

Brussels-Austin Nonequilibrium Statistical Mechanics in the Early Years: Similarity Transformations between Deterministic and Probabilistic Descriptions

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Abstract

The fundamental problem on which Ilya Prigogine and the Brussels-Austin Group have focused can be stated briefly as follows. Our observations indicate that there is an arrow of time in our experience of the world (e.g., decay of unstable radioactive atoms like Uranium, or the mixing of cream in coffee). Most of the fundamental equations of physics are time reversible, however, presenting an apparent conflict between our theoretical descriptions and experimental observations. Many have thought that the observed arrow of time was either an artifact of our observations or due to very special initial conditions. An alternative approach, followed by the Brussels-Austin Group, is to consider the observed direction of time to be a basic physical phenomenon and to develop a mathematical formalism that can describe this direction as being due to the dynamics of physical systems. In part I of this essay, I review and assess an attempt to carry out an approach that received much of their attention from the early 1970s to the mid 1980s. In part II, I will discuss their more recent approach using rigged Hilbert spaces.

Keywords: Thermodynamics, Statistical Mechanics, Dynamical Systems, Probability, Arrow of Time

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How and to what extent the irreversible phenomena observed in the macroscopic domain can be reconciled with the reversible dynamical laws of classical (or quantum) mechanics is the fundamental question of statistical mechanics (Misra 1978, p. 1627).

1 Introduction

The work of Ilya Prigogine and his group is difficult to understand and assess, being highly mathematical in nature. Moreover although their fundamental intuitions have remained essentially unchanged over the course of several decades, the approach has changed with time making their views difficult to pin down with precision. The ideas Prigogine and his colleagues have been pursuing in various forms were sketched in his (1962). He along with George, Henin and Rosenfeld gave the earliest mathematically detailed description in their (1973; see also George 1973a, 1973b).

The core idea is the following. The conventional approach to describing physical systems within classical mechanics (CM) relies on a representation of states ω (e.g. of particles) as points in an appropriate state space Ω . This means that the dynamics of a system are derivable from the time-parameterized trajectories of these points. The equations governing the dynamics of conservative systems are reversible with respect to time. When there are too many states involved to make solving these equations feasible (as in gases or liquids), coarse-grained averages—*i.e.* macrolevel averages ignoring microlevel details (so-called fine-grained level)—are used to develop a statistical picture of how the system behaves rather than focusing on the behavior of individual states. In contrast the Brussels-Austin Group argues these systems should be approached in terms of models based on distributions ρ over an appropriate state space. These distribution functions may be understood in terms of the probability density $\rho(\vec{q}_1, \vec{q}_2, \vec{q}_3, \dots, \vec{p}_1, \vec{p}_2, \vec{p}_3, \dots, t)$ of finding a set of molecules (say) with coordinates $\vec{q}_1, \vec{q}_2, \vec{q}_3, \dots$ and momenta $\vec{p}_1, \vec{p}_2, \vec{p}_3, \dots$ at time t on the relevant energy surface and are analogous to the microcanonical distribution. In the Brussels-Austin approach, the dynamics of a system is calculated from *distribution functions* directly. The equations governing the dynamics of these distributions are generally *time-irreversible*. In addition interpreting the distribution functions as probability densities suggests that macroscopic classical statistical mechanics models are irreducibly probabilistic. This would mean that probabilities are as much an ontologically fundamental element of the macroscopic world, as successfully described by physics, as they are usually taken to be for the microscopic world of quantum mechanics (QM).

The extent to which the Brussels-Austin program, as just sketched, is distinguishable from a coarse-grained approach to statistical mechanics is a delicate question. As this two-part essay develops, I will point out how their work differs from typical coarse-grained approaches. My task in part I will be to review Prigogine and co-workers' motivations (§2) and then discuss their various approaches to nonequilibrium systems, focusing on the period from the 1960s to

the mid 1980s, covering their subdynamics and similarity transformation approaches (§§3-4). Part II will focus on the more recent rigged Hilbert space approach.

2 Motivations

A crucial motivation is the question of how classical dynamical systems, described in conventional CM by deterministic, time-reversible equations of motion, are related to time-irreversible processes. The central questions are: What connections, if any, exist between these two types of systems; and Why is it we never observe such processes going “in reverse?”

A key concern is the status of the second law of thermodynamics: When a constraint internal to a closed system is removed, the total entropy must increase or at best stay constant. As one of the fundamental laws of conventional equilibrium thermodynamics, it is valid only at or near *thermodynamic equilibrium*. Prigogine and his colleagues believe that some appropriate generalization of the second law should be applicable to nonequilibrium systems as well.

Typically coarse-grained descriptions of systems involve calculating macro-level averages of quantities over finite volumes and are considered to provide less specific information than descriptions involving points in state space. Probabilistic processes in such models are irreversible, but are usually interpreted as reducible; that is to say, the probabilities are considered to be consequences of our calculation techniques and measurement limitations. Irreversibility could then be understood as a consequence of a coarse-grained description rather than as a fundamental feature of systems.

The second law is considered time-irreversible in so far as the process of entropy increase cannot be reversed (a cube of ice melting and diffusing in a glass of tea does not reconstitute itself into a cube of ice again). If the second law is taken to be a fundamental law (not a consequence of coarse-grained descriptions), then there is a puzzling conflict with our fundamental time-symmetric equations, a particularly sharp conflict in the case of conservative systems. Thus,

[T]he elucidation of the relation between conservative and dissipative dynamical systems necessarily involves a clarification of the relation between deterministic dynamics and probabilities. Because of the close relation that exists between entropy and probability, once this is clarified the relation that exists between dynamics and the second law will also be made clear (Nicolis and Prigogine 1989, p. 199).

In all fundamental theories (be it classical dynamics, quantum mechanics or relativity theory) entropy is conserved as a result of the unitary (or measure-preserving) character of the evolution, in flagrant contradiction with the formulation of the second law of thermodynamics. As a result, the second law has usually been regarded as an approximation or even as being subjective in character. By

contrast, in the approach to the problem of irreversibility developed by us, the law of entropy increase and, therefore, the existence of an “arrow of time” is taken to be a fundamental fact. The task of a satisfactory theory of irreversibility is thus conceived as the study of the fundamental change in the conceptual structure of dynamics, which the law of entropy increase implies (Misra and Prigogine 1983, p. 421).

We can distinguish two types of irreversibility: *extrinsic* and *intrinsic* (e.g. Atmanspacher, Bishop and Amann 2002). Extrinsic irreversibility is irreversible behavior of a physical system due to its interaction with an environment, where in the absence of an environment, the system itself would be reversible. Examples of extrinsic irreversibility are given by any open-system evolution described by a master equation. By contrast, intrinsic irreversibility refers to irreversible behavior originating in the dynamics of a physical system without explicit reference to an environment. An example of intrinsic irreversibility would be kaon decay. In contrast to most views on statistical mechanics (SM), the Brussels-Austin Group believes that intrinsic irreversibility is fundamental and has been searching for an intrinsically irreversible formulation of SM.¹

3 Subdynamics and Similarity Transformations

3.1 Koopman Formulation of Classical Mechanics and its Extension

Most of the Brussels-Austin Group’s results are developed in a Hilbert space (HS) in part due to matters of elegance as well as out of a desire to unify CM and QM within one formalism. They relied heavily upon Koopman’s extension of HS and linear transformations to the study of steady n -dimensional fluid flow with positive density (Koopman 1931). Originally, Koopman studied the dynamics of state space volumes, where the elements ϕ of $L^\infty(\Omega)$ are defined on the state space Ω (the natural dual space being $L^1(\Omega)$). In CM, physical observables (e.g. energy) are usually associated with real-valued functions defined on Ω . Koopman’s formulation generalizes this feature in analogy with QM by associating linear operators on $L^\infty(\Omega)$ with physical observables. Thus the expectation value of an observable corresponding to the operator F is defined as $(\phi, F\phi)$, where $F(\phi)(\omega) = f(\omega)\phi(\omega)$ is unitary and $f : \Omega \rightarrow \mathcal{R}$ is defined on state space points $\omega \in \Omega$ referring to states.

An important relevant example is Liouville’s equation describing the evolution of a distribution function ρ in state space. Liouville’s equation can be converted to an operator equation with the unitary² form $U_t = e^{-iLt}$ and, in

¹Their original focus was on open systems. More recently they have focused on closed systems (Part II).

²Koopman uses the Hilbert space generator representation for U_t which is formulated for elements of L^2 . This has led to some confusion as to what mathematical spaces to which Koopman’s formulation is applicable.

Hamiltonian form,

$$L = \sum_k \left[\frac{\partial H}{\partial p_k} \frac{\partial}{\partial q_k} - \frac{\partial H}{\partial q_k} \frac{\partial}{\partial p_k} \right], \quad (1)$$

where (1) is the Poisson bracket, p and q representing generalized momenta and positions respectively, and t representing time. The operator U_t is self-adjoint and is generally unbounded on $L^\infty(\Omega)$. The physical interpretation of the Koopman formulation of Liouville’s equation is the same as in CM. In the so-called Lagrangian picture, the motion of state space points can be treated like a flowing fluid. In both conventional SM and the modified Koopman formulation, Liouville’s equation describes the evolution of the distribution ρ as it moves through state space from the perspective of an observer at rest.

Koopman’s formalism is defined on the state space $L^\infty(\Omega)$. The Brussels-Austin Group wanted to use this formalism to study the evolution of state space points themselves and, so, extended Koopman’s formalism to the space $L^2_\mu(\Omega)$ (square integrable functions using measure μ ; e.g. Misra 1978), although no formal justification for these extensions was ever worked out rigorously.

3.2 Subdynamics

The first approach developed in this early phase was called *subdynamics*, the idea being to split the state space $L^2_\mu(\Omega)$ of the system dynamics into distinct thermodynamic and non-thermodynamic subspaces *via* an appropriate projection operator, and then to enumerate the conditions under which the non-thermodynamic subspace made no contribution to the evolution of the thermodynamic features of the system (Prigogine, George and Henin 1969; Prigogine et al. 1973; Obce-mea and Brändas 1983; Dougherty 1993; Karakostas 1996). Karakostas (1996, pp. 383-4) argues that the 1973 version of subdynamics represents a generalization of coarse-graining, in that it merely amounts to a reduced description of the system.³ Ultimately, however, subdynamics turned out to be dependent on the Brussels-Austin conception of the relationship between deterministic dynamics and probabilistic dynamics—e.g. similarity transformations—so I will not say anything more about subdynamics here.

3.3 Similarity Transformations

The second approach developed during this period was based on a similarity transformation Λ mapping a trajectory description of “unstable” classical systems—systems exhibiting exponential trajectory divergence—into a description in terms of probabilistic Markov processes. The existence of such a Λ would then provide a means of translating between the trajectory and the Markov descriptions. In a problematic sense to be discussed below, this would establish an “equivalence” between trajectory and probabilistic descriptions and, hence, an equivalence between time-reversible and time-irreversible dynamics for such

³Versions of subdynamics derived from a Lyapunov variable are not so easily classified as coarse-grainings (see below).

systems. Furthermore, although the amount of information in the trajectory description is supposedly preserved in moving to the probabilistic description, Prigogine and coworkers also claimed that there was new physics contained in the latter description that was not contained in the former. It is this additional physics in the probabilistic description that they believed resulted in new physical features, rendered elements of the trajectory description (e.g. “exact trajectories”) unphysical idealizations.

The technical details may be summarized as follows: When mathematically defined on $L^2_\mu(\Omega)$, the evolution of particular types of Markov processes can be shown to correspond to nonunitary semigroup operators $W_t^* = \Lambda U_t \Lambda^{-1}$ via a similarity transformation $\Lambda : L^2_\mu(\Omega) \rightarrow L^2_\mu(\Omega)$, where Λ is closed, densely defined on $L^2_\mu(\Omega)$ and invertible.⁴ The crucial result is that W_t^* be positivity preserving on the positive t -axis only, guaranteeing that W_t^* leads to a monotonic, time-irreversible approach to a unique final state (conjectured in (Misra, Prigogine and Courbage 1979, p. 12) and proven in (Goodrich, Gustafson and Misra 1980)).⁵ Any system characterized by Λ would then be asymptotically stable: Any initial state will evolve irreversibly to a unique equilibrium distribution as $t \rightarrow \infty$. By contrast in Koopman’s original formulation, dynamical systems are characterized by a unitary group U_t defined for both the positive and negative t -axes, preserving the time reversibility of the governing dynamical equations.⁶

By constructing a nonunitary similarity transformation Λ acting on the distribution function ρ in the trajectory description defined on $L^2_\mu(\Omega)$ at time t , a distribution function in the Markov description is then given by $\rho' = \Lambda\rho$. The time-reversible Liouville equation in Koopman’s original formulation,

$$i\frac{\partial\rho}{\partial t} = U_t\rho, \quad -\infty \leq t \leq \infty, \quad (2)$$

where ρ and U_t are defined on $L^2_\mu(\Omega)$, is then transformed into a time-irreversible equation

$$i\frac{\partial\rho'}{\partial t} = W_t^*\rho', \quad t \geq 0 \quad (3)$$

where W_t^* and ρ' are also defined on $L^2_\mu(\Omega)$. The interpretation of (3) is similar to that of the Liouville equation in the Koopman description: It describes the evolution of the density function ρ' in state space, but only for the positive time direction. The dynamics under U_t is time-reversible. However in (3), the evolution governed by W_t^* is *time-irreversible*. This is the key for time-irreversibility in the similarity transformation approach and leads to the definition of intrinsic

⁴Karakostas (1996) gives a detailed discussion of these and related operators defined in the subdynamics approach developed in (Prigogine *et al.* 1973). The transformation discussed in Karakostas (1996) is related to, but different from the similarity transformation I discuss here as Prigogine and coworkers have made several modifications to their program since publication of (Prigogine *et al.* 1973). For example Λ in this latter publication is star-unitary, but the Λ developed later in the approach I am reviewing is nonunitary.

⁵The proof is not constructive, however, so Λ must still be constructed for every system.

⁶Originally the Brussels-Austin Group treated the operators Λ and W_t^* , along with the distribution ρ , as being defined on SHS. This turns out to be inadequate, however, as I will explain below.

randomness: A model is intrinsically random if there exists a nonunitary Λ such that the unitary group U_t is transformed to the Markov semigroup W_t^* (Goldstein, Misra and Courbage 1981, pp. 114-8; Courbage and Prigogine 1983, p. 2412).

The strategy was to use a nonunitary similarity transformation Λ to move from the trajectory description characterized by U_t to the Markov description characterized by W_t^* . Since similarity transformations preserve all structural features, the hope was that the two descriptions would be shown to be "equivalent" *via* Λ .

3.4 Microentropy Operator

Following a suggestion by Misra (1978), Λ was derived from the so-called *microentropy operator* M , a positive linear operator defined on $L_\mu^2(\Omega)$ that, according to Misra, fulfils the conditions for a *Lyapunov variable*, i.e., a variable that increases monotonically to an asymptotically stable value (Misra 1978; e.g. Hale and Koçak 1991, pp. 277-92).⁷ A system must have at least the property of strong mixing in order for Lyapunov variables to exist. Lyapunov variables can be formally constructed for Kolmogorov or K-flows (1978, pp. 1629-30). Strong mixing is a necessary condition, while being a K-flow is a sufficient condition for the existence of such variables. For unstable systems Misra's proposed that M be identified with an appropriate Lyapunov variable. Later Gustafson showed that the Λ transformation so defined exists only for K-flows (1997, pp. 61-4).

The operator M obeys the following properties (Misra 1978; Brauuss 1984):

- (i) If $\rho \in L_\mu^2(\Omega)$, then $M\rho \in L_\mu^2(\Omega)$.
- (ii) M is nonnegative; that is, $(\rho_t, M\rho_t) > 0$ for all $t \geq 0$ and decreases monotonically to a minimum value for the equilibrium distribution ρ_{eq} , where $\rho_t = U_t\rho$.
- (iii) $d/dt(\rho_t, M\rho_t) \leq 0$ for all $t \geq 0$.

Property (i) expresses closure: M never leads outside $L_\mu^2(\Omega)$. Properties (ii) and (iii) characterize a Lyapunov variable, implying that M is monotonically increasing. Since M is positive, it can be factorized (*i.e.* $M = \Lambda^*\Lambda$), so $\Lambda = M^{\frac{1}{2}}$. Furthermore as Brauuss pointed out, the microentropy operator illuminates the Brussels-Austin definition of intrinsic randomness. Suppose the dynamics for a K-flow in the trajectory description is given by U_t and that M is a Lyapunov variable for this dynamics. Then $(\rho_t, M\rho_t)^{1/2}$ defines a contractive semigroup W_t^* (namely $W_t^* = \Lambda U_t \Lambda^{-1}$), that can act to convert smooth, Hamiltonian trajectories into Brownian trajectories (1985, p. 9-11).

The factorization of M is not unique, however, because in general operators Λ differ by phase factors, where $W_t^* \varphi_\Lambda |\Lambda| = |\Lambda| U_t$ and φ_Λ is the phase factor for Λ . So the class of Λ transformations must be restricted to *admissible factorizations*,

⁷That M be a Lyapunov variable is important for a generalization of the concept of entropy discussed below.

i.e. where $W_t^* \Lambda = \Lambda U_t$ holds (Braunss 1985, 19). Furthermore, there is a practical difficulty in identifying an appropriate positive definite variable serving as a basis for M , there being no constructive guidance for choosing appropriate variables.

Misra's proposal of relating Λ to M also allows Λ to be related to a time operator T for K-flows (Misra 1978; Misra, Prigogine and Courbage 1979; Goldstein, Misra and Courbage 1981). Let \mathcal{H}_0 denote the one-dimensional subspace spanned by constant-valued functions on a given energy surface, P_0 the projections from $L_\mu^2(\Omega)$ onto this subspace, \mathcal{H}_0^\perp the orthogonal complement of \mathcal{H}_0 and P_0^\perp the projections from $L_\mu^2(\Omega)$ onto \mathcal{H}_0^\perp . For dynamical systems that are K-flows, there exists a family of projection operators F_η , $-\infty < \eta < \infty$, with the following properties (Misra 1978, p. 1629):

- (i) $F_\eta \leq F_\kappa$ if $\eta < \kappa$.
- (ii) $\lim_{\eta \rightarrow \infty} F_\eta = P_0^\perp$.
- (iii) $\lim_{\eta \rightarrow -\infty} F_\eta = 0$.
- (iv) F_η is strongly continuous in η .
- (v) $U_t F_\eta U_t^\dagger = F_{\eta+t}$.

Conditions (ii) and (iii) are to be understood in the strong operator limit. It is then possible to construct a self-adjoint operator

$$T = \int_{-\infty}^{\infty} \eta dF_\eta, \quad (4)$$

which has F_η as its spectral family of projections. T is self-adjoint and canonically conjugate to L via the commutation relation $[L, T] = -iI$, where I is the identity operator and the eigenvalues of T are determined by the parameter time t when applied to eigenfunctions of T . Then M can be constructed as a function of T as

$$M = h(T) + \alpha P_0, \quad (5)$$

where $\alpha \geq 0$ and $h(T)$ is an operator defined through the relation

$$(\psi, h(T)\phi) = \int_{-\infty}^{\infty} h(\eta) d(\psi, F_\eta \phi), \quad (6)$$

where ψ, ϕ are vectors in \mathcal{H}_0^\perp and $h(\eta)$ is any monotone decreasing, positive, bounded, continuous and differentiable function, whose derivative is always negative and bounded (Misra 1978, p. 1629). The inner product in (6) is to be understood in the following way. To each vector ψ in \mathcal{H}_0^\perp , there is a corresponding family of functions $\{\psi_n(\eta)\}$, where $n = 1, 2, 3, \dots$ and where $\psi_n(\eta) \in L_\mu^2$, such that

$$(\psi, \phi) = \sum_{n=1}^{\infty} \left(\int_{-\infty}^{\infty} \psi_n^*(\eta) \phi(\eta) d\eta \right). \quad (7)$$

The operator M as defined in (5) satisfies all the properties listed above.

The time operator T associates an “age” or “internal time” with a well defined distribution function $\bar{\rho} \equiv \rho - \rho_{eq}$. If $\bar{\rho}$ is an eigenfunction of T , the corresponding eigenvalue gives the “age” associated with ρ and is determined by an external (i.e. observer’s) time that serves to label the dynamics. If $\bar{\rho}$ is not an eigenfunction of T , but a combination of eigenfunctions corresponding to two or more distinct eigenvalues, then only an “average age” can be associated with ρ (Misra, Prigogine and Courbage 1979, pp. 17-8).

The discovery of a time operator was one of the Brussels-Austin Group’s significant contributions to SM and systems theory (c.f. Atmanspacher and Scheingraber 1987, where an alternative derivation of a time operator is given and compared with the Brussels-Austin version). This “internal time” operator, according to Misra, Prigogine and Courbage, expresses the ‘inherent (but hidden) stochastic and nondeterministic character of the evolution’ of such unstable systems (1979, p.5). It is this hidden ‘stochastic and nondeterministic’ character of the evolution that the change of representation *via* Λ is supposed to reveal.

Furthermore, the existence of Λ leads to the claim that for unstable CM systems, one can find a representation in which the dynamics are irreducibly probabilistic in that Λ transforms a trajectory representation into a probabilistic one, so that unstable classical systems do not possess exact smooth (i.e., everywhere differentiable) trajectories in the probabilistic description (see §3.5 below).

In addition to finding a time-irreversible dynamics, Prigogine and co-workers were also interested in far from equilibrium SM. In conventional equilibrium SM, the concept of entropy is defined at equilibrium. For example starting with the canonical probability distribution, the fine-grained Gibbsian entropy may be expressed as

$$- \int_{\Omega} \rho \ln \rho d\Omega . \quad (8)$$

As a first step toward a conception of entropy valid for nonequilibrium as well as equilibrium cases, Misra proposed a generalization of the conventional definition (8),

$$- \ln(\rho, M\rho) , \quad (9)$$

where ψ represents normalized functions on $L^2_{\mu}(\Omega)$ and

$$\rho(\omega) = |\psi(\omega)|^2, \quad (10)$$

where (10) can be interpreted as the Gibbsian ensemble. Since near equilibrium the thermodynamic entropy of a system increases monotonically until equilibrium is reached, the idea is that any function used to model thermodynamic entropy far from equilibrium should also have the property of increasing monotonically in the neighborhood of a nonequilibrium stable state.⁸ Misra’s sugges-

⁸For example, (8) is not monotonically increasing for Hamiltonian models (in fact it is an invariant of Hamiltonian evolution). A coarse-grained average version of (8) combined with

tion is that functionals like (9) may be interpreted as a nonequilibrium entropy since they monotonically increase with time (1978, p. 1627).⁹

The quantity

$$(\psi, F\psi) = \int_{\Omega} f(\omega)\rho(\omega)d\mu(\Omega) \quad (11)$$

can be interpreted as an expectation value of the observable F in the state ψ , where F is the operator of multiplication by the state space function $f(\omega)$. For observables corresponding to state space functions $f(\omega)$, the expression (11) represents an ensemble average of $f(\omega)$ in the ensemble (10). The correspondence between functions F and the ensembles $\rho(\omega)$ is one-to-one because $(\psi, F\psi)$ is single-valued when F is an operator of multiplication on state space (Misra 1978, p. 1628). By contrast the functional $(\psi, M\psi)$ is *not* a single-valued functional of $\rho(\omega)$, though it may be possible to ensure that the rate of change of such a functional remains a single-valued functional of $\rho(\omega)$ (Misra 1978, p. 1628). A further consequence is that Lyapunov variables such as M must fail to commute with at least some of the operators that are multiplications by functions defined on state space (Misra 1978, p. 1628). This implies that unstable systems possess noncommuting observables (see below).

To summarize, according to the Brussels-Austin Group, provided such a Λ can be found, the deterministic dynamics of unstable systems are equivalent to time-irreversible, (irreducibly) probabilistic Markov processes. The first concrete example they gave was for a simplified Baker's transformation.¹⁰ Although it is conservative and time reversible, the question naturally arises: Are there any realistic physical systems for which Λ could be constructed? Generic prescriptions for constructing time operators for Bernoulli systems and Kolmogorov flows were given in (Courbage and Misra 1980; Goldstein, Misra and Courbage 1981). These constructions, however, are purely formal and, hence, Λ also remains formal.¹¹

More recently, concrete examples of time operators have been constructed for unilateral shift representations of dynamics for Renyi maps, where T for such maps is densely defined on a HS (Antoniou, Sadovnichii and Shkarin 1999; Antoniou and Suchanecki 2000; Mercik and Weron 2000). Furthermore, a generic prescription for constructing T for exact systems, where the dynamics is noninvertible, was given in (Antoniou and Suchanecki 2000). Time operators for the semigroups associated with the nonrelativistic and relativistic one-dimensional diffusion equations have also been constructed (Antoniou, Prigogine, Sadovnichii and Shkarin 2000). Nevertheless, in all these cases Λ appears only as a formal object assumed to be densely defined on a HS.

some probabilistic assumptions yields a monotonically increasing function for Hamiltonian models (Misra 1978, p. 1630). The proposal in (9) is monotonically increasing in these models without resorting to such assumptions.

⁹Atmanspacher and Scheingraber (1987) proposes characterizing nonequilibrium systems without utilizing the concept of entropy.

¹⁰The Baker's transformation is discussed in more detail in §3.5.

¹¹An alternative derivation of Λ and its relationship to time operators and the evolution of states is given in (Suchanecki 1992).

3.5 Trajectories

Another of the Brussels-Austin Group’s claims is that the exact deterministic trajectories of unstable dynamical systems are *idealizations*. There has been a great deal of confusion in understanding precisely what Prigogine and collaborators have meant when they write that exact deterministic trajectories do not exist or are unrealizable in unstable systems. Many have interpreted their statements and arguments to mean the *total absence* of trajectories for such systems (e.g. Bricmont 1995). But the Brussels-Austin Group only meant to be arguing against a *particular type* of trajectory, namely those which have unchanging width and are everywhere differentiable (“exact and smooth” in the Brussels-Austin nomenclature). However, this distinction did not receive sufficient emphasis in the similarity transformation approach and was easily misunderstood.

Misra, Prigogine and Courbage (1979) argued for the “unreality” of these exact deterministic trajectories in the following way. In unstable systems, viewed from a Lagrangian point of view, where the state space points are in motion, small regions of state space contain points moving along ‘rapidly diverging or qualitatively distinct types of trajectories.’ The conclusion they draw is that

[o]bviously, in this situation, the concept of deterministic evolution along state space trajectories cannot be defined operationally and hence, constitutes a physically unrealizable idealization. Therefore, in dealing with dynamically unstable systems, classical mechanics seems to have reached the limit of the applicability of some of its own concepts. This limitation on the applicability of the classical concept of state space trajectories is—it seems to us—of a fundamental character. It forces upon us the necessity of a new approach to the theory of dynamical evolution of such systems which involves the use of distribution functions in an essential manner (Misra, Prigogine and Courbage 1979, pp. 4-5).

Leaving aside the questionable association of physical processes with operational definitions, there are two things to note about this passage. First, at the time of the above quotation, the Brussels-Austin Group had not given detailed arguments that the concept of exact, smooth trajectories was physically unrealizable. Rather they viewed the failure of the concept as “obvious” for unstable systems, the classical concept of exact, smooth trajectory having “reached the limit of applicability” in such systems. Second, they took this failure to mean that such dynamical systems must be described by distribution functions implying *probabilistic descriptions are fundamental for such systems*—i.e., intrinsic randomness.

Their argument against the reality of exact, smooth trajectories later took the following form:

- (A) Deterministic dynamics and Markov processes are “equivalent” descriptions for unstable systems via the existence of the transformation Λ .

- (B) However, the concepts of point-like states and exact, smooth trajectories are physically unrealizable idealizations for unstable systems.
- (C) On the other hand, Markov processes are operationally well defined for unstable systems.
- (D) Therefore, evolution of probabilistic distributions, not state space point trajectories, represent the fundamental descriptions of such systems.

In (D) Prigogine and his colleagues are urging upon us a fundamentally different way of conceiving classical unstable systems, not merely a new formalism for calculating results on such systems. Premises (A) and (B) are both required for (D). Premise (A) comes from the “equivalence” thesis between deterministic dynamics and probabilistic processes mentioned above. The requirement of (B) is more subtle. Recall that the classical conception of state space is a space of points each of which represents a possible state of the system in terms of particular values of the positions and momenta of the system constituents. The failure of the concept of smooth deterministic trajectories implies that exact states for such systems are also *unphysical idealizations*, meaning probabilities can arise in some fashion other than coarse-graining. The unreality of exact states means that the state space points in CM are also unphysical idealizations: ‘The concept of state space point and state space trajectories, which are regarded in the classical theory as simple and basic notions, must be viewed now as a mathematical reconstruction, and this reconstruction requires infinite precision’ (Misra and Prigogine 1983, p. 427; see also Goldstein, Misra and Courbage 1981, pp. 112-3). Prigogine and coworkers considered infinite precision to be physically impossible, hence their appeal to premise (B) as well for the conclusion that probability is irreducible in unstable systems.

Given such far-reaching claims, the similarity transformation approach warrants closer examination. I will first assess premises (A) and (B) independently and then spell out what conclusions I believe the approach licenses. Along the way, I will indicate revisions the Brussels-Austin Group made to their approach.

Although some in the Brussels-Austin Group have taken it as “obvious” that the concepts of exact states and smooth trajectories fail for unstable systems, the failure of these concepts is not so obvious. Simply invoking operationalism is no longer a convincing argument. This attempt to justify (B) is particularly weak since it can at best mean that *in practice* our operational definition suffers an empirical breakdown for unstable systems. Our usual procedures in classical mechanics will not allow us to predict with accuracy the trajectories of the system arbitrarily far into the future because of our inability to either measure or represent the initial conditions to infinite accuracy (Bishop, forthcoming). One cannot conclude from this, however, that exact trajectories and state space points do not exist.

A revised argument involves extending Λ and W_t^* to generalized distribution functions from the theory of distributions (i.e. using the theory of distributions; c.f. Schwartz 1950, 1951). Originally Λ and W_t^* were supposedly defined as acting on distribution functions ρ defined on $L^2_\mu(\Omega)$. Misra and Prigogine (1983)

claimed that since ‘we are interested in studying the evolution (under $[W_t^*]$) of phase points, we need to extend the action of Λ and $[W_t^*]$ to singular (Dirac δ -functions type) distributions concentrated on a given state space point’ (Misra and Prigogine 1983, pp. 423-5).¹² They explicitly constructed U_t , Λ and W_t^* and a complete set of orthonormal eigenvectors for W_t^* for the Baker transformation. It turns out that both regular and singular distribution functions can be expanded as linear combinations of these eigenvectors. This allows the action of Λ and W_t^* to be applied to singular distributions like $\delta(p - p_0)\delta(q - q_0)$, representing a distribution concentrated at the point (p_0, q_0) in state space. Applying Λ to $\delta(p - p_0)\delta(q - q_0)$ transforms it from a function taking a nonzero value *only* at the point (p_0, q_0) to a function taking nonzero values over a subset of state space points (Goldstein, Misra and Courbage 1981, 121). Something similar happens under the action of W_t^* . Misra and Prigogine pointed out ‘that *even if one could start* with an initial condition corresponding to a point on the state space, it will cease to be a state space point under the physical evolution $[W_t^*]$ and the transformation Λ ’ (1983, 424). From these results they concluded that

The basic object of the theory must now be not the state space points and their dynamical evolution along state space trajectories, but the transformation of points under the transformation Λ and their evolution under $[W_t^*]$. One might still argue that at least in the case when Λ is invertible, one could reconstruct the motion of state space points along trajectories from a knowledge of the evolution under $[W_t^*]$ of the transformed object $[\delta(p - p_0)\delta(q - q_0)]$ (Misra and Prigogine 1983, 425).

They go on to argue that such a reconstruction is not possible for arbitrarily large time ‘except if one assumes infinite accuracy in the observation of the physically evolving states’ (p. 425). This is consistent with the fact that the dynamics of state space points and trajectories are not the “fundamental objects” of their physical theory. Rather, under the action of Λ , the distributions are now fundamental.

However, Batterman pointed out that this confused the evolution of Dirac-type functions with that of points in state space (1991, pp. 259-260). state space points $\omega \in \Omega$ are not the same type of mathematical objects as distributions. So nothing was actually demonstrated about the dynamics of state space points. Indeed no such line of demonstration can work, because the operator Λ in these cases maps singular distributions defined *on* Ω into distributions with finite support on Ω , so the probabilistic description describes the evolution of distributions on state space points and not the evolution of the points themselves. Furthermore, technically M , Λ and W_t^* are defined not for points, because the vectors of L_μ^2 are not points, but equivalence classes of functions

¹²Mathematically this extension requires that the Hilbert space be extended as well. Initially they were unaware of this point, but extended spaces becomes important in their more recent work discussed in Part II.

that are equal almost everywhere. This is a crucial point for the Brussels-Austin Group because state space points represent the exact states of the system. The latter simply drop out of the description, implying nothing about the nature of their trajectories.

Note as well that this arguments confuses an epistemological claim (i.e. the inability to attain infinite measurement accuracy) with an ontological one (i.e. the ultimate nature of trajectories), a conflation of epistemology with ontology plaguing nearly every one of the group’s arguments regarding trajectories in their older approach.

Misra (1978, pp. 1628-9) hints at another possible argument in support of (B). In the Koopman formalism, classical observables are often associated with linear operators that are multiplications by state space functions at least some of which, according to Misra (1978), fail to commute with the microentropy operator M . Sufficiently unstable classical models, so the argument goes, would possess complementary observables in analogy with the position and momentum operators in QM. Therefore the simultaneous determination of some classical observables and a nonequilibrium entropy of the form (9) would be subject to a Heisenberg-like relation. Misra states that for conditions where the dynamics are described in terms of smooth state space trajectories with all classical observables completely determined, the concept of nonequilibrium entropy would be inapplicable. Alternatively, conditions permitting the precise determination of the nonequilibrium entropy would preclude the possibility of accurately determining the state space trajectories (Misra 1978, p. 1629). The deterministic description in terms of trajectories would then be complementary to the probabilistic description in terms of nonequilibrium entropy.

The argument needs to be spelled out in more detail. First it needs to be demonstrated that in the extended Koopman formalism all the physically relevant classical observables can be representable as multiplications by state space functions. As Misra points out, there are many more operators in L^2_μ that are not multiplications, but these other operators are considered to have no physically meaningful interpretation in terms of classical observable quantities (1978, p. 1628). The physically meaningful operator M , however, cannot be represented as a multiplication operator on state space due to the requirement that it be monotonically increasing (Misra 1978, pp. 1627-8), so additional argumentation is needed to show that all *other* relevant classical observables must be represented by multiplications on state space. An additional complication is that although in the “momentum representation” in the extended Koopman formalism, the momentum is represented by a multiplication operator, in the “position representation”, momentum is represented by a differential operator. So the form of some physically meaningful operators are representation dependent. Furthermore viable candidates for the mathematical descriptions of the supposed nonequilibrium entropy need to be constructed for any realistic physical systems. That question is related to the truth of (A) insofar as Λ is a function of M .

It is possible to give a less radical reinterpretation of (D) based on an operationalist view of unobservable entities implicit in (Nicolis and Prigogine 1989):

(D') Probabilistic descriptions represent the proper descriptions consistent with observability and computability.

It then remains to be seen what can be made of the claim that the probabilistic description represents no “loss of information” with respect to the trajectory description. In this context I need to examine a more recent version of the argument for *indiscernibility* of trajectories put forward by Nicolis and Prigogine (1989, pp. 204-8). This argument begins by noting that the Baker’s transformation,

$$x' = 2x, \quad y' = \frac{y}{2} \quad 0 \leq x \leq \frac{1}{2} \quad (12a)$$

$$x' = 2x - 1, \quad y' = \frac{y+1}{2} \quad \frac{1}{2} \leq x \leq 1, \quad (12b)$$

is measure-preserving in the sense that the unit square remains invariant under repeated iterations. The action of (12) stretches the square in the x -direction as much as it compresses it in the y -direction. This contraction plays a crucial role in Nicolis and Prigogine’s indiscernibility argument regarding the supposed “irrelevance” of Liouville’s theorem for a given sub-area of the unit square.

Suppose ρ is confined initially to a sub-area Δ of state space (e.g. the shaded region in Figure 1). The sub-area Δ remains invariant through the first few iterations. According to Nicolis and Prigogine, the contracting dimension decreases exponentially to some ε and remains constant thereafter, because *this represents the limit of our ability to measure or localize this dimension accurately*. They refer to the decreasing dimension as a fiber which eventually gets distributed evenly throughout state space and cannot be localized. Hence the support of Δ would increase until it reaches the support of a larger subset of the state space and, from an *empirical* standpoint, render Liouville’s theorem on preservation of the area of sub-regions of state space “irrelevant”. Nicolis and Prigogine interpret this as due to the fact that measurements (or, more generally, effects of physical interactions) refer to regions of finite support in state space, not to mathematical points. Supposedly the conclusion regarding the indiscernibility of contracting fibers (analogous to state space trajectories) follows from the fact that measurements are only finitely accurate. Hence the support of the sub-region Δ is not area preserving below the observational threshold ε , so they conclude that Liouville’s theorem is inapplicable below this threshold.

Clearly the argument confuses ontology with epistemology. Obviously, given (12), the contracting dimension will never reach a constant ε ; rather, the fiber will asymptotically approach zero thickness. Hence the density of Δ will remain invariant as its support varies. The “irrelevance” of Liouville’s theorem, according to Nicolis and Prigogine, is due to our inability to localize/measure the fiber below ε thickness. But this is an epistemological point as the fibers of the Baker’s transformation remain ontologically precise according to (12). Therefore, while there may be some epistemic bound on our ability to precisely measure fibers of decreasing thickness, such a bound would not support the ontological claim (B).

Figure 1: Figure 1. The first steps in the stretching and folding action of the Baker's transformation.

The existence of this epistemic bound does imply a loss of information about the trajectories, so how can Prigogine and coworkers claim that their approach suffers no loss of information when it is unable to demonstrate the unreality of exact state space points and smooth trajectories and, hence, support (A)? This argument can only be seen as supporting (A) if one adopts an operational attitude: Unobservable trajectories will have the same observational consequences as if there were no exact smooth trajectories at all. Since the observational outcomes are the same, the concepts of smooth trajectories and exact states can be dropped from the theoretical description as so much excess baggage. This operational attitude is the only consideration that can be offered in support of (D) and, of course, is compatible with (D').

In my judgment, the ontological conclusion (D) is not licensed in the similarity transformation approach. The Brussels-Austin Group formalism does not show the nonexistence of exact states or smooth trajectories in unstable systems.¹³ Rather, like the coarse-grained approaches from which the Prigogine school seeks to distinguish itself, their new formalism substitutes a probabilistic description in place of point-like states and trajectories in state space. In contrast their formalism emphasizes physics ignored in typical coarse-graining techniques. Furthermore standard coarse-graining replaces individual states ω with distributions defined uniformly over a finite cell of Ω without distinguishing points belonging to different stable manifolds in unstable systems. The Brussels-Austin probability distributions are constructed to distinguish points belonging to stable manifolds from unstable ones. Furthermore the Markovian semigroups derived from Λ are not related to local point transformations in state space in contrast to those semigroups derived from coarse-graining projections (Suchanecki, Antoniou and Tasaki 1994). So the similarity transformation approach can be viewed as an alternative calculational approach to coarse-graining provided Λ can be constructed for real-world systems.

3.6 Directions in Time

One acclaimed virtue of this version of the Brussels-Austin approach is the ability of Λ to provide time-asymmetry. The transformation Λ is chosen so that

¹³As the Brussels-Austin Group shifted away from the similarity transformation approach, they dropped terms like "nonexistent" in favor of terms like "irrelevant" when discussing trajectories (Part II).

time-asymmetry is guaranteed under its action. There exist, nevertheless, two distinct transformations, Λ_+ and Λ_- , corresponding to two distinct semigroups, W_t^{+*} and W_t^{-*} , respectively. Λ_+ corresponds to future-directed evolution toward equilibrium along the positive t -axis and Λ_- corresponds to past-directed evolution toward equilibrium along the negative t -axis (Misra and Prigogine 1983, p.422). This implies that there are two possible probabilistic descriptions.

Why then do we not observe evolutions of the W_t^{-*} -type? To answer this question the Brussels-Austin Group uses singular initial probability distributions since nonsingular distributions can approach equilibrium in either direction in time under Λ_+ and Λ_- . By translating their conception of entropy into information-theoretic language, Courbage and Prigogine (1983, p. 2414-5) showed that their formulation of the second law requires infinite information for specifying the initial states of a singular distribution evolving in the negative t -direction, but only finite information for specifying the initial states for evolution in the positive t -direction. This would render the initial conditions for systems to approach equilibrium along the negative t -axis physically unrealizable: ‘Of course, even a regular function close to a contracting fiber [Λ_- -type description] will require such a high information content that it will be practically impossible to realize it for a given state of technology’ (Courbage and Prigogine 1983, p. 2416). Since singular probability distributions are supposedly operationally unrealizable, they argue it is physically impossible for unstable systems to evolve to equilibrium in the negative t -direction. Hence their version of the second law acts as a selection rule for initial states.

This argument is supposed to show why anti-thermodynamic behavior in the real world is impossible (for a slightly different version, see Misra and Prigogine 1983). Nevertheless, the argument is problematic. The most fundamental difficulty is that it conflates epistemic concepts (e.g. information, empirical accessibility of states) with ontic concepts (e.g. actual states and behaviors of systems).

Second, Courbage and Prigogine claimed that, ‘this selection rule expresses the unrealizability of experiences in which a set of particles that undergo several collisions will asymptotically emerge with parallel velocities’ (1983, p. 2413). As Sklar points out, however, spin-spin echo experiments represent systems apparently exhibiting just the anti-thermodynamic behavior the Brussels-Austin selection principle rules out (Sklar 1993, pp. 219-22). In these experiments a number of molecules with a magnetic moment are initially in a state where all the moments are aligned in the same direction. A nonuniform magnetic field is then applied. In response to the field, the magnetic moments begin to spin, but since the field is nonuniform, some moments spin faster than others due to their spatial location with respect to the field. After a time period t_a , the orientations of the magnetic moments are completely random. At this point the nonuniform magnetic field is reversed. The moments begin to spin in the opposite direction such that after time $2t_a$, all the spins are aligned in the same initial direction. It looks as if the system has been thermodynamically reversed.

The Brussels-Austin Group has a response to this objection. If the system is left to itself, the orientations of the magnetic moments will continue to be

random and entropy continues to increase monotonically. If the magnetic field is reversed at time t_a , the entropy of the system is decreased to a value *below* its initial value (it actually makes a discontinuous jump) due to the external intervention of reversing the field (i.e. the system was opened to an outside influence). As the moments reverse themselves, however, the entropy continues its monotonic increase from its newly lowered value and returns to its initial value at the point in time when the moments return to their initial alignments.¹⁴

A more fundamental problem with the selection principle argument is that it turns on the definition of entropy. The conditions for the existence of the microscopic entropy operator M and, hence, for Λ , admit alternative notions of entropy that have the opposite temporal behavior to the Brussels-Austin Group definition ($\Lambda_+ = M_+^{\frac{1}{2}}$). Recall that the microentropy operator M is related to the existence of a time operator T for K-flows. There is a relationship between such time operators and the Kolmogorov-Sinai entropy (Atmanspacher and Scheingraber 1987), and since K-flows are reversible, one could select an alternative “entropy” (e.g. characterized by negative rather than positive Lyapunov exponents) with the opposite temporal direction endowing T with the opposite temporal direction and, then, construct an M_- . On this basis an argument similar to that of Courbage and Prigogine could be formulated whose conclusion is that the approach to equilibrium along the positive t -axis is “impossible” (e.g. Misra and Prigogine 1983, p. 427; Karakostas 1996, pp. 393-4). On what basis is one definition privileged over another? Why do we not see about half of the systems approaching equilibrium in one time direction, while the other half approach equilibrium in the opposite time direction?

The Brussels-Austin Group often responds to this type of objection by appealing to experimental observations of time asymmetry. This amounts to taking phenomenological laws as fundamental and thereby excludes all definitions of entropy that licensed anti-thermodynamic behavior. Obviously such a move comes at an explanatory cost. It is precisely these observations that need explanation, but by taking them as fundamental the Brussels-Austin Group gives up the ability to offer an explanation for the thermodynamic arrow of time. In other words the acclaimed link between classical deterministic systems and Markov processes, which was supposed to illuminate the mystery of irreversibility, affords us no gain in understanding the puzzle of the second law and is in danger of becoming circular.

3.7 Problems with the “Equivalence” Thesis

The “equivalence” between trajectory and probabilistic descriptions of unstable system *via* Λ stands in need of further clarification. If Λ is a similarity transformation, it must preserve the spacetime features of the physical system. In this approach, however, the ontological elements of the two descriptions are supposed to be so different (point states and trajectories vs. probability dis-

¹⁴A discussion of a generic time reversal experiment in the context of a two state system (a ground state and an excited state) is given in (Petrosky, Prigogine and Tasaki 1991, 200-202).

tributions) that the implication should be that we have two different physical descriptions or models of the system. Assume for the sake of argument that in unstable systems smooth state space trajectories are physically irrelevant idealizations. This view calls into question the validity of the classical deterministic description which assumes such trajectories are physically meaningful.

Some insight into the “equivalence” thesis and the physical significance of the similarity transformation can be found in the work by Gustafson and colleagues (Gustafson and Goodrich 1980; Antoniou and Gustafson 1993; Gustafson 1997; Antoniou, Gustafson and Suchanecki 1998). They have shown that any Markovian semigroup dynamics arising from a coarse-grained projection of a K-flow can be embedded into a larger Kolmogorov dynamical system. Moreover many other kinds of Markovian semigroup dynamics can also be embedded into a larger Kolmogorov system regardless of their origin (Gustafson 1997, pp.66-8 and references therein; Antoniou, Gustafson and Suchanecki 1998, pp. 114-8). No specific results for embedding a Markovian dynamics induced by similarity transformations exist at present as no concrete realizations of Λ for physical systems have been developed nor are many physical properties of such transformations known (e.g. Antoniou, Gustafson and Suchanecki 1998, p. 119). From this perspective, then, the equivalence of deterministic and probabilistic descriptions *via* Λ needs further specification. The physical significance of Λ for unstable systems can be understood minimally as a change of representation from the deterministic description to a dynamics distinguishing stable and unstable manifolds of such systems.

In my judgment, the Brussels-Austin Group ought to have been arguing that the probability description is the primary physical picture of the behavior of unstable systems. After all, according to them the ontological elements of the deterministic description are unrealizable and the probability description—being irreducibly probabilistic—captures the dynamical behavior of the probability distribution and the collective and long-range effects within such systems that are missing from a trajectory description. In addition it is precisely this irreducible probability that gives rise to the claim that unstable classical systems can be intrinsically random or indeterministic (Misra, Prigogine and Courbage 1979; Goldstein, Misra and Courbage 1981). Finally Gustafson has demonstrated that the inverse transformation Λ^{-1} cannot be positivity preserving for K-flows, so any reverse transformation (“embedding”) from the probabilistic description induced by Λ to a deterministic Kolmogorov dynamics must violate positivity of probability (Gustafson 1997, pp. 61-2). So it appears that a case can be made that under Λ , probabilistic models are more physically accurate or appropriate for these systems. The similarity transformation, then, should not be viewed as yielding an equivalence between the two descriptions.¹⁵

¹⁵In more recent work, Prigogine and colleagues explicitly argue that the trajectory description and the distribution description are not equivalent for a class of models known as large Poincaré systems (Petrosky and Prigogine 1996 and 1997; Part II).

4 Discussion

Part of the explanation for the difficulties in the similarity transformation approach lies in the fact that the Brussels-Austin Group started to work in an inappropriate mathematical framework. They treated the operators Λ and W_t^* as if they were defined on HS in the modified Koopman approach, when what was actually needed was an extended space such as a rigged Hilbert space (Bohm 1981, 2814; Obcemea and Brändas 1983; Petrosky and Prigogine 1996, pp. 481-2; Part II). Indeed Ordóñez has recently shown that the similarity transformation approach amounts to rigging a HS (1998). Furthermore the fact that they were tacitly working in an extended space all along is indicated by their interests in the evolution of distribution functions and densities, the use of delta functions in the arguments on trajectories I rehearsed above, as well as the presence of the semigroup operators W_t^* and the unbounded nature of the operators U_t and W_t^* . None of these elements are well defined on the whole of HS.

Although serious questions remain regarding how to demonstrate conclusively that the past-directed semigroups are somehow unphysical and regarding the mathematical difficulty of the similarity transformation approach, this earlier attempt by the Brussels-Austin Group to develop a new approach to thermodynamics and SM does achieve some milestones. It provides a generalized formalism allowing a unified mathematical treatment of deterministic and probabilistic systems and has potential application to QM systems as well, holding out the possibility of a unified treatment for statistical physics at both the microphysical and macrophysical levels. In addition the framework appears equally suitable to QM and CM suggesting that the two levels of description may themselves become unified. Provided the transformation Λ can be found for the unstable SM systems in question, the Brussels-Austin Group demonstrated a *mathematical* relation between the time-reversible dynamics of the trajectory description and the time-irreversible dynamics of the Markov description. This suggests that if they could produce an alternative justification for taking the Markov description as primary, they may still be able to reconcile the irreversible behavior with the standard time-reversible SM. Along the way there were new mathematical developments, particularly in the area of time operators.

The realization that this formalism was tacitly assuming an extension beyond HS was one of the reasons that motivated the Brussels-Austin Group to move to rigged Hilbert spaces. Another motivation for switching formalisms was that realistic physical models become almost mathematically intractable in the similarity transformation approach. Results were only obtained for discrete mathematical systems like the Baker's transformation, never for continuous mathematical systems much less realistic physical models. The more recent work in rigged Hilbert spaces holds forth the promise of overcoming many of these difficulties, so I will discuss it in Part II.

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