THOUGHTS ON *THE END OF CERTAINTY*, CHAPTER 4, SECTION II

By Bill Daniel

As I struggle through *The End of Certainty*, I keep wondering who its intended audience is. There is not enough detail for it to be a technical book intended for experts in thermodynamics, yet there are too many references to concepts unfamiliar to the general reader for it to be targeted at a popular audience. There's a glossary, but it's pretty brief and not very helpful. I found myself chasing many different threads through Wikipedia and textbooks trying to get a better grasp on the many ideas (some of them deeply insightful, I think…) that Prigogine presents. I have not done an exhaustive job of this by any means (I actually do have a life!), and a lot remains impenetrable to me. But I thought I would share what I have learned about one obscure part of the book that was a bit easier for me because I have a little previous knowledge about it.

That area is the relationship between some of the foundational mathematics of non-equilibrium thermodynamics and quantum mechanics – specifically the vector spaces that are home to the state vectors of continuous operators. I have not yet read Chapter 6 where Prigogine presumably goes into this topic in more depth, but his introductory remarks in Chapter 4 were enough to pique my interest in thinking about his ideas. He had me at "rigged Hilbert space!" (p. 96)

So, for what it's worth, here are some thoughts about that very limited slice of this wide-ranging book that I hope will be helpful to some in the group. I think that what follows is correct, but if I have screwed up anything, please let me know. I offer this in the hope that it might stimulate others whose expertise lies elsewhere to do something similar for other areas of the book.

I tried to "begin at the beginning," and write something that would include the applicable quantum mechanics basics in order to ensure that we are all on the same quantum page. Maybe I'll do that some other time, but it became so overwhelming that I gave up that project for now. If you need explanation of some of the ideas I had hoped to cover, but wound up having to assume familiarity with (such as those in ***bold italics*** below), I urge you to look them up. Or we can talk briefly about some of them in our meeting.

That said, here goes…

In quantum mechanics, ***observables*** are represented by ***operators***. Actually, the situation is a bit more restrictive than that. Quantum mechanical observables are represented by ***Hermitian operators***. I'm not going to go into what makes an operator Hermitian, but let's just say that Hermitian operators have "nice" properties that make them suitable models for physical observables.

We call the set of ***eigenfunctions*** of a Hermitian operator it's ***spectrum***. It can have a ***discrete*** or a ***continuous*** spectrum, depending on its ***eigenvalues***. If there is "space" between the eigenvalues (in the sense that you can find a number between any two of them – admittedly a concept that needs careful definition for complex eigenvalues, though we will sidestep that mathematical issue) the spectrum is discrete. The eigenfunctions of a Hermitian operator with a discrete spectrum occupy a ***Hilbert space*** whose dimension is determined by the operator[1] and represent ***physically realizable states***. If its spectrum is continuous, though, its eigenfunctions may not be ***normalizable*** and therefore don't themselves correspond to physical states. More on that in a bit.

The discrete case is the easiest to handle because the eigenfunctions of discrete Hermitian operators have three important properties: 1) they have *real* eigenvalues, 2) eigenfunctions with different eigenvalues are ***orthogonal***,[2] and, if the state space of a Hermitian operator is finite-dimensional, its eigenfunctions ***span*** the space.[3] These properties make them ideal for the description of quantum systems and allow any state function in the Hilbert space of the operator to be written as a ***superposition*** of its eigenfunctions.

Prigogine draws an analogy between the discrete quantum mechanical case and the thermodynamic description of a reversible process. The eigenfunctions of its ***Perron-Frobenius*** (or "transfer") ***operator***, U, are the "nice" functions Prigogine mentions at the bottom of p. 92 and describes in more detail on p. 93 for the ***Bernoulli map***. He mentions one eigenfunction in particular, the second of the [Bernoulli polynomials, $B_n(x)$], of the U operator: $B_1(x) = x - ½$ with eigenvalue ½. He points out that the ***distribution function***, ρ, analogously to the quantum state of an operator with discrete eigenvalues, can be "written as a superposition of Bernoulli polynomials." (p. 93)

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[1] It's probably obvious, but just in case it's not, I want to point out that operators with finite-dimensional eigenspaces must be discrete and continuous operators must have infinite-dimensional eigenspaces. However, the converse of those statements are not true. Operators with infinite-dimensional eigenspaces may be continuous or discrete. This is analogous to the set of real numbers and the set of integers: both have an infinite number of elements, but are respectively continuous and discrete.

[2] It turns out that, even if eigenfunctions share the same eigenvalue, there is a straightforward process for extracting eigenfunctions that *are* orthogonal, so everything is particularly simple with discrete Hermitian operators.

[3] We say that the set of eigenfunctions of such an operator is ***complete***. Fortunately, completeness, while not a property of all infinite-dimensional Hermitian operators with discrete spectra, is always true for the ones physicists care about – those that correspond to observables. So, I will cavalierly and unapologetically assume that all discrete Hermitian operators have a complete set of eigenfunctions.

So, all is rainbows and unicorns in the world of discrete Hermitian operators – even ones modeled by infinite-dimensional Hilbert spaces. Eigenfunctions are well-behaved and superpositions are clearly defined.

The quantum mechanical problem gets thornier, though, in the case of continuous spectra. The state vectors of operators with continuous spectra must, of course, live in an infinite-dimensional space, but that's not the crux of the problem. For continuous operators, the three properties we have come to covet so dearly for the discrete case (reality, orthonormality, and completeness) *all fail*:

1) Operators with a continuous spectrum can (and almost always do) have <u>*complex eigenvalues*</u>.
2) Eigenfunctions may <u>*not be normalizable*</u> (or orthogonal, for that matter) because inner products may not exist.
3) The all-important position and momentum operators are examples of Hermitian operators with continuous spectra that are <u>*not complete*</u> in Hilbert space. In fact, *none* of their eigenfunctions live there.[4]

The situation is dire. But, in his 1930 book, *The Principles of Quantum Mechanics*, a book that even today remains one of the clearest and most insightful expositions of the subject, Dirac realized that there is a solution. It's a two-part approach. First, we must expand the space of state vectors from Hilbert space (still fine for *discrete* operators) to a larger vector space. ("Ultimately," as Prigogine says, "to grasp the real world, we must leave Hilbert space." p. 95) Second, we must also restrict the continuous operators covered by this expanded space to those whose eigenvectors have *real* eigenvalues.

If we do this, it can be shown that the remaining operators occupy a space referred to by Prigogine as "***rigged Hilbert space***,[5] or ***Gelfand space***." (p. 96) Their eigenfunctions don't represent physical states anymore, but because: 1) they have real eigenvalues (because of our restriction), 2) they exhibit what

[4]The eigenfunctions of the derivative operator (and hence the momentum operator), e^{ikx}, are certainly not square-integrable (and hence not normalizable) because they blow up as $x \to \infty$, and the eigenfunctions of the position operator involve the Dirac delta function, $\delta(x - x_0)$, which, as Prigogine points out (p. 103) isn't normalizable either. Neither of these functions are elements of Hilbert space.

[5] I always thought Leslie Ballentine in *Quantum Mechanics, A Modern Development* (1998) was the original source of this term, but since Prigogine used it in this book published the previous year, clearly I was wrong. Anyway, Ballentine says that by "rigged" he means "'equipped and ready for action' in analogy with the rigging of a sailing ship." (p. 28) In any case, rigged Hilbert space (what Ballentine denotes as $\Omega^{\times}$) contains vectors "whose coefficients… blow up no faster than a power of n as $n \to \infty$," (p. 27) if you care.

Griffiths[6] calls "***Dirac orthonormality***,"[7] and 3) they form a complete set, they thereby recover (sort of) the three vital properties that make the Hilbert space structure so useful in the discrete case.

These individual eigenfunctions with exactly determined eigenvalues are not physically real, though. A free particle cannot exist in a state with definite energy, for example. The wave function of such a particle is not normalizable. However, we can construct a normalizable wave function by integrating the eigenfunctions over a range of frequencies. The result is a ***wave packet*** that is physical. That said, let's get back to our hero, Dr. Prigogine.

He says (p. 94) that the eigenfunctions of the ***Perron-Frobenius operator***, U, that advances the distribution function in time,[8] lives in this same rigged Hilbert space. In fact, the eigenfunctions of continuous quantum operators are the same "generalized functions" that correspond to the ones Prigogine calls $\tilde{B}_n(x)$ that (apparently – I'm not familiar with this notation) are Bernoulli distributions expressed as delta functions and their derivatives that are, like the eigenfunctions of the operators of quantum mechanics with continuous spectra, only normalizable in the Dirac sense. Prigogine says (p. 92-4) that these are necessary to describe thermodynamic irreversibility, just as they are necessary to describe continuous quantum operators.

He goes on to say (p. 94-5) that "the statistical formulation for the Bernoulli map is applicable only to nice probability functions ρ and not to single trajectories that correspond to singular distribution functions represented by δ-functions." I read this to mean that the eigenfunctions of U that reside outside Hilbert space (yet still in the rigged version), like the similar ones in quantum mechanics, do not correspond to physical situations. Non-equilibrium systems do not follow predictable trajectories in phase space any more than quantum observables with continuous spectra admit unique descriptions of their state. In Prigogine's words, "[t]he description of deterministic chaos in terms of trajectories corresponds to an overidealization and is unable to express the approach to equilibrium." (p. 95)

This is truly beautiful! I just love it when nature repeats the same ideas in different contexts. It certainly helps my understanding when I can apply so directly what I've learned in one area of physics to another that, at first look, seems very dissimilar. I hope you feel the same pleasure I do when you see this happen, and will help me to decode the many other sections of this book that may contain similar pleasures, but which remain mysterious to me because they don't overlap with anything I know! Thanks for reading!

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[6] *Introduction to Quantum Mechanics*, Second edition, p. 103.

[7] This requires adopting the ***Dirac delta function*** that Prigogine talks about on pages 94-95 in place of the more familiar ***Kronecker delta function*** used in the discrete case.

[8] I think that Prigogine is making an analogy between the unitary Perron-Frobenius operator and the unitary ***time-evolution operator*** that advances quantum mechanical states in time, but I haven't yet found where he says this explicitly.