Linear response in the nonequilibrium zero range process

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Abstract:
We explore a number of explicit response formulæ around the boundary driven zero range process to changes in the exit and entrance rates. In such a nonequilibrium regime kinetic (and not only thermodynamic) aspects make a difference in the response. Apart from a number of formal approaches, we illustrate a general decomposition of the linear response into entropic and frenetic contributions, the latter being realized from changes in the dynamical activity at the boundaries. In particular we so obtain nonlinear modifications to the Green-Kubo relation. We end by bringing some general remarks about the situation where that nonequilibrium response remains given by the (equilibrium) Kubo formula such as for the density profile in the boundary driven Lorentz gas.

1 Introduction

Linear response theory for nonequilibrium systems is slowly emerging from a great variety of formal approaches — see [1] for a recent review. It remains however very important in nonequilibrium to concentrate more on the physical-operational meaning of the response expressions. Obviously, it is very practical to have experimental access to the various terms in a response formula and to learn in general to recognize facts of the unperturbed system that are responsible for the particular response. That at least is what has made the fluctuation-dissipation theorem so useful in equilibrium. For example, transport properties as summarised in the mobility or conductivity, can be obtained from the diffusion in the unperturbed equilibrium system. In other words, not only is there a unifying response relation in equilibrium, it also possesses a general meaning in terms of fluctuations and dissipation. Such is not yet quite the situation for nonequilibrium systems and extra examples, in particular for spatially extended systems will therefore be useful.

The present paper gives the response systematics for the zero range process. The zero range process regularly appears in nonequilibrium studies and has the simplifying structure that its stationary distribution is simple (and remains a product distribution even away from equilibrium) while it shows a rich and quite realistic phenomenology. We refer to [2, 3] for a general introduction and nonequilibrium study of the model. We refer to Section 3 in [3] for a review of applications, in particular for the correspondence with shaken granular gases. We will repeat the set-up in Section 3. Interestingly, the time-reversed zero range process has an external field and particle currents directed opposite to the density profile. To start however we repeat in the next section some more formal aspects of the nonequilibrium linear response. Our point of view is to look in particular for the decomposition of the response into a frenetic and an entropic contribution. The entropic part is expressed in terms of (time-antisymmetric) currents and the frenetic part gets related to the (time-symmetric) dynamical activity. The latter refers to the number of exits and entrances of particles at the boundaries of the system. Section 4 is doing that decomposition for the boundary driven zero range process, and gives a number of response formulæ for density and current. There we find our main results, in particular
modified Green-Kubo relations. Finally, in Section 5 we treat some special cases which bring the nonequilibrium response to resemble the equilibrium Kubo formula. That opens the separate theme of trying to understand under what physical conditions nonequilibrium features remain largely absent.

2 Nonequilibrium response

We restrict ourselves to open systems connected to various different equilibrium reservoirs. Their nonequilibrium is passive in the sense that they do not affect the reservoirs directly and that all nonequilibrium forcing works directly on the particles of the system.

The state of the open system is described by values $x$ for some reduced variables, e.g. (some) particle positions. In the course of time $[0,t]$ there is a path or trajectory $\omega := (x_s, 0 \leq s \leq t)$ for which we have a well-defined entropy flux $S(\omega)$, that is the change of entropy in the equilibrium reservoirs. That $S(\omega)$ typically depends on the elementary changes in $x$ and how that affects the energy and particle number of the reservoirs. Of course $S(\omega)$ also depends on parameters such as the temperature, the chemical potentials of the reservoir and coupling coefficients of interaction. It will thus change under perturbations.

Similarly, for every state $x$ there is a notion of reactivity, like the escape rate from $x$. For the path $\omega$ there will then be a dynamical activity $D(\omega)$ which reflects the expected amount of changes along the path $\omega$, again function of the system and reservoir parameters.

Consider now a perturbation of that same system in which parameters are changed. Clearly, for any path $\omega$ the entropy flux $S$ and the dynamical activity $D$ will change. We can look for the linear excess, that is the amount by which the perturbation has changed these observables to first order. The linear response for a path-observable $O(\omega)$ is the difference in expectation $\langle \cdot \rangle^h$ between the perturbed process (with small time-dependent amplitude $h_s$, $s \in [0,t]$) and the original steady expectation $\langle \cdot \rangle$. It has the form

$$\langle O(\omega) \rangle^h - \langle O(\omega) \rangle = \frac{1}{2} (\langle \text{Ent}^0_{[0,t]}(\omega) O(\omega) \rangle - \langle \text{Esc}^0_{[0,t]}(\omega) O(\omega) \rangle) \quad (1)$$

where $\text{Ent}^0_{[0,t]}$ is the excess in entropy flux per $k_B$ over the trajectory due to the perturbation and $\text{Esc}^0_{[0,t]}$ is the excess in dynamical activity over the trajectory. The latter and second term on the right-hand side of (1) is the frenetic contribution; in many nonequilibrium situations the physical challenge is to learn to guess or to find and evaluate that $\text{Esc}^0_{[0,t]}$ from partial information on the dynamics. We refer to [4, 5] for the general introduction, and to [6] for complementary aspects to entropy. The present paper takes the opportunity to explore this question and to make such task more specific for the zero range process. Let us however first give the more general formal structure, restricting ourselves to Markov jump processes. For a more general review of various recent approaches, see [1].

On the finite state space $K$ we consider transition rates $k(x, y), x, y \in K$. We assume irreducibility so that there is exponentially fast convergence to a unique stationary distribution $\rho(x), x \in K$, satisfying

$$\sum_{y \in K} [\rho(x) k(x, y) - \rho(y) k(y, x)] = 0, \quad x \in K$$

Still, in general, there are nonzero currents of the form $j(x, y) := \rho(x) k(x, y) - \rho(y) k(y, x) \neq 0$ for some pairs $x \neq y \in K$, so that the stationary process is not time-reversible.

For physical models the rates carry a specific meaning. Following the condition of local detailed balance the ratio

$$\log \frac{k(x, y)}{k(y, x)} = \sigma(x, y)$$

should be the entropy flux (in units of $k_B$) in the transition $x \rightarrow y$. Consider now again the path $\omega := (x_s, 0 \leq s \leq t)$. It consists of jumps (transitions) at specific times $s_i$ and waiting times over
$s_{i+1} - s_i$. The total entropy flux $S$ (in units of $k_B$) is

$$S(\omega) = \sum_{s_i} \sigma(x_{s_i^-}, x_{s_i^+}) \quad (2)$$

where the sum takes the two states $x_{s_i^-} \rightarrow x_{s_i^+}$ over which the transition occurs at jump time $s_i$.

For the dynamical activity we need a reference process. Writing

$$k(x, y) = \psi(x, y)e^{\sigma(x,y)/2} \text{ with } \psi(x, y) = \psi(y, x)$$

we take the reference rates $k_0(x, y) = 1$ whenever $\psi(x, y) \neq 0$ and zero otherwise. That reference process will not matter in the end but it is useful to keep it for a while. With respect to that reference we do not only have a change in “potential barrier” $-\log 1 = 0 \rightarrow -\log \psi(x, y)$ for each transition, but also a change in the escape rates for each state $x$:

$$\xi(x) = \sum_{y|\psi(x,y) > 0} [k(x, y) - 1]$$

We then take the dynamical activity $D$ over the path $\omega$ be the combination

$$D(\omega) = \int_0^t ds \xi(x_s) - \sum_{s_i} \log \psi(x_{s_i^-}, x_{s_i^+}). \quad (3)$$

Perturbations change $S$ and $D$. Let us look at a specific example of perturbed transition rates considered in [7, 8]:

$$k_s(x, y) = k(x, y)e^{h_s[V(y) - aV(x)]}, \quad t > s \geq 0 \quad (4)$$

where the $a, b \in \mathbb{R}$ are independent of the perturbing potential $V$ and the $h_s \ll 1$ is small. One standard possible choice is taking $a = b = 1/2T$ where $T$ is the temperature of the environment which exchanges the energy $V$ with the system. We continue however with the more general perturbation [4]. It is instructive to rewrite the perturbation [4] as

$$k_s(x, y) = k(x, y)e^{h_s [\frac{1}{2}(V(x) + V(y)) - \frac{1}{2}(V(y) - V(x))]} e^{h_s(a+b)(V(y) - V(x))/2} \quad (5)$$

again being split in a symmetric prefactor (between square brackets) and an anti-symmetric part in the exponential. From here it is easy to see the excess for the entropy flux at a transition $x \rightarrow y$ to be

$$h_s(a + b)(V(y) - V(x)) \quad (6)$$

We use [3] to find the perturbation to $S$ in [2] yielding

$$\text{Ent}^{[0,t]}(\omega) = (a + b) \sum_{s_i} h_s [V(x_{s_i^+}) - V(x_{s_i^-})]$$

$$= (a + b) \{ h_t V(x_t) - h_0 V(x_0) - \int_0^t ds h_s V(x_s) \}. \quad (7)$$

For the dynamical activity we should use again the reference process with rates $k_0(x, y)$ as above. Then, at least for the change in escape rates (first term in [3]) at state $x$,

$$\sum_y [k_s(x, y) - k(x, y)] = h_s \sum_y k(x, y) \{ \frac{b - a}{2}(V(x) + V(y)) + \frac{a + b}{2}(V(y) - V(x)) \}$$

$$= h_s \sum_y k(x, y) [bV(y) - aV(x)] \quad (8)$$
to first order in \( h_s \). The total change to \( D \) of (8) is thus

\[
\text{Esc}^{[0,t]}(\omega) = \int_0^t ds \, h_s \sum_y k(x_s, y) [bV(y) - aV(x_s)] + \frac{a-b}{2} \sum_{s_i} h_{s_i} [V(x_{s_i}) + V(x_{s_i}^-)] \tag{9}
\]

where the last term corresponds to the change in the second term of \( D \) in (8), as from (5). In all, the expressions (7) and (9) completely specify the response (1) for the example (4).

We can still rewrite the previous formulæ, losing somewhat the physical interpretation but gaining somewhat formal elegance. To start, let us restrict ourselves to the more simple situation where the observable \( O \) is just a state function \( O(x), x \in K \). The response then investigates the change to first order in the \( h_s \), where the first expectation \( \langle \cdot \rangle^h \) is under the perturbed Markov dynamics \((s \geq 0)\) and the second \( \langle \cdot \rangle \) is the original steady expectation. To say it differently, linear response wants to compute the generalized susceptibility \( h \) to first order in \( (\vee) \), but they should in the end all coincide with (1) for (7)–(9). For example, in terms of the backward generator \( L \) of the jump process,

\[
Lf(x) = \frac{d}{ds} \bigg|_{s=0} \langle f(x_s) \rangle_{x_0=x} = \sum_y k(x,y) [f(y) - f(x)]
\]

we have for (7) that

\[
\langle \{ h_t V(x_t) - h_0 V(x_0) - \int_0^t ds \, h_s V(x_s) \} O(x_t) \rangle = \int_0^t ds \, h_s \frac{d}{ds} \langle V(x_s) O(x_t) \rangle = -\int_0^t ds \, h_s \langle V(x_s) LO(x_t) \rangle
\]

On the other hand, for (9),

\[
\text{Esc}^{[0,t]}(\omega) = b \int_0^t ds \, h_s LV(x_s) + (b-a) \{ \int_0^t ds \, h_s \sum_y k(x_s, y) V(x_s) - \sum_{s_i} h_{s_i} \frac{V(x_{s_i}) + V(x_{s_i}^-)}{2} \}
\]

We must substitute that expression together with (11) into (11), which leads to

\[
R(t,s) = a \frac{\partial}{\partial s} \langle V(x_s) O(x_t) \rangle - b(LV(x_s) O(x_t)) \tag{10}
\]

for all times \( 0 \leq s \leq t \), which recovers a result of (5). Of course, these expectations are stationary and only depend on the time-difference \( t-s \). For the case \( b = a = 1/(2T) \) in (11), the response formula thus becomes

\[
R(t,s) = \frac{1}{2T} \frac{\partial}{\partial s} \langle V(x_s) O(x_t) \rangle - \frac{1}{2T} \langle LV(x_s) O(x_t) \rangle
\]

In equilibrium, i.e., under stationary time-reversal symmetry where all currents \( j(x, y) = 0 \), we have for \( t > s \)

\[
\langle LV(x_s) O(x_t) \rangle = \langle V(x_s) LO(x_t) \rangle = \frac{\partial}{\partial t} \langle V(x_s) O(x_t) \rangle
\]
and hence the two terms in the right-hand side of (10) coincide and we recover the Kubo-formula, \[ R_{eq}(t,s) = \frac{1}{T} \frac{\partial}{\partial s} (V(s)O(t))_{eq}, \quad 0 < s < t \] (11) whenever \( a + b = 1/T \).

Such formal systematics in nonequilibrium as in (10) is useful as it is generally available, but its physical interpretation relies on the equivalence (as discussed above for the example (4)) with (1), much in the same way as, for equilibrium, the Kubo-formula can be called a fluctuation–dissipation relation. Note that in nonequilibrium, from (1), the response formula has become a fluctuation–dissipation–activity relation. We refer to [4, 5, 8, 1] for more details.

Another (again more formal) possibility of writing the linear response formula (10) uses the adjoint \( L^\ast \) of the backward generator with respect to the stationary distribution \( \rho \); \( \langle (Lf)g \rangle = \langle f(L^\ast g) \rangle \) or

\[ L^\ast g(x) = \sum_y k(y,x) \frac{\rho(y)}{\rho(x)} [g(y) - g(x)] \] (12)

which generates the time-reversed stationary process. With this notation, for \( s < t \) and in the stationary regime,

\[ \frac{\partial}{\partial s} (V(x_s)O(x_t)) = -\frac{\partial}{\partial t} (V(x_s)O(x_t)) = -\langle V(x_s)LO(x_t) \rangle = -\langle L^\ast V(x_s)O(x_t) \rangle \] (13)

so that

\[ \frac{\partial}{\partial s} (V(x_s)O(x_t)) + \langle LV(x_s)O(x_t) \rangle = \langle (L - L^\ast)V(x_s)O(x_t) \rangle \]

Therefore, referring to the response (10),

\[ a \frac{\partial}{\partial s} (V(x_s)O(x_t)) - b(LV(x_s)O(x_t)) = (a + b) \frac{\partial}{\partial s} (V(x_s)O(x_t)) - b((L - L^\ast)V(x_s)O(x_t)) \]

or

\[ R(t,s) = (a + b) \frac{\partial}{\partial s} (V(x_s)O(x_t)) - b((L - L^\ast)V(x_s)O(x_t)) \] (14)

The first term is the Kubo expression (11). The second term will be useful whenever we know more about the time-reversed process. If wanted, one can still substitute there

\[ \langle (L - L^\ast)f \rangle(x) = 2 \sum_y \frac{j(x,y)}{\rho(x)} [f(y) - f(x)] \]

to obtain the interpretation of (10) in terms of the moving frame.

Let us finally mention the Agarwal-Kubo procedure for arriving at a linear response expression, see e.g. formula 13 in [1]. That is first order perturbation theory on the level of forward generators. We consider the unperturbed forward generator

\[ L^+ g(x) = \sum_y [k(y,x)g(y) - k(x,y)g(x)] \]

and its perturbation is denoted by \( L^h^+ \). Then, we have in general

\[ R(t,s) = \left( \frac{(L^h^+ - L^+)}{\rho} \right)(x_s)O(x_t) \] (15)

The obvious disadvantage here is that one should know the stationary density \( \rho \); in contrast, all observables in (10) are explicit and known and in (11) they even have a meaning.
3 Formal elements of the zero range process

3.1 Steady state

On the lattice interval \( \{1, 2, \ldots, N\} \), each site \( i \) carries a number \( x(i) \in \mathbb{N} \) of indistinguishable particles. The dynamics is characterized by the rate \( w(k) \) at which a particle jumps from site \( i \) when \( x(i) = k \), and parameters \( \alpha, \beta, \gamma, \delta \) for the rates of exits and entrances at the boundaries. More specifically, a particle moves from \( i \) to a neighboring site \( j = i \pm 1 \) at rate \( w(x(i)) \). We need that \( w(0) = 0 \) and \( w(k) > 0 \) for \( k > 0 \). At the boundary site \( i = 1 \) a particle is added at rate \( \alpha \) and at \( i = N \) is added at rate \( \delta \), while a particle moves out from \( i = 1 \) at rate \( \gamma w(x(1)) \) and moves out from \( i = N \) at rate \( \beta w(x(N)) \). As reference for more details using mostly the same notation, we refer to [3].

It is well-known that the product distribution \( \rho = \rho_{N, \alpha, \beta, \gamma, \delta} \) is invariant,

\[
\rho(x) = \prod_{i=1}^{N} \nu_i(x(i)), \quad \nu_i(k) = \frac{z_i^k}{Z_i} \frac{1}{w(1)w(2)\ldots w(k)}, \quad k > 0
\]

\( Z_i = 1 + \sum_{k=1}^{\infty} \frac{z_i^k}{w(1)w(2)\ldots w(k)} \) (16)

The “fugacities” \( z_i \) are of the form \( z_i = C_i + B = z_1 + C(i-1) \) where

\[
B := \frac{\alpha + (1 - \gamma)C}{\gamma}, \quad C := \frac{\delta \gamma - \beta \alpha}{\beta \gamma N + \beta (1 - \gamma) + \gamma} = \frac{e^{\mu_r/T} - e^{\mu_i/T}}{N} \left(1 + \frac{\beta + \gamma - 3 \gamma}{\beta \gamma N}\right)^{-1}
\]

We have introduced “chemical potentials” \( \mu_i := T \log \alpha/\gamma \) and \( \mu_r := T \log \delta/\beta \) with \( T \) the environment temperature. When \( \mu_i = \mu_r, \alpha/\gamma = \delta/\beta \), then \( C = 0, B = z_1 = \alpha/\gamma \); and detailed balance is satisfied. If not, we get a stationary particle current (to the right) equal to \( \langle J_i \rangle = -C = \alpha - \gamma z_1 = \beta z_N - \delta \) and thermodynamic driving force \( \langle \mu_i - \mu_r \rangle/T = \log \alpha/\gamma - \log \delta/\beta \). Note however that for \( C \neq 0 \) the (then nonequilibrium) stationary distribution \( \rho \) also depends on purely kinetic (and not only on thermodynamic) aspects; they will again enter the response in terms of the dynamical activity. For example, fixing \( \alpha/\gamma \) and \( \delta/\beta \) does not determine \( C \), trivially but importantly.

3.2 Time-reversal

To make explicit use of the formula (14), we need to know the time-reversed process, which is interesting in itself.

In general for a Markov process as we had it described in Section 2 the time-reversed process is again a Markov jump process with generator \( L^* \) in (12) and with rates

\[
k^{rev}(x, y) = k(y, x) \frac{\rho(y)}{\rho(x)}
\]

for the stationary distribution \( \rho \). Because we know the stationary distribution \( \rho \) of the zero range process as the product distribution (16), it is actually easy to determine explicitly the time-reversed process. This is interesting also because, by time-reversing, the particle current will be reversed/change sign but the stationary density profile, as given in terms of the fugacities \( z_i \), will remain the same. As can be guessed, that only works because by time-reversing one actually generates an external field. Let us see the details.
First we take a bulk transition in which a particle hops to a neighboring site. Take $y = x - e_i + e_{i+1}$ where $e_i$ stands for the particle configuration with exactly one particle at site $i$. Then,

$$\frac{\rho(y)}{\rho(x)} = \frac{w(x(i))}{w(x(i+1))} \quad k(y, x) = w(x(i+1))$$

which means that in the time-reversed process a particle moves from site $i$ to $i+1$ at rate $k^{rev}(x, x - e_i + e_{i+1}) = z_{i+1} w(x(i))/z_i$ while similarly for a jump from $i$ to $i-1$, $k^{rev}(x, x - e_i + e_{i-1}) = z_{i-1} w(x(i))/z_i$. We have therefore for the time-reversed process again a zero range process but now in an inhomogeneous bulk field

$$E_i := 2 \log \frac{z_{i+1}}{z_i}$$

over the bond $(i, i+1)$, having the sign of $C$, i.e., pushing the particles towards the boundary where the chemical potential was largest. At the boundaries we find the creation and annihilation parameters for the time-reversed process to be

$$\alpha^{rev} = \gamma z_1, \quad \beta^{rev} = \frac{\delta}{z_1}, \quad \gamma^{rev} = \frac{\alpha}{z_1}, \quad \delta^{rev} = \beta z_N.$$

That means that the chemical potentials for the reversed process have become

$$\mu_i^{rev} = -\mu_i + 2T \log(e^{\mu_i/T} + C/\gamma)$$
$$\mu_r^{rev} = -\mu_r + 2T \log(e^{\mu_r/T} - C/\beta)$$

Note of course that in the case of detailed balance $E_i \equiv 0$ and $\alpha^{rev} = \alpha$ etc., so that the equilibrium process is unchanged by time-reversal.

We can now write down the explicit expression for the second term in (14):

$$(L - L^*)V(x) = \left(\gamma - \frac{\alpha}{z_1}\right) w(x(1)) [V(x - e_1) - V(x)] + \left(\alpha - \gamma z_1\right) [V(x + e_1) - V(x)]$$

$$+ \left(\beta - \frac{\delta}{z_N}\right) w(x(N)) [V(x - e_N) - V(x)] + \left(\delta - \beta z_N\right) [V(x + e_N) - V(x)]$$

$$-C \sum_{i=1}^{N-1} \frac{w(x(i))}{z_i} [V(x - e_i + e_{i+1}) - V(x)]$$

$$+C \sum_{i=2}^{N} \frac{w(x(i))}{z_i} [V(x - e_i + e_{i-1}) - V(x)]$$

Applying that for $V(x) = N(x) := x(1) + x(2) + \ldots + x(N)$ the total number of particles in the system, we get

$$(L - L^*)N(x) = \left(\frac{\alpha}{z_1} - \gamma\right) w(x(1)) + \left(\frac{\delta}{z_N} - \beta\right) w(x(N))$$

(17)

where we have also used that $\gamma z_1 + \beta z_N = \alpha + \delta$.

### 4 Responses in the zero range process

Let us consider the perturbation

$$\alpha \to q \alpha, \quad \beta \to p' \beta, \quad \gamma \to p' \gamma, \quad \delta \to q' \delta$$

(18)

to the parameters governing the entrance and exit rates at the boundaries of the system. Their thermodynamic meaning is to shift the chemical potentials by $h_\ell = T \log q/p$ for the left and by $h_r = T \log q'/p'$ for the right reservoir. Depending on the remaining freedom how to choose the $p, p'$ we can distinguish still several “kinetic” possibilities.
4.1 “Potential” perturbation

A first possible perturbation that we consider is that

$$\frac{q}{p} = \frac{q'}{p'} = e^{h/T}$$  \hfill (19)

with $h$ the small (equal) shift in left and right chemical potential. Even while the zero range process is not formulated directly in terms of a potential, even at detailed balance, it is still easy to fit (19) into the scheme of (4), in particular by choosing $h \equiv h$ (time-independent), $a = b = 1/(2T)$, potential $V = N$ equal to the particle number, and

$$e^{h/(2T)} = q = q', \quad e^{-h/(2T)} = p = p'.$$  \hfill (20)

We can thus apply (14) with formula (17) to give the correct modification of the Kubo formula as

$$\frac{\langle O(x_1) \rangle^h - \langle O \rangle}{h} = \frac{1}{T} \langle N \rangle - \frac{1}{T} \langle N(x_0) O(x_1) \rangle$$

$$+ \frac{1}{2T} \int_0^t ds \{ \frac{\alpha}{z_1} - \gamma \} \langle w(x_0(1)) O(x_s) \rangle + \frac{\delta}{z_N} \langle w(x_0(N)) O(x_s) \rangle \}$$  \hfill (21)

Of course we could also have used (10) with $L \langle N \rangle = \alpha + \delta - \gamma w(x(1)) - \beta w(x(N))$ to obtain

$$\frac{\langle O(x_1) \rangle^h - \langle O \rangle}{h} = \frac{1}{2T} \langle N(x_t) - N(x_0); O(x_1) \rangle$$

$$+ \frac{1}{2T} \int_0^t ds \{ \gamma \langle w(x_0(1)); O(x_s) \rangle + \beta \langle w(x_0(N)); O(x_s) \rangle \}$$  \hfill (22)

where we have used connected correlation functions $\langle A; B \rangle := \langle A B \rangle - \langle A \rangle \langle B \rangle$. The first term in the right-hand side is the entropic or dissipative part of the response, since in that correlation one sees the observable $O$ correlated with the particle loss; the last term may be called the frenetic part of the response, since one meets there the correlation with the time-integrated escape rates.

Finally one finds place for the Agarwal-Kubo formula (15), which here is explicit because the stationary density $\rho$ is given in (16). For the “potential” perturbation (19)–(20) given by $\alpha \to (1 + h/(2T))\alpha$, $\beta \to (1 - h/(2T))\beta$, $\gamma \to (1 - h/(2T))\gamma$, $\delta \to (1 + h/(2T))\delta$ and under discussion so far, that gives

$$\frac{L^+ \rho - L \rho}{\rho} (x) = \alpha \frac{h}{2T} \left[ \frac{\rho(x - e_1)}{\rho(x)} - 1 \right] + \delta \frac{h}{2T} \left[ \frac{\rho(x - e_N)}{\rho(x)} - 1 \right] + \gamma \frac{h}{2T} w(x(1))$$

$$- \gamma \frac{h}{2T} w(x(1) + 1) \frac{\rho(x + e_1)}{\rho(x)} + \beta \frac{h}{2T} w(x(N)) - \beta \frac{h}{2T} w(x(N) + 1) \frac{\rho(x + e_N)}{\rho(x)}$$

$$= \frac{h}{2T} \left[ \frac{\alpha}{z_1} (w(x(1)) - z_1) + \frac{\delta}{z_N} (w(x(N)) - z_N) + \gamma (w(x(1)) - z_1) + \beta (w(x(N)) - z_N) \right]$$  \hfill (23)

This calculation results in the linear response formula

$$\frac{\langle O(x_1) \rangle^h - \langle O \rangle}{h} = \frac{1}{2T} \int_0^t ds \{ \frac{\alpha}{z_1} + \gamma \} \langle w(x_0(1)); O(x_s) \rangle + \frac{\delta}{z_N} + \beta \} \langle w(x_0(N)); O(x_s) \rangle \}$$  \hfill (24)
4.2 General perturbation

We emphasize that the three response formulæ (21)–(22)–(24) are mathematically identical. They all start from the “potential perturbation” (4) as realized in (19)–(20). They are however not to be applied for other perturbations even consistent with (19), except in equilibrium where the response does not pick up the detailed kinetics. Let us therefore do better (more general) and illustrate the systematic interpretation with unique formula (1) to the perturbation (18).

We only need experience with entropy and no calculation to find the first term in (1). For the perturbation (18) the entropic part in the response follows the usual (irreversible) thermodynamics and we must have the excess in entropy flux given by

\[ \text{Ent}^{[0,t]}(\omega) = -\frac{h_r}{T} J_r(\omega) - \frac{h_\ell}{T} J_\ell(\omega) \]  

(25)

where \( J_r \) (\( J_\ell \)) is the net number of particles that have exited to the right (left) reservoir (time-integrated current). When we specify to a perturbation like (19) in which the chemical potentials get shifted together, \( h = h_r = h_\ell \), we can use that

\[ J_\ell(\omega) + J_r(\omega) = N(x_0) - N(x_t) \]

so that the excess in entropy flux becomes

\[ \text{Ent}^{[0,t]}(\omega) = \frac{h}{T} (N_t - N_0) \]  

(26)

proportional to the change over time in particle number.

For the second term in (1) we lack the experience and calculation will guide us. The point is that the dynamical activity (3) exactly picks up the time-symmetric part in the action for path-integration. More specifically, let us now call \( P^h \) the process started from the unperturbed stationary zero range process (16) but under the perturbed dynamics for a time \([0,t]\). The unperturbed stationary process is denoted by \( P \). We can compute the action \( A^h \) for which

\[ P^h = e^{-A^h} P \simeq (1 - A^h) P \]

with

\[
A^h = -I_\ell^L \log p - \log q - I_\ell^- \log p' - \log q' + \int_0^t ds \left\{ (p - 1) \gamma w(x_s(1)) + (p' - 1) \beta w(x_s(N)) + (q - 1)\alpha + (q' - 1)\delta \right\}
\]  

(27)

where for example \( I_\ell^L \) equals the total number of particles that have entered the system from the left, and \( I^-_\ell \) is the total number of particles that have escaped to the right reservoir. We decompose this action with the time-reversal \( \theta \) which makes \((\theta x)_s = x_{t-s}\), so that the response (up to higher order in \( h \)) can be obtained from

\[
P^h - P = \frac{1}{2} [A^h \theta - A^h] P - \frac{1}{2} [A^h \theta + A^h] P
\]

\[
= \left\{ \frac{1}{2} \text{Ent}^{[0,t]} - \text{Esc}^{[0,t]} \right\} P
\]

(28)

where we indicate the general relation with (1).

In particular, we verify that

\[
A^h \theta - A^h = \log q' p \left( I_\ell^L - I_\ell^- \right) + \log p' q \left( I^-_\ell - I^-_\ell \right)
\]
of C range process. Observe that it is the correlation between current is given by a difference between variances of the current and dynamical activity, where indeed exactly equals (25) (using for example $I^\ell_\alpha - I^\ell_{-\alpha} = -J_\ell$). On the other hand, for the time-symmetric part

$$A^h \theta + A^h = -\log(pq) I^\ell - \log(p'q') I^\ell + 2(p - 1)\gamma \int_0^t ds w(x_s(1))$$

$$+ 2(p' - 1)\beta \int_0^t ds w(x_s(N)) + 2(q - 1)\alpha t + 2(q' - 1)\delta t$$

(29)

with left activity $I^\ell := I^\ell_\alpha + I^\ell_{-\alpha}$ the total number of transitions at the left boundary and similarly for $I^\ell$ at site N. The excess in dynamical activity $\text{Esc}^{[0,t]} = (A^h \theta + A^h)/2$ that we need for the general response in (11) is thus

$$\text{Esc}^{[0,t]}(\omega) = -\log\sqrt{pq} I^\ell - \log\sqrt{p'q'} I^\ell + (p - 1)\gamma \int_0^t ds w(x_s(1))$$

$$+ (p' - 1)\beta \int_0^t ds w(x_s(N)) + (q - 1)\alpha t + (q' - 1)\delta t$$

(30)

Note that of course here the separate $p, p'$ and $q, q'$ play a role, and not just their ratio $p/q, p'/q'$ as for (25) — that is how the frenetic contribution picks up kinetic information, while the entropic part is purely thermodynamic. Substituting (25) and (30) into (11) gives the general response of the zero range process under (18). A natural application is to look at how the current into the left reservoir changes when $h_r = 0, h_L = -\alpha$ or $q' = p = p' = 1$ but $q = 1 - a/T$, decreasing (for $a > 0$) the chemical potential of the left reservoir. Then, for that choice, (25) and (30) give

$$\langle J_\ell \rangle^h - \langle J_\ell \rangle = \frac{a}{2T} \langle J_\ell; J_\ell \rangle - \frac{a}{2T} \langle J_\ell; I^\ell \rangle$$

(31)

which is the modification to the Green-Kubo relation (11), for all times $t > 0$, for the boundary driven zero range process. Observe that it is the correlation between current $J_\ell$ and dynamical activity $I^\ell$ that governs the correction. When $t \uparrow +\infty$, the conductivity will of course coincide with the change of $C$ in (18) under $\alpha$. There is a similar relation for the change in expected dynamical activity, so that in fact

$$\langle J_\ell + I^\ell \rangle^h - \langle J_\ell + I^\ell \rangle = \frac{a}{2T} \langle J_\ell; J_\ell \rangle - \frac{a}{2T} \langle I^\ell; I^\ell \rangle$$

is given by a difference between variances of the current and dynamical activity, where still $\langle J_\ell \rangle = C = -\alpha + \gamma z_1$, $\langle I^\ell \rangle = \alpha + \gamma z_1$.

Formulae (26)–(30) in (11) will of course also lead again to a formula equal to each of the (21)–(22)–(24) when restricting to (19)–(20).

4.3 “External” perturbation

Shifting the chemical potentials (from the outside) realistically means to change $\alpha \to q \alpha$ and $\delta \to q' \delta$ but not the exit rates $\beta$ and $\gamma$. That is thermodynamically the same (in the shift of chemical potentials) as for the “potential” perturbation in Section 4.1 but it is kinetically different. The response formulae (21)–(22)–(24) are then invalid except at equilibrium. Here we look when we change only the rates of the incoming particles in (18) but restricting ourselves to (19):

$$p = 1 = p', \quad q = q' = 1 + h/T$$

(32)

Note that the expected total activity in the unperturbed steady regime equals

$$\langle I^\ell + I^\ell \rangle = (a + \gamma z_1 + \beta z_N + \delta)t = 2(\alpha + \delta)t$$
because the stationary current equals \( \alpha - \gamma z_1 = \beta z_N - \delta \). That means that the excess dynamical activity (30) (for perturbation (32)) simply equals
\[
\text{Esc}^{[0,t]}(\omega) = \frac{\hbar}{2T} \{ (I^f + I^r) - [I^f + I^r] \}
\]
which is now very visibly related to the dynamical activity. We therefore find the linear response formula (11) to become
\[
\frac{\langle O(\omega) \rangle_h - \langle O(\omega) \rangle}{\hbar} = \frac{1}{2T} \langle (N_t - N_0); O(\omega) \rangle + \frac{1}{2T} \langle (I^f + I^r); O(x) \rangle
\]
which is another result for the linear response of the boundary driven zero range model when both left and right entrance rates have been increased with the same small amount. Note that from (11) it is here also possible to take a general path-observable \( O(\omega) \) that depends on the whole trajectory \( \omega \). The first term is entropic corresponding to the dissipation of particles and the second term is frenetic with the total dynamical activity \( I := I^f + I^r = I^L + I^L + I^R + I^R \).

Let us check the formula (34) for the linear response around equilibrium \( (C = 0, \text{detailed balance}) \), and with \( O = I \) the total activity. Then, since the first term \( \langle (N_t - N_0); O(\omega) \rangle = 0 \) for time-symmetric \( O \), we have a Green-Kubo type formula for the linear response of the dynamical activity around equilibrium:
\[
\frac{\langle I \rangle^h - \langle I \rangle^0}{\hbar} = \frac{1}{2T} \text{Var} I > 0
\]
with, in the right-hand side, the unperturbed equilibrium variance of the dynamical activity giving the expected change in that same dynamical activity when the left and right chemical potentials get slightly shifted. Whether, say for positive \( h \), the change in dynamical activity remains positive also for boundary driven zero range processes depends apparently on whether the dynamical activity is positively or negatively correlated with the dissipation of particles. One could guess that for very small \( \alpha, \delta \leq 1 \) while keeping \( \gamma, \beta w(k) \approx 1 \) (low temperature reservoirs) there is a negative correlation between \( N_t - N_0 \) and \( I \) which would make at least the first term in (34) for \( O = I \) negative.

In any event however, be it equilibrium or nonequilibrium, we have the positivity of
\[
\frac{\langle N(x_t) + I \rangle^h - \langle N(x_0) + I \rangle}{\hbar} = \frac{1}{2T} \text{Var}(N_t - N_0 + I) > 0
\]
by taking the observable \( O = N_t - N_0 + I \) in (34).

Let us further simplify and take \( O \) in (34) a state function. It is then relevant to see how the stationary distribution (10) gets modified under (32). It is straightforward to check that \( C, B \rightarrow qC, qB \) so that the new “ fugacities” become equal to \( qz_1 \). The stationary distribution thus simply changes by multiplying \( \exp[\hbar \mathcal{N}(x)/T] \) to the weights \( \rho(x) \). It is therefore not so surprising that the linear response drastically simplifies. To check it we take the opportunity to illustrate again the Agarwal-Kubo procedure (15) but now for the perturbation (32):
\[
L^+ \rho - L^+ \rho(x) = \frac{\alpha(q - 1)}{\rho(x)} \frac{\rho(x - e_1)}{\rho(x)} - 1 + \delta(q' - 1) \frac{\rho(x - e_N)}{\rho(x)} - 1
\]
\[
= \frac{\alpha h}{T} \left[ \frac{w(x(1))}{z_1} - 1 \right] + \delta \frac{h}{T} \left[ \frac{w(x(N))}{z_N} - 1 \right]
\]
where we substituted the known stationary distribution \( \rho \) from (10). On the other hand, the backward generator of the time-reversed process equals
\[
L^* \mathcal{N}(x) = -\frac{\alpha}{z_1} w(x(1)) + \gamma z_1 + \beta z_N - \frac{\delta}{z_N} w(x(N))
\]
and $\alpha - \gamma z_1 + \delta - \beta z_N = 0$. Therefore,

$$\frac{L^h \rho - L^t \rho}{\rho} = -\frac{1}{T} L^* N \tag{37}$$

As a consequence, using (15) results in the linear response exactly of the same form (11) as in equilibrium, because (with $V = N$ in (13)),

$$\frac{d}{ds} \langle N(x_s) O(x_t) \rangle = -\frac{d}{dt} \langle N(x_0) O(x_{t-s}) \rangle = -\langle N(x_0) L O(x_{t-s}) \rangle = -\langle L^* N(x_0) O(x_{t-s}) \rangle \tag{38}$$

In other words, for state observables, the linear response of any boundary driven zero range process to “external” perturbations (32) has always the same equilibrium Kubo-form (11), independent of being close or far from detailed balance.

## 5 Intersections of equilibrium and nonequilibrium evolutions

One of the less understood facts of nonequilibrium physics is that the regime of linear response around equilibrium appears to extend sometimes quite beyond its theoretical boundaries. Depending on the situation, that is the case for certain transport equations like the Fourier or even sometimes Ohm’s law, but also for the more general regime of hydrodynamics where local equilibrium often appears to be a very good approximation. In nonequilibrium and irreversible thermodynamics, Green-Kubo relations and general principles like the minimum/maximum entropy production principle often continue to work and are used beyond their theoretical limits of validity. The difference between equilibrium and nonequilibrium processes is not always so crystal clear. For example, if one starts with a dynamics for which the Gibbs distribution $\sim e^{-\beta H}$ is invariant, for some Hamiltonian $H$, then that distribution is also obviously unchanged when adding extra transformations or updating that leave the Hamiltonian $H$ invariant. On a more formal level, suppose we modify the Liouville equation to

$$\frac{\partial}{\partial t} \rho(x,t) + \{\rho, H\} = \int dx [k(y,x) \rho(y) - k(x,y) \rho(x)] \tag{39}$$

where the right-hand side involves transition rates $k(x,y)$ between states $x \rightarrow y$. If these $k(x,y)$ are zero unless $H(x) = H(y)$, then $\rho \sim \exp[-\beta H]$ remains of course invariant. On the other hand, the modified dynamics need not at all to satisfy detailed balance and then the resulting stationary regime will not be time-reversal invariant.

In fact, one of the reasons for not having yet an established nonequilibrium statistical mechanics may well be the lack of urgent questions as irreversible thermodynamics continues to work surprisingly well in a large range of transport and rate processes in physical or chemical systems. Much of standard thermodynamics can even be mimicked for relatively small systems without feeling the urge for new concepts beyond those available in close-to-equilibrium regimes. Only with turbulence and very-far-from-equilibrium processes where new phenomena such as pattern formation and self-organization appear, do we really see major modifications with respect to the traditional approach.

The above is also true for linear response, where in equilibrium the Kubo formula (11) summarizes the response in terms of a fluctuation-dissipation formula. As we have seen in the previous section with the combination (37)–(38), the Kubo formula extends for the zero range process and for perturbations (32) to the nonequilibrium case. In the present section we look at that from a more general perspective.

### 5.1 Special perturbations

A special case arises when $b = 0$ and $a = 1/T$ in (4), because then the response is of the equilibrium form (11).
Figure 1: The boundary driven Lorentz gas. A flat rectangular slab is placed between two thermochemical reservoirs and contains an array of fixed discs, which scatter particles (red dots) via elastic collisions. The centers of the scatterers are placed in a regular triangular lattice with finite horizon; that is, the distance among the centers of contiguous disks $(4R/\sqrt{3})$ ensures that a particle cannot cross a unit cell without colliding at least once with the scatterer contained in such cell. There is a uniform temperature in the reservoirs $T$, which determines the velocities of all gas particles. If a particle hits a boundary wall it disappears from the system, while other particles are injected to the system at given rates, proportional to each reservoir density.

Suppose we have (quite arbitrary) a Markov jump process with rates $k(x, y)$ that we perturb by adding a time-dependent potential into

$$k_t(x, y) = k(x, y) e^{-h_t V(x)/T}$$

where $h_t$ is the small parameter. The linear response formula is obtained by putting $b = 0$ in (10) which gives the Kubo-equilibrium formula. That can also be seen from the following consideration. Take $h$ to be constant; the law $\rho^h$ defined by $\rho^h(x) \propto \rho(x) e^{h V(x)/T}$ is stationary for the new dynamics (to all orders in $h$). In other words, here the resulting behavior under this perturbation is like in equilibrium, even though the unperturbed dynamics can be far from equilibrium.

The case of perturbation (32) for zero range is just slightly different and is summarized in (37), which is the condition that there exists a function $V$ for which

$$(L^h - L)^+ \rho = h \rho L^+ V = h L^+ (V \rho)$$

for the stationary density $\rho$. That is equivalent with finding a potential $V$ so that for all functions $f$

$$\sum_x ((L^h - L)f)(x) \rho(x) = h \sum_x (Lf)(x) V(x) \rho(x)$$

It is easily seen that (41) exactly follows when $L^h = (1 + hV) L$ which (basically) is (40). Therefore, (37) or (41) is only slightly weaker than (40).

5.2 Density response in the boundary driven Lorentz gas

The Lorentz gas is a well known mechanical model of particle scattering that reproduces electron transport in metals [12,13]. Concerning our present focus and subject what becomes important is the fact that in the appropriate scales of time and energy the Lorentz gas is diffusive, see [14,15] and references therein. Moreover, when the system is connected to reservoirs, the “external” perturbations (32) become very natural. Thus, one can expect that the response for the density profile follows
the zero range process as studied in the previous sections. We have performed extensive numerical experiments in such model to corroborate our expectations.

To be more precise, we consider the two-dimensional slab containing a Lorentz gas illustrated in Fig 1. There is a cloud of point particles which move freely in the space between the array of scatterers and collide elastically with them. The vertical coordinate is periodic and in the horizontal direction there are left and right boundary walls, which connect the system to thermo-chemical reservoirs, characterized by chemical potential \(\mu_l, \mu_r\) and uniform temperature \(T\). In terms of the mean reservoir density \(\rho\), the reservoir chemical potential \(\mu \propto T \ln(\rho/T)\). During time evolution, as a particle hits the boundaries, it moves into a reservoir; additionally, other particles are emitted to the system at given rates \(\pi_{l,r} \sim \rho \sqrt{T}\). The complete model of stochastic thermal and particle reservoirs with the Lorentz slab is borrowed from a similar work on a modified Lorentz gas; a detailed description about the choice of emission rates and chemical potential, temperature and incoming particle velocities from the reservoirs can be found there [16]. In our present case we are interested in independent particles with constant temperature \(T\); with this setting the planar Lorentz gas slab of Fig. 1 evolves to a nonequilibrium stationary state with diffusive transport of particles, whenever \(\Delta \mu \equiv \mu_l - \mu_r \neq 0\).

We now wish to connect this model with the zero range model. The rates at which particles enter (like \(\alpha\) and \(\delta\) in the zero range process) are controlled externally by the nominal reservoir temperature and the chemical potentials. For the rates at which individual particles leave, that is only controlled by the temperature and the local (boundary) density. Thus, one is under perturbation (32). We have therefore proceeded to test whether our boundary driven Lorentz gas satisfies the response as predicted by the Kubo-formula (11) independent of the distance to equilibrium. The simulation result is indeed positive.

In the nonequilibrium molecular dynamics simulations, we have taken as observable the total number \(N\) of particles in the system. The perturbation simply consists of modifying the reservoir densities, so that the entrance rates \(\pi_{l,r}\) are shifted by the same small amount \(\pi_{l,r} \rightarrow \pi_{l,r} e^{h/T}\) (depending also on the constant temperature). The response of \(N\) to this perturbation is shown in Fig 2 for a nonequilibrium stationary regime with moderate driving of \(\Delta \mu/T = 0.2\) and \(T = 150\). The perturbation is applied at time \(t = 0\) and the system is then observed in transient states which evolve to the new stationary state. Each response curve consists of averages over an ensemble of \(1.5 \times 10^3\) initial conditions from the steady regime; relaxation to the final (stationary) state takes about \(9.15 \times 10^4\) collisions in the gas. The response for a higher driving \(\Delta \mu/T = 2.0\), and using either of the terms in (38), gives similar outcomes; indeed we see that the Kubo-relation (11) follows no matter how far from equilibrium we are. That is not surprising because of the independence of the particles; actually we can predict all density responses simply from solving the linear diffusion equation. This is also shown in Fig. 2 with the curve in crosses. Yet, one must note that this interesting example is just a special case of what happens more generally in the zero range model (possibly showing non-linear hydrodynamics).

6 Conclusions

We have studied response in the nonequilibrium zero range process, giving explicit expressions of the entropic and frenetic terms in which such response is formally decomposed. That was done for various types of perturbations to the boundary rates. We have found systematic contributions of correlation functions with the dynamical activity to correct in general the Kubo-equilibrium formula. There are in particular modified Green-Kubo relations where the current and the dynamical activity
$\Delta \mu / T = 0.20, \ T = 150; \ h / T = 0.02$

Figure 2: The response in the number of particles $N$ of the driven Lorentz gas when both reservoir chemical potentials are shifted, $\mu_{\ell,r} \rightarrow \mu_{\ell,r} + h$. The full curve is the Kubo-equilibrium formula, calculated with $\Delta \mu / T = 0.2$, $T = 150$. The dotted curve corresponds to direct measurements of $N$ while performing the shift at $t = 0$. These curves are obtained from averages over $1.5 \times 10^6$ initial conditions. Also in the plot, the crosses (blue) show the response obtained by solving the diffusion equation $\partial_t \rho(x, t) = \lambda \partial_{xx} \rho(x, t)$, with $\lambda$ diffusivity, taking the stationary unperturbed particle density profile as initial condition, and perturbed densities as boundary conditions.
complement their responses. There is however also an important case of “external” perturbations where the response retains the equilibrium form, which can also be checked for the driven Lorentz gas. We may expect similar behavior for other boundary driven systems with diffusive transport for which the analogy with certain aspects of the zero range process can be argued.

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