

the microscopic states of macroscopic systems to such interactions with their environments strongly indicates that simultaneously existing *opposite arrows of time* in different regions of the Universe would be inconsistent with one another. This universality of the arrow of time seems to be its most important property. Time asymmetry has therefore been regarded as a global *symmetry breaking*. However, such a conclusion would *not* exclude the far more probable situation of thermal equilibrium.

Lawrence Schulman (1999) has challenged the usual assumption of a universal arrow of time by suggesting explicit counterexamples. Most of them are indeed quite illustrative in emphasizing the role of initial or final conditions, but they appear unrealistic in our Universe (see Zeh 2005b). The situation is similar to the symmetric boundary conditions suggested by Wheeler and Feynman in electrodynamics, and discussed in Sect. 2.4. Local final conditions at the present stage of the Universe or in the near future can hardly be retro-caused by a low entropy condition at the big crunch (see also Casati, Chirikov and Zhirov 2000), but may be essential during a conceivable recontraction era of the Universe (see Sect. 5.3).

In order to reverse the thermodynamical arrow of time in a bounded system, it would not therefore suffice to “go ahead and reverse all momenta” in the system itself, as ironically suggested by Boltzmann as an answer to Loschmidt. In an interacting Laplacean universe, the Poincaré cycles of its subsystems could in general only be those of the whole Universe, since their exact Hamiltonians must always depend on their time-dependent environment.

Time reversal including thermodynamical aspects has been achieved even in practice for very weakly interacting spin waves (Rhim, Pines and Waugh 1971). The latter can be regarded as isolated systems to a very good approximation (similar to electromagnetic waves in the absence of absorbers), while allowing a sudden sign reversal of their spinor Hamiltonian in order to simulate time reversal ($dt \rightarrow -dt$). These spin wave experiments demonstrate that a closed system in thermodynamical equilibrium may preserve an arrow of time in the form of *hidden correlations*. When a closed system has reached macroscopic equilibrium, it *appears* T -symmetric, although its fine-grained information determines the distance and direction in time to its low-entropy state in the past (see also the Appendix for a numerical example). In contrast to such rare almost-closed systems, generic ones are strongly affected by Borel's argument, and *cannot* be reversed by local manipulations.

3.2 Zwanzig's General Formalism of Master Equations

Boltzmann's *Stoßzahlansatz* (3.6) for μ -space distributions and the master equation (3.31) for coarse-grained Γ -space distributions can thus be understood in a similar way. They describe the transformation of *special* macroscopic states into more probable ones, whereby the higher information con-

tent of the former is transformed into macroscopically irrelevant information. There are many other master equations based on the same strategy, and designed to suit various purposes. Zwanzig (1960) succeeded in formalizing them in a general and instructive manner that also reveals their analogy with retarded electrodynamics as another manifestation of the arrow of time – see (3.40)–(3.49) below.

The basic concept of Zwanzig’s formalism is defined by idempotent mappings \hat{P} , acting on probability distributions $\rho(p, q)$:

$$\rho \rightarrow \rho_{\text{rel}} := \hat{P}\rho, \quad \text{with} \quad \hat{P}^2 = \hat{P} \quad \text{and} \quad \rho_{\text{irrel}} := (1 - \hat{P})\rho. \quad (3.32)$$

Their meaning will be illustrated by means of several examples below, before explaining the dynamical formalism. If these mappings *reduce* the information content of ρ to what is then called its ‘relevant’ part ρ_{rel} , they may be regarded as a *generalized coarse-graining*. In order to interpret ρ_{rel} as a probability density again, one has to require its non-negativity and, for convenience,

$$\int \rho_{\text{rel}} dp dq = \int \rho dp dq = 1, \quad (3.33)$$

that is,

$$\int \rho_{\text{irrel}} dp dq = \int (1 - \hat{P})\rho dp dq = 0. \quad (3.34)$$

Reduction of information means

$$S_{\Gamma}[\hat{P}\rho] \geq S_{\Gamma}[\rho] \quad (3.35)$$

(or similarly for any other measure of ensemble entropy).

Using this concept, Lewis’ master equation (3.31), for example, may be written in the generalized form

$$\left\{ \frac{\partial \rho_{\text{rel}}}{\partial t} \right\}_{\text{master}} := \frac{\hat{P}e^{-i\hat{L}\Delta t} \rho_{\text{rel}} - \rho_{\text{rel}}}{\Delta t}. \quad (3.36)$$

It would then describe a monotonic increase in the corresponding entropy $S[\rho_{\text{rel}}]$. In contrast to Zwanzig’s approach, to be described below, phenomenological master equations such as Lewis’s unifying principle have often been meant to describe a *fundamental* indeterminism that would replace reversible Laplacean determinism.

In most applications, Zwanzig’s idempotent operations \hat{P} are linear and Hermitean with respect to the inner product for probability distributions defined above (3.27). In this case they are projection operators, which preserve only some ‘relevant component’ of the original information. If such a projection obeys (3.33) for every ρ , it must leave the equipartition invariant, $\hat{P}1 = 1$, as can be shown by writing down the above-mentioned inner product of this equation with an *arbitrary* distribution ρ and using the hermiticity of \hat{P} .

Zwanzig's dynamical formalism may also be useful for non-Hermitean or even non-linear idempotent mappings \hat{P} (see Lewis 1967, Willis and Picard 1974). These mappings are then not projections any more: they may even *create new information*. A trivial example for the creation of information is the nonlinear mapping of all probability distributions onto a fixed one, $\hat{P}\rho := \rho_0$ for all ρ , regardless of whether or not they contain a component proportional to ρ_0 . The physical meaning of such generalizations of Zwanzig's formalism will be discussed in Sects. 3.4 and 4.4. In the following we shall consider information-reducing mappings.

Zwanzig's 'projection' concept is deliberately kept general in order to permit a wealth of applications. Examples introduced so far are coarse-graining, $\hat{P}_{\text{cg}}\rho := \rho^{\text{cg}}$, as defined in (3.28), and the neglect of correlations between particles by means of μ -space densities:

$$\hat{P}_\mu\rho(p, q) := \prod_{i=1}^N \frac{\rho_\mu(\mathbf{p}_i, \mathbf{q}_i)}{N},$$

with

$$\rho_\mu(\mathbf{p}, \mathbf{q}) := \sum_{i=1}^N \int \rho(p, q) \delta^3(\mathbf{p} - \mathbf{p}_i) \delta^3(\mathbf{q} - \mathbf{q}_i) dp dq. \quad (3.37)$$

(As before, boldface letters represent three-dimensional vectors, while p, q is a point in Γ -space.) The latter example defines a *non-linear* though information-reducing 'Zwanzig projection'. Most arguments applying to linear operators \hat{P} remain valid in this case when applied to the linearly resulting μ -space distributions $\rho_\mu(\mathbf{p}, \mathbf{q})$ (which do not live in Γ -space) rather than to their products $\hat{P}_\mu\rho(p, q)$ (which do). In quantum theory, this approach is related to the Hartree or mean field approximation. Boltzmann's 'relevance concept', which, when written as a Zwanzig projection, would map real states onto products of *smooth* μ -space distributions, can then be written as $\hat{P}_{\text{Boltzmann}} = \hat{P}_\mu\hat{P}_{\text{cg}}$. An obvious generalization of $\hat{P}_{\text{Boltzmann}}$ can be defined by a projection onto two-particle correlation functions. In this way, a complete hierarchy of relevance concepts in terms of *n-point functions* (equivalent to a cluster expansion) can be defined.

A particularly important concept of relevance, that is often not even noticed, is *locality* (see, e.g., Penrose and Percival 1962). It is required in order to define entropy as an extensive quantity – in accordance with the phenomenological equation (3.1) and with the concept of an entropy *density* $s(\mathbf{r})$, such that $S = \int s(\mathbf{r})d^3r$. The corresponding Zwanzig projection of locality may be symbolically written as

$$\hat{P}_{\text{local}}\rho := \prod_k \rho_{\Delta V_k}. \quad (3.38)$$

The RHS here is meant to describe the neglect of all statistical correlations beyond a distance defined by the size of volume elements ΔV_k . The probability distributions $\rho_{\Delta V_k}$ would here be defined by integrating over all external

degrees of freedom. The volume elements have to be chosen large enough to contain a sufficient number of particles in order to preserve dynamically relevant short range correlations (as required for real gases, for example). In order to allow volume elements ΔV_k with physically open boundaries, their probability distributions $\rho_{\Delta V_k}$ in (3.38) have to admit variable particle number (density fluctuations) – as in a grand canonical ensemble.

Locality is presumed, in particular, when writing (3.1) in its differential (local) form as a ‘continuity inequality’ for the entropy density $s(\mathbf{r}, t)$,

$$\frac{\partial s}{\partial t} + \text{div} \mathbf{j}_s \geq 0, \quad (3.39)$$

with an entropy current density $\mathbf{j}_s(\mathbf{r}, t)$. This form allows the definition of phenomenological entropy-producing (hence positive) terms on the RHS in order to replace the inequality by an *equation* (see Landau and Lifschitz 1959 or Glansdorff and Prigogine 1971). An example is the source term $\kappa(\nabla T)^2/T^2$ in the case of heat conduction, where κ is the heat conductivity.

The general applicability of (3.39) demonstrates that the concept of *physical entropy* is always based on the neglect of nonlocal correlations. Therefore, the production of entropy can be usually understood as the transformation of local information into nonlocal correlations (as depicted in Fig. 3.1). This description is in accordance with the conservation of ensemble entropy (determinism) *and* with intuitive causality. The Second Law thus depends crucially on the dynamical irrelevance of microscopic correlations *for the future* (as assumed in the *Stoßzahlansatz*, for example). Since this ‘microscopic causality’ cannot be observed as easily and directly as the causal correlations which define retardation of macroscopic radiation, its validity under all circumstances has been questioned (Price 1996). However, it is not only indirectly confirmed by the success of the *Stoßzahlansatz*, but also (in its quantum mechanical form – see Sect. 4.2) by the validity of a Sommerfeld radiation condition (see Sect. 2.1) for microscopic scattering experiments, or by the validity of exponential decay (Sect. 4.5).

The Zwanzig projection of locality is again ineffective on real states, which are always local in the sense of defining the states of all their subsystems. Therefore, applying \hat{P}_{local} to an individual state (a δ -function or sum of them) would not lead to a non-singular entropy S_Γ . This will drastically change in quantum mechanics, because it is kinematically non-local (Chap. 4).

As already mentioned on p. 55, coarse-graining as a relevance concept may also enter in a hidden form, corresponding to its nontrivial limit $\Delta V_\Gamma \rightarrow 0$, by considering only *non-singular measures* on phase space (thus excluding δ -functions). This strong idealization may be mathematically signalled by the ‘unitary inequivalence’ of the original Liouville equation and the master equations resulting in this limit (see Misra 1978 or Mackey 1989).

Further examples of Zwanzig projections will be defined throughout the book, in particular in Chap. 4 for quantum mechanical applications, where the relevance of locality leads to the important concept of decoherence. Dif-

ferent schools and methods of irreversible thermodynamics may even be distinguished according to the concepts of relevance which they are using, and which they typically regard as 'natural' or 'fundamental' (see Grad 1961).

However, the mere *conceptual* foundation of a relevance concept ('paying attention' only to certain aspects) is insufficient for justifying its *dynamical* autonomy in the form of a master equation (3.36) – see the Appendix for an explicit example. Locality *is* usually dynamically relevant in this sense because of the locality of all interactions. This dynamical locality is essential even for the very concept of physical *systems*, including those of local observers as the ultimate referees for what is relevant.

Zwanzig reformulated the exact Hamiltonian dynamics for ρ_{rel} regardless of any specific choice of \hat{P} instead of simply *postulating* a phenomenological master equation (3.36) in analogy to Boltzmann or Lewis. It can then in general not be autonomous⁵, that is, of the form $\partial\rho_{\text{rel}}/\partial t = f(\rho_{\text{rel}})$, but has to be written as

$$\frac{\partial\rho_{\text{rel}}}{\partial t} = f(\rho_{\text{rel}}, \rho_{\text{irrel}}) \quad (3.40)$$

in order to eliminate ρ_{irrel} by means of certain assumptions. The procedure is analogous to the elimination of the electromagnetic degrees of freedom by means of the condition $A_{\text{in}}^{\mu} = 0$ when deriving a retarded action-at-a-distance theory (Sect. 2.2). In both cases, empirically justified boundary conditions which specify a time direction are assumed to hold for the degrees of freedom that are to be eliminated.

To this end the Liouville equation $i\partial\rho/\partial t = \hat{L}\rho$ is decomposed into its relevant and irrelevant parts by multiplying it by \hat{P} or $1 - \hat{P}$, respectively:

$$i\frac{\partial\rho_{\text{rel}}}{\partial t} = \hat{P}\hat{L}\rho_{\text{rel}} + \hat{P}\hat{L}\rho_{\text{irrel}}, \quad (3.41a)$$

$$i\frac{\partial\rho_{\text{irrel}}}{\partial t} = (1 - \hat{P})\hat{L}\rho_{\text{rel}} + (1 - \hat{P})\hat{L}\rho_{\text{irrel}}. \quad (3.41b)$$

This corresponds to representing the Liouville operator by a matrix of operators

$$\hat{L} = \begin{pmatrix} \hat{P}\hat{L}\hat{P} & \hat{P}\hat{L}(1 - \hat{P}) \\ (1 - \hat{P})\hat{L}\hat{P} & (1 - \hat{P})\hat{L}(1 - \hat{P}) \end{pmatrix}. \quad (3.42)$$

Equation (3.41b) for ρ_{irrel} , with $(1 - \hat{P})\hat{L}\rho_{\text{rel}}$ regarded as an inhomogeneity, may then be formally solved by the method of the variation of constants (interaction representation). This leads to

$$\rho_{\text{irrel}}(t) = e^{-i(1-\hat{P})\hat{L}(t-t_0)}\rho_{\text{irrel}}(t_0) - i \int_0^{t-t_0} e^{-i(1-\hat{P})\hat{L}\tau} (1 - \hat{P})\hat{L}\rho_{\text{rel}}(t - \tau) d\tau, \quad (3.43)$$

⁵ In mathematical physics, 'autonomous dynamics' is often defined as the absence of any explicit time dependence in the dynamics – regardless of whether it is fundamental or caused by a time-dependent environment.

as may be confirmed by differentiation.

If $t > t_0$, (3.43) is analogous to the *retarded form* (2.9) of the boundary value problem in electrodynamics. In this case, $\tau \geq 0$, and $\rho_{\text{rel}}(t - \tau)$ may be interpreted as an advanced source for the ‘retarded’ $\rho_{\text{irrel}}(t)$. Substituting this formal solution (3.43) into (3.41a) leads to three terms on the RHS, viz.,

$$\begin{aligned} i \frac{\partial \rho_{\text{rel}}(t)}{\partial t} &= \text{I} + \text{II} + \text{III} \\ &\equiv \hat{P} \hat{L} \rho_{\text{rel}}(t) + \hat{P} \hat{L} e^{-i(1-\hat{P})\hat{L}(t-t_0)} \rho_{\text{irrel}}(t_0) - i \int_0^{t-t_0} \hat{G}(\tau) \rho_{\text{rel}}(t - \tau) d\tau . \end{aligned} \quad (3.44)$$

The integral kernel of the last term,

$$\hat{G}(\tau) := \hat{P} \hat{L} e^{-i(1-\hat{P})\hat{L}\tau} (1 - \hat{P}) \hat{L} \hat{P} , \quad (3.45)$$

corresponds to the retarded Green’s function of Sect. 2.1.

Equation (3.44) is exact and, therefore, cannot yet describe time asymmetric dynamics. Since it forms the first step in this derivation of master equations, it is known as a *pre-master equation*. The meanings of its three terms are illustrated in Fig. 3.2. The first one describes the internal dynamics of ρ_{rel} . In Boltzmann’s μ -space dynamics (3.3), it would correspond to $\{\partial \rho_{\mu} / \partial t\}_{\text{free+ext}}$. It vanishes if $\hat{P} \hat{L} \hat{P} = 0$ (as is often the case).⁶

The second term of (3.44) is usually omitted by presuming the absence of irrelevant initial information: $\rho_{\text{irrel}}(t_0) = 0$. If *relevant* information happens to be present initially, it can then be dynamically transformed into irrelevant information. (Because of the asymmetry between \hat{P} and $1 - \hat{P}$, irrelevant information would have to be measured by $-S_{\Gamma}[\rho] + S_{\Gamma}[\rho_{\text{rel}}]$ rather than by $-S_{\Gamma}[\rho_{\text{irrel}}]$.)

The vital third term is *non-Markovian* (non-local in time), as it depends on the whole time interval between t_0 and t . Its retarded form (valid for $t > t_0$) is compatible with the intuitive concept of causality. This term becomes approximately *Markovian* if $\rho_{\text{rel}}(t - \tau)$ varies slowly for a small ‘relaxation time’ τ_0 during which $\hat{G}(\tau)$ becomes negligible for reasons to be discussed. In (3.44), $\hat{G}(\tau)$ may then be regarded to lowest order as being proportional to a δ -function in τ . This assumption is also contained in Boltzmann’s *Stoßzahlansatz*, where it means that correlations arising by scattering

⁶ Since the (indirectly acting) non-trivial terms contribute only in second and higher orders of time, the time derivative defined by the master equation (3.36) would then vanish in the limit $\Delta t \rightarrow 0$. This corresponds to what in quantum theory is known as the *quantum Zeno paradox* (Misra and Sudarshan 1977), also called *watched pot behavior* or the *watchdog effect*. It describes an *immediate* loss of information from the irrelevant channel (or its dynamically relevant parts – see later in the discussion), such that it has no chance of affecting its relevant counterpart any more. Fast information loss may be caused by a strong coupling to the environment, for example. Since this efficiency depends on the energy level density (Joos 1984), the Zeno effect is relevant mainly in quantum theory.

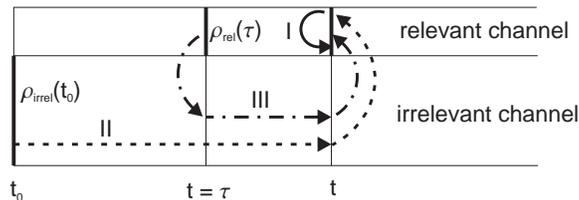


Fig. 3.2. Retarded form of the exact dynamics for the relevant information according to Zwanzig's *pre-master equation* (3.24). In addition to the instantaneous direct interaction I, there is the contribution II arising from the 'incoming' irrelevant information, and the retarded term III in analogy to electromagnetic action at a distance, resulting from 'advanced sources' in the whole time interval between t_0 and t (cf. the left part of Fig. 2.2)

are irrelevant for the forward dynamics of ρ_{rel} . In analogy to retarded electromagnetic forces, this third term of the pre-master equation then assumes the form of an effective direct interaction between the relevant degrees of freedom (though instantaneous in this nonrelativistic treatment). In electrodynamics, the charged sources would represent the 'relevant' variables, while their effective interactions act 'at a distance'. In statistical physics, this 'interaction' describes the dynamics of *ensembles*.

The Markovian approximation may be understood by means of assumptions which simultaneously explain the applicability of the initial condition $\rho_{\text{irrel}} \approx 0$ at *all* times – provided it holds in an appropriate form in the very distant past. This is again analogous to the condition in electrodynamics that A_{in}^μ either vanishes or can be well understood in terms of a limited number of known or at least plausible sources *at all times*.

Consider the action of the operator $(1 - \hat{P})\hat{L}\hat{P}$ appearing on the RHS of the kernel (3.45). Because of the structure of a typical Liouville operator, it transforms information from ρ_{rel} only into *specific* parts of ρ_{irrel} . In the scattering theory of complex objects, similar formal parts are called *doorway states* (Feshbach 1962). For example, if the Hamiltonian contains no more than two-particle interactions, $\hat{L}\hat{P}_\mu$ creates two-particle correlations. Only the subsequent application of the propagator $\exp[-i(1 - \hat{P})\hat{L}\tau]$ is then able to produce states 'deeper' in the irrelevant channel (many-particle correlations in this case) – see Fig. 3.3. Recurrence from the depth of the irrelevant channel is related to Poincaré recurrence times, and may in general be neglected (as exemplified by the success of Boltzmann's collision equation). If the *relaxation time*, now defined as the time required for the transfer of information from the doorway 'states' into deeper parts of the irrelevant channel, is of the order τ_0 , say, one may assume $\hat{G}(\tau) \approx 0$ for $\tau \gg \tau_0$, as required for the Markovian δ -function approximation $\hat{G}(\tau) \approx \hat{G}_0\delta(\tau)$.

Essential for the validity of this approximation is the large information capacity of the irrelevant channel (similar to that of the electromagnetic field

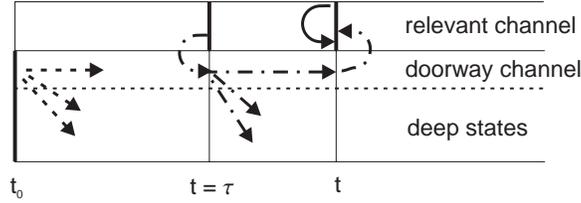


Fig. 3.3. The large information capacity of the irrelevant channel and the specific structure of the interaction together enforce the disappearance of information into the depth of the irrelevant channel if an appropriate initial condition holds

in Chap. 2, but far exceeding it). For example, correlations between particles may describe far more information than the single-particle distribution ρ_μ . A fundamental *cosmological* assumption,

$$\rho_{\text{irrel}}(t_0) = 0, \quad (3.46)$$

at a time t_0 in the *finite* past (similar to the cosmological $A_{\text{in}}^t = 0$ at the big bang) is therefore quite powerful – even though it is a *probable* condition. Any irrelevant information formed later from the initial ‘information’ contained in $\rho_{\text{rel}}(t_0)$ (that is, from any specification of the initial state) may be expected to remain dynamically negligible in (3.44) for a very long time. It would be essential, however, for calculating backwards in time under these conditions.

The assumption $\rho_{\text{irrel}} \approx 0$ has thus to be understood in a *dynamical* sense: any newly formed contribution to ρ_{irrel} must remain irrelevant in the ‘forward’ direction of time. The dynamics for ρ_{rel} may then appear autonomous (while it cannot be exact). For example, all correlations between subsystems seem to require advanced local *causes*, but no similar (retarded) *effects*. Otherwise they would be interpreted as a *conspiracy*, the deterministic version of *causae finales*.

Under these *assumptions*, one obtains from (3.44), as a first step, the non-Markovian dynamics

$$\frac{\partial \rho_{\text{rel}}(t)}{\partial t} = - \int_0^{t-t_0} \hat{G}(\tau) \rho_{\text{rel}}(t-\tau) d\tau. \quad (3.47)$$

The upper boundary of the integral can here be replaced by a constant T that is large compared to τ_0 , but small compared to any (theoretical) recurrence time for $\hat{G}(\tau)$. If $\rho_{\text{rel}}(t)$ is now assumed to remain constant over time intervals of the order of the relaxation time τ_0 , corresponding to an already prevailing partial (e.g., local) equilibrium, one obtains the time-asymmetric Markovian limit:

$$\frac{\partial \rho_{\text{rel}}(t)}{\partial t} \approx -\hat{G}_{\text{ret}} \rho_{\text{rel}}(t), \quad (3.48)$$

with

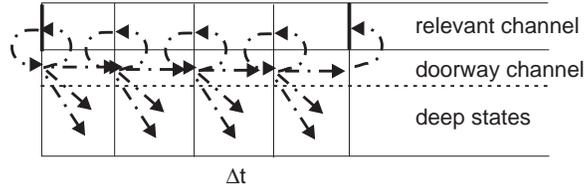


Fig. 3.4. The master equation represents ‘alternating dynamics’, usually describing a monotonic loss of relevant information

$$\hat{G}_{\text{ret}} := \int_0^T \hat{G}(\tau) d\tau. \quad (3.49)$$

A similar nontrivial limit of vanishing retardation ($\tau_0 \rightarrow +0$) led to the LAD equation with its asymmetric radiation reaction in Sect. 2.3. The integral (3.49) could be formally evaluated when inserting (3.45), but it is usually more conveniently computed after this operator has been applied to a specific $\rho(t)$. (See the explicit evaluation for discrete quantum mechanical states in Sect. 4.1.2.)

The autonomous master equation (3.48) again describes *alternating dynamics* of the type (3.36) (see Fig. 3.4). Irrelevant information is disregarded after short time intervals Δt (now representing the relaxation time τ_0). If \hat{P} only *destroys* information, the master equation describes never-decreasing entropy:

$$\frac{dS_{\Gamma}[\rho_{\text{rel}}]}{dt} \geq 0. \quad (3.50)$$

This corresponds to a *positive* operator \hat{G}_{ret} (as can most easily be shown by means of the *linear* measure of entropy).

A phenomenological probability-conserving Markovian master equation for a system with ‘macroscopic states’ described by a (set of) ‘relevant’ variable(s) α , that is, $\rho_{\text{rel}}(t) \equiv \rho(\alpha, t)$ (see also Sects. 3.3 and 3.4) can be written in the general form

$$\frac{\partial \rho(\alpha, t)}{\partial t} = \int [w(\alpha, \alpha') \rho(\alpha', t) - w(\alpha', \alpha) \rho(\alpha, t)] d\alpha'. \quad (3.51)$$

The transition rates $w(\alpha, \alpha')$ here define the phenomenological operator \hat{G}_{ret} by means of its integral kernel $\hat{G}_{\text{ret}}(\alpha, \alpha') = -w(\alpha, \alpha') + \delta(\alpha, \alpha') \int w(\alpha, \alpha'') d\alpha''$. They often satisfy a generalized time inversion symmetry,

$$\frac{w(\alpha, \alpha')}{\sigma(\alpha)} = \frac{w(\alpha', \alpha)}{\sigma(\alpha')}, \quad (3.52)$$

where $\sigma(\alpha)$ may represent the density of the (‘irrelevant’) microscopic states with respect to the variable α – that is, $\sigma := dn/d\alpha$, where n is the number of microscopic states as a function of α . In this case one may again derive an *H*-theorem, in analogy to (3.12), for the *generalized H-functional*

$$H_{\text{gen}}[\rho(\alpha)] := \int \rho(\alpha) \ln \frac{\rho(\alpha)}{\sigma(\alpha)} d\alpha = \overline{\ln p}. \quad (3.53)$$

The final form on the RHS is appropriate, since the mean probability $p(\alpha)$ for individual microscopic states and for given $\rho(\alpha)$ is then $p(\alpha) = \rho(\alpha)/\sigma(\alpha)$. The entropy defined by $-kH_{\text{gen}}$ is also known as the *relative entropy* of $\rho(\alpha)$ with respect to the measure $\sigma(\alpha)$. The latter is often introduced *ad hoc* as part of a phenomenological description.

Under the approximation $w(\alpha', \alpha) = f(\alpha)\delta'(\alpha - \alpha')$ one now obtains the deterministic ‘drift’ limit of the master equation (3.51) – usually representing the first term of (3.44). It defines the first order of the *Kramers–Moyal expansion* for $w(\alpha, \alpha')$, equivalent to an expansion of $\rho(\alpha', t)$ in terms of powers of $\alpha' - \alpha$ at $\alpha' = \alpha$. The second order, $w(\alpha', \alpha) = f(\alpha)\delta'(\alpha - \alpha') + g(\alpha)\delta''(\alpha - \alpha')$, leads to the *Fokker–Planck equation* as the lowest non-trivial approximation that leads to an irreversible equation (see de Groot and Mazur 1962, Röpke 1987). In this respect, it is analogous to the LAD equation as the lowest non-trivial order in the Taylor expansion of the Caldirola equation (2.31). A master equation is generally equivalent to a (stochastic) *Langevin equation* for *individual* macroscopic trajectories $\alpha(t)$ which may form a dynamical ensemble represented by $\rho(\alpha, t)$.

In contrast to the Liouville equation (3.26), the master equation (3.48) or (3.36) cannot be unitary with respect to the inner product for probability distributions defined above (3.27). While total probability must be conserved by these equations, that of the individual trajectories *cannot* (see also Sect. 3.4). Information-reducing master equations describe an indeterministic evolution, which in general only determines an ever-increasing ensemble of different *potential* successors for each macroscopic state (such as a point in α -space).⁷ As discussed above, this macroscopic indeterminism is compatible with microscopic determinism if that information which is transformed from relevant

⁷ The frequently used picture of a ‘fork’ in configuration space, characterizing a dynamical indeterminism, may be misleading, since it seems to imply unique predecessors. This would be wrong, as can be recognized, for example, in an equilibrium situation. In the case of a stochastic dynamical law that is defined on a finite set of states, a state must in general also have different possible predecessors, corresponding to an inverse fork. Inverse forks by themselves would represent a pure forward determinism (a ‘semigroup’, that may describe *attractors*). All these structures are meant to characterize the *dynamical law*. They are neither properties of the (f)actual history (which is assumed to evolve along a *definite* trajectory regardless of the nature of the dynamical law), nor of an evolving ensemble that represents a specific state of knowledge.

However, only dynamically unique predecessors may give rise to recordable histories (consisting of ‘facts’ that are redundantly documented). The *historical nature* of our world is thus based on a uniquely determined or even overdetermined macroscopic past – see also footnote 1 of Chap. 2, Fig. 3.8, and Sect. 3.5. A macroscopic history that was completely determined from its macroscopic *past* would be in conflict with the notion of an (apparent) free will.