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Deriving GENERIC from a Generalized Fluctuation Symmetry

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Abstract Much of the structure of macroscopic evolution equations for relaxation to equilibrium can be derived from symmetries in the dynamical fluctuations around the most typical trajectory. For example, detailed balance as expressed in terms of the Lagrangian for the path-space action leads to gradient zero-cost flow. We expose a new such fluctuation symmetry that implies GENERIC, an extension of gradient flow where a Hamiltonian part is added to the dissipative term in such a way as to retain the free energy as Lyapunov function.

Keywords Gradient flow · GENERIC · Dynamical large deviations · Fluctuation symmetry

1 Main Result

Evolution equations for macroscopic densities may enjoy a certain geometric interpretation making them to resemble mechanical equations of motion with friction. As main example, the kinetic and macroscopic return to equilibrium can be described as a gradient flow on the manifold of possible density profiles. In general that means we can identify a free energy functional on those profiles and the evolution on the manifold is one of steepest descent: it follows the fastest decrease of the free energy. The metric determining steepness is given in terms of the positive Onsager matrix of mobilities under the scheme of local equilibrium. There has been a lot of mathematical work around such variational evolutions related to optimal transport; see e.g. [1]. Moving closer to statistical mechanics and looking in the physics literature it has been less explained how gradient flow is directly connected with

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detailed balance as expressed on the level of dynamical fluctuations. We therefore start this paper by giving examples and general theory (on a physical level) of gradient flow; see Sects. 3.1 and 4.1 . We show how the structure of the Lagrangian (the dynamical fluctuation functional) determines the return to equilibrium. In other words, how the equations obtained from a law of large numbers structurally depend on the fluctuations around that law.

The main new result of the present paper is however the logical continuation of that idea when inertia plays a role. We have identified a symmetry for the dynamical fluctuations of underdamped systems from which the structure of GENERIC appears. That symmetry is not involved mathematically as we hint at immediately below, and is valid under very general and natural conditions. Still it is the essential link to move from gradient flow to GENERIC on the level of dynamical fluctuations. The Generalised Equation for Non-Equilibrium Reversible-Irreversible Coupling (GENERIC, [2–4]) corresponds to a class of evolution equations describing return to equilibrium, where besides the dissipative and gradient part in the equation there is also a Hamiltonian part. We explain the structure via some illustrative examples in Sect. 3.2 and our main result there is found in Sect. 4.2.

To introduce the "new" fluctuation symmetry on the level of dynamical fluctuations which leads to GENERIC, we can already consider a Newtonian particle of mass m in one dimension with position x and velocity v. Assume there is a stochastic component in the motion in the sense that the acceleration $\dot{v}$ is noisy. We leave the physical origin of that noise unspecified here but we suppose that the variance goes to zero as some parameter $N \uparrow +\infty$; it could e.g. refer to an inverse temperature or to some macroscopic limit. Suppose now that we are able to find a force $F(x, v)$ so that for any given phase space point (x, v) the symmetry

$$\text{Prob}_N\,[m\dot{v} = F(x,v) + b \,|\, v, x] = \text{Prob}_N[m\dot{v} = F(x,v) - b \,|\, v, x] \tag{1}$$

holds for all possible forces b, in the sense of probability densities. The reason for that symmetry could simply be that the distribution of $m\dot{v} - F(x, v)$ is even, as it would be for a Gaussian noise, e.g. with $F(x, v) = -\partial_x V(x) - \gamma\, v$ for some potential V and friction $\gamma \geq 0$. Let us further assume that as $N \uparrow \infty$ the acceleration becomes deterministic so that for sure, e.g. via the law of large numbers, there is a unique force b^* for which $m\dot{v} = F(x, v) + b^*$. Then, by the symmetry (1), we conclude that necessarily $b^* = 0$ and hence we must have that $m\dot{v} = F(x, v)$ (Newton's law) in the deterministic limit. To say it differently, if we discover a force F for which the symmetry in fluctuations (1) holds, then the deterministic limit must be Newton's force law with that F. Similarly, in the case of return to equilibrium where inertial effects remain visible, the symplectic or Hamiltonian part will appear in evolution equations.

The above simple reasoning is expected to apply under a wide range of natural situations, and some further sophistication (e.g. by rewriting (1) for time-integrals) leads to the GENERIC contribution in relaxation equations as we will show in Sect. 4.2.

Apart from the derivation of GENERIC from the dynamical fluctuation structure, this paper wants to emphasize in physical terms the transfer of structures from mesoscopic to macroscopic level. It is interesting to see that theme developed in various stages of nonequilibrium statistical mechanics as the subject of the next section.

2 Context and Some Historical Remarks

While macroscopic equations describing the return to equilibrium have been conceived and applied even before the atomistic picture of matter was widely accepted, their derivation shows important mathematical and conceptual difficulties. After all, hydrodynamic and ther-

modynamic behavior is described autonomously in only a few macroscopic variables and it must be understood how these variables get effectively decoupled from the many microscopic degrees of freedom. Moreover, in modifying the scale of description, the character of the dynamics could drastically change, from a unitary or a Hamiltonian to a dissipative evolution as possibly one of the most remarkable features.[1] In Boltzmann's microscopic derivation of irreversibility he introduced a third scale of description in which the fluctuations are still visible and he understood the macroscopic limit as a law of large numbers. Even when we cannot derive and even when we do not know the precise macroscopic evolution equation, fluctuation theory still tells us that the entropy functional must be increasing in time along that evolution. The point is that the entropy is the large deviation rate function for macroscopic fluctuations and is therefore *always* increasing along the first-order evolution equation for the macroscopic variable. It was the first time that, paradoxically, an object appearing in the theory of *large deviations* played a major role in the characterization of *typical macroscopic behavior*. The result has been made precise and illustrated in various contexts [5–10].

A very famous next result was that of Lars Onsager in 1931 [11,12], showing that the linearized macroscopic evolution has a symmetry, called reciprocity and appearing in the matrix of the linear response coefficients as a consequence of microscopic reversibility. Again fluctuations entered, as reversibility implies that the typical return path to equilibrium can be obtained from the small fluctuations away from that equilibrium. That study was continued by Onsager and Machlup in 1953 on the same level of linearized hydrodynamics pioneering there the description in terms of probabilities on path-space [13]. The connection between response theory and fluctuation theory on path-space was taken back up in the derivation of response relations around nonequilibrium, [14].

The mathematical literature on path–wise fluctuations started in the 1970s. It resulted in large deviation theory for Markov processes and for stochastic perturbations of dynamical systems [15–17]. For all those results one usually starts from more microscopic considerations or from mesoscopic models and moves on to show aspects of the structure of dynamical fluctuations. There is however also the other side, to learn about the structure of the macroscopic evolution equations *directly from* the path-wise large deviations. Our main example there and inspiration for the present paper is [10] which is perhaps still less-known and which we will present in a statistical physics language in Sect. 4.1.

3 Gradient and GENERIC Dynamics

In this section, we introduce the notions of gradient flow and GENERIC, and illustrate them through several simple examples. More involved examples for complex fluids are found in the original [2–4]. Besides the review aspect we also present our first result, which is the characterization of a general form, in Eq. (20), of nonlinear relaxation to equilibrium.

3.1 Gradient Flow

Gradient flow refers to a certain structure in the relaxation to equilibrium. The equilibrium itself is characterized in terms of a (set of) macroscopic variable(s), which we denote by z in all abstract generality, but which we will replace within specific examples, depending on

[1] Perhaps the earliest example where that question became manifest is through d'Alembert's paradox (1752) for reconciling, what we call today, Euler's equation with that of Navier-Stokes. As d'Alembert wrote indeed, "It seems to me that the theory (potential flow), developed in all possible rigor, gives, at least in several cases, a strictly vanishing resistance, a singular paradox which I leave to future Geometers to elucidate."

the context, by ρ for densities of matter or by x for magnetization, etc. The evolution of the variable z is determined by the current j_z through an equation of the form

$$\dot{z} = D j_z \tag{2}$$

where the operator D can be minus the divergence, the identity operator, or a stoichiometry matrix, depending on the type of dynamics being considered (respectively: type-B, typically for a density; type-A, like for magnetization; chemical reactive systems).

Quite abstractly an evolution has traditionally been called a gradient flow if the displacement of the dynamical variable z can be written in the form

$$\dot{z} = M \, \mathrm{d}S, \qquad M = D \, X \, D^\dagger, \qquad j_z = X \, D^\dagger \, \mathrm{d}S \tag{3}$$

for a symmetric positive semi-definite operator X and the adjoint $D^\dagger$ defined by the relation $a \cdot Db = b \cdot D^\dagger a$. Here $\mathrm{d}S$ stands for the derivative of a state function $S(z)$ with respect to z (being a functional derivative if $z = \rho$). S might be an entropy, minus a free energy or some other thermodynamic potential depending on the context, etc. Examining the time-derivative of S, we find

$$\dot{S} = \mathrm{d}S \cdot \dot{z} = \mathrm{d}S \cdot M \, \mathrm{d}S \geq 0 \tag{4}$$

so that S is always increasing and the equilibrium state is obtained by maximizing S. Mathematically it makes sense to think of z as a point of a Riemannian manifold, moving by steepest descent of the functional $-S$. The descent is measured in a metric provided by the operator X, which is in general related to the physical mobility.

In [10], the notion of gradient flow was extended from (3) to nonlinear evolutions, which appear for instance when considering reactive processes or jump processes on a discrete state space, with Poissonian statistics [18]. The nonlinear gradient flow equation, which still describes relaxation towards equilibrium but with a nonlinear operator 'X', is obtained by replacing (3) with

$$\dot{z} = D \, \partial\psi^\star(D^\dagger \mathrm{d}S/2; z) \tag{5}$$

for a convex functional $f \mapsto \psi^\star(f; z)$ where f stands for a thermodynamic force, and $\partial\psi^\star$ is the derivative with respect to f. We can call $\psi^\star$ a nonlinear mobility operator [19] since the Onsager reciprocity property $X = X^T$ in (3) is equivalent to the property that $Xf = \partial\psi^\star(f)/2$ for $\psi^\star(f) = f \cdot Xf$. An essential requirement here is that

$$\psi^\star(f; z) \geq \psi^\star(0; z) = 0, \tag{6}$$

and that $\psi^\star$ is symmetric in $\pm f$.

The inequality in (4) can also be extended since

$$\dot{S} = \mathrm{d}S \cdot \dot{z} = 2 \, D^\dagger \mathrm{d}S/2 \cdot \partial\psi^\star(D^\dagger \mathrm{d}S/2) \overset{(6)}{\geq} 0, \tag{7}$$

which gives again the monotonicity of $S(z(t))$ in time.

3.1.1 Example 1: Type-B Dynamics

The most standard example of gradient flow is given by a conservative relaxational dynamics (type-B) in the form of a continuity equation for a scalar density $\rho(r, t)$ defined for every position in a fixed volume, $r \in \Lambda \subset \mathbb{R}^3$, and with fixed boundary conditions $\rho(r, t) = \bar{\rho}$, $r \in \partial\Lambda$:

$$\dot{\rho} = -\nabla \cdot j_\rho \tag{8}$$

where $D = -\nabla\cdot$ is (minus) the divergence with respect to r so that $D^\dagger = \nabla$ is the gradient. The current is given in terms of a density-dependent mobility χ (being a 3×3 symmetric non-negative matrix) and the thermodynamic force F, as

$$j_\rho(r) = \chi\,(\rho(r))\;F(r), \quad F(r) = -\nabla\,\mu(r), \quad \mu(r) = \frac{\delta\mathcal{F}[\rho]}{\delta\rho(r)} \tag{9}$$

for local chemical potential μ expressed as a variational derivative from free energy functional $\mathcal{F}[\rho]$ up to a constant. Such a dynamics (8)–(9) gives a description of hydrodynamic relaxation to equilibrium, or, ignoring space–time rescaling, it can be part of a description in dynamical density functional theory [20,21] to describe an inhomogeneous fluid. Given (9) we can rewrite (8) as

$$\dot\rho(r,t) = \nabla\cdot\left(\chi(\rho(r,t))\nabla\left(\frac{\delta\mathcal{F}[\rho]}{\delta\rho(r)}\right)\right) \tag{10}$$

to recognize the gradient flow structure (3) with $M = -\nabla\cdot\chi\nabla$ and $S = -\mathcal{F}$. The monotonicity of the entropy, or equivalently of the free energy, is

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{F}[\rho] = -\int \mu(r)\,\nabla\cdot j\,(\rho(r))\,\mathrm{d}r = -\int \nabla\mu(r)\cdot\chi\,(\rho(r))\,\nabla\mu(r)\mathrm{d}r \le 0$$

where the second equality uses partial integration with vanishing boundary term, and the final inequality is obtained by the non-negativity and symmetry of the mobility matrix $X = \chi$ as in (4).

For example, on the unit interval $\Lambda = [0,1]$ with $\rho(0,t) = \rho(1,t) = \bar\rho$ we can take the grand potential at temperature T,

$$\mathcal{F}[\rho] = k_B T\int_0^1\left(\rho(r)\,\log\frac{\rho(r)}{\bar\rho} - \rho(r) + \bar\rho\right)\mathrm{d}r, \quad \text{for which } \mu(r) = k_B T\log\frac{\rho(r)}{\bar\rho}$$

and (10) is then the linear diffusion equation for the mobility $\chi = \rho$.

3.1.2 Example 2: Markov Jump Process

We next look at a detailed-balanced Markov jump process as an example of a type-A relaxational dynamics on a discrete state space. The macroscopic equation is here the Master equation, obtained for the density of independent random walkers following the Markov transitions:

$$\dot\rho(c) = \sum_{c'} k(c',c)\rho(c') - k(c,c')\rho(c) \tag{11}$$

for the time-dependent density $\rho(c) = \rho(c;t)$ on configurations c, with transition rate $k(c,c')$ for the jump $c \to c'$. Detailed balance at inverse temperature β with respect to a potential $V(c)$ is enforced by requiring $k(c,c') = \varphi(c',c)\mathrm{e}^{\frac{\beta}{2}(V(c)-V(c'))}$, where $\varphi(c',c) = \varphi(c,c') \ge 0$ are symmetric activity parameters for the transitions $c \leftrightarrow c'$.

The operator D of (3) is here minus the discrete divergence acting on antisymmetric functions b, and $D^\dagger$ acts as a gradient on functions a of configurations c:

$$(Db)(c) = -\sum_{c':\varphi(c',c)\neq 0} b(c,c'), \quad a\cdot Db = \sum_{c\sim c'} a(c)b(c',c), \quad (D^\dagger a)(c,c') = a(c') - a(c) \tag{12}$$

where the sum in the middle is over all (c, c') where $\varphi(c, c') \neq 0$. The current in (11) over $c \to c'$ is

$$j(c, c') = k(c, c')\rho(c) - k(c', c)\rho(c')$$

but can also be written as

$$j(c, c') = \varphi(c, c')\sqrt{\rho(c)\rho(c')}\left(\mathrm{e}^{-\frac{1}{2}D^\dagger[\log\rho+\beta V](c,c')} - \mathrm{e}^{\frac{1}{2}D^\dagger[\log\rho+\beta V](c,c')}\right) \tag{13}$$

We therefore take

$$S[\rho] = -\sum_c \rho(c)\left[\log\rho(c) + \beta V(c)\right] \tag{14}$$

to express the Master Eq. (11) in its nonlinear gradient flow form (5), with

$$\psi^\star(f;\rho) = 2\sum_{c,c'}\varphi(c, c')\sqrt{\rho(c)\rho(c')}\,\left(\cosh f_{c,c'} - 1\right) \tag{15}$$

as function of a force $f_{c,c'}$, function of (c, c').

3.2 GENERIC and Pre-GENERIC

GENERIC (the General Equation for Non-Equilibrium Reversible-Irreversible Coupling [2]), in its original form, is an additive combination of a Hamiltonian and a gradient flow. Symbolically, it extends (3) to

$$\dot{z} = A\,\mathrm{d}E + M\,\mathrm{d}S \tag{16}$$

where $E = E(z)$ and $S = S(z)$ are interpreted as energy and entropy functionals, with $\mathrm{d}E$ and $\mathrm{d}S$ the appropriate derivatives. $A = A(z)$ is an antisymmetric operator while $M = M(z)$ is a symmetric, non-negative definite operator. Finally, E, S, M, A are assumed to satisfy the orthogonality conditions

$$A\,\mathrm{d}S = 0, \qquad M\,\mathrm{d}E = 0 \tag{17}$$

As a consequence, along the flow,

$$\dot{S} = \mathrm{d}S \cdot A\,\mathrm{d}E + \mathrm{d}S \cdot M\,\mathrm{d}S = \mathrm{d}S \cdot M\,\mathrm{d}S \geq 0$$
$$\dot{E} = \mathrm{d}E \cdot A\,\mathrm{d}E + \mathrm{d}E \cdot M\,\mathrm{d}S = 0$$

In other terms, GENERIC characterizes a dynamics of return to equilibrium consisting of two orthogonal parts, the first being dissipative (the gradient flow along the entropy S), whereas the second is Hamiltonian and conserves the energy E. In the book [2] one finds a wealth of topics for the dynamical relaxation towards equilibrium going beyond the purely dissipative evolutions. We refer to that book and to the original papers [3,4] for further information on that extension of irreversible thermodynamics.

We consider here a less constrained version of those equations, which can be seen as a precursor to GENERIC, which we call *pre*-GENERIC. It consists in renouncing to the existence of a conserved energy E, but instead considering a general flow $\mathcal{D}J$ instead of $A\,\mathrm{d}E$,

$$\dot{z} = \mathcal{D}J + M\,\mathrm{d}S, \qquad M = DXD^\dagger \tag{18}$$

with the operator $\mathcal{D}$ acting on J, a given function of z, similar to (2), and where the second part is the gradient flow of Eq. (3). The first constraint in (17) can then be replaced by the less constraining orthogonality condition

$$\mathcal{D}J \cdot \mathrm{d}S = 0 \tag{19}$$

leading as before to the monotonicity of S. The second constraint in (17), as well as the conservation resulting from it, are removed as unnecessary for the structure. A mathematical argument will be formulated elsewhere [22].

Like in the case of gradient flow, (pre-)GENERIC can and in fact should be extended to nonlinear flows (see also [23]) as

$$\dot{z} = \mathcal{D}J + D\,\partial\psi^\star(D^\dagger \mathrm{d}S/2; z) \tag{20}$$

The monotonicity of the entropy follows as in (7),

$$\dot{S} = \mathrm{d}S \cdot \mathcal{D}J + 2\,\mathrm{d}S/2 \cdot D\partial\psi^\star(D^\dagger \mathrm{d}S/2) \geq 0 \tag{21}$$

Recognizing the structure (20) as the typical behavior unifying various types of relaxation to equilibrium is one of the main results of this paper.

The appeal of pre-GENERIC is first somewhat pragmatic and secondly mathematical. First, as we will see, it appears in examples in a direct way. GENERIC often requires adding extra variables to the models which nicely complete the structure, but are not directly or physically given. Secondly, as shown in [22], it turns out that the aforementioned extension is systematically possible, meaning that pre-GENERIC formally implies GENERIC. We are therefore mostly interested here in working with pre-GENERIC. In order to get the full GENERIC structure, we have to add an auxiliary scalar variable E to the system, in order to fix the two conditions that were not satisfied above. We refer to [22] for one systematic way to do that.

3.2.1 Example 3: Underdamped Diffusions

As shown in [24], the underdamped Vlasov–Fokker–Planck equation naturally gives rise to GENERIC and hence to a triple (J, M, S). It provides us with an opportunity to illustrate the formal notation of (18).

The variable z is, as in Example IIIA 1 above, a time-dependent density $\rho(q, p; t)$, but in its underdamped version, depending on positions $q \in \mathbb{R}^d$ and momenta $p \in \mathbb{R}^d$. The Vlasov–Fokker–Planck equation is given by

$$\dot{\rho} = -\nabla_q \cdot \rho \frac{p}{m} + \nabla_p \cdot \rho \left(\nabla_q V + \nabla_q (\Phi \star \rho) + \gamma \frac{p}{m} \right) + \gamma\, \beta^{-1}\, \Delta_p \rho \tag{22}$$

for damping coefficient γ, mass m and inverse temperature $\beta = (k_B T)^{-1}$. The convolution is defined as

$$\Phi \star \rho\ (q) = \int_{\mathbb{R}^{2d}} \Phi(q - q')\, \rho(q', p')\, \mathrm{d}q'\, \mathrm{d}p'$$

That equation arises as a mean-field limit of underdamped diffusions interacting through a potential Φ, with friction γ and at inverse temperature β [25]. The Kramers equation describing the evolution of a probability density for underdamped Markov diffusions is recovered for $\Phi = 0$.

In order to unravel the structure of (22), we rewrite it in matrix form, separating the q and p directions. For instance, the operator $D = \mathcal{D}$ is given by minus the divergence

$$D = -\nabla = -\begin{bmatrix} \nabla_q & \nabla_p \end{bmatrix} \tag{23}$$

Moreover, this being an equilibrium system, we can define the Gibbs entropy

$$\mathcal{S}[\rho] = -k_B \int_{\mathbb{R}^{2d}} \rho \log \rho \, \mathrm{d}q\mathrm{d}p \tag{24}$$

and the energy (including kinetic energy, potential self-energy and interaction energy)

$$\mathcal{H}[\rho] = \int_{\mathbb{R}^{2d}} \left(\frac{p^2}{2m} + V(q) + \frac{1}{2}(\psi \star \rho)(q) \right) \rho \, \mathrm{d}q\mathrm{d}p \tag{25}$$

and combine them into the free energy functional $\mathcal{F}[\rho] = \mathcal{H}[\rho] - T\,\mathcal{S}[\rho]$.

Equation (22) can be then written as

$$\dot{\rho} = -\nabla \cdot \rho K \nabla \frac{\delta \mathcal{H}[\rho]}{\delta \rho(r)} + \nabla \cdot \chi \nabla \frac{\delta \mathcal{F}[\rho]}{\delta \rho(r)} \tag{26}$$

with $2d \times 2d$ matrices

$$K = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \quad \text{and} \quad \chi = \rho\gamma \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \tag{27}$$

The system evolution (26) (and thus also (22)) has the pre-GENERIC structure (18), with $S = -\mathcal{F}$, $M = -\nabla \cdot \chi \nabla$, and with $J = \rho K \nabla \frac{\delta \mathcal{H}[\rho]}{\delta \rho(r)}$. Indeed, as required for (21) we have the orthogonality

$$\begin{aligned} J \cdot D^\dagger \mathrm{d}S &= \int_{\mathbb{R}^{2d}} \frac{\delta \mathcal{H}[\rho]}{\delta \rho(r)} \nabla \cdot \rho K \nabla \frac{\delta \mathcal{F}[\rho]}{\delta \rho(r)} \, \mathrm{d}q\mathrm{d} \\ &= \int_{\mathbb{R}^{2d}} \frac{\delta \mathcal{H}[\rho]}{\delta \rho(r)} \nabla \cdot \rho K \nabla \frac{\delta \mathcal{H}[\rho]}{\delta \rho(r)} \, \mathrm{d}q\mathrm{d}p - \beta^{-1} \int_{\mathbb{R}^{2d}} \frac{\delta \mathcal{H}[\rho]}{\delta \rho(r)} \nabla \cdot \rho K \nabla \frac{\delta \mathcal{S}[\rho]}{\delta \rho(r)} \, \mathrm{d}q\mathrm{d}p \\ &= 0 \end{aligned} \tag{28}$$

because of the antisymmetry of K for the first term, and the fact that $\nabla \cdot \rho K \nabla \frac{\delta \mathcal{S}[\rho]}{\delta \rho(r)} = (\nabla_q \nabla_p - \nabla_p \nabla_q)\rho = 0$ for the second term in (28).

3.2.2 Example 4: Andersen Thermostat

A good example of a nonlinear GENERIC system is the so-called Andersen thermostat [26], often used for numerical simulations of Hamiltonian systems subject to thermal fluctuations. In this model, independent massive particles with positions q and momenta p, of mass m and subject to a potential $V(q)$, are perturbed in their Hamiltonian motion by having their momentum randomized according to their natural Maxwellian distribution at constant rate $\varphi \geq 0$. The evolution of the density of particles ρ is then given by

$$\dot{\rho}(q,p) = -\nabla \cdot \rho(q,p) K \nabla \frac{\delta \mathcal{H}[\rho]}{\delta \rho(q,p)} + \varphi \, \frac{e^{-\frac{p^2}{2m}}}{\sqrt{2\pi m}} \int \mathrm{d}p' \, \rho(q,p') - \varphi \, \rho(q,p) \tag{29}$$

which is a combination of a Hamiltonian flow and a jump process on p for inverse temperature $\beta = 1$. The Hamiltonian is given by

$$\mathcal{H}[\rho] = \int_{\mathbb{R}^{2d}} \left(\frac{p^2}{2m} + V(q) \right) \rho(q,p) \, \mathrm{d}q\mathrm{d}p$$

and the symplectic matrix K is the same as in (27). We can also use the same entropy $\mathcal{S}$ and free energy $\mathcal{F}$ as there.

For the jump part we imagine replacing all sums by integrals in Sect. 3.1.2 getting a nonlinear gradient flow (20) with $S = -\mathcal{F}$ and

$$\psi^\star(f;\rho) = \frac{2\varphi}{\sqrt{2\pi m}} \int e^{-\frac{p^2+p'^2}{4m}} \sqrt{\rho(q,p)\rho(q,p')}\,(\cosh f - 1)\,\mathrm{d}p\mathrm{d}p' \tag{30}$$

The corresponding negative divergence D and gradient $D^\dagger$ are as in (12),

$$Db\,(p) = -\int b(p,p')\,\mathrm{d}p', \qquad D^\dagger a(p,p') = a(p') - a(p)$$

That allows us to write (29) as

$$\dot\rho + \nabla\cdot J = D\,\partial\psi^\star(D^\dagger \mathrm{d}S/2; z) \tag{31}$$

which is of the pre-GENERIC form (20) with $\mathcal{D} = -\nabla\cdot$, and $J = \rho K\,\nabla\frac{\delta\mathcal{H}[\rho]}{\delta\rho(r)}$ and the orthogonality (19) as before in (28).

This example can be easily extended to more general jumps and even to a combination of diffusions and jumps, as long as the rates satisfy detailed balance with respect to $\mathcal{H}$. This type of system was considered in [27] and interpreted as being in equilibrium with work-producing reservoirs, where it is necessary to factor out that work in order to obtain the physical entropy production of the system. As we see here, that is equivalent to writing the fluctuation symmetry around the average flux J present in the system.

3.2.3 Example 5: Nonlinear Friction

The equation of motion

$$\begin{aligned}\dot q &= \frac{p}{m}\\ \dot p &= -\nabla_q V(q) - 2\varphi\,\sinh\left(\frac{p}{2m}\right)\end{aligned} \tag{32}$$

shows nonlinear friction.

Defining the energy $h(q,p) = \frac{p^2}{2m} + V(q)$, we rewrite it as

$$\begin{bmatrix}\dot q\\ \dot p\end{bmatrix} = K\nabla h + \partial\psi^\star\left(-\frac{1}{2}\nabla h\right) \tag{33}$$

with

$$\psi^\star(f_q, f_p; q, p) = 2\varphi\,\left(\cosh f_p - 1\right) \tag{34}$$

which is of pre-GENERIC form (20) with $D = \mathcal{D} = 1$, $J = K\nabla h$ and $S = -h$. The orthogonality (19) is verified as

$$J\cdot D^\dagger \mathrm{d}S = -(K\nabla h)\cdot\nabla h = 0 \tag{35}$$

by the antisymmetry of K.

4 Large Deviations Approach to Equilibrium Flows

Dynamical ensembles give the probabilities of trajectories for particle systems [17,28,29]. Those probabilities can arise from random initial conditions and/or coarse graining where the integrated degrees of freedom have been assigned a statistical distribution. For the present paper we place ourselves at a mesoscopic level, looking at the fluctuation dynamics of macroscopic degrees of freedom in a system with a large parameter N (usually size, number of elements, inverse temperature or number of copies), as could be obtained via the theory of large deviations [7,16,17,28,30,31]. The main objects of interest are then the Lagrangian L and the Hamiltonian H.

We consider in a time-interval $[0, t]$ all possible evolutions of the variable z and of a current variable j which are compatible with the microscopic system; we thus have a flow of state and current variables $(z(s), j(s)), s \in [0, t])$ verifying, at each moment, the equation

$$\dot{z}(s) - \mathcal{D}J(z(s)) = Dj(s) \tag{36}$$

for a given fixed current J and operators $\mathcal{D}$ and D as we had them before in the examples. In many interesting cases however $\mathcal{D} = D$, and we can then in fact stick to the constraint

$$\dot{z}(s) = Dj(s) \tag{37}$$

where the J of (36) is possibly to be part of the j.

There are many possible trajectories all satisfying the constraint (36) or (37), and we investigate the structure of their probability. At time zero we start in equilibrium so that the probabilities are given by an entropy functional $S(z(0))$, while for later times the probability will also involve the currents j.

The Lagrangian $L(j; z) \geq 0$ of the system governs the path probabilities of the macroscopic variable, via

$$\text{Prob}[(z(s), j(s)), s \in [0, t]] \simeq e^{NS(z(0))}\, e^{-N\int_0^t \mathrm{d}s\, L(j(s);z(s))}, \qquad N \uparrow +\infty \tag{38}$$

which is to say that L determines the plausibility of the various possible trajectories. Note that all fluctuations are exponentially damped in N with respect to the zero cost flow j_z where $L(j_z; z) = 0$. Properties that can be assumed from the outset are that $L(j, z) \geq 0$, is convex in j for all z, and that $L = 0$ induces a unique evolution equation, the so called zero-cost flow. Finding the differential equation for the typical macroscopic trajectory is thus equivalent to finding for any given z the solution j_z of $L(j_z; z) = 0$, and then to substitute that solution into (36) or (37) to get an autonomous equation for $z(t)$. The question we ask here more specifically is

> Can we identify the $\psi^\star$ in (20) from properties of the Lagrangian L, for S given in (38)?

In particular, which symmetries of the Lagrangian naturally lead to gradient flow and to pre-GENERIC?

Note also that from the Lagrangian L we define the Hamiltonian H through a Legendre transform:

$$H(f; z) = \sup_j \left[j \cdot f - L(j; z)\right], \tag{39}$$

where f, the variable dual to the current j, is a thermodynamic force. By construction, $L(j_z; z) = 0$ is equivalent with H verifying

$$j_z = \partial H(0; z) \tag{40}$$

Symmetries of the Lagrangian will be translated in properties of H.

4.1 From Detailed Balance to Gradient Flow

We first address the question above in the context of detailed balance (time-reversibility). Here we assume the constraint (37) for some operator D as appears in (2)–(5) (or, $J = 0$ in (36)). We will see how under detailed balance conditions the time-symmetric part of the Lagrangian, $L(-j; z) + L(j; z)$, determines the zero-cost flow j_z for given entropy S, and in such a way that the autonomous evolution is a gradient flow with respect to the entropy S, as in (5) or as in the examples of Sect. 3.1.

By detailed balance (on the mesoscopic level of (38) and for a variable z which is even under kinematic time-reversal) we mean that the probability of any trajectory, including the initial condition distributed with respect to the entropy S, is equal to that of its time-reversal. That is the condition that

$$\int_0^t \mathrm{d}s \ [L(-j(s); z(s)) - L(j(s); z(s))] = S(z(t)) - S(z(0)) \tag{41}$$

which, if true for all times t, is nothing else than requiring $L(-j; z) - L(j; z) = \dot{S}$, or that

$$L(-j; z) - L(j; z) = j \cdot D^\dagger \mathrm{d}S(z) \tag{42}$$

Similarly, under detailed balance (42) and from (39) we have

$$H(f; z) = H(-f - D^\dagger \mathrm{d}S; z) \tag{43}$$

Clearly now, at zero-cost flow j_z where $L(j_z; z) = 0$, the time-symmetric part must equal the antisymmetric part of the Lagrangian, which under (42) yields

$$L(-j_z, z) + L(j_z, z) = j_z \cdot D^\dagger \mathrm{d}S(z) \tag{44}$$

which is an equation for j_z. In order to solve it, we will decompose the time-symmetric part $L(-j; z) + L(j; z)$, as in the left-hand side, in a pair of convex conjugates.

Define

$$\begin{aligned} \psi(j; z) &= \frac{1}{2}\big[L(-j; z) + L(j; z)\big] - L(0; z) \\ &= \frac{1}{2}\, j \cdot D^\dagger \mathrm{d}S(z) + L(j; z) - L(0; z) \end{aligned} \tag{45}$$

where the second line uses (42) and implies that $\psi(j; z)$ is convex in j. From the first line we see that ψ is symmetric in $\pm j$ and vanishes at $j = 0$. It is therefore also positive, $\psi(j; z) \geq 0$. The Legendre transform of ψ is

$$\psi^\star(f; z) = \sup_j [j \cdot f - \psi(j; z)] \tag{46}$$

and we will show that it is the same function as appears in (5). Note indeed that by replacing here ψ via (45) we find a convex

$$\psi^\star(f; z) = H(f - D^\dagger \mathrm{d}S/2; z) + L(0; z) \tag{47}$$

which is symmetric in $\pm f$, positive and vanishes only at $f = 0$. Moreover,

$$L(0; z) = \psi^\star(D^\dagger \mathrm{d}S/2; z), \qquad L(j; z) = -\frac{1}{2}\, j \cdot D^\dagger \mathrm{d}S(z) + \psi(j; z) + \psi^\star(D^\dagger \mathrm{d}S/2; z) \tag{48}$$

which implies that the zero-cost flow must satisfy

$$j_z = \partial H(0; z) = \partial \psi^\star(D^\dagger \mathrm{d}S/2; z) \tag{49}$$

(If say in one dimension for $j \in \mathbb{R}$ we find $f \in \mathbb{R}$ for which $\psi(j) + \psi^\star(f) = jf$ for Legendre convex pairs ψ and $\psi^\star$, then $j = (\psi^\star)'(f)$.) We conclude from (49) that the typical path $\dot{z} = Dj_z$ has indeed the generalized gradient flow structure (5).

Additional insight can be gained from adding to (48) that

$$\begin{aligned} \psi^\star(f; z) &= H(f - D^\dagger \mathrm{d}S/2; z) - H(-D^\dagger \mathrm{d}S/2; z) \\ H(f; z) &= \psi^\star(f + D^\dagger \mathrm{d}S/2; z) - \psi^\star(D^\dagger \mathrm{d}S/2; z) \end{aligned} \tag{50}$$

We see that ψ and $\psi^\star$ are the re-centred symmetric parts of L and H respectively, identical to L and H for $\mathrm{d}S(z) = 0$.

We now revisit the examples presented in Sect. 3.1 in the context of large deviations.

4.1.1 Example 1 Continued: Diffusion Limits

We start with the first example from Sect. 3.1.1, namely the overdamped diffusion. We consider N independent such diffusions. That leads to a quadratic Lagrangian, as encountered in macroscopic fluctuation theory [7,32], more generally as diffusion limits of interacting particle systems,

$$L(j; \rho) = j \cdot \frac{\chi^{-1}}{4} j - \frac{\mathrm{d}S}{2} \cdot \nabla \chi \nabla \frac{\mathrm{d}S}{2} - \frac{1}{2} j \cdot \nabla \mathrm{d}S \tag{51}$$

where χ^{-1} should be understood as a pseudo-inverse. The associated Hamiltonian is

$$H(f; \rho) = f \cdot \chi(f + \nabla \mathrm{d}S) \tag{52}$$

It is straightforward to check that L and H verify all the properties discussed above, with functions

$$\psi(j; \rho) = j \cdot \frac{\chi^{-1}}{4} j \quad \text{and} \quad \psi^\star(f; \rho) = f \cdot \chi f. \tag{53}$$

4.1.2 Example 2 Continued: Jump Processes

The example from Sect. 3.1.2 considers a large number N of particles jumping on the graph with vertices (states) c over bonds where $\varphi(c, , c') \neq 0$ with detailed balanced rates $k(c, c') = \varphi(c', c)\, \mathrm{e}^{\frac{\beta}{2}(V(c) - V(c'))}$ for $\varphi(c', c) = \varphi(c, c')$. Instead of the Gaussian noise appropriate for a diffusion process, all the currents here have Poissonian statistics, leading to the Lagrangian found in [33],

$$\begin{aligned} L(j; \rho) = 2 \sum_{c \sim c'} \varphi(c', c) \sqrt{\rho(c)\rho(c')}\, \lambda\left(\frac{j(c, c')}{2\varphi(c', c)\sqrt{\rho(c)\rho(c')}} \right) \\ + k(c, c')\rho(c) + k(c', c)\rho(c') + \frac{1}{2} j(c, c')\, \log\left(\frac{k(c, c')\, \rho(c)}{k(c', c)\, \rho(c')} \right) \end{aligned} \tag{54}$$

with function

$$\lambda(j) = j \log\left(j + \sqrt{1 + j^2} \right) - \sqrt{1 + j^2} \tag{55}$$

having Legendre transform $\lambda^\star(f) = \cosh f$. The corresponding Hamiltonian is

$$H(f;\rho) = 2\sum_{c\sim c'} \varphi(c',c)\sqrt{\rho(c)\rho(c')}\cosh\left(f_{c',c} + \frac{1}{2}\log\frac{k(c,c')\,\rho(c)}{k(c',c)\,\rho(c')}\right) - k(c,c')\rho(c) - k(c',c)\rho(c')$$

where the sum is taken over every pair of neighboring states, and which can be written more compactly as

$$H(f;\rho) = \sum_{c,c'} k(c,c')\rho(c)\left(\mathrm{e}^{f_{c',c}} - 1\right) \tag{56}$$

with $f_{c,c'} = -f_{c',c}$. It is straightforward to check that (45) and (50) hold with

$$\psi(j;\rho) = 2\varphi(c',c)\sqrt{\rho(c)\rho(c')}\,\lambda\left(\frac{j}{2\varphi(c',c)\sqrt{\rho(c)\rho(c')}}\right) + 2\varphi(c',c)\sqrt{\rho(c)\rho(c')} \tag{57}$$

and

$$\psi^\star(f;\rho) = 2\sum_{c\sim c'} \varphi(c',c)\sqrt{\rho(c)\rho(c')}\left(\cosh f_{c,c'} - 1\right) \tag{58}$$

and with S given by (14), and $\mathrm{d}S$ in the cosh in (56).

4.2 To GENERIC

An essential ingredient in the previous analysis and examples was the (standard) condition of detailed balance (42). Looking back at the Examples IIIB1–IIIB3 for GENERIC flow we see that it is important to introduce momentum or velocity degrees of freedom to naturally give rise to the additional Hamiltonian flow. While such systems remain generalized reversible—one needs to flip the velocities when reversing the spatial trajectory—the condition (42) must be revisited.

Let us start with the constraint (37) on (38). We no longer require (42) but we suppose indeed very similarly to (1) that the Lagrangian satisfies

$$L(J-j;z) - L(J+j;z) = j\cdot D^\dagger \mathrm{d}S \tag{59}$$

for some function $J(z)$, to be derived from the Lagrangian as well. The reasoning of Sect. 4.1 can then be repeated by replacing L with $\tilde{L}(j;z) = L(J+j;z)$. The new Lagrangian $\tilde{L}$ inherits the relevant properties of L: non-negativity, convexity in its first argument, and unique minimization. The Hamiltonian H is obtained as before in (39), but the generalized detailed balance condition (59) leads to a modified version of (43),

$$H(-D^\dagger \mathrm{d}S/2 - f;z) - H(-D^\dagger \mathrm{d}S/2 + f;z) = -2f\cdot J \tag{60}$$

making the duality between L and H more symmetric than before.

The functions ψ and $\psi^\star$ are still defined as the re-centered symmetric parts of L and H, and are still Legendre transforms of one another. They verify

$$L(j;z) = \psi(j-J;z) + \psi^\star(D^\dagger \mathrm{d}S/2;z) - \frac{1}{2}(j-J)\cdot D^\dagger \mathrm{d}S \tag{61}$$

$$H(f;z) = \psi^\star(f + D^\dagger \mathrm{d}S/2;z) - \psi^\star(D^\dagger \mathrm{d}S/2;z) + f\cdot J \tag{62}$$

and the typical current j_z or zero-cost flow is given by

$$j_z = \partial H(0; z) = J + \partial\psi^\star(D^\dagger \mathrm{d}S/2; z) \tag{63}$$

Adding the orthogonality condition $J \cdot D^\dagger \mathrm{d}S = 0$ leads naturally to the nonlinear version of pre-GENERIC, with $\dot{z}$ given by (20) for $\mathcal{D} = D$,

$$\dot{z} = DJ + D\partial\psi^\star(D^\dagger \mathrm{d}S/2; z). \tag{64}$$

Note that, in the case of diffusions, where H is quadratic in f, there are many symmetries of the type of (60) with a linear right-hand side but no special orthogonality relation between the shift in the argument H and the linear prefactor, so that only this one connects to a gradient flow [34]. On the other hand, for driven jump processes, a similar orthogonality can be defined without the same type of symmetry for H (the right-hand side is no longer linear), which again does not lead to a gradient flow [35].

We see next how that structure arises from the large deviations of the examples in Sect. 3.2.

4.2.1 Example 3 Continued: Underdamped Diffusions

Concerning the Vlasov–Fokker–Planck equation of Sect. 3.2.1 we can use the fluctuation theory in [24]. We have a quadratic Lagrangian,

$$L(j; \rho) = (j - J) \cdot \frac{\chi^{-1}}{4}(j - J) - \frac{\mathrm{d}S}{2} \cdot \nabla\chi\nabla\frac{\mathrm{d}S}{2} - \frac{1}{2} j \cdot \nabla \mathrm{d}S \tag{65}$$

with Hamiltonian current,

$$J = \begin{bmatrix} \rho \frac{p}{m} \\ -\rho(\nabla_q V + \nabla_q \Phi \star \rho) \end{bmatrix} \tag{66}$$

The associated Hamiltonian to (65) is

$$H(f; \rho) = f \cdot \chi(f + \nabla \mathrm{d}S) + f \cdot J \tag{67}$$

We thus recover the structure of (61) and (62), with the same functions ψ and $\psi^\star$ as for the detailed balanced overdamped case in Sect. 4.1.1:

$$\psi(j; \rho) = j \cdot \frac{\chi^{-1}}{4} j, \qquad \psi^\star(f; \rho) = f \cdot \chi f \tag{68}$$

from which the Eq. (26) derives its structure.

4.2.2 Example 4 Continued: Andersen Thermostat

We now consider N particles evolving according to the thermostat dynamics of Sect. 3.2.2, i.e., according to (29). The only origin of randomness is the momentum resetting in the jump-part, while the Hamiltonian flow continues. We are therefore in the situation of (36) where $J = \rho K \nabla \frac{\delta \mathcal{H}[\rho]}{\delta \rho(r)}$ is the Hamiltonian current corresponding to

$$\begin{bmatrix} \dot{q} \\ \dot{p} \end{bmatrix} = K \nabla \frac{\delta \mathcal{H}[\rho]}{\delta \rho(r)} = \begin{bmatrix} \frac{p}{m} \\ -\nabla_q V(q) \end{bmatrix} \tag{69}$$

For (38) we only need to estimate the probability of Poisson-distributed jumps but that is the same as for the Markov jump processes in Sect. 4.1.2. We thus have for the current j

corresponding to the momentum jumps the expressions

$$\psi(j;\rho) = 2\varphi \int \frac{e^{-\frac{p^2+p'^2}{4m}}}{\sqrt{2\pi m}} \sqrt{\rho(q,p)\rho(q,p')} \left(\lambda \left(\frac{\sqrt{2\pi m} e^{\frac{p^2+p'^2}{4m}} j_{q,p;q,p'}}{2\varphi \sqrt{\rho(q,p)\rho(q,p')}} \right) + 1 \right) \mathrm{d}p\mathrm{d}p' \tag{70}$$

and

$$\psi^\star(f;\rho) = 2\varphi \int \frac{e^{-\frac{p^2+p'^2}{4m}}}{2\sqrt{\pi m}} \sqrt{\rho(q,p)\rho(q,p')} \left(\cosh f_{q,p;q,p'} - 1\right) \mathrm{d}p\mathrm{d}p' \tag{71}$$

as before in (58).

4.2.3 Example 5 Continued: Nonlinear Friction

In the example from Sect. 3.2.3 we have $\mathcal{D} = D = I$ and we are in the case with constraint (37) in (38). We can directly write the Lagrangian for the dynamics with a Hamiltonian flow and jumps of the form $p \to p \pm N^{-1}$ at fixed q, with rates $k^{\pm}(q,p) = N\varphi\, e^{-N\frac{(p\pm N^{-1})^2 - p^2}{4m}}$:

$$L(\dot{q},\dot{p};q,p) = 2\varphi\, \lambda\left(\frac{\dot{p} + \nabla_q V(q)}{2\varphi}\right) + 2\varphi\, \cosh\left(\frac{p}{2m}\right) + \dot{p}\frac{p}{2m} \tag{72}$$

with constraint $\dot{q} = \frac{p}{m}$ and λ as in (55). The associated Hamiltonian is

$$H(f_q, f_p; q, p) = 2\varphi\, \cosh\left(f_p + \frac{p}{2m}\right) - 2\varphi\, \cosh\left(\frac{p}{2m}\right) + f_q\, \frac{p}{m} - f_p \nabla_q V(q) \tag{73}$$

These can be decomposed along Eqs. (61) and (62), with functions

$$\psi(\dot{q},\dot{p};q,p) = 2\varphi\, \lambda\left(\frac{\dot{p}}{2\varphi}\right) + 2\varphi \quad \text{and} \quad \psi^\star(f_q, f_p; q, p) = 2\varphi\left(\cosh f_p - 1\right) \tag{74}$$

giving the required structure of (32).

5 Conclusions

We have followed the tradition of establishing structural facts about the macroscopic evolution towards equilibrium from symmetries in the dynamical fluctuations. Our case was that of identifying the appropriate fluctuation symmetry that yields (nonlinear) gradient flow and (generalized) GENERIC. The latter are equations where a gradient flow is added to the Hamiltonian part in the evolution. Such evolutions occur when apart from underdamped translational motion of particles there is also a reaction mechanism, such as resetting of momentum, friction or dissipative Langevin forces. We have given the dynamical fluctuation functions from which the structure of the zero-cost flow can be derived. An essential ingredient here is the decomposition of the Lagrangian in the path-space action in its entropic and frenetic contributions [36]. The entropic part is antisymmetric under time-reversal. The frenetic part is the time-symmetric counterpart and contains the nonlinear mobility governing the speed at which the free energy is going to decrease.

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