entropy production associated with the process with probability p_n . It is natural to expect that $\sigma_0 = 0$, $\{\sigma_n > 0, n = 1, 2, ...\}$ and $\{\sigma_n < 0, n = -1, -2, ...\}$.

Summarising, both processes with positive and negative entropy production occur at the microscopic level. It is clear that the sequences (15) fully codify the entropy production in the system. So, the problem is to determine P and Σ . We will show below that both P and Σ can be extracted from the probability distribution $\varrho[\dot{S}]$ generated by the correlation functions

$$\mathcal{M}_n[\dot{S}] = \langle \dot{S}(t_1) \cdots \dot{S}(t_n) \rangle_{\Omega}. \tag{16}$$

The based observation now is that $\mathcal{M}_n[\dot{S}]$ are the moments of $\varrho[\dot{S}]$, namely

$$\mathcal{M}_n[\dot{S}] = \int_{\mathcal{D}} d\sigma \, \sigma^n \varrho[\dot{S}](\sigma) \,, \tag{17}$$

where \mathcal{D} is the range of entropy production. The strategy at this point consists of three steps:

- derivation of the correlation functions $\mathcal{M}_n[\dot{S}]$ given by (16);
- reconstruction of the distribution $\varrho[\dot{S}]$ from its moments $\mathcal{M}_n[\dot{S}]$ (also known as moment problem [16]);
- derivation of the sequences P and Σ from $\varrho[\dot{S}]$.

Although conceptually very clear, the first two steps are practically quite involved. They include the derivation of the infinite sequence of correlation functions (16), followed by the solution of the moment problem. Nevertheless we give in the next section two examples where this program can be taken to the end. We describe one fermionic and one bosonic model, where the interaction domain $\mathbb D$ is reduced to a point x=0. We show that with such point-like interaction one can determine $\varrho[\dot S]$ and consequently P and Σ in exact and explicit form and discuss the physical implications of the solution.

4. Fermionic/bosonic Schrödinger junction

We analyse in this section two examples with point-like interaction described by a unitary scattering matrix $\mathbb S$ as shown in Fig. 2. The dynamics along the leads L_i with coordinates $\{(x,i): x<0, i=1,2\}$, where |x| is the distance from the interaction and i labels the lead, is defined by the Schrödinger equation

$$\left(i\partial_t + \frac{1}{2m}\partial_x^2\right)\psi(t,x,i) = 0, \qquad (18)$$

where ψ is a quantum field satisfying the equal-time canonical (anti)com-

$$\beta_1, \mu_1$$
 C_1 C_2 C_2

Figure 2: System with point-like interaction S at x = 0.

mutation relations

$$[\psi(t,x,i), \psi^*(t,y,j)]_{\pm} = \delta_{ij} \,\delta(x-y) \tag{19}$$

and * stands for Hermitian conjugation. The interaction is fixed by the boundary condition

$$\lim_{x \to 0^{-}} \sum_{j=1}^{2} \left[\lambda (\mathbb{I} - \mathbb{U})_{ij} + i(\mathbb{I} + \mathbb{U})_{ij} \partial_{x} \right] \psi(t, x, j) = 0, \qquad (20)$$

where λ is a free parameter with dimension of mass and \mathbb{U} is an arbitrary unitary matrix $\mathbb{U} \in U(2)$. This is [17] the most general boundary condition ensuring the self-adjointness of the Hamiltonian. In momentum space the associated scattering matrix is given by [17, 18]

$$\mathbb{S}(k) = -\frac{\left[\lambda(\mathbb{I} - \mathbb{U}) - k(\mathbb{I} + \mathbb{U})\right]}{\left[\lambda(\mathbb{I} - \mathbb{U}) + k(\mathbb{I} + \mathbb{U})\right]},\tag{21}$$

where the matrices in the numerator and denominator commute. One can easily verify that this scattering matrix is unitary $\mathbb{S}(k)\mathbb{S}^*(k) = \mathbb{I}$ and satisfies Hermitian analyticity $\mathbb{S}^*(k) = \mathbb{S}(-k)$. The dynamics fixed by (18-20) is invariant under time-reversal if and only if \mathbb{U} and consequently $\mathbb{S}(k)$ are symmetric.

We will show below that the above system, called in what follows Schrödinger junction, nicely illustrates the program from the previous section and works simultaneously for both Fermi (+) and Bose (-) statistics.

For simplicity we assume in what follows that $\mathbb{S}(k)$ has no bound states, referring for the general case to [19]. Then, the general solution of (18-20) is given by

$$\psi(t, x, i) = \sum_{j=1}^{2} \int_{0}^{\infty} \frac{dk}{2\pi} e^{-i\omega(k)t} \left[e^{-ikx} \delta_{ij} + e^{ikx} \mathbb{S}_{ij}^{*}(k) \right] a_{j}(k), \qquad (22)$$

where $\omega(k) = \frac{k^2}{2m}$ is the dispersion relation and the oscillators

$${a_i(k), a_i^*(k), :, k > 0, i = 1, 2}$$
 (23)

generate a standard canonical (anti)commutation relation algebra A_{\pm}

$$[a_i(k), a_j^*(p)]_{\pm} = \delta_{ij} 2\pi \delta(k-p).$$
 (24)

Notice that (23) annihilate and create only in-coming particles because k > 0. The contribution of the out-going excitations is generated by the second term in the integrand of (22), which involves the scattering matrix $\mathbb{S}(k)$.

The basic physical observables, we are interested in, are

$$j_x(t,x,i) = \frac{\mathrm{i}}{2m} \left[\psi^*(\partial_x \psi) - (\partial_x \psi^*) \psi \right] (t,x,i), \qquad (25)$$

$$\vartheta_x(t, x, i) = \frac{1}{4m} [(\partial_t \psi^*) (\partial_x \psi) + (\partial_x \psi^*) (\partial_t \psi) - (\partial_t \partial_x \psi^*) \psi - \psi^* (\partial_t \partial_x \psi)](t, x, i),$$
(26)

$$\dot{S}(t,x) = -\sum_{i=1}^{2} \beta_i \, q(t,x,i) \,, \qquad q_x(t,x,i) = \vartheta_x(t,x,i) - \mu_i j_x(t,x,i) \,. \tag{27}$$

In order to compute the correlation functions of the entropy production operator $\dot{S}(t,x)$ one must fix a representation of the oscillator algebras \mathcal{A}_{\pm} . We choose the Landauer-Büttiker (LB) representation [20, 21] { \mathcal{H}_{LB} , Ω_{LB} }, which represents a non-equilibrium generalisation of the Gibbs representation [22] to the case of systems which exchange particles and energy with more then one heat reservoir. Adopting the field-theoretical construction [23] of { \mathcal{H}_{LB} , Ω_{LB} }, one can derive in explicit form the expectation values

$$\langle a_{l_1}^*(k_1)a_{m_1}(p_1)\cdots a_{l_n}^*(k_n)a_{m_n}(p_n)\rangle_{LB}^{\pm}, \qquad k_i, p_i > 0,$$
 (28)

in the LB steady state $\Omega_{\rm LB}$. It is convenient for this purpose to introduce the matrix

$$\mathbb{M}_{ij}^{\pm} = \begin{cases}
2\pi\delta(k_i - p_j)\delta_{l_i m_j} d_{l_i}^{\pm}[\omega(k_i)], & i \leq j, \\
\mp 2\pi\delta(k_i - p_j)\delta_{l_i m_j} \left(1 \mp d_{l_i}^{\pm}[\omega(k_i)]\right), & i > j,
\end{cases}$$
(29)

where

$$d_l^{\pm}(\omega) = \frac{1}{e^{\beta_l(\omega - \mu_l)} \pm 1}, \qquad \text{(for bosons } \mu_l < 0\text{)}$$

are the Fermi/Bose distribution of the reservoir R_l . Then one has [23]

$$\langle a_{l_1}^*(k_1)a_{m_1}(p_1)\cdots a_{l_n}^*(k_n)a_{m_n}(p_n)\rangle_{LB}^{\pm} = \begin{cases} \mathbf{det}\left[\mathbb{M}^+\right], & k_i, p_i > 0, \\ \mathbf{perm}\left[\mathbb{M}^-\right], & k_i, p_i > 0, \end{cases}$$
(31)

where **det** and **perm** indicate the determinant and the permanent of the corresponding matrices. It is perhaps useful to recall that

$$\mathbf{perm}\left[\mathbb{M}\right] = \sum_{\sigma_i \in \mathcal{P}_n} \prod_{i=1}^n \mathbb{M}_{i\sigma_i}, \qquad \mathcal{P}_n - \text{set of all permutations of } n \text{ elements.}$$

Equations (29-31) are the basic ingredients for deriving the correlation functions in the LB representation. Our first step in this direction will be to compute some one-point functions. In particular, we will check that time-reversal is spontaneously broken, namely that $T\Omega_{\rm LB} \neq \Omega_{\rm LB}$. Following the argument in section 1, it is enough to control the mean value of the particle current (25). One finds

$$\langle j(t,x,i)\rangle_{\text{LB}}^{\pm} = \int_0^{\infty} \frac{d\omega}{2\pi} \sum_{l=1}^2 \left[\delta_{il} - |\mathbb{S}_{il}(\sqrt{2m\omega})|^2 \right] d_l^{\pm}(\omega) \neq 0,$$
 (33)

which confirms the spontaneous T-breaking.

For the mean value of the entropy production one has

$$\langle \dot{S}(t,x) \rangle_{\text{LB}}^{\pm} = \int_0^{\infty} \frac{d\omega}{2\pi} |\mathbb{S}_{12}(\sqrt{2m\omega})|^2 [\gamma_2(\omega) - \gamma_1(\omega)] [d_1^{\pm}(\omega) - d_2^{\pm}(\omega)] \ge 0,$$
(34)

where

$$\gamma_i(\omega) \equiv \beta_i(\omega - \mu_i) \,. \tag{35}$$

(32)

The positivity follows directly from the fact that the two square brackets in the integrand have always the same sign. The bound (34) is a special case of the general result of Nenciu [24] for systems in the LB state and in contact with arbitrary number of heat reservoirs.

We turn now to the n-point correlation functions

$$\langle \dot{S}(t_1, x_1) \cdots \dot{S}(t_n, x_n) \rangle_{LP}^{\pm},$$
 (36)

which, due to the total energy conservation, depend only on the time differences $\{\hat{t}_i \equiv t_i - t_{i+1} : i = 1, ..., n-1\}$. This fact allows to introduce for

 $n \geq 2$ the frequency ν via the Fourier transform

$$w_n^{\pm}[\dot{S}](x_1, ..., x_n; \nu) = \int_{-\infty}^{\infty} d\hat{t}_1 \cdots \int_{-\infty}^{\infty} d\hat{t}_{n-1} e^{-i\nu(\hat{t}_1 + \cdots \hat{t}_{n-1})} \langle \dot{S}(t_1, x_1) \cdots \dot{S}(t_n, x_n) \rangle_{LB}^{\pm}.$$
 (37)

Following the classical studies [25]-[29] in quantum noise and full counting statistics, we perform the zero-frequency limit in which the quantum fluctuations are integrated over the whole time axes. It turns out [1, 2] that in this limit the position dependence in (37) drops out and one finds

$$\lim_{\nu \to 0^{+}} w_{n}^{\pm} [\dot{S}](x_{1}, ..., x_{n}; \nu) = \int_{0}^{\infty} \frac{d\omega}{2\pi} \,\mathcal{M}_{n}^{\pm} [\dot{S}](\omega) \,, \tag{38}$$

where $\mathcal{M}_n^{\pm}[\dot{S}]$ are precisely the moments (17) of the probability distribution $\varrho_n^{\pm}[\dot{S}]$ we are looking for. Using (29-31), one gets

$$\mathcal{M}_{n}^{\pm}[\dot{S}] = \begin{cases} \gamma_{21}^{n}(\omega) \det[\mathbb{D}^{+}(\omega; l_{1}, ..., l_{n})], \\ \gamma_{21}^{n}(\omega) \operatorname{\mathbf{perm}}[\mathbb{D}^{-}(\omega; l_{1}, ..., l_{n})], \end{cases}$$
(39)

where

$$\gamma_{ij}(\omega) \equiv \gamma_i(\omega) - \gamma_j(\omega) = (\beta_i - \beta_j)\omega - (\beta_i\mu_i - \beta_j\mu_j), \qquad (40)$$

is a basic dimensionless parameter defining the entropy generated by transporting a particle with energy ω from the reservoir R_i to R_j . Moreover the \mathbb{D}^{\pm} -matrices are given by

$$\mathbb{D}_{ij}^{\pm}(\omega; l_1, ..., l_n) = \begin{cases} \mathbb{J}_{l_j l_i}(\omega) d_{l_j}^{\pm}(\omega), & i \leq j, \\ \mp \mathbb{J}_{l_j l_i}(\omega) \left[1 \mp d_{l_j}^{\pm}(\omega) \right], & i > j, \end{cases}$$
(41)

with

$$\mathbb{J}_{11}(\omega) = -\mathbb{J}_{22}(\omega) = |\mathbb{S}_{12}(\sqrt{2m\omega})|^2 \equiv \tau(\omega), \tag{42}$$

$$\mathbb{J}_{12}(\omega) = \overline{\mathbb{J}}_{21}(\omega) = -\mathbb{S}_{11}(\sqrt{2m\omega})\,\overline{\mathbb{S}}_{12}(\sqrt{2m\omega})\,,\tag{43}$$

where $\tau(\omega)$ is the transmission probability. For $\tau(\omega) = 0$ the leads are isolated and the system is in equilibrium.

At this stage, using (39-43) one can derive the inequality

$$\mathcal{M}_{n}^{\pm}[\dot{S}] \ge 0, \qquad n = 1, 2, \dots$$
 (44)

which is one of our main results. The rigorous proof of the bound (44) can be found in [1] for fermions and in [2] for bosons. Referring to these papers for the details, we will give below an alternative intuitive explanation, which has the advantage of providing a simple physical interpretation in terms of

the sequence of probabilities P in (15). In order to derive P we introduce the moment generating function [16]

$$\chi^{\pm}[\dot{S}](\lambda) = \sum_{n=0}^{\infty} \frac{(\mathrm{i}\lambda)^n}{n!} \mathcal{M}_n^{\pm}[\dot{S}], \qquad (45)$$

where the ω -dependence is implicit. After some algebra one finds

$$\chi^{+}[\dot{S}](\lambda) = 1 + ic_{1}^{+}\sqrt{\tau}\sin(\lambda\gamma_{21}\sqrt{\tau}) + c_{2}^{+}\left[\cos(\lambda\gamma_{21}\sqrt{\tau}) - 1\right],$$
 (46)

$$\chi^{-}[\dot{S}](\lambda) = \frac{1}{1 - ic_{1}^{-}\sqrt{\tau}\sin(\lambda\gamma_{21}\sqrt{\tau}) - c_{2}^{-}\left[\cos(\lambda\gamma_{21}\sqrt{\tau}) - 1\right]},$$
 (47)

where c_i^{\pm} are expresses via the reservoir distributions d_i^{\pm} as follows

$$c_1^{\pm} \equiv d_1^{\pm} - d_2^{\pm}, \qquad c_2^{\pm} \equiv d_1^{\pm} + d_2^{\pm} \mp 2d_1^{\pm}d_2^{\pm}.$$
 (48)

The final step towards the entropy production distributions $\varrho^{\pm}[\dot{S}]$ is the Fourier transform

$$\varrho^{\pm}[\dot{S}](\sigma) = \int_0^\infty \frac{\mathrm{d}\lambda}{2\pi} \mathrm{e}^{-\mathrm{i}\lambda\sigma} \chi^{\pm}[\dot{S}](\lambda) \,. \tag{49}$$

Since according to (46,47) $\chi^{\pm}[\dot{S}]$ are periodic functions in λ with period $2\pi/\sqrt{\tau}$, the Fourier transform is a superposition of δ -functions - the so called "Dirac comb". The fermionic comb has only three "teeth"

$$\varrho^{+}[\dot{S}](\sigma) = \sum_{k=-1}^{1} p_{k}^{+} \delta(\sigma - k\gamma_{21}\sqrt{\tau}), \qquad (50)$$

because only single particle processes are allowed by Pauli's principle since the energy ω is fixed and there is no degeneracy in spin and momentum in the Schrödinger junction. In (50)

$$p_{\pm 1}^{+} = \frac{1}{2} \left(c_2^{+} \mp c_1^{+} \sqrt{\tau} \right) , \qquad p_0^{+} = 1 - c_2^{+} ,$$
 (51)

and

$$\sigma_{\pm 1} = \pm \gamma_{21} \sqrt{\tau} \,, \qquad \sigma_0 = 0 \,, \tag{52}$$

are precisely the elements of the sequences P^+ and Σ^+ we are looking for. In fact one can easily verify that

$$p_k^+ \ge 0, \qquad \sum_{k=-1}^1 p_k^+ = 1.$$
 (53)

The bosonic case is technically more involved since the comb has infinite "teeth"

$$\varrho^{-}[\dot{S}](\sigma) = \sum_{k=-\infty}^{\infty} p_{k}^{-} \delta(\sigma - k\gamma_{21}\sqrt{\tau}), \qquad (54)$$

because multi-particle processes are allowed. The computation, performed in [2], gives

$$p_{\pm n}^{-} = \frac{(c_{2}^{-} \pm c_{1}^{-} \sqrt{\tau})^{n}}{2^{n} (1 + c_{2}^{-})^{n+1}} {}_{2}F_{1} \left[\frac{1+n}{2}, \frac{2+n}{2}, n+1, \frac{(c_{2}^{-})^{2} - \tau(c_{1}^{-})^{2}}{(1+c_{2}^{-})^{2}} \right], \quad (55)$$

$$\sigma_{\pm n} = \pm n \gamma_{21} \sqrt{\tau}, \qquad n = 0, \pm 1, \pm 2, \dots$$
 (56)

where ${}_2F_1$ is the Gauss hypergeometric function. Equations (55,56) define the sequences P^- and Σ^- in the bosonic case. In analogy with (53) one has [2]

$$p_k^- \ge 0, \qquad \sum_{k=-\infty}^{\infty} p_k^- = 1.$$
 (57)

Summarising, (53,57) imply that both $\varrho^{\pm}[\dot{S}]$ are well defined probability distributions. Equations (51,55) provide in explicit form the probabilities p_k^{\pm} for the basic emission and absorption processes in terms of the Dirac/Bose distributions d_i^{\pm} and the interaction τ . All quantum fluctuations in the zero frequency limit are taken into account. The relative simplicity of p_k^{+} with respect to p_k^{-} is a consequence of the Pauli principle. In order to compare p_k^{\pm} for different k and to get a more precise idea about the distributions $\varrho^{\pm}[\dot{S}]$ it is convenient to introduce the smeared versions $\varrho^{\pm}_{\alpha}[\dot{S}]$ by the substitution

$$\delta(\sigma) \longmapsto \delta_{\alpha}(\sigma) \equiv \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 \sigma^2}, \qquad \alpha > 0,$$
 (58)

in (50,54). By construction $\varrho_{\alpha}^{\pm}[\dot{S}] \to \varrho^{\pm}[\dot{S}]$ for $\alpha \to \infty$ in the sense of generalised functions. The advantage of $\varrho_{\alpha}^{\pm}[\dot{S}]$ is that they are not singular and can be easily plotted for some value of α and the parameters β_i , μ_i and τ . Typical plots are shown in Fig. 3, where the left and right panel display the fermionic and bosonic distribution respectively.

The relative height of the peaks in Fig. 3 allows to compare the different probabilities of the fundamental emission-absorption processes described in points (a)-(c) in section 3. We see that the predominant process is the emission and reabsorption by the same reservoir with vanishing entropy production $\sigma = 0$. For $\sigma \neq 0$ the peaks are symmetric with respect to the origin and the right ones $(\sigma > 0)$ always dominate the left ones $(\sigma < 0)$. This observation provides the physical explanation for the positivity bound (44) on the moments $\mathcal{M}_n^{\pm}[\dot{S}]$.

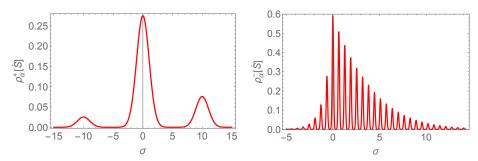


Figure 3: Fermionic and bosonic entropy production distributions.

The knowledge of the sequences P^{\pm} and Σ^{\pm} in explicit form (51, 52, 55, 56) has relevant physical applications. Using this microscopic information one can establish the fluctuation relations [30]-[32] governing the entropy production in the LB state. Moreover, one can introduce a concept of efficiency of the quantum transport, which goes beyond the meal value description and takes into account all quantum fluctuations. For more details about these applications we refer the reader to [1, 2].

In conclusion, for non-equilibrium quantum systems in the LB state microscopic processes with negative entropy production occur with some non-vanishing probability. For each such process however, there exists a more probable one with the opposite positive entropy production, which dominates. This feature can be interpreted in our context as a quantum version of the second law of thermodynamics.

5. Conclusions

The above study develops a field theoretic approach to the entropy production in non-equilibrium quantum systems in a state Ω , which breaks spontaneously time-reversal invariance. The parameter which controls this phenomenon is the expectation value of the particle current in Ω . The mechanism allows for non-trivial entropy production even in absence of dissipation. The basic idea of the framework is to derive and investigate the probability distribution $\rho[S]$, generated by the n-point correlation functions of the entropy production operator \hat{S} in the state Ω . One can extract from $\rho[S]$ the sequence P of probabilities, associated with the fundamental processes of emission and absorption of particles from the heat reservoirs, driving the system away from equilibrium. In this way one obtains a microscopic picture of the quantum transport and entropy production, which takes into account all quantum fluctuations. These general ideas have been illustrated in the paper on the example of two exactly solvable models - the fermionic and bosonic Schrödinger junctions with point-like interaction. We show that in these two cases one can derive in exact and closed form the probability distribution $\varrho[\dot{S}]$ and prove that all its moments $\mathcal{M}_n[\dot{S}]$ are

non-negative in the zero frequency limit, which provides a bridge with the second law of non-equilibrium classical thermodynamics.

Our investigation demonstrates that the entropy production operator plays a fundamental role in non-equilibrium quantum physics. For this reason it will be important to test the above ideas in other models and within alternative frameworks. Among others, non-equilibrium conformal field theory [33]-[35], generalised quantum hydrodynamics [36]-[39] and the theory of periodically driven quantum systems [40] could be adopted. Studies in this direction will certainly contribute for better understanding the fascinating properties of the quantum world away from equilibrium.

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