Brussels-Austin Nonequilibrium Statistical Mechanics: Large Poincaré Systems and Rigged Hilbert Space

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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 due to the dynamics of physical systems. This essay focuses mainly on recent developments in the Brussels-Austin Group after the mid 1980s. The fundamental concerns are the same as in their earlier approaches (subdynamics, similarity transformations), but the contemporary approach utilizes rigged Hilbert space (whereas the older approaches used Hilbert space). While the emphasis on nonequilibrium statistical mechanics remains the same, their more recent approach addresses the physical features of large Poincaré systems, nonlinear dynamics and the mathematical tools necessary to analyze them.

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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 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).

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 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 $\rho(\vec{q}_1, \vec{q}_2, \vec{q}_3, ..., \vec{p}_1, \vec{p}_2, \vec{p}_3..., t)$ of finding a set of molecules (say) with coordinates $\vec{q}_1, \vec{q}_2, \vec{q}_3, ...$ and momenta $\vec{p}_1, \vec{p}_2, \vec{p}_3...$ at time t on the relevant energy surface and are analogous to the microcanonical distribution. In this latter 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 essay develops, I will point out how their work differs from typical coarse-grained approaches. First, I will review Prigogine and co-workers' motivations (Section 2) and then discuss their various approaches to nonequilibrium systems. This discussion will be divided into two parts. The first, briefer part will cover the period from the 1960s to the mid 1980s, discussing their subdynamics and similarity transformation approaches (Section 3). The second part will cover their more recent work on large Poincaré systems in rigged Hilbert space. Large Poincaré systems are defined and illustrated in Section 4 using nonintegrable Hamiltonians and classical perturbation theory as a way of motivating some of the key physical and mathematical problems for such systems. The rigged Hilbert space approach to these systems is outlined in Section 5, and the corresponding time-ordering rule and semigroup operators governing the dynamics are introduced. Particular details of the approach are discussed in Section 6, where an alternative interpretation of Prigogine's treatment of trajectories and their relationship to the dynamics of distributions is discussed. I will conclude with some remarks on probabilistic dynamics (Section 7).

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, 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.

3 The Early Years: Subdynamics and Similarity Transformations

Most of the Brussels-Austin Group's results during this period are developed in Hilbert space (HS) in part due to matters of elegance as well as out of a desire to unify CM and quantum mechanics (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 $L^1(\Omega)$). The Brussels-Austin Group wanted to use this formalism to study the evolution of state space points themselves and, so, applied Koopman's formalism to the space $L^2_\mu(\Omega)$ (square integrable functions using measure μ), although no rigorous justification for this extension was ever given.

3.1 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; Obcemea and Brändas 1983; Dougherty 1993; Karakostas 1996). Karakostas (1996, pp. 383-384) 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.[1] 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.

3.2 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 for such 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. It is this additional physics in the probabilistic description that they believed resulted in new physical features and rendered elements of the trajectory description 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.[2] 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)).[3] 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 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

[1]Versions of subdynamics derived from a Lyapunov variable are not so easily classified as coarse-grainings (Section 3.2).

[2]In (Prigogine et al. 1973), a star-unitary Λ was assumed, but the Λ developed afterwards is nonunitary.

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

time-reversible Liouville equation in Koopman's original formulation,

$$i\frac{\partial\rho}{\partial t} = U_t\rho,\ -\infty \leq t \leq \infty\ , \tag{1}$$

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

$$i\frac{\partial\rho'}{\partial t} = W_t^*\rho',\ t \geq 0\ , \tag{2}$$

where W_t^* and ρ' are also defined on $L^2_\mu(\Omega)$. This is the key for time-irreversibility in the similarity transformation approach and leads to the definition of intrinsic 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. 114-118).

Following a suggestion by Misra (1978), Λ was derived from the so-called *microentropy operator* M, a positive linear operator defined on $L^2_\mu(\Omega)$ that, according to Misra, fulfils the conditions for a *Lyapunov variable*, i.e., a variable that increases monotonically to an asymptotically stable value. 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. 1629-1630). 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. 61-64).

Since M is positive (Misra 1978; Braunss 1984), it can be factorized ($M = \Lambda^*\Lambda$), so $\Lambda = M^{\frac{1}{2}}$. Furthermore as Braunss 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, pp. 9-11).

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

$$-\ln(\rho, M\rho)\ . \tag{3}$$

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, a feature that functionals like (3) possess (1978, p. 1627).

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*, 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.

3.3 Trajectories

There has been a great deal of confusion over what Prigogine and collaborators mean when they write that exact deterministic trajectories do not exist or are unrealizable for unstable dynamical systems. Many have interpreted such statements to mean the *total absence* of trajectories for such systems (e.g., Bricmont 1995, pp. 165-6). 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 ("smooth" in the Brussels-Austin nomenclature).[4] However, this distinction did not receive sufficient emphasis in the similarity transformation approach and was easily misunderstood.

Most of the group's early statements and arguments regarding trajectories tend to be operationalist in character (e.g., Misra, Prigogine and Courbage 1979, pp. 4-5). But as they developed their program, they also developed other arguments, one of which I will consider briefly involving extending Λ and W_t^* to generalized distribution functions. 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' (p. 423). For example 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) into 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 then continue:

> *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...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 $[\delta(p-p_0)\delta(q-q_0)]$ (p. 425).

But, since such a construction is not possible for arbitrarily large time 'except if one assumes infinite accuracy in the observation of the physically evolving states' (p. 425), they conclude that smooth trajectories are unrealizable in unstable systems.

[4] Private communication. See Section 6.3.

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. The latter simply drop out of the description, implying nothing about the nature of their trajectories.

Two remarks are in order here. First, M, Λ and W_t^* are defined not for points (the vectors of L^2_μ are not points), but equivalence classes of functions that are equal almost everywhere. This is crucial for the Brussels-Austin Group because state space points represent the exact states of systems. Second, 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). The conflation of epistemology with ontology plagues nearly every one of the group's arguments regarding trajectories in their older approach (e.g., Nicolis and Prigogine 1989, pp. 204-208, where observational limitations are argued to lead to a violation of Liouville's theorem in the case of the Baker's transformation).

The similarity transformation approach, then, does not show the nonexistence of exact states or smooth trajectories in unstable systems. Rather, like the coarse-grained approaches from which the Prigogine school seeks to distinguish itself, this approach substitutes a probabilistic description in place of point-like states and trajectories. 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 a more rigorous alternative to coarse-graining provided Λ can be constructed.

3.4 Directions in Time

One claimed virtue of this version of the Brussels-Austin approach is the ability of Λ to provide time-asymmetry. 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, pp. 2414-2415) 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). 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, the entropy of the system decreases discontinuously to a value *below* its initial value 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.

A third 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 M is related to the existence of K-flows; one could simply select an alternative "entropy" (e.g., characterized by negative rather than positive Lyapunov exponents) with the opposite temporal direction endowing M with the opposite temporal direction. 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. 393-394).

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 licensing 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 claimed link between classical deterministic systems and Markov processes, which was supposed to illuminate the mystery of irreversibility, affords us no gain in understanding and is in danger of becoming circular.

3.5 Problems with the "Equivalence" Thesis

The "equivalence" between trajectory and probabilistic descriptions of unstable systems *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 distributions) 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. Furthermore, it is the 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).

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.66-68; Antoniou, Gustafson and Suchanecki 1998, pp. 114-118). 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. 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. Furthermore, Gustafson (1997, pp. 61-26) 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.

4 The Later Years: Large Poincaré Systems and Rigged Hilbert Space

One of the most serious difficulties with the Brussels-Austin Group's early approaches, unnoticed for many years, was the use of an inappropriate mathematical framework. They treated the operators Λ and W_t^* as being 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, p. 2814; Obcemea and Brändas 1983). 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, 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 HS. This realization, among other considerations discussed below, led Prigogine and coworkers to significantly revise their approach to reconciling deterministic microscopic dynamics with probabilistic macroscopic dynamics in unstable systems.

It has been argued that no current approaches to microscopic dynamics can explain or derive the second law of thermodynamics, since it is both necessary and sufficient for such a derivation that the microscopic dynamics be exact (e.g., Mackey 1992, pp. 98-100; 2002).[5] Although it can be shown that the coarse-grained projection operator arising from the earlier Brussels-Austin approach yields an exact dynamics, whether their similarity transformation yields exact dynamics is unknown (Antoniou and Gustafson 1993; Antoniou, Gustafson and Suchanecki 1998, p. 119). Nevertheless, one of the crucial claims of the earlier approach was that trajectory descriptions at the microscopic level and probabilistic descriptions at the macroscopic level of thermodynamic behavior are related via a transformation.

This way of viewing the relationship between trajectory and probabilistic descriptions is de-emphasized in their more recent work. So the core point is no longer to derive irreversible thermodynamic behavior from reversible microscopic descriptions, so much as to argue for the *priority* of irreversible macroscopic descriptions for a particular class of systems known as Large Poincaré systems. However, the core intuitions of the new approach remain continuous with their earlier work; namely, that irreversibility is fundamentally dynamical in character and that distributions are ontologically fundamental explanatory elements for unstable systems.

[5] A dynamics on a state space Ω with a transfer operator P_t is *exact* if and only if $\lim_{t\to\infty} |P_t\rho - \rho_{eq}|_{L^1} = 0$ for every initial density ρ, where ρ_{eq} is the unique stationary density (i.e., equilibrium density), P_t governs the dynamics (e.g., Liouville or the Frobenius-Perron operators), and the norm is in the sense of Lebesgue integrable functions. Among other properties, exact dynamics are noninvertible.

The Brussels-Austin Group's recent work develops a method for constructing a complete set of eigenvectors for the model equations describing the thermodynamic approach to equilibrium in a Large Poincaré system (LPS) as well as nonlinear dynamics more generally. This approach reformulates the question of how to relate reversible trajectory and irreversible probabilistic descriptions as follows: How can the trajectory dynamics of an LPS yield necessary conditions for the thermodynamics approach to equilibrium and What further mechanisms account for the sufficient conditions for such behavior?

4.1 Integrable Systems

Toward the end of the 19th century, Poincaré was investigating planetary motion, among other things. Solving the equations of motion for the solar system is extremely difficult because all the planets interact with each other through gravitational forces. One of the questions Poincaré pursued was whether there was a suitable way to transform these equations of motion into a system of equations where the gravitational interaction would vanish and one could solve the evolution equations for the angle variables of each planet independently of the others. What Poincaré showed was that in general such a transformation was impossible for systems of N mutually interacting bodies. If a canonical transformation exists carrying a system of equations describing a set of interacting particles into a set where the interactions vanish, then the system is classified as *integrable*. This means that the original system of equations can be transformed into one where each particle's behavior is fully described by an equation that is independent of any other particle.

Poincaré showed that systems of equations were nonintegrable when they contained *resonances* between various degrees of freedom. Roughly a resonance is a transient metastable state establishing a narrow, precise frequency gateway through which energy can be efficiently transferred from one element of a physical system to another. Physical examples of resonances include bound states produced in particle collisions and intermediates in chemical reactions.

4.2 Perturbation Theory

In order to make these notions of resonances and nonintegrability more precise, consider Hamiltonian systems in CM. While models with completely integrable Hamiltonians are rare, they are still very useful in the study of physical systems. For many systems can be modeled using Hamiltonians of the form

$$H = H_0(\vec{J}) + \lambda V(\vec{J}, \vec{\alpha}), \tag{4}$$

where H_0 is assumed to be completely integrable, $\vec{J}$ represents the action variables (e.g., generalized momentum vectors), $\vec{\alpha}$ the angle variables (e.g., generalized coordinate vectors) and λ (assumed $\ll 1$) is the coupling coefficient roughly describing the strength of the interactions through the potential V. The question of whether or not a Hamiltonian system is integrable is equivalent to being able to find a canonical transformation from the old state space coordinates $(\vec{J}, \vec{\alpha})$ to new coordinates $(\vec{I}, \vec{\beta})$ decoupling all the equations for the angle variables (in essence turning off all the interactions by making λ zero). When such a transformation can be found, the Hamiltonian is said to be completely integrable and I will refer to this type of integrability as complete integrability (to be distinguished from the Brussels-Austin sense of integrability below).

In general one then must proceed using a perturbation method where the strategy is to find approximate solutions of (4) in terms of $H_o(\vec{I})$ plus small perturbations due to $V(\vec{I}, \vec{\beta})$. In the course of standard perturbation (e.g., Tabor 1989, 89-108), terms of the form

$$\frac{V_{n_i,n_j,n_k...}}{n_i\beta_i + n_j\beta_j + n_k\beta_k + ...} \tag{5}$$

emerge where, i, j, and k are integers labeling the particles, $V_{n_i n_j n_k}$ represents the Fourier transformed potential, the n_l indicate the (discrete) degrees of freedom of the particles in the Fourier expansion, and the β_l can be negative and are often interpreted as generalized frequencies. Clearly terms like (5) increase without bounds when the denominator approaches zero. The denominator being zero represents a resonance. It is the presence of a sufficient number of these resonances that blocks the standard canonical transformation techniques for producing a completely integrable system of equations. For an N-body problem, the resonance condition takes the form that the finite sum $n_i\beta_i + n_j\beta_j + n_k\beta_k + ... + n_N\beta_N = 0$. In general there are several combinations of n_l's and β_l's satisfying this condition.

4.3 Large Poincaré Systems

First consider an integrable Hamiltonian for a system with two degrees of freedom. The state space trajectories will then be confined to the surfaces of nested tori, where each surface corresponds to a different combination of the values of the two constants of the motion. Now add perturbations λV to this Hamiltonian where $\lambda \ll 1$. If the perturbations leave the Hamiltonian integrable, then the model dynamics are not appreciably affected. In contrast, if the perturbations render the Hamiltonian nonintegrable (e.g., resonance phenomena), then these periodic orbits will be disrupted because such perturbations are as physically important as the unperturbed orbits of the integrable part of the model, due to the transfer of energy involved. The KAM theorem specifies the conditions under which tori associated with quasi-periodic trajectories survive and constitute the majority of motions realized in state space, so that most regions in state space for nonintegrable models close to integrable models show stable nonperiodic orbits (e.g., Hilborn 1994, 337-9).

There are two types of fixed points for the state space trajectories in Hamiltonians of the form (4): elliptic and hyperbolic (saddle points). Elliptic fixed points correspond to stable periodic orbits which are disrupted by resonances. Hyperbolic fixed points present complex behavior: Trajectories exhibiting sensitive dependence on initial conditions and which wander erratically over large regions of state space. These structures also exhibit self-similarity. However, since Hamiltonian systems do not contract to some fixed point as do dissipative systems, orbits near hyperbolic fixed points will become unstable leading to exponentially diverging trajectories. It should be pointed out that stable and chaotic orbits can coexist simultaneously in state space.

Large Poincaré systems are of interest to Prigogine and coworkers. Consider a typical Hamiltonian of the form

$$H(p,q) = \sum_{i=1}^{N} \frac{\vec{P}_i^2}{2m_i} + \lambda \sum_{j>i}^{N} V(|\vec{q}_i - \vec{q}_j|), \tag{6}$$

where $\vec{q}$ and $\vec{p}$ are N-component vectors representing generalized coordinates and momenta respectively, and the system is in a large box with volume L^3. The Brussels-Austin group is interested in "large" systems, meaning they work in the limit $L^3 \to \infty$ (the number of particles N may be finite or infinite). A LPS is obtained when the system is large and the number of degrees of freedom of the system tends to infinity. An example of a LPS with a finite number of particles would be a finite number of charges interacting with an electromagnetic field, while an example with an infinite number of particles would be the *thermodynamic limit* ($L^3 \to \infty$, $N \to \infty$, N/L^3 finite). Such systems possess "continuous sets of resonances". By continuous sets of resonances, the Brussels-Austin Group means that in the Fourier transformed representation, the eigenfrequencies are continuous functions of the wave vector k, so that the summation operations over terms like (5) must be replaced by integrals and the denominators of such terms can be arbitrarily close to zero.

The resonance condition for a continuous set of resonances for a LPS in the context of perturbation theory takes the form

$$\int \int b\beta db d\beta = 0, \tag{7}$$

where b (representing degrees of freedom) and β are continuous functions defined over the real numbers. Under condition (7) motion will not even be quasi-periodic so that variables have a continuous spectrum.[6] No canonical transformation exists turning these LPS models into completely integrable models (Prigogine et al. 1991, pp. 6-7). Such models exhibit the type of randomness associated with mixing, K-flows and Bernoulli systems, but are usually interpreted as deterministic.

As an example of a LPS, imagine a gas containing an infinite number of particles continually undergoing collisions, where the collision processes never cease. A more realistic example is an electromagnetic oscillator with frequency

[6] As Koopman and von Neumann first pointed out, for dynamical systems with continuous spectra, 'the states of motion corresponding to any set become more and more spread out into an amorphous everywhere dense *chaos*. Periodic orbits, and such like, appear only as very special possibilities of negligible probability' (Koopman and von Neumann 1932, p. 61). This is generally acknowledged to be the first reference to the term "chaos" in the context of dynamics.

ω_{osc} interacting with an electromagnetic field. The field has an infinite number of degrees of freedom and the frequency ω_k of the field varies continuously with k, giving rise to an infinite number of resonances. Continuous resonances like those in an LPS are involved in fundamental phenomena such as absorption and emission of light, decay of unstable particles and the scattering of electromagnetic waves off of fluids or other forms of matter, and are found in both CM and QM.

The rigged Hilbert space (RHS) approach of the Prigogine school is a method for solving the equations of a LPS (in both CM and QM) consisting in constructing a complete set of eigenvalues and eigenvectors for the Liouville operator acting on distribution functions ρ. The construction of such eigenvalues and eigenfunctions is what Prigogine and colleagues call the 'generalized problem of integration' (Prigogine et al. 1991, p. 4). To be clear about terminology, finding a transformation that decouples the Hamiltonian in (4) is what is required to show that the system is completely integrable in the sense described earlier. Constructing the complete set of eigenvalues and eigenvectors for a set of equations derived from (4) is what Prigogine and colleagues refer to as 'integrating' or solving the equations of motion. Although initially motivated in the context of perturbation theory (as sketched here), the RHS approach is more general in nature and applicable to any LPS (e.g., most systems in SM, systems involving interacting fields).

5 The Rigged Hilbert Space Approach

There are three key elements in the Brussels-Austin method to solving LPS equations. First, they utilize distribution functions to describe the dynamics. Second, they adopt extended spaces as a mathematical framework for solving the equations. Third, they introduce an "appropriate" time ordering of the dynamical states of the system.

5.1 The Need for Distributions

When solutions of the generalized integration problem exist, they reduce to classical trajectories for most CM systems and to state vectors for most QM systems. In the context of a LPS, however, Prigogine and colleagues argue solutions are not reducible beyond distributions for CM systems (density operators for QM systems). Examples include systems in kinetic theory, radiation damping and interacting fields. One important feature of such physical contexts is that they are characterized by *persistent interactions*. According to Petrosky and Prigogine, a system's interactions are persistent if there are no asymptotic states such that the interactions finally cease (1997, pp. 33-35). For example in kinetic theory, the molecules of a gas are in constant interaction with one another because they are undergoing continuous collisions. This physical situation should be contrasted with the idealized case of a single neutral particle scattering off a fixed target. In the latter situation, there is a *transitory interaction* because the particle undergoes an interaction only in a finite region near the target over a very short time interval, while the particle spends the majority of its life in the so-called asymptotic in and out states free of any interactions with the target. Since interactions never cease for systems with persistent interactions, the model equations typically will not be completely integrable.

The presence of persistent interactions is one of the features giving rise to the continuous set of resonances in a LPS. In a gas containing a large number of particles, these resonances allow for energy to be transferred and leveled throughout the system. Through persistent interactions and the resulting resonances, any ordered patterns are destroyed through *diffusion* (Section 6.2 below).

A further consequence is that the physical dynamics are no longer localized, but are spread throughout the space occupied by the LPS. For the gas example, these nonlocal dynamics will take the form of correlations as described in Section 6.2 below. In addition if the number of particles is large enough, then the degrees of freedom for such a gas of particles will have a continuous spectrum qualifying it as a LPS. This implies that we should expect the dynamical description of such systems to be in terms of distributions of particles rather than in terms of individual particles, because the effects of long-range and higher-order correlations due to such interactions become at least as important as the trajectory dynamics. The particles remain coupled to one another through their interactions resulting in collective effects (Section 6.2 below). This type of long-range coupling at least implies that the global or collective dynamics of the system cannot be accurately represented by trajectory dynamics alone (Section 6.3 below). As a consequence, Prigogine and colleagues believe we must view irreversibility as a property of a system that emerges at the global level which is not derivable from the trajectory description, meaning that distributions are the natural elements for representing statistical phenomena rather than trajectories.[7]

5.2 The Need for RHS

A RHS is an extended mathematical space first introduced by the Russian mathematician Gel'fand and his collaborators (Gel'fand and Vilenkin 1964). Briefly a RHS can be understood in the following way (see Bohm 1967). Let Ψ be an abstract linear scalar product space and complete it with respect to two topologies. The first topology is the standard HS topology, $\tau_{\mathcal{H}}$, and the second topology, τ_{Φ}, is defined by a countable set of norms such that τ_{Φ} is finer than $\tau_{\mathcal{H}}$. A Gel'fand triplet is obtained by completing Ψ with respect to τ_{Φ} to obtain Φ and with respect to $\tau_{\mathcal{H}}$ to obtain $\mathcal{H}$. In addition we consider the dual spaces of continuous linear functionals $\Phi^{\times}$ and $\mathcal{H}^{\times}$ respectively. Since $\mathcal{H}$ is self dual, we obtain

$$\Phi \subset \mathcal{H} \subset \Phi^{\times}, \tag{8}$$

[7]To avoid a simple confusion (e.g., Bricmont 1995, pp. 165-166), note that singular distributions such as delta functions *are not* used to represent probability distributions in the rigged Hilbert space approach.

where $\Phi^{\times}$ is characterized by the induced topology $\tau_{\times}$.[8]

For the Brussels-Austin Group, the chief reason to work in a RHS is the ability to naturally model unstable physical phenomena such as decay, scattering and the irreversible approach to equilibrium lacking in HS (e.g., Bishop 2003a). These kinds of time-dependent processes require complex eigenvalues and generalized eigenfunctions (Gel'fand and Shilov 1967). Such mathematical quantities are not well-defined in HS, but are given rigorous justification in a suitable RHS. In particular the Liouville operator, which characterizes a LPS's approach to equilibrium, does not have a complete set of eigenvalues and eigenfunctions in a HS. The Brussels-Austin Group has demonstrated that a complete set of eigenvalues and eigenvectors for this important operator can be defined and calculated for several chaotic models in extended spaces (Antoniou and Tasaki 1992 and 1993; Hasegawa and Shapir 1992; Hasegawa and Driebe 1993). An additional motivation for switching to a RHS is that the equations of motion defined on a HS are time-symmetric. Time-asymmetric equations may be defined and solved in a RHS making the latter type of space a natural choice for modeling intrinsic irreversible processes. Intrinsic irreversibility is of prime interest to the Brussels-Austin Group because these types of irreversible processes are related to intrinsic arrows of time in physics (i.e., arrows of time which are independent of human intervention or approximation).[9]

5.3 Semigroup Operators in RHS and Irreversibility

One of the important features of RHS is that evolution operators are often elements of semigroups rather than groups, so that irreversible behavior can be modeled naturally. The case of simple (idealized) scattering is a good example for illustrating the concepts. There is a preparation apparatus which prepares particles in a particular state (energy, angular momentum, etc.). The particles are emitted at a target (assumed to be fixed in this analysis). The free particle Hamiltonian in (4) is H_0 while the potential in the interaction region surrounding the scattering center is V. After the interaction with the target, the detector registers the particle measuring quantities such as the angle of scattering relative to the initial direction of the particle as emitted from the accelerator or the energy of the particle after the scattering event.

Each interaction involves a resonance which can be described as

$$|E^{\pm}>=\left(1+\frac{1}{E-H\pm i\varepsilon}V\right)|E>\,, \tag{9}$$

[8]To say that τ_{Φ}, is *finer* than $\tau_{\mathcal{H}}$ means there are fewer τ_{Φ}-convergent Cauchy sequences in Φ than there are $\tau_{\mathcal{H}}$-convergent Cauchy sequences in $\mathcal{H}$. (Likewise to say that the topology of $\Phi^{\times}$, denoted by $\tau_{\times}$, is *coarser* than $\tau_{\mathcal{H}}$ means there are more $\tau_{\times}$-convergent Cauchy sequences in $\Phi^{\times}$ than $\tau_{\mathcal{H}}$-convergent Cauchy sequences in $\mathcal{H}$.) Therefore the space Φ is a dense linear subspace of $\mathcal{H}$.

[9]In more recent work Petrosky and Prigogine (1997) have explored rigging "Liouville space"–the space of density functions or density operators–for dynamics. Ordóñez (1998) has demonstrated that these Liouville spaces can be rigged as a Gel'fand triplet, yielding semi-group operators and generalized eigenvectors.

a Lippmann-Schwinger-type equation for the evolution of the energy eigenstates as they pass through the scattering region. Whenever the operator on the right hand side of (9) applied to the energy eigenstate $|E>$ goes to infinity, we have a resonance. According to the Brussels-Austin Group, if, given a sufficiently large number of interacting particles, the number of resonances in a system is sufficiently large, then the system will evolve from a highly ordered state to a completely randomized or equilibrium state. This evolution is intrinsically irreversible, due to the internal dynamics of the system.

The intrinsic irreversibility of LPS models must be described by semigroups. This necessitates leaving the HS framework and working in a broader mathematical space such as a RHS which Antoniou and Prigogine (1993) adopt in their analysis of the Friedrich's model for scattering. In the Gel'fand triplet $\Phi \subset \mathcal{H} \subset \Phi^{\times}$, $\Phi^{\times}$ is the space of particle distribution functions. Furthermore Antoniou and Prigogine adopt the following time ordering condition: Any excitations or preparations are to be interpreted as events taking place before $t = 0$ while any de-excitations or detections are to be interpreted as events taking place after $t = 0$ (1993, pp. 445 and 455).

At the point in the analysis of the scattering experiment where choices have to be made regarding how to interpret the directions of integration for the analytic functions involved in the upper and lower complex half-planes, they choose the following interpretations (1993, pp. 454-455): Excitations are identified with extensions from the lower to the upper half-plane, while de-excitations are identified with extensions from the upper to the lower half-plane. So the time-ordering rule is applied with respect to the choice of how to deform the contours in the complex plane with respect to the choice of direction of integration along the contours. Proceeding in this fashion Antoniou and Prigogine derive concrete realizations for the space Φ involving Hardy class function spaces (1993 pp. 457-459; see also Bishop 2003a and 2003b).

Antoniou and Prigogine discuss two semigroups of evolution operators. The first is $U^{\dagger}(t) = e^{-iHt}$, initially defined on $\mathcal{H}$ for $-\infty < t < \infty$, extended to $\Phi^{\times}$. It is continuous and complete in the topology $\tau_{\times}$ of $\Phi^{\times}$ only for $t \geq 0$, and they identify its temporal direction as carrying states into the forward direction of time. This operator describes evolution reaching equilibrium in the future. The second operator is $U^{\dagger}(t)$ extended to $\Phi^{\times}$, continuous and complete in the topology $\tau_{\times}$, but only for $t \leq 0$.[10] They identify the temporal direction of this latter operator as carrying states into the *backward direction* of time ($-t$ increasing), so this operator describes evolution reaching equilibrium in the past. Since no physical systems are ever observed evolving to equilibrium from the future into the past, they *select* $U^{\dagger}(t)$ extended to $\Phi^{\times}$ for $t \geq 0$ as the physically relevant semigroup of evolution operators for modeling statistical mechanical systems. This selection is taken to be an expression of the second law of thermodynamics based on our empirical observations (Antoniou and Prigogine 1993, p. 461).

The approach sketched in this section for the case of transient scattering can

[10]The requirements of continuity and completeness force the unitary group extended to $\Phi^{\times}$ to be restricted to the separate time ranges $t \leq 0$ and $t \geq 0$ (Bohm and Gadella 1989, pp. 35-119).

be extended to the case where the interactions are continuous and persistent, yielding similar results (Petrosky and Prigogine 1996 and 1997).

6 Discussion of the RHS Approach

The Brussels-Austin Group's RHS approach has yielded solutions (mostly numerical) to nonequilibrium statistical mechanical system equations. Based on these solutions and the insights gained from the new approach, Prigogine and coworkers make a number of claims needing detailed discussion.

6.1 Thermodynamic Arrow of Time

One of the claimed virtues of the approach is that it provides an explanation for the thermodynamic arrow of time. This has been one of the central goals of Prigogine since he began his work in SM. One feature that both the earlier similarity transformation approach and the RHS approach share in this quest is a kind of vacillation between seeking an explanation of the thermodynamic arrow in the dynamics of the physical system, and taking the empirically observed direction of the arrow as a fundamental principle.

In the RHS approach, the types of mechanisms to which the Brussels-Austin Group appeals for explaining the thermodynamic arrow are diffusion, the growth of correlations and collective effects, all of which are generated by Poincaré resonances (Antoniou and Prigogine 1993; Petrosky and Prigogine 1996 and 1997). The extension of the description of a LPS, with Poincaré resonances, persistent interactions and chaotic dynamics, to Gel'fand triplet spaces allows the eigenvector equations to be solved. In the course of analyzing these solutions, characteristically there are two semigroups that emerge as sketched in Section 5.3. At this point in the analysis, one semigroup is selected because it represents systems approaching equilibrium in the temporal direction of the future, while the other semigroup is disregarded because it describes systems approaching equilibrium in the temporal direction of the past which is never observed and, therefore, deemed to be unphysical (Antoniou and Prigogine 1993, p. 461; Petrosky and Prigogine 1996, p. 453 and 1997, p. 13). By making this latter appeal to observations, the Brussels-Austin Group is appealing to the very facts they seek to explain *via* the dynamics of the physical system.

The model equations alone do not uniquely determine which semigroup is the appropriate one, so some kind of appeal to physical considerations is needed. As discussed in Section 5.3 above, the Brussels-Austin Group does make an appeal to a criterion for choosing a temporal ordering: Any excitations are to be interpreted as events taking place before $t = 0$ while any de-excitations are to be interpreted as events taking place after $t = 0$. While there is a clear ordering of time from excitation to de-excitation, the criterion invoked still ultimately rests upon our observations that a system is excited before it undergoes de-excitation. The *physical* reason why the thermodynamic arrow runs from the past toward the future is still undiscovered in the RHS approach, though the approach gives us the mathematical tools to explore and describe the arrow precisely.

6.2 Correlation Dynamics

The RHS approach highlights the role of nonlocal and collective effects due to long-range correlations, introducing new dynamics in the probabilistic description not expressed in the trajectory description of a LPS.[11] The term "collective effects" is used to describe the behavior of an aggregate of particles coupled together in some fashion that is distinct from the behavior of individual particles. Collective effects can arise from long-range forces such as electromagnetism and gravity, or from spatial correlations caused by interactions.

Spatial correlations play an important role in the temporal ordering of the dynamics of SM systems. In atomic or molecular gases, collective effects are due to collisions. Consider the idealized textbook situation, where we start with an isolated gas of N particles in a volume V that have yet to interact with one another. If the initial distribution of the particles is homogeneous and isotropic, then the particles are equally likely to be at any point $\vec{r}$ in V.[12] This result holds for each individual particle under the condition that the positions of the other particles are arbitrary. In a typical gas or liquid, this latter condition is not fulfilled in general, however. Consider two particles at a time in our gas. Given the position of one particle, different positions of the second particle are not equally likely to obtain; namely, the second particle cannot occupy the position of the first particle. Due to interparticle interactions and the symmetry properties of the state vectors, different values of the relative position $(\vec{r}_2 - \vec{r}_1)$ between our two test particles in the entire gas do not appear with equal likelihood. This feature is known as a *spatial correlation* between the simultaneous positions $\vec{r}_1$ and $\vec{r}_2$ of the two particles.

In a plasma, for example, where the gas is composed of charged particles, spatial correlations are the tendencies of unlike charges to cluster together and the tendencies of like charges to repel each other. The simultaneous positions of the particles in the plasma are not all equally likely. It turns out that there is a simple relationship between the spatial integral of the correlation function representing spatial correlation and the mean square fluctuation of the density of the gas particles (Pathria 1972, pp. 447-450), meaning the spatial distribution of the particles is influenced by the presence of such correlations. In addition these correlations are directly dependent on the density of particles in the gas. As the density decreases, such collective effects disappear because the *mean free path* of the particle, a measure of the likelihood of a collision during a given distance traveled, becomes comparable to V. This means collision events will be very rare and correlations will be kept to a minimum when the mean free

[11] Prigogine (1962, pp. 138-195) introduced a simplified version of correlation dynamics and George (1973) developed the idea in the direction indicated in this section.

[12] Of course, in this idealized example the assumption of equiprobability of states is reasonable. In a LPS, by contrast, interactions are persistent, so this assumption cannot be made.

path is large.

Collisions are frequent in dense gases and the spatial correlations induced by collisions couple each particle with many (possibly all) other particles in the gas. It is this coupling due to correlations that leads to collective behavior responsible for gas particles being collected into coherent structures rather than being uniformly spread throughout the volume. Examples would be turbulence and shock waves.

To see how these correlations develop, start with the particles in the gas before they have interacted with each other. As they begin colliding, the first interactions set up binary correlations between particles. As the interactions persist, ternary correlations begin to appear. The process will continue by establishing quaternary correlations and so on through N-ary correlations as more and more particles become involved others through collisions. The progression from lower order correlations (which appear first) to higher order correlations (which appear later) corresponds to a natural temporal ordering for the evolution of the states of the gas. Correlations and other collective effects can rival or exceed the role of individual particle trajectories and be masked by a dynamical description that treats trajectories as its basic explanatory element.

For example the electromagnetic force is a long-range force. It is the dominant force in many situations in a plasma, so the behavior of a plasma is not reducible to the dynamics of the trajectories of the individual particles alone. In the case of a plasma, the energy of the plasma is affected by the presence of correlations, such that one of the differences between the energy of a plasma and that of an ideal gas (noninteracting particles) is given by a correction term due to correlation effects (Krall and Trivelpiece 1986, pp. 63-65). Not only do these effects interact with the electromagnetic fields of the plasma itself, but they also generate new electromagnetic fields that react back on the plasma leading to very complex dynamics.

Long-range correlations are another effect in the dynamics of correlations that become apparent in the RHS approach (discussed in its earliest form in Prigogine 1962 and George 1973). As gas particles begin to interact, correlations develop among the particles due to interactions (recall that in a LPS these interactions are associated with resonances). Along with the growing order of correlations, long-range correlations develop as particles interact with one another and then separate over long distances while carrying the "memory" of their prior interactions (correlations) with them to other parts of the gas. Over short time scales, the growing order of correlations appears to be the more dominant of the two effects. As time goes on, the long-range correlations due to resonances are built up so that collective effects become influential. These long-range correlations are associated with nonequilibrium modes of energy transfer (Petrosky and Prigogine 1996, p. 468).

Over longer time-scales, another very interesting phenomenon occurs. Equilibrium short-range binary correlations remain finite, but nonzero around each particle. In turn ternary nonequilibrium correlations are built up among particles in a small region. These correlations diffuse throughout the system, leaving the equilibrium correlations, while quartinary nonequilibrium correlations are built up among the local particles. These correlations diffuse throughout the system while quintinary nonequilibrium correlations build up and so forth. As time continues the variously ordered nonequilibrium correlations can propagate over large distances due to diffusion so that the corresponding information is transferred globally among the particles of the gas. The end result is a "sea" of multiple incoherent correlations (Petrosky and Prigogine 1996, p. 468). This effect provides a natural temporal direction for the flow of entropy and is revealed in the types of complex spectral representations of the operators governing statistical evolution made possible by working in an RHS.

In this sense one might argue that as the order of correlations increases, as long-range correlations grow and as higher-order nonequilibrium correlations propagate throughout the gas, the effects of individual trajectories on the global dynamics of the gas become less important relative to the effects of the dynamics of correlations. This does not mean that particles lack trajectories and positions in state space as these types of interaction events are parasitic on these concepts (e.g., mean free path between collisions). In my view correlations and collective effects make the significant contributions to the global dynamics while the effects of trajectories play a role only locally (see below).[13]

One might object that the dynamics of correlations can somehow be reversed even though the probability of the right kinds of reversals to run the whole evolution backwards (like a film in reverse) is extremely small. If true, then the situation is still the same as in standard thermodynamics where the increase in entropy in systems is viewed as being reversible though the probability is vanishingly small.

The Brussels-Austin response to such an objection for open systems was given in Section 3.4. For closed systems they have shown that as the dynamics of correlations continue, an "entropy barrier" against inversion develops. This barrier can be defined as the value of the H-function[14] after such an inversion minus its value before such an inversion. This difference increases exponentially with time, so the longer the LPS evolves, the higher the barrier to inversion. Essentially this means that the energy requirements to invert the system of particles increases very rapidly with time. As the system approaches equilibrium, this energy barrier diverges, hence, there is no physical way of "going back" in the anti-thermodynamic direction (Petrosky and Prigogine 1996, pp. 468-469 and 494-495).

Among the physical mechanisms playing a role in a LPS, correlations appear to play a crucial role in irreversibility. As was apparent in the earlier similarity transformation approach, the progression of correlations suggests a natural direction for the thermodynamic arrow (George 1973). But this is not simply another way of saying that entropy increases for such systems because in an

[13]Of course I have used idealized examples in this section in the sense that we imagined starting with a gas of noninteracting particles and then "turning on" the interactions. Recall that interactions are persistent in a LPS so there is never a time in such systems when the microscopic dynamics can be characterized by smooth, smooth trajectories.

[14]This is a thermodynamic function related to entropy, which does not require coarse graining or the invocation of an environment in the Brussels-Austin approach.

open system the order of correlations may continue to grow while the measure of disorder in the system may remain constant or decrease. So correlations are not the complete explanation for the thermodynamic arrow of time.

6.3 "Collapse of Trajectories"

In the similarity transformation approach, Prigogine and collaborators put forward several arguments to the effect that smooth (i.e., everywhere differentiable), deterministic trajectories do not exist for unstable statistical mechanical systems. These arguments were fundamentally flawed in similar ways in that epistemological claims were treated as ontological claims. In the new approach, this bias against such smooth trajectories and the dynamics derivable from trajectories resurfaces in a different form that clarifies the Brussels-Austin attitude toward trajectories.

It is well known that in the traditional description, the trajectory of a point particle free of any external forces can be represented mathematically as a superposition of "plane waves" by taking the position of the particle and applying a Fourier transform from (q, p) space to (k, p) space. In this latter space, a trajectory is a coherent superposition of plane waves and this superposition is modeled by a Dirac delta function. For a particle undergoing free motion, this distribution function is a solution to the equation of motion, has unchanging width and is everywhere differentiable throughout its deterministic evolution ("smooth" trajectory).

For a finite number of particles with normalizable distributions, the trajectory description in (k, p) space and the Brussels-Austin probabilistic description agree.[15] In the thermodynamic limit, however, Prigogine and coworkers argue that resonances destroy smooth trajectories in the following way. In the thermodynamic limit, the Dirac delta function describing the trajectories of particles at $t = 0$, once evolution begins, immediately begins spreading throughout a subspace of (k, p) space under the action of resonances, though maintaining a delta function singularity[16] (Petrosky and Prigogine 1996, pp. 479-481 and 1997, pp. 35-37). The trajectories are no longer representable as delta functions, but by broader kinds of distribution functions. Petrosky and Prigogine unfortunately described this phenomenon as the "collapse of trajectories", but all they really mean is that a different notion of trajectory is required in a LPS.

In (q, p) space, this implies that there are no longer any smooth (everywhere differentiable) trajectories, but, rather, trajectories exhibiting *Brownian motion*. A simple way to see this is to return to our idealized gas example. As before,

[15] Some critics, such as Bricmont (1995, pp. 165 and 175), have overlooked the way in which the RHS approach reduces to standard SM approaches for small numbers of particles when LPS conditions are not fulfilled.

[16] The significance of the delta function singularity appears to be more mathematical than physical. Mathematically it means that so-called reduced distribution functions–where the distribution function refers to a subset s of the total number of particles in the system–exists in the thermodynamic limit, but such distribution functions almost always exist for molecules under most realistic forces. Reduced distributions were introduced into nonequilibrium contexts by (Brout and Prigogine 1956; Prigogine and Balescu 1959).

assume initially that the particles have not interacted with each other. Prior to any collisions, the motion of the particles can be characterized by smooth trajectories. As they begin interacting, the particle trajectories become piece-wise continuous as instantaneous discontinuities arise associated with each collision. Continuous interactions of this type would then prevent trajectories from being everywhere differentiable, resulting in particles exhibiting Brownian trajectories rather than smooth ones, but this in no way implies that there are no trajectories whatsoever.

Consider the special case of a single smooth trajectory represented as

$$\gamma(p,q) = \prod_{i=1}^{N} \delta(\vec{q}_i - \vec{q}_i^0)\delta(\vec{p}_i - \vec{p}_i^0) \tag{10}$$

in a LPS model where the superscript 0 indicates the contribution from the unperturbed Hamiltonian. To first order the time evolution of the momentum for the component $i = 1$ is giving by

$$\vec{p}_1(t) = \vec{p}_1^0 + \lim_{\Omega\to\infty} \frac{\lambda}{\Omega} \sum_k \sum_{n=2}^{N} (-\vec{k}) \frac{V_k}{\vec{k}\cdot(\vec{v}_1^0 - \vec{v}_n^0) - i\varepsilon} \left(e^{-i\vec{k}\cdot(\vec{v}_1^0-\vec{v}_n^0)t} - 1\right) e^{-i\vec{k}\cdot(\vec{q}_1^0-\vec{q}_n^0)}, \tag{11}$$

where Ω is the volume, $\vec{k}$ is the wave vector, $\vec{v}_1$ is the velocity vector of particle 1, $\vec{v}_n$ is the velocity vector of particle n, and ε is an infinitesimal positive constant. The first term represents the contribution from the unperturbed Hamiltonian and the second term represents contributions from the interactions. If N is finite, (11) becomes

$$\vec{p}_1(t) = \vec{p}_1^0 + \lambda \sum_{n=2}^{N} \int d\vec{k} \frac{V_k}{\vec{k}\cdot(\vec{v}_1^0 - \vec{v}_n^0) - i\varepsilon} \vec{k} e^{-i\vec{k}\cdot(\vec{q}_1^0-\vec{q}_n^0)} + O(\lambda^2), \tag{12}$$

in the limit $t \to \infty$ because the pole at $\vec{k}\cdot(\vec{v}_1^0 - \vec{v}_n^0) = i\varepsilon$ vanishes as $\Omega \to \infty$, the LPS condition. According to (12) the value of the momentum to first order asymptotically approaches a constant and the time dependence drops out. Note that in the limit $|\vec{q}_1^0 - \vec{q}_n^0| \to \infty$, the interactions from particles n remains finite even if such interactions are short-ranged due to resonances, so that long-range correlations are built up. In the thermodynamic limit, (11) generally diverges and Petrosky and Prigogine conclude that point distributions such as (10) representing trajectories are not physically admissible and, therefore, smooth trajectories are inconsistent with the thermodynamic limit in a LPS (1996, p. 480). Only singular nonlocal distributions appear to be consistent with the thermodynamic limit and such distributions lie outside of HS (Petrosky and Prigogine 1996, pp. 479-481).

These results are related to the nonlocal nature of the collective effects of the entire distribution described in Section 6.2 above. If any arbitrary finite number of particles were selected within the system and treated in isolation, all nonlocal diffusion and correlation effects become negligible and we are left with the standard description (however, the trajectories in these descriptions would not necessarily be everywhere differentiable).

In more realistic situations, the nonexistence of smooth trajectories leads directly to the Brussels-Austin claim that a LPS exhibits behavior that *cannot be derived from trajectory dynamics*. Such effects include the breaking of time symmetry (i.e., the appearance of semigroups of operators governing the evolution), diffusion and correlation dynamics. Prigogine and coworkers refer to these effects as "non-Newtonian" to emphasize the fact that the trajectory description is inadequate to account for them. The existence of collision operators such as the Fokker-Planck operator is only a necessary condition for irreversibility and other "non-Newtonian" effects. Particular types of distributions (namely singular nonlocal distributions) must also be present in order to have sufficient conditions for such behavior. The class of singular distribution functions is quite broad and applicable to many ordinary situations in SM (the canonical distribution is an example; see also Prigogine 1962 and 1997). Algebraic and computer modeling demonstrating that the trajectory and distribution descriptions yield different results for systems fulfilling LPS conditions have been carried out (e.g., Petrosky and Prigogine 1993, 1994 and 1996).

I believe the appropriate way to understand this new approach with its "non-Newtonian" effects is to agree with them that these distribution descriptions cannot be reduced to point-wise descriptions. However, both descriptions should be viewed as valid within their domains. The trajectory description is valid for local regions of a LPS, where there are relatively few particles. Here trajectory dynamics is the dominant feature. Interactions take place among particles at this local level and to the extent that we can ignore higher-order and long-range correlations, trajectory and distribution descriptions agree in their account of physical behavior as was noted earlier.

Where my interpretation differs from many within the Brussels-Austin Group is when the conditions for a LPS are met (large number of particles, continuous frequencies, etc.). I agree that in examining the global evolution of an LPS, higher-order correlations and collective effects due to long-range, persistent interactions are the dominant features, which are not reducible to trajectory dynamics alone. Trajectories are not irrelevant, however, because such features as correlations and collective effects presuppose particle positions and trajectories. For example, collective effects in ordinary gases do not disconfirm the existence of trajectories, though the effects of correlations can rival or exceed the effects of individual particle trajectories and be masked by a dynamical description that treats trajectories as the sole explanatory element. Note that (12) does not imply smooth point trajectories are immediately expunged from a LPS. Physically smooth trajectories are converted into random walks due to the persistent interactions and the long-range, higher-order correlations that diffuse throughout the system over time. As described above, resonances are closely related to long-range correlations and collective effects, behavioral features of unstable systems for which the trajectory description alone cannot adequately account. For LPS models the whole is more than the sum of its parts. Particle trajectories are necessary for global distributions to exist, but are insufficient for determining how such global distributions evolve in time. The thermodynamic paradox might be dissolved because (1) the time-symmetric behavior of the trajectory dynamics contributes nothing more to the global evolution of the SM system than the necessary conditions for the existence of such a system and (2) in a LPS trajectories exhibit Brownian motion and correlation dynamics dominate the macroscopic dynamics. Thermodynamic behavior would then be an emergent global phenomenon possessing a temporal direction.

My interpretation suggests a way to reduce the tension in their view between operationalism with respect to trajectories and realism with respect to distributions (see Section 3.3), where the Brownian trajectories of the system give the *necessary* conditions for the existence of the distribution ρ, but *not sufficient* conditions for its evolution. In my judgement the new approach the Brussels-Austin Group has been exploring illuminates some of the underlying physical mechanisms of thermodynamic behavior. Focusing on the growth and dynamics of correlations and collective effects are important physical insights which have advanced our understanding of thermodynamic processes. And by employing extended mathematical structures such as RHS, they have developed powerful tools for describing such processes which will doubtless lead to further insights.

As a last comment, I should point out that this RHS approach does not represent a kind of coarse-graining approach, at least as normally understood. Emphasis shifts away from trajectories because they are only a part of the story of the behavior of a LPS. Coarse-grained accounts typically assume that trajectory dynamics is the whole story, but involve some kind of averaging process over this underlying dynamics. In contrast, no averaging procedures have been used in the RHS approach. And, as in the similarity transformation approach, the RHS approach distinguishes between manifolds of stable and unstable motions (in contrast to typical coarse-grained accounts). Furthermore, if the global behavior of a LPS is not only emergent, but also constrains the motion of individual particles (say by restricting the modes of energy transfer), then an appropriate mathematical description should be able to describe this kind of feedback between levels in a system. The RHS approach can describe such feedback effects, whereas coarse-grained accounts cannot because they deal with only one level of a given system. Finally, whether trajectories that are not everywhere continuous nor everywhere differentiable are deterministic or not is an open question in the RHS approach, as I discuss in the concluding section (coarse-grained accounts typically assume trajectories are deterministic, though usually no explicit assumptions are made regarding continuity and differentiablility).

7 Possibility Rather than Certainty?

Prigogine's provocatively titled book, *The End of Certainty* (1997), sums up one of arguably the most important and far reaching consequences of the Brussels-Austin Group's work: Namely, that the certainty of the deterministic, time-symmetric trajectory description is not applicable to the global dynamics of a

LPS. Instead only a statistical description of probability densities remains. In conventional CM and SM models, particle positions and trajectories are treated as the fundamental ontological entities determining the dynamical evolution of the system. In the RHS approach for LPS models, by contrast, the fundamental ontological feature is the probability distribution, i.e., the large-scale arrangement of the particles themselves. To reformulate the laws of classical dynamics along the statistical lines suggested by Prigogine and co-workers leads to the conclusion that such laws now 'express "possibilities" and no more "certainties"' (Petrosky and Prigogine 1997, p. 1).

Where there are relatively few numbers of particles, this approach to dynamics reduces to the standard results of CM, so the trajectory picture with its deterministic and time-reversible character is preserved as a limiting case. In non-LPS cases, the RHS approach recovers the usual results of SM (e.g., Fokker-Planck equations, Boltzmann equations, non-Markovian master equations). It is in cases where the LPS criteria apply that probability becomes the fundamental notion, irreducible to the trajectory description. Systems must be treated holistically, at least to some degree (not to be confused with coarse-grained averages). If any subset of the total number of particles N is treated by itself all the "non-Newtonian" effects disappear and the conventional descriptions are recovered. It is in this sense that Prigogine believes, 'What is now emerging is an "intermediate" description that lies somewhere between the two alienating images of a deterministic world and an arbitrary world of pure chance...[T]he new laws of nature deal with the possibility of events, but do not reduce these events to deductible, predictable consequences' (Prigogine 1997, p. 189).

The nature of this possibility supposedly represents a new conception which remains to be clarified, however. It is clearly not the kind of irreducible indeterminism described in von Neumann collapse, where some sort of collapse from multiple possibilities to a single actuality is envisioned. As Prigogine and colleagues describe it, their probabilistic formulation of physics is also to be distinguished from chaotic dynamics, where the underlying dynamics is deterministic, but the outcomes of the system are not predictable. The latter is *epistemically* indeterminable but not *ontically* indeterministic.[17] Instead the dynamics envisioned by Prigogine and his colleagues involves an interplay between unitary reversible processes and irreversible processes.

But the relationship of this probabilistic evolution to deterministic dynamics remains unclear and requires attention because under some conditions the dynamics of probability distributions can be "embedded" into completely deterministic dynamics and Markov processes can almost always be "embedded" into deterministic Kolmogorov processes (Section 3.5). This leaves open the possibility that there is no *significant fundamental difference between this new conception of probabilistic evolution and the conventional conception of deterministic evolution*, or so one could plausibly argue.[18]

[17]Understanding what it means for a system or a description to be ontically indeterministic is by no means straightforward (e.g., Bishop 2002).

[18]The larger deterministic systems into which probabilistic processes are embedded could be fictitious (Primas 2002). Furthermore, the existence of theorems showing that Markov

Though more needs to be said regarding the notion of probabilistic dynamics they are working out, it must be internally generated by the dynamics of the system (e.g., *via* correlation dynamics) rather than imposed from the outside by observers, measuring apparatuses or the environment. I do not take it that this need for more clarification is a serious weakness of their program. On the contrary, it could be analogous to the early days of quantum theory where many concepts (indeterminacy being one of them) were very hazy at the start inviting serious reflection and exploration.

The RHS formalism gives us a unified description of dynamics and thermodynamics within a statistical framework and a consistent, rigorous description of irreversible processes. The mathematical developments are indeed impressive, including new results regarding the theory of complex spectral representations of operators. Furthermore this framework is powerful enough to allow a unification between CM and QM (Prigogine et al. 1991; Petrosky, Prigogine and Tasaki 1991; Petrosky and Prigogine 1994). However, the promise of the recent Brussels-Austin work must be balanced against two important open questions: (1) What is the physical and mathematical status of the past-directed $t \leq 0$ semigroup (Section 5.3) and (2) What is the precise nature of the probability lying at the heart of an LPS? Answering these two questions holds the key to their being able to offer an explanation for the thermodynamic arrow of time and for their developing a notion of indeterminism that is different in kind from that discussed in conventional QM developments that would be truly revolutionary.

As things stand, the Brussels-Austin Group has given us a powerful descriptive tool for irreversible processes, and nonlinear dynamics more generally, but they have not given us an explanation for the origination of the irreversibility we observe in our world. One might object that the RHS approach is ultimately only of mathematical interest since there is nothing philosophically interesting given the current state of the above open questions. This response is too quick, however. These open questions can also be viewed as opportunities for exploration of the underlying concepts of the approach in order to attempt to answer these questions. For example, by adopting a different arrow of time in the context of scattering in a RHS formulation of QM, one can show that the $t \leq 0$ semigroup is also future oriented (this time arrow is, however, highly operational in character and not generally applicable outside of laboratory contexts; for discussion, see Bishop 2003a and 2003b). So interesting conceptual questions are raised by the Brussels-Austin work. Besides, even if questions (1) and (2) should ultimately be answered in a way that closes off this avenue for nonequilibrium SM, that information is also valuable to philosophers.

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processes can be embedded in a larger deterministic process does not necessarily mean that a given Markov process is deterministic. Whether or not a given Markov process is deterministic or not is an ontological rather than a mathematical question. It should also be clear, however, that simply characterizing the probability densities via Kolmogorov measures is insufficient because this cannot settle the ontological nature of the probability.

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