RECOLLECTIONS OF AN INDEPENDENT THINKER

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Let me first point out that my title is consciously ambiguous. It reflects the marvelous imprecision that is possible with language. Am I the independent thinker or is someone else? Whose recollections are these anyway? And is the "of" equivalent to "about" or to "by"? And who here is "independent," of what, or of whom?

In apposition to this observation, let me quote one for whom ambiguity is anathema:

"*This may seem like an inflexible, cavalier attitude; I am convinced that nothing short of it can ever remove the ambiguity of 'what is the problem?' that has plagued probability theory for two centuries.*" E.T. Jaynes

I will touch upon the work of several independent thinkers tonight, but what I have to say is mostly, of course, about E. T. Jaynes. Those in this roomful of independent thinkers surely recognize both his independence and his originality. He is a man who has marched to a different drummer upon a road less traveled by. Those of us gathered here tonight, and many others in the world of science and engineering, now find themselves following in his footsteps.

Where many of us have had one career in one field, Ed Jaynes has had several. The broad collection of expertise from a wide variety of different disciplines in this gathering reflects this diversity of his ideas and their applications. Part of what I have to say is verifiable fact, part is subjective speculation, and part is derived from the recollection of others – however suitably filtered. I trust that Ed will correct the more egregious of my mistakes.

I came to Washington University in the fall of 1961 as a green graduate student, after three years in the Navy's Nuclear Submarine Program in New London, Connecticut. I was strongly motivated toward theoretical physics. I had dabbled in theater, English literature, philosophy and journalism before ending up in physics. My mentor, Eugen Merzbacher, had impressed me with his mastery of many fields and with the power and beauty of the interplay of theory and experiment in physics. The resident theorists at Washington University were Edward Condon, Eugene Feenberg, and Ed Jaynes – all three notably independent thinkers with unique and original things to say. All three, by chance, had a personal linkage to Princeton and to Eugene Wigner.

Ed had come to Washington University in 1960 after ten years at Stanford, after graduate study first at Berkeley and later at Princeton. This brief summary masks, however, the story of his intellectual development and his contact with some of the leading eminences of contemporary physics. He spent the war years first at the Sperry Gyroscope Company and later at the Naval Research Laboratory working on the development of microwave radar equipment. He went to Berkeley to work with J. Robert Oppenheimer, drawn as were many other bright, young men just after the War by the legendary reputation of the leading contemporary figure in science and public affairs. When Oppenheimer moved to the Institute for Advanced Study in Princeton, only three graduate students were taken with him. Oppenheimer wrote personal "Dear Harry" letters to Harry Smythe, the chairman of the Princeton Physics Department and author of the famous *Smythe Report* about the development of nuclear weapons, asking that these students be admitted to the Princeton Physics Department. Others who wished to follow had to make it as best they could. Ed Jaynes was one of the three selected. According to his contemporaries, he already exhibited characteristics that we now widely recognize. He was quiet, private, conservative, and very independent in his thinking. He harbored some skepticism about the quantum theory and its conceptual and philosophical foundations.

Apparently none of the students who followed Oppenheimer to Princeton ended up finishing their dissertations with him as their advisor. Some gravitated to David Bohm; others to Eugene Wigner, both of whom, themselves, were highly independent and original thinkers and respected those qualities in others. Both Bohm and Wigner had by that time made important and seminal contributions to the development of quantum theory. One contemporary reports that "Ed Jaynes was always interested in things from first principles and skeptical of many of the things repeated in the textbooks of the times, but was too polite to be out-and-out disagreeable about it."

As was the case with John Bardeen ten years earlier, the problem Jaynes worked on with Wigner was highly contemporary and also involved a quite demanding calculation. The title of his first publication, which was on the displacement of the oxygen in barium titanate, hardly reveals that this was the basis for explaining the fundamental properties of the whole class of materials called ferroelectrics. These materials are crystalline substances that have a permanent, spontaneous electric polarization; that is, an electric dipole moment per unit volume, that can be reversed by an electric field. This is a pretty odd property, since this internal electric polarization implies a charge separation that in most materials would be wiped out due to the enormous mobility of electrons. Ferroelectric materials have not become as important to technology as the analogous ferromagnetic materials, but Jaynes' calculations on barium titanate were evidently a *tour de force*. The description of the occurrence of this phenomenon, which is due to minute changes in the location of ions within the crystal, proved highly convincing and in good agreement with a variety of electrical and thermodynamic data. This work led directly to Jaynes' first book, *Ferroelectricity*, published by Princeton University Press in 1953 and was Volume I in a prestigious new series called *Investigations in Physics*. Ten years later – when I took solid state physics from him – this book was still the principal work in the field.

A review in *Physics Today* stated, "... an excellent survey of the diverse theories of ferroelectricity of $BaTiO_3$, with a particular emphasis on the electronic theory first proposed by Wigner, and later more fully developed by Jaynes. Of particular merit is the objectivity and conscientiousness with which the author evaluates the pros and cons of various theories and their experimental justification." That's pretty fine praise for a first effort.

His book was also notable by the company it kept. Volume II in this series was *The Mathematical Foundations of Quantum Mechanics* by John von Neumann; Volume III, *The Shell Theory of the Nucleus* by Eugene Feenberg; Volume IV, *Angular Momentum* by A.R. Edmonds; and Volume V, *Nuclear Structure* by Leonard Eisenbud and E.P. Wigner. This was an assortment of leading monographs by major figures at the time in their fields of physics. As one of his contemporaries has commented, "Ed was the only one of that group of Princeton graduate students who got a good job at a good institution."

Jaynes' thesis problem has a remarkable contemporary flavor. Barium titanate and its close relatives occur in what is called the perovskite structure. The ferroelectricity corresponds to a displacement of oxygen ions by only about 1% of the dimension of the crystalline unit cell. The resulting phase transition results from an instability – a softening – of one of the normal lattice vibration modes, a property that is associated with pairing in strong-coupling superconductors. Somewhat related electronic phenomena may also occur in the much more recently discovered high-temperature superconductors that also have the perovskite structure. Jaynes' advisor Eugene Wigner, himself one of the truly creative and independent thinkers of our time, is said to have later characterized Jaynes as "one of the two most under-appreciated people in physics." My source for that comment also said that "people who have their own way of doing things always got along best with Wigner."

One of the attractions of Stanford for Jaynes and Jaynes for Stanford, may well have been due to his war-time experience developing microwave devices. He had spent a summer working in the microwave laboratory of the W.W. Hanson Laboratories of Physics at Stanford before going to Princeton. Jaynes became an assistant professor in applied physics, and several publications from this period deal with nonlinear dielectric materials, electromagnetic propagation, and waveguides. He was extensively involved as a consultant, particularly with the Varian brothers. He was the resident guru on the behavior of electrons in cavity resonators and other phenomena and also worked on magnetic resonance. His calculations were only replaced much later with the advent of powerful computers. At the same time, he must have been well along in the development of the information theoretic approach to statistical mechanics, since the two very significant and profound papers on that subject were published in *The Physical Review* in 1957. Although some of the older faculty were apparently not enamored of Ed Jaynes' formulation of statistical mechanics, a lot of younger faculty and graduate students found it much more appealing than more standard approaches.

Electromagnetic theory and statistical mechanics might seem like very different fields. They are linked, however, through the fundamental concept of radar – to launch electromagnetic radiation which propagates through various media, is scattered, and the scattered radiation is detected. The resulting inverse scattering problem is a natural arena for Bayesian methods.

By about this time, Jaynes' work with Varian resulted in his buying a quite large house. When he moved to St. Louis, he purchased an even larger house, quite close to the university campus, which he generously shared with visiting friends, and on occasion with graduate students. When George Pake returned to Washington University from Stanford as Provost in 1962, Ed invited the entire Pake family to come and stay with him until they found a place to live. The Pake children explored the house from top to bottom and, in the process, it is claimed that they found a bathroom in the house that Ed did not even know that he had. By the time I began working with Ed in 1964, one graduate student's family was in residence helping around the property, and Ed was inviting other students and their families to join him on Friday afternoons around the pool. It was a warm and much appreciated gesture.

Ed was an extraordinarily effective teacher. He was quite the antithesis of the professor whose well-worn lecture notes finally are transformed into a textbook summation of the standard dogmas of the day. I can recall taking quantum mechanics, solid state physics, statistical mechanics – twice– probability theory, and quantum electronics during my six years as a graduate student and auditing many of his individual lectures as well. Even when covering seemingly well-known standard material, Ed's lectures always had a distinct flavor of having been freshly rethought. Though mathematical techniques were there as needed, discussions of the physics were always firmly rooted in experiment or in logical developments from first principles. This was particularly the case in his approach to statistical mechanics, where a whole variety of experiments of a purely macroscopic character by 1900 had exposed the inadequacy of the classical description of matter. Gibbs' formulation of statistical mechanics provided the natural linkage between the various macroscopic experiments and the behavior of particles at the microscopic level. Indeed one commentator on the work of Gibbs some 30 years later observed, "Gibbs' definition of the phase of the statistical system (in counter distinction to that given by eminent contemporary Boltzmann) is the one which clearly leads to the modern quantum statistics as created on the one hand by Einstein and Bose and on the other by Fermi and Dirac."

Ed's lectures invariably began with an historical perspective developing the fundamental ideas in the context of their time of origin, with the line of argument often seeming transparently simple. In retrospect I can see in Jaynes' lectures of the early 1960's the well-developed roots of his major lines of investigation that have been so original and so fruitful. His early skepticism about some aspects of the quantum theory of electromagnetic processes led to a whole series of masterful analyses of quantum electronic systems on semiclassical grounds. His highly original formulation of statistical mechanics, using information theoretic arguments, directly extended the fundamental ideas of Gibbs and provided the basis of a whole series of fundamental investigations of statistical mechanics. Along the way he clarified a number of puzzling, and sometimes out-and-out incorrect, conclusions that have propagated in the literature. His investigations of issues connected with statistical inference in science, rooted in many respects in the work of Sir Harold Jeffreys, not only plowed a lot of new ground with regard to principles in physics, but also developed powerful techniques usable in many other areas of science. Much of his work on the foundations of mathematical statistics, particularly on the generalized inverse Bayesian technique, touches on many of the most interesting issues involving the use of incompletely characterized or simply incomplete data for the purpose of drawing practically useful conclusions. We thus see this Princeton-trained physicist lecturing at companies and in business schools to economists and mathematical statisticians on the foundations of their own subjects. It is a tribute to the clarity of Jaynes' thinking and his recognition of the universality of the principles with which he has dealt that he has been able to translate so much of his work into other domains, totally different from those that originally motivated his work.

Jaynes' papers are invariably lucid and often seem more in the manner of a friendly blackboard chat than the somewhat terse, forbidding, and stylized presentations affected by many physicists. He does not simply write up every new idea, but thinks things through, often seeking the more general, more elegant, or clearer way. Some of his speculative pastries never get fully baked. I recall a draft about formulating theories in macroeconomics and another about the muscle as an engine that were privately circulated and never seem to have made it through his filter.† His extension of the information theory formalism to irreversible processes ("Nonlocal Transport Theory" with Douglas Scalapino) never seems to have been published, although it was included in his lectures. Some simple calculations applying this technique to sound attenuation in ideal and weakly interacting quantum gases were included in my thesis and also not published. Analyses that took several weeks of work in 1964 with an IBM-704 can nowadays be done as student problems with a hand-held HP in an afternoon, so posterity is no less rich. Thoughts of Jaynes' that I recall on the approach to equilibrium and on the degree to which reversible thermodynamic cycles are unattainable, I saw later much more fully developed by the very independent thinking chemist Steve Berry.

Jaynes is a member of that illustrious company of independent thinkers who contradict the notion that a theorist should properly be concerned only with fundamental principles and their mathematical elaboration and thereby eschew practical problems, realistic situations, and experimental realities. Indeed, many of the truly great theorists have been involved extensively with the design and analysis of experiments. Einstein, after all, formulated much of his statistical mechanics to analyze a series of experiments which allowed him, among other things, to determine Avogadro's number in several different ways, establish concretely the atomistic nature of matter, and build a goodly part of the foundations for the development of quantum mechanics.

Perhaps more surprisingly, Einstein and Leo Szilard in 1928 applied for a patent for a refrigerator using a pumped liquid metal as a working fluid. Such electromagnetic pumps are now incorporated in the cooling circuit in liquid-metal-cooled reactors. Szilard apparently originated the notion of a liquid-metal-cooled pile, which he pushed as a candidate for the first plutonium production reactors. The official AEC historian has noted drily: "For Szilard, the new and unusual held no cause for hesitation." (Szilard, very much an independent thinker, also explored the relationship between information and statistical mechanics, but did not fully recognize the advantage of generalizing the approach of Gibbs that was later discovered by Jaynes.) Eugene Wigner, although renowned for his work on group theory and quantum mechanics, on nuclear structure, on R-matrix theory, other fundamental developments in nuclear and particle physics, and helping to found modern solid state theory, also was the principal designer of the plutonium production reactors that were built at Hanford during World War II. These were an enormous scale-up from very small scale experiments to what nowadays would be multibillion dollar investments. He also designed the "Clinton pile" at Oak Ridge. Wigner's original training was in chemical engineering, although his Nobel Prize was for work in theoretical physics. John Bardeen, also a Wigner student, was almost as deeply involved in electrical engineering as he was in theoretical physics, as attested to by articles in the April 1992 issue of *Physics Today*. Bardeen, as did Wigner, worked and consulted with a variety of industrial companies while still advancing the frontiers of theory.

Jaynes, as noted before, had practical experience with radar and other microwave devices early in his career and has maintained a continuing interest in quantum electronics. Concurrently, he has maintained an interest for many years in the physics of music.

Even Jaynes' intellectual forebear, J. Willard Gibbs, had a practical side. The scientific writings of J. Willard Gibbs were noted for their conciseness and difficulty and were

† *Editors' note:* The work on the muscle as an engine finally appeared in 1989, included in reference [64] in the Jaynes bibliography at the end of this volume.

often published in little-known local journals. Some 33 years after Gibbs' death in 1903, Yale University Press published an extended commentary on his scientific writings. It was considerably longer than the two bound volumes of the scientific works themselves. Typical statements by the distinguished authors include, "In this immortal work, . . . the originality, power, and beauty of Gibb's work in the domain of thermodynamics have never been surpassed" and "the greatest mathematical physicist of the American nation."

But the earliest work of J. Willard Gibbs, which includes his Ph.D. thesis, is of a rather different character. His dissertation bears the title "Of the Form of the Teeth of Wheels in Spur Gearing." It is primarily an exercise in applied geometry. His 1863 Ph.D. was the fifth such degree granted in the United States, the first in engineering, and arguably the second in science. Immediately after receiving his degree, Gibbs served as a tutor at Yale, initially in Latin and only later in natural philosophy. The only original work that he seems to have completed during this period was an improved railway car brake, which was patented in 1866.

Shortly after receipt of this patent, Gibbs left for a three-year sojourn in Europe, which brought him into contact with the most advanced thinking in the most advanced scientific capitals in the world. Nonetheless, upon returning to Yale, Gibbs focused his attention on improving the conical pendulum governor for steam engines, originally invented by James Watt. A model embodying this improvement was apparently made in about 1872 and still exists in New Haven. (It is noteworthy in these times that Gibbs was initially appointed professor of mathematical physics without salary in 1871 and only received a formal salary from Yale after receiving an offer from Bowdoin College of $1800 per year for a "chair of mathematics, or of physics.")

It is perhaps inevitable that the work of a truly independent thinker may take some time to be fully recognized. As the diversity of participants at this meeting attests, Edwin T. Jaynes' work has become increasingly recognized as well as respected. In their introduction to the book *Maximum Entropy and Bayesian Methods in Inverse Problems*, Smith and Grandy point out, reflecting work up to about ten years ago, "The sheer number of citations of his works indicates the considerable influence that he has had on this subject. His influence through personal interaction is even greater." More recent comments reinforce this view. Half a dozen years earlier in an essay in tribute to another truly and original independent thinker, George Gamow, Wolfgang Yourgrau and Alwyn Van der Merwe state, "Finally, a decade after the birth of information theory, Edwin Jaynes drew from it the one important lesson for physics, which has since given rise to highly significant simplified treatment of the foundation of statistical mechanics." These authors began the last paragraph in their 37-page paean to the information theory approach: "But more important than the didactical advantages is the unification, simplification, and clarification which information theory has wrought of the foundation of statistical mechanics." They end with the statement, "To us with a philosophic bias in scientific matters, this in itself is a genuine achievement, although the pragmatic physical scientist will rightly discern the crowning glory of the information approach is in the fresh answers to old problems, which it is starting to provide in the study of irreversible phenomena." Such praise is much the sort that, some thirty years after his death, devolved upon J.Willard Gibbs. Ed Jaynes fully deserves to be recognized as Gibbs' modern heir.

Some of the nuances must, however, get lost in translation. In a work entitled *Energy and Entropy* by G.N. Alekseev, first published in Moscow in 1978 (in English in 1987), it is stated, ". . . difficulties stem from the application of a method, based on the superficial similarity between information and Boltzmann's formula for entropy to areas for which the latter was never intended. . . It is thus much easier for theorists to proclaim a relationship between entropy and information than to demonstrate it by practical numerical examples. Nevertheless, 22 or 27 years ago this relation was so thoroughly developed that information theory became the basis (not vice versa) for the development of a sophisticated system of universal thermodynamics which was derived from a group of original equations. (The theory belongs to M. Tribus, an American scientist.)"

Finally, it should be said that Ed Jaynes encouraged his students, both by example and sometimes by his comments, to indulge in some of his extracurricular habits. One of these is certainly music and the appreciation of the physics of music; another is an appreciation of history and of old books, wherever they may be found. In the thirty years since I first met Ed Jaynes, I have suffered from the rampant spread of the old-book disease. Scratching that old-book itch has led me to many classics, including a little volume on the early work of J. Willard Gibbs, including the aforementioned thesis, which I have brought here for Ed tonight. I would like to present it to Ed at this time, with the suggestion that his work is quite likely to have the same kind of long history and the same kind of future as that of his illustrious predecessor.

A LOOK BACK: EARLY APPLICATIONS OF MAXIMUM ENTROPY ESTIMATION TO QUANTUM STATISTICAL MECHANICS

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ABSTRACT. E.T. Jaynes has been the central figure for over three decades in showing how maximum entropy estimation (MEE) provides an extension of logic to cases where one cannot carry out Aristotelian deductive reasoning. Here I will review two early applications of MEE which I hope will provide some insight into how these ideas were being used in quantum and statistical mechanics around 1960.

In May of '61 I turned in my Ph.D. thesis (Scalapino, 1961) to Stanford University and, following a well-known dictum, went on to work on other problems. Now, three decades later, on this, the occasion of Ed Jaynes' seventieth birthday, I decided to look back to see what we were doing when I was first getting to know Ed and his special approach to problems.

Not surprisingly, my thesis contains several applications of the principle of Maximum Entropy Estimation (MEE). In 1957 Ed had written two seminal articles (Jaynes, 1957(a), 1957(b)) showing how one could use Shannon's (1948) Information Theory to construct density matrices for a variety of different problems in equilibrium statistical mechanics. I had been very much taken with this work and wanted to understand how it could be applied to other systems.

Ed had shown how the MEE formalism could be used to generate ensembles in statistical mechanics when there was only partial knowledge available about a system with many degrees of freedom. It seemed natural to wonder what this formalism would predict for a microscopic quantum system with a small number of degrees of freedom, particularly when the measurement provided sufficient information to specify the state uniquely. Ed may have known, but I had no idea what to expect when I started out to apply MEE for the first time.

The problem was certainly basic enough. Consider a spinless particle moving in one dimension, and imagine that experimentally one knows that

$$\begin{aligned} &\operatorname{Tr}\rho x = \operatorname{Tr}\rho p = 0 \\ &\operatorname{Tr}\rho x^2 = \Delta x^2, \qquad \operatorname{Tr}\rho p^2 = \Delta p^2. \end{aligned} \tag{1}$$

According to the MEE formalism, ρ is determined by maximizing $S = -\mathrm{Tr}\,\rho \ln \rho$, subject to the constraints of Eq. (1). This leads in the usual way to the density matrix

$$\rho = \frac{e^{-\lambda_1 x^2 - \lambda_2 p^2 - \lambda_3 x - \lambda_4 p}}{Z(\lambda_i)} \tag{2}$$

with

$$Z(\lambda_i) = \mathrm{Tr}\,\rho. \tag{3}$$

The λ_i are determined so as to satisfy the constraints of Eq. (1),

$$\begin{aligned} 0 &= \frac{\partial}{\partial \lambda_3} \ln Z = \frac{\partial}{\partial \lambda_4} \ln Z \\ \Delta x^2 &= -\frac{\partial}{\partial \lambda_1} \ln Z, \qquad \Delta p^2 = -\frac{\partial}{\partial \lambda_2} \ln Z. \end{aligned} \tag{4}$$

Now λ_3 and λ_4 vanish by inspection, and using a harmonic oscillator basis in which

$$\left(\lambda_1 x^2 + \lambda_2 p^2\right) |n\rangle = 2\left(\lambda_1 \lambda_2\right)^{1/2} \hbar \left(n + \frac{1}{2}\right) |n\rangle, \tag{5}$$

one can show that

$$Z = \sum_n e^{-2(\lambda_1\lambda_2)^{1/2}\hbar(n+\frac{1}{2})} = \frac{1}{2\sinh\left(\hbar(\lambda_1\lambda_2)^{1/2}\right)}. \tag{6}$$

Then solving Eq. (4), one obtains

$$\begin{aligned} \lambda_1 &= \frac{1}{\hbar}\frac{\Delta p}{\Delta x} \coth^{-1}\left(\frac{2}{\hbar}\Delta p \Delta x\right) \\ \lambda_2 &= \frac{1}{\hbar}\frac{\Delta x}{\Delta p} \coth^{-1}\left(\frac{2}{\hbar}\Delta p \Delta x\right) \end{aligned} \tag{7}$$

so that

$$Z = \left(\left(\frac{2}{\hbar}\right)^2 \Delta x^2 \Delta p^2 - 1\right)^{1/2}. \tag{8}$$

Now the probability of being in the n^{th} harmonic oscillator state is

$$P_n = \langle n|\rho|n\rangle = \frac{1}{Z} e^{-2(\lambda_1\lambda_2)^{1/2}\hbar(n+\frac{1}{2})} = \frac{\left(\frac{2}{\hbar}\Delta p \Delta x - 1\right)^n}{\left(\frac{2}{\hbar}\Delta p \Delta x + 1\right)^{n+1}}. \tag{9}$$

In the limit of a *complete measurement* in which Δx and Δp are determined as accurately as the Heisenberg uncertainty principle allows so that $\Delta x \Delta p = \hbar/2$, Eq. (9) becomes

$$P_n = \delta_{n,0}. \tag{10}$$

Thus in this case the MEE density matrix $\rho = |0\rangle\langle 0|$ corresponds to the pure state

$$|0\rangle = \frac{1}{(2\pi)^{1/4}(\Delta x)^{1/2}}\, e^{-x^2/4\Delta x^2}. \tag{11}$$

One can note that if $\Delta x \Delta p < \hbar/2$, the probabilities associated with the odd n states are negative, clearly indicating the fact that one has moved into an unphysical regime.

Finally, evaluating the entropy one obtains

$$S = \left(\frac{\Delta x \Delta p}{\hbar} + \frac{1}{2}\right) \ln\left(\frac{\Delta x \Delta p}{\hbar} + \frac{1}{2}\right) - \left(\frac{\Delta x \Delta p}{\hbar} - \frac{1}{2}\right) \ln\left(\frac{\Delta x \Delta p}{\hbar} - \frac{1}{2}\right). \tag{12}$$

For $\Delta x \Delta p = \hbar/2$, $S = 0$ as expected, while for $\Delta x \Delta p < \hbar/2$, S becomes complex. For $\Delta x \Delta p \gg \hbar/2$,

$$S \simeq \ln\left(\frac{\Delta x \Delta p}{\hbar}\right). \tag{13}$$

This is just the usual Boltzmann results in which S is the log of the number of states in the reasonably probable part of phase space.

All of this seems obvious now, but I can assure you, for a graduate student trying to understand Ed's MEE formalism, it was very reassuring.

With this background, I turned to the main problem of interest, which was extending the MEE formalism to non-equilibrium problems. Here the goal was to find an algorithm for constructing density matrices appropriate to non-equilibrium conditions. If this could be done, then, for example, transport properties could be obtained by simply tracing the desired operators over the density matrix exactly as in equilibrium statistical mechanics. In particular, there would be no need to integrate ρ forward over an "induction time" or to carry out some coarse-graining procedure (Mori, 1958). As it was to turn out, this algorithm had already been stated by Gibbs (1960): find the distribution which, while agreeing with what is known, "gives the least value of the average index of probability of phase." Ed had clearly understood how this applied to equilibrium statistical mechanics, but what should be done in the non-equilibrium case? I began by studying a steady-state non-equilibrium problem.

Suppose one knows in addition to $\langle H\rangle$, the average value of another operator $\langle F\rangle$; then applying MEE to determine the density matrix gives

$$\rho = \frac{e^{-\beta H - \lambda F}}{Z(\beta, \lambda)} \tag{14}$$

with

$$Z = \mathrm{Tr}\, e^{-\beta H - \lambda F}. \tag{15}$$

Here β and λ are determined, so that one obtains the known expectation values of H and F. However, if one also knows that the system is in a steady state but that F does not commute with H, one has a new and interesting problem. Clearly in this case the expression for ρ, given by Eq. (15), is not stationary, so that the expectation values of typical operators will evolve in time. In addition, they will be found to have been evolving in the past. Thus $\langle F(t)\rangle = \mathrm{Tr}\,\rho\left(e^{iHt}Fe^{-iHt}\right)$ will not have been stationary for $t < 0$, contrary to the information one has.