Some Philosophical Influences on Ilya Prigogine's Statistical Mechanics

(Running head: Philosophy and the Statistical Mechanics of Ilya Prigogine)

Abstract:

During a long and distinguished career, Belgian physical chemist Ilya Prigogine (1917-2003) pursued a coherent research program in thermodynamics, statistical mechanics, and related scientific areas. The main goal of this effort was establishing the origin of thermodynamic irreversibility (the "arrow of time") as local (residing in the details of the interaction of interest), rather than as global (being solely a consequence of properties of the initial singularity – the "Big Bang"). In many publications for general audiences, he stated the opinion that this scientific research had great philosophical importance. Prigogine and his colleagues considered that the most recent stages of this research program have been successful, so that the local origins of the arrow of time are now established. There is no scientific consensus as to whether or not this claim is valid. Similarly, there is no consensus on whether the competing global (initial singularity) explanation has been proven.

End of Abstract

Belgian chemist and physicist Ilya Prigogine (1917-2003) made substantial advances in the science of non-equilibrium thermodynamics — recognized by the Nobel Prize in Chemistry for 1977. He also published a number of books for general audiences, developing themes related to his scientific work. Prigogine's publications were received with high enthusiasm in many parts of the world[1] — but also generated widespread unease (particularly among physicists), and some overt opposition.

Prigogine's family had fled Russia (where his father had been a chemical engineer) in 1921, and eventually settled in Belgium in 1929. Ilya's brother Alexander (four years older) studied chemistry at the Université Libre de Bruxelles (ULB, the Free University of Brussels). The younger Prigogine decided not to pursue his interest in history, archaeology, and music (he was an outstanding pianist) but rather to follow his brother into the ULB chemistry curriculum. However, he maintained a lively interest in phases of culture other than science throughout his career.

The importance of formal philosophy to his intellectual development is evident from a short autobiography that he prepared in connection with his Nobel Prize.

> Since my adolescence, I have read many philosophical texts. I still remember the spell *L'évolution créatrice* cast on me. More specifically, I felt that some essential message was embedded, still to be made explicit, in Bergson's remark: "The more deeply we study the nature of time, the better we understand that duration means invention, creation of forms, continuous elaboration of the absolutely new." (Prigogine, 1977)

French philosopher Henri Bergson (1859-1941) was the recipient of the 1929 Nobel Prize for Literature. His influence was strong in the French-speaking parts of Belgium when Ilya Prigogine was in secondary school there. Bergson is said to have been the first to elaborate a "process" philosophy. He held that classical science had excessively "spatialized" time, to the neglect of duration, including "lived time." A consuming interest in time — and especially its relationship to the emergence of new types of organization — became a salient characteristic of Prigogine's work, both in his science and in his books for general audiences.

As a young chemistry student at ULB, Prigogine came under the influence of Théophile De Donder (1873-1957) who had earned his Ph.D. in science while teaching secondary school, and then was appointed to teach a course in theoretical thermodynamics for engineers at the same university, bringing mathematical theory to bear on practical problems. The autobiography continues:

> …since the fundamental work by Clausius, the second principle of thermodynamics has been formulated as an inequality: entropy production is positive. … Given my interest in the concept of time, it was only natural that my attention was focused on the second principle, as I felt from the start that it would introduce a new, unexpected element into the description of the evolution of the physical world. … A huge part of my scientific career would then be devoted to the elucidation of macroscopic as well as microscopic aspects of the second principle, in order to extend its validity to new situations…(Prigogine, 1977)

German physicist Ludwig Boltzmann (1844-1906), who as a senior scientist had also held a chair of natural philosophy (Fasol-Boltzman, 1990), was another of the young Prigogine's favorite authors.

> Since the time of my first graduation in science, I have been an enthusiastic reader of Boltzmann, whose dynamical vision of physical becoming was for me a model of intuition and penetration. Nonetheless, I could not but notice some unsatisfying aspects. It was clear to me that Boltzmann introduced hypotheses foreign to dynamics; under such assumptions, to talk about a dynamical justification of thermodynamics seemed to me an excessive conclusion, to say the least. In my opinion, the identification of entropy with molecular disorder could contain only one part of the truth if, as I persisted in thinking, irreversible processes were endowed with the constructive role that I never cease to attribute to them. For another part, the applications of Boltzmann's methods were restricted to dilute gases, while I was most interested in condensed systems. (Prigogine, 1977)

The fundamental laws of both classical mechanics and quantum mechanics have time-reversal symmetry — it would not be possible to decide whether a video of a collision of billiard balls (or of an interaction involving a single atom and a photon) were running forwards or backwards. This being the case, it is a problem to understand the origin of the irreversibility of most events that we observe in ordinary life — even such a seemingly simple process as the loss of heat from a cup of hot liquid. Boltzmann made a major contribution in recognizing that spontaneous changes (such as cooling coffee) involve transition from less probable (more highly organized, low entropy) arrangements to more probable (less highly organized, higher entropy) ones. Boltzmann also made the further inference that since all spontaneous changes lead to lower net organization (higher entropy), the early stages of the universe must have been highly organized indeed (very low entropy).

Prigogine's teacher De Donder was the founder of "The Brussels School of Thermodynamics" which focused on the thermodynamic treatment of irreversible processes, including chemical reactions. Much of the work of the Brussels School was connected with rates of entropy production of systems that are not at equilibrium. One of Prigogine's early achievements, after he was appointed to the ULB physical chemistry faculty, was to demonstrate that non-equilibrium systems that are close to equilibrium will evolve so as to approach the equilibrium state in such a way that the rate of entropy production is as low as is possible.

The Prigogine autobiography reports:

> De Donder related the entropy production in a precise way to the pace of a chemical reaction, through the use of a new function that he was to call "affinity." (Prigogine, 1977)

De Donder’s affinity quantity[2] is well defined for any particular sample, but with respect to a particular chemical reaction. Each sample has a different value of affinity for each chemical reaction that might possibly occur.[3] Affinity is the measure of the distance (in energy units) of the actual state of a system from some one (specified) equilibrium condition of the same system. This complex notion disturbs many. Affinity was not used or referred to in the textbook (Lewis, 1923) that dominated American thermodynamics education for the middle years of the twentieth century. Affinity is still regarded with suspicion by many scientists, as it was when De Donder introduced the term. The autobiography continues:

> It is difficult today to give an account of the hostility that such an approach was to meet. For example, I remember that towards the end of 1946, at the Brussels IUPAP meeting, after a presentation of the thermodynamics of irreversible processes, a specialist of great repute said to me, in substance: “I am surprised

> that you give more attention to irreversible phenomena, which are essentially transitory, than to the final result of their evolution, equilibrium.” (Prigogine, 1977)

The time-reversal symmetry of basic physical laws is sometimes taken to suggest that time is somehow unreal — dependent on the perceptions of human observers. This impression is strengthened by the usual method used for dealing with systems that are not at equilibrium. Since calculation of the microscopic state of such a system is generally impossible, average values of quantities of interest are computed for small but macroscopic volumes. Such models produce irreversibility, but that result may be (and is generally considered) an artifact of the approximation ("coarse graining") that has been used.

Prigogine (facetiously) displayed a statement of Albert Einstein on his office wall(Edens, 1991).

> For us believing physicists, the distinction between past, present and future is only an illusion, however persistent.

Prigogine regarded this point of view as wrong, and also pernicious, since it implies radical separation between human concerns and fundamental physical reality. Prigogine (as Bergson had done) considered time to be objective, real, and creative — rather than a result of human inadequacy, or of some peculiarity of the early state of the universe.

The standard understanding of the origin of the second law of thermodynamics (the second principle of Clausius mentioned above) is that the universe emerged from an initial singularity that had an extraordinarily high degree of organization. Prigogine held that the origin of many types of irreversibility is ‘local’ (residing in the details of the interaction of interest) rather than ‘global’ (ultimately related to some peculiarity of the initial singularity at the origin of universe).

In July 1974, Prigogine, together with Isabelle Stengers (then a philosophy graduate student at ULB and also a member of his physical chemistry research group there), prepared a presentation under the auspices of the Council of Europe. The French title of that piece is *La Nouvelle Alliance,* translated as "‘The New Covenant." In support of the choice of that English noun, with its religious overtones, the title page of the original Prigogine and Stengers paper carries an epigram from pages 194-195 of Jacques Monod’s book, *Le Hazard at la Necessité* (“Chance and Necessity”). The translation of that epigram given in the English version of the paper is:

> The old covenant is broken; at last man knows that he is alone in the indifferent immensity of the universe, whence he emerged by chance.

In the original article, in the book of the same title published in French in 1979, and in the English version (*Order out of Chaos*) Prigogine and Stengers made their objection to this point of view explicit:

> The denial of becoming by physics estranged science from philosophy ... [and] ... became a dogmatic assertion directed against all those (chemists, biologists, physicians) for whom a qualitative diversity existed in nature … Today we believe that the epoch of certainties and absolute oppositions is over. Physicists belong to their culture, to which, in their turn, they make an essential contribution. (Prigogine, 1984)

Philosopher Huw Price (1996) strongly recommends that reality be viewed from an "Archimedean point" — "an untainted perspective" that transcends all special situations — the view from nowhere and "nowhen." After discussing difficulties that are encountered by attempts to deal with the mind-body problem on such an atemporal basis, Kim (2003) concluded that a "functional" approach is necessary to deal with relationships between mental states and their physical substratum. This implies that (as Bergson had taught) taking duration into accopunt is essential for philosophy. Taking time as seriously as Prigogine recommends would suggest that satisfactory resolution of the mind-body problem, and other major questions of human interest will require a even longer historical perspective than Kim envisions, including attention to developmental processes. Prigogine maintained that his approach marks a break with the style of science that has been dominant for several centuries, and signals a turning point in human appreciation of the physical world. Prof. Prigogine's work may be seen as an important contribution to a major intellectual transition that is now underway in several areas of culture through which long dominant presuppositions are undergoing revision. For instance, the type of economics that has been dominant for much of the second half of the twentieth century is being strongly challenged by an approach that takes the detailed evolutionary history of far-from-equilibrium multi-agent systems much more seriously (Bowles and Gintis, 2000). In many ways this (apparently independent) development in economic theory is quite parallel to the change in physical understanding of thermodynamics that Prigogine advocated.

Jean Bricmont (1995), professor of theoretical physics at the Catholic University at Louvaine-la-neuve — a short distance from Brussels — believes that Prigogine's philosophical conclusions are not supported by his results in statistical mechanics, and that his interpretations are seriously misleading. Bricmont's main point is that Boltzmann's late-nineteen-century explanation of irreversible processes is fully satisfactory. On this basis, there is no justification for regarding recent work on the thermodynamics of irreversible processes as bringing about radical change in fundamental physical understanding. Bricmont states:

> There are two fundamental ingredients in the classical explanation of irreversibility, in addition to the microscopic laws: .. initial conditions and .. many degrees of freedom: we have to distinguish between microscopic and macroscopic variables. (Bricmont, 1995).

Bricmont would probably put the emphasis on the words "have to" in the last clause in this statement. Prigogine, in contrast, would surely have read this sentence with emphasis on the word "we." Prigogine would not accept the view that the irreversibility of the processes that chemists and engineers encounter is based only on human ignorance. He held that the source of irreversibility was in the dynamics of interactions involved in those processes, rather than in the choice of variables used in a description, the ignorance of some human investigator, or some residue of the primordial fireball. His principal goal, throughout his long and active scientific career, was to demonstrate a local origin for irreversibility. The divergence of this goal from the aims of most physicists may account for a good deal of the unease that his work occasioned.

With this in mind, it is important to examine the present state of Boltzmann's inference that the original state of the universe was highly organized (low entropy). David Albert (2000) given an endorsement of that position, but Eric Winsberg (2004) claimed that endorsement is based on philosophic presuppositions, rather than on other arguments. Roger Penrose considered the same question on a more technical and scientific basis. He discusses (1989) cosmological singularities (such as the black holes and the original singularity – "the big bang") in terms of two tensors that he calls RICCI and WEYL. With respect to an initially spherical object, WEYL would correspond to a tidal distortion, changing the symmetry but preserving the volume; conversely RICCI refers to a symmetry-preserving contraction that reduces the volume of the sphere. He then reports:

> We generally find that [in spatiotemporal singularities] WEYL is much larger than RICCI…. Such behaviour is associated with a singularity of *high entropy.* However the situation with respect to the big bang seems to be quite different… As we approach the initial singularity we find that it is RICCI that becomes infinite rather than WEYL… This provides us with a singularity of *low entropy.* (Penrose, 1989)

Steven Hawking (1985, p. 2490.) comments on Penrose's proposal "[i]n effect, one is putting in the thermodynamic arrow by hand". Penrose concedes that the main argument for considering RICCI much larger than WEYL for the big bang is that is what needs to be the case in order for that singularity to have the low entropy that thermodynamics seems to require. Hawking's own suggestions for the cosmological origins of the arrow of time are also subject to objections (Price, 1996). It thus seems that the presumption that the arrow of time derives exclusively from the initial singularity is subject to the Scotch verdict — “not proven”. If Prigogine's quest for a local origin for thermodynamic irreversibility were to succeed, it might also contribute to progress in cosmology.

Bram Edens (1991) produced a thesis in philosophy of science that reviewed the work of Prigogine and his associates at ULB and Austin[4] (the Brussels–Austin group, or BAG) Edens suggested that Prigogine had a complex and non-standard fundamental outlook that issued in a quite unusual research program dealing with systems that are far from equilibrium.

> For the direction of time to be a problem we need to presuppose a certain kind of reductionism.. [that] macroscopic laws are reducible to microscopic laws. …Prigogine advocates a non-statistical (intrinsic) universally valid (at all levels) interpretation of irreversibility. (Edens, 1991)

Edens outlined several stages in the early research of Prigogine and his colleagues: a) Non-equilibrium Statistical Mechanics: near to equilibrium, entropy production is a minimum. 1946-~1971. b) Causal Dynamics: projection operators were used to derive generalized master equations. 1966-1977. c) The New Complementarity (of probabilistic and deterministic descriptions of non-equilibrium systems). ~1969-1989. Edens reports that, in the late 1960s, Prigogine shifted the center of his attention away from systems near equilibrium to those that are far from equilibrium — for those high-affinity sytems, entropy production was identified as the source of novel order. This shift in emphasis coincided with the development of widespread interest in instabilities and oscillations in chemical systems. The theoretical work of the Prigogine group, particularly that connected with the abstract chemical reaction-network model called "the Brusselator," was centrally important in understanding oscillations, self-organization, and pattern formation in chemical and biological systems.

Far-from-equilibrium chemical systems are governed by complex sets of differential equations, concerned with many chemical reactions and with diffusion of reagents and products. Even though the fundamental laws that describe the underlying physical processes all are fully reversible, such systems exhibit irreversible evolution in the direction that increases total entropy — the direction that leads to the future and not to the past. What is the origin of this symmetry-breaking? Edams identifies a series of phases in the Prigogine groups' answers to such questions: a) entropy as a selector (some initial states require infinite information and therefore are impossible), 1983-2004. b) an alternative to quantum theory. Far-from equilibrium symmetry-breaking eliminates wave-function collapse: ~1988. c) embedding—every function in phase space is a *trace* of a function in space of higher dimensionality: 1980-1998. (This approach derived from suggestions of Mackey (1992)) d) rigged Hilbert space: eigenfunctions for systems involving persistent interactions lie outside Hilbert space, and have intrinsically broken time-symmetry, ~1986-2004. Prigogine and his coworkers considered that their results from these several research initiatives were mutually reinforcing — and that their most recent research definitely established that the origin of irreversibility is local rather than global in character.

Robert C. Bishop (2004) recently published an independent analysis of the development of Prigogine's research program, with emphasis on work since the mid-1980s. He reports how aspects of work of the BAG did not fit comfortably into the mathematical framework of Hilbert space (HS) in which it had been cast. Eventually it was realized that a different framework — the "rigged Hilbert space" (RHS) that had been developed earlier for other purposes — was more appropriate for dealing with dynamic systems of the type that the BAG was interested in.

In the late 19th century, Henri Poincaré (1854-1912) had found that calculation of trajectories of objects in the solar system were complicated by "resonances" — transient associations of objects that prevented integration of differential equations. Systems of interest in statistical mechanics are generally "large Poincaré systems" (LPS) for which resonances are ubiquitous. In such cases, the BAG found that calculations using RHS yield probability distributions rather than trajectories. This led to the assertion that when resonances are present, probability distributions are basic, and trajectories are derivative and approximate (to the extent that they exist at all). Prigogine concluded that the local origin of time reversal asymmetry had been established by these investigations.

Bishop proposes a variant interpretation of Prigogine's claim that trajectories do not exist, so that probabilistic descriptions are fundamental.

> The thermodynamic paradox might be resolved because: (1) the time-symmetric behaviour of the trajectory dynamics contributes nothing more to the global evolution of the statistical mechanical system than the necessary conditions for the existence of such a system and (2) in a large Poincare system trajectories exhibit Brownian motion, and correlation dynamics dominate the macroscopic dynamics. Thermodynamics is then an emergent global phenomenon possessing a temporal direction. (Bishop, 2004)

Both Edams and Bishop are much impressed by the extent, quality, and significance of the work of the BAG, but do not agree that the local origin of irreversibility has yet been unambiguously established. In their view, the work of the BAG, has greatly advanced description and understanding of far-from-equilibrium systems, but it is not yet clear whether or not the arrow of time has been "put in by hand" for basically philosophic reasons (as Hawking suggested is the case with Penrose's proposals on the initial singularity). Given the ambitious nature of the research program of the BAG, it is not at all surprising that adequate assessment of the results of their work is not quickly done. It well may be that the tension between the positions of Prigogine and his compatriot Bricmont (for example) may be a continuation of a perennial, basically metaphysical, debate (Hein, c. 1980).

It seems appropriate to quote at some length from what may be the last paper that Prof. Prigogine personally saw through the press.

> In his famous book on quantum mechanics, Dirac stated that chemistry can be reduced to problems in quantum mechanics. It is true that many aspects of

chemistry depend on quantum mechanical formulations. Nevertheless, there is a basic difference. Quantum mechanics, in its orthodox form, corresponds to a deterministic time reversible description. This is not so for chemistry. Chemical reactions correspond to irreversible processes creating entropy. That is, of course, a very basic aspect of chemistry, which shows that it is not reducible to classical dynamics or quantum mechanics. Chemical reactions belong to the same category as transport processes, viscosity, and thermal conductivity, which are all related to irreversible processes.

As far back as in 1870 Maxwell considered the kinetic equations in chemistry, as well as the kinetic equations in the kinetic theory of gases, as *incomplete* dynamics. From his point of view, kinetic equations for chemistry would be the result of adding "ignorance" to the physical description. This is indeed still the opinion of the majority of physicists today. However, it would be paradoxical if chemistry, which plays a fundamental role in the description of nature, were the result of our own mistakes.

The basic [result] is that the fundamental description of nonintegrable systems is no longer precisely in terms of Hamiltonian equations, but in terms of kinetic equations with broken time symmetry. Once we have the kinetic equation, it is easy to show that we have irreversible processes and entropy production. It seems to me therefore very natural to consider that chemistry is indeed a very important example of nonintegrable Poincare systems, where the non-integrability is due to resonances. I hope that this new aspect will continue to be explored by future generations of physicists and chemists." (Prigogine, 2003)

Due in part to the philosophic influences at its origins, Prigogine's scientific work makes contact with the complex problems that are encountered by engineers, chemists, biologists and social scientists in a way that physical science rarely does. This may account for the large number of enthusiastic readers his general-interest books have attracted. But in so doing it has called into question notions that have long been considered by physicists to be well established — thereby engendering cool or even hostile reception.

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[1] See, for example: http://www.unisi.it/eventi/prigogine/awards.htm

[2] RT ln Q/K — where K is the equilibrium constant for a specific reaction and Q has the same form as an equilibrium constant but involves actual rather than equilibrium concentrations.

[3] Similarly, each place has a different value of "distance" depending on what possible destination is considered. Some philosophers hold that distance does not exist.

[4] At the Prigogine Center for Statistical Mechanics of the University of Texas, Austin.