

THERMODYNAMICS AND QUANTUM MECHANICS NOTES

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THOUGHTS ON QUANTUM MECHANICS

We have a variety of experimental facts to account for. Minimal list is [see Tomonga]:

- (1) Emmission (or absorption) of EM radiation at (?) discrete [or at least bunched] frequencies.
- (2) Planck black body radiation spectrum.

Why is this independent of the material used? Is it really? The specific heats aren't.

How is spectrum related to power? Can it be used to \implies autocorrelation function?

- (3) Variation of specific heats with temperature.

This is related to (2), and its important to note that there are differences (though small) with the material.

- (4) Photoelectric effect.
- (5) Compton effect.

IDEA. We need to find a SDS with a discrete set of allowed frequencies (or energies?) $\nu_i(\alpha)$ [or $E_i(\alpha)$], $\alpha = 1, 2, \dots$.
 α plays the role of a bifurcation parameter \ni for given $\alpha \exists$ only one globally stable solution $\nu_i(\alpha)$

or

Maybe as α varies the solutions are chaotic but for a given $\alpha \exists$ a characteristic $\langle \nu_i \rangle$ [$\langle \cdot \rangle$ denotes average over path].

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HOW TO JUSTIFY USE OF THE MAXIMAL ENTROPY PRINCIPLE

- (1) Note that by use of the MEP its possible to derive a variety of the existing definitions used in SM and QM. This seems important because this only requires that we use the facts from QM that are experimentally observed, e.g., discrete frequency of radiation, etc. Furthermore, e.g., if derive the density appropriate for discrete frequencies [Plank form, see later] then by calculating the maximal entropy we get the Einstein equation for specific heat (heat capacity).
- (2) Therefore, in searching for a possible QM alternative it might by important to delineate the systems for which max entropy will be reached, i.e. if could show that a system $\rightarrow H_{max}$ then we have a justification for the MEP.
- (3) Note for finite μ space and S invertible and measure preserving then (T9.3.1) H is constant. Further, using the arguments on pp. 263-4, if S is not μ preserving can have a new space with $\tilde{\mu}$ and again H_c is constant. Therefore we have the important and general fact that:

Dynamical Systems (reversible) $\implies H$ constant \implies DS not the answer

This is the basis of the objections raised by Loschmidt (Umkehrinwand) against Boltzmann. Other objection to Boltzmann by Zermelo (Wiederkehrinwand) was based on the Poincaré recurrence theorem for ergodic systems.

- (4) (T9.3.2 + T9.4.2) \implies SDS Exact $\iff H(P^t f) \rightarrow 0$.

Discussion pp263-4 \implies SDS is AS $\iff H_c(P^t f|g) \rightarrow 0$.

Therefore there are 2 classes of SDS in which H or H_c goes to 0 as $t \rightarrow \infty$.

- (5) What about SDS in general? SDS are irreversible. From T9.9.2, for *any* Markov operator P we have

$$H_c(Pf|Pg) \geq H_c(f|g),$$

so at least H_c can't decrease for SDS.

Further, from T5.3.2 if we have a *constrictive* MO then P is AP and therefore AP SDS have constant or increasing H_c , but never decreasing. However, note that the increase in H_c could be only due to the ϵ part of $P^n f \rightarrow 0$. In general the maximum entropy will depend on the initial density f_0 .

- (6) Also from T9.4.1 if P is a MO with $P1 = 1$ then if $\exists c > 0 \ni$

$$H(P^n f) \geq -c \forall n \text{ sufficiently large} \implies P \text{ constrictive.}$$

- (7) DS: K flow, Mixing, Weakly mixing, Ergodic, All ODE, some PDE.

SDS: K flow, Mixing, Weakly mixing, Ergodic, PLUS Asymptotically stable, exact, asymptotically periodic (some), Some PDE, ?? DDE

- (8) Take trace of a DS. If trace is intersecting and nonperiodic, then entropy of trace is constant or increasing in spite of fact that entropy of parent system was constant.

Idea of Proof: Trace intersecting and periodic \implies for a given $x \exists t \ni S^{-t}(x)$ is not unique $\implies S$ not invertible \implies Trace is a SDS \implies result by item 5 above. Therefore, taking away information may \implies that get an increase in H .

- (9) In justifying the MEP forget about DS \implies no point in dealing with systems of ODE's, whether they have stable SS's, LC's, or "chaotic" behaviour.
 (10) Therefore, to justify the MEP we need to concentrate on SDS and have an H theorem where we can prove

$$\lim_{t \rightarrow \infty} H_c(P^t f|P^t g) = H_{max}(f|g).$$

This goes back to Andy's idea of using H_c to get an H theorem.

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 ENTROPY AND ADDED NOISE

For Maps.

- (1) **Randomly Applied Stochastic Perturbations**, pp. 227 et seq.

S non-singular, $P_S + \text{noise} \rightarrow P_\epsilon$. Then $\{P_\epsilon^n\}$ is AS \implies by Result 4 above [pp263-4] that

$$H_c(P_\epsilon^n f|g) \rightarrow 0.$$

Therefore, adding noise to any system (constant entropy or not) \implies get increasing entropy. [BUT, adding noise can give AP too, with different entropy behaviour.]

If μ space is finite and S is measure preserving, then T10.4.2 \implies

$$\text{limiting density} = f_* = \frac{1}{\mu(X)} \implies H \rightarrow H_{max}$$

(see Chapter 9).

- (2) **Constantly Applied Stochastic Processes**, pp282 et seq.

From C10.5.1 (p287) if \exists a Liapunov function for \bar{P} then $\{\bar{P}^n\}$ is AS \implies again that entropy $\rightarrow 0$.

For Continuous Time Systems.

- (1) For the Fokker Planck equation T11.9.1 (p330) gives conditions for the AS of $\{P_t\}$.

Does AS in a continuous time system $\implies H_c \rightarrow 0$? YES.

- (2) Look at Andy Lasota and J. Traple results for continuous time systems with noise.

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 THE MAXIMAL ENTROPY PRINCIPLE

CHAPTER 2. MAXIMAL ENTROPY PRINCIPLES.

In this chapter we examine the surprising consequences of maximizing the Boltzmann Gibbs entropy subject to various constraints. In Section A we show that for a system operating in a phase space of finite measure with no other constraints, the entropy will assume a maximal value if and only if the density (in the terminology of Gibbs) is the density of the microcanonical ensemble. Further, in Section B for a general phase space it is demonstrated that given the expectation value of a particular observable, the Boltzmann-Gibbs entropy of a density will attain its maximum if and only if the density is a generalization of the density of the canonical ensemble.

In Section C we show that the mathematical definition of the Boltzmann-Gibbs entropy of a density can be plausibly argued to coincide with the thermodynamic entropy of a system characterized by that density, and that all of equilibrium thermodynamics follows.

Section D shows how other constraints, coupled with the maximal entropy principle, yield the densities of the Maxwell Boltzmann or other distributions. Section E shows how the use of a maximal entropy principle can be used to derive the Planck blackbody radiation law. Section F briefly considers how the maximal entropy principle can be extended to situations in which there are known expectation values of several observables.

A. MICROCANONICAL ENSEMBLES.

Armed only with the integrated version of the Gibbs inequality (1.5) we may immediately understand the origin of the classical Gibbs microcanonical ensemble as reflecting a manifestation of extremal properties of the entropy. Consider a given space X with finite Lebesgue measure, $\mu_L(X) < \infty$ (forgo the normalization $\mu_L(X) = 1$ temporarily), and all possible densities f . Then the only density that maximizes the entropy is the (uniform) density of the Lebesgue measure of X . More precisely,

Theorem 2.1. *When $\mu_L(X) < \infty$, the density that maximizes the Boltzmann-Gibbs entropy is the uniform density*

$$f_*(x) = \frac{1}{\mu_L(X)}. \quad (2.1)$$

For any other density $f \neq f_*$, $H(f) < H(f_*)$.

Proof. Pick an arbitrary density f so, by definition, the entropy of f is

$$H(f) = - \int_X f(x) \log(f(x)) dx.$$

However, with $g(x) = 1/\mu_L(X)$ the integrated Gibbs inequality (1.5) gives

$$H(f) \leq - \int_X f(x) \log g(x) dx = - \log \left[\frac{1}{\mu_L(X)} \right] \int_X f(x) dx,$$

or $H(f) \leq - \log \left[\frac{1}{\mu_L(X)} \right]$ since f is a density. The equality holds if and only if $f = f_*$. However, the entropy of f_* is easily calculated to be

$$H(f_*) = - \int_X \frac{1}{\mu_L(X)} \log \left[\frac{1}{\mu_L(X)} \right] dx = - \log \left[\frac{1}{\mu_L(X)} \right],$$

so $H(f) \leq H(f_*)$ for any density f , or $H(f) < H(f_*)$ for $f \neq f_*$. Clearly, if X is normalized so $\mu_L(X) = 1$, then $H(f) \leq 0$. \square

Example 2.1. The uniform density f_* defined by (2.1) is a generalization of the density of the microcanonical ensemble introduced by Gibbs in his work on the foundations of thermodynamics.

Specifically, Gibbs considered the special case of a conservative mechanical system, *i.e.* one in which the forces are such that the work $W(x_1, x_2)$ required to move a particle between two points x_1 and x_2 in the phase space X is independent of the path connecting x_1 and x_2 . For conservative systems the energy U is a constant of the motion, which simply means U is constant along any given trajectory. Furthermore, any density f which is a function of the energy U alone, $f(U)$, will also be a constant of the motion. (This invariance of the density along trajectories is what Gibbs referred to as *conservation of extension in phase*.) Inasmuch as it is necessary to have an ensemble with an

(ultimately) time independent density to describe the behaviour of a system in thermal equilibrium, Gibbs reasoned that a natural first choice would be to pick an ensemble characterized by the density

$$f(U) = \begin{cases} \text{Constant} & U = U_0 \\ 0 & \text{otherwise,} \end{cases} \quad (2.2)$$

where the energy U_0 is to be specified.

The density in equation (2.2) is the density of what Gibbs called the **microcanonical ensemble**, and it is clearly a special case of the uniform density (2.1) which maximized the entropy of a finite space. In the microcanonical ensemble the phase space X is taken to be the space X^* of conjugate position and momenta (q, p) restricted by the requirement that $U(p, q) = U_0$. The constant appearing in the density (2.2) is simply related to the measure of the restricted space X^* by $\text{Constant} = 1/\mu_L(X^*)$. •

Notice that in the derivation of the density (2.1) maximizing the entropy on a finite space, there was no reference to the nature of the dynamics of the system generating the density. This is in sharp contrast to the usual approach in thermodynamics in which the dynamics are quite specifically used to argue for the plausibility of the microcanonical density (2.1). The fact that a generalization of this density appears in such a natural way merely illustrates the generality of both the density and the method used to obtain it, and that the existence of the density of the microcanonical ensemble is independent of the system dynamics.

B. CANONICAL ENSEMBLES.

Even more fascinating consequences can emerge from the extremal properties of entropy that offer insight into the basic foundation of thermodynamics of both classical and quantum systems. In this section we state and prove a theorem that is used to deduce all of conventional equilibrium thermodynamics in the next section.

Theorem 2.2. *Assume that an (observable) nonnegative measurable function $\mathcal{O}(x)$ is given as well as the average $\langle \mathcal{O} \rangle$ of that function over the entire space X , weighted by the density f :*

$$\langle \mathcal{O} \rangle = \int_X \mathcal{O}(x) f(x) dx. \quad (2.3)$$

(Note that $\langle \mathcal{O} \rangle$ is nonnegative and may be time dependent.) Then the maximum of the entropy $H(f)$, subject to the constraint (2.3), occurs for the density

$$f_*(x) = Z^{-1} e^{-\nu \mathcal{O}(x)} \quad (2.4)$$

where Z is defined by

$$Z = \int_X e^{-\nu \mathcal{O}(x)} dx, \quad (2.5)$$

and ν is implicitly determined from

$$\langle \mathcal{O} \rangle = Z^{-1} \int_X \mathcal{O}(x) e^{-\nu \mathcal{O}(x)} dx. \quad (2.6)$$

Proof. The proof again uses the integrated Gibbs inequality. From (1.5), for densities f and f_* ,

$$\begin{aligned} H(f) &\leq - \int_X f(x) \log f_*(x) dx \\ &= - \int_X f(x) [-\log Z - \nu \mathcal{O}(x)] dx \\ &= \log Z + \nu \int_X f(x) \mathcal{O}(x) dx \\ &= \log Z + \nu \langle \mathcal{O} \rangle. \end{aligned}$$

However it is easy to show that

$$H(f_*) = \log Z + \nu \langle \mathcal{O} \rangle \quad (2.7)$$

and therefore $H(f) \leq H(f_*)$, with the equality holding if and only if $f = f_*$. □

The choice of notation in (2.4) and (2.5) was intentional to draw the connection with the density of the Gibbs canonical ensemble.

Example 2.2. If X^* is the conjugate position-momentum (q, p) space, $\mathcal{O}(x)$ is the system energy functional, and $\langle \mathcal{O} \rangle$ the average (over the phase space) energy of the system, then Z as given by (2.5) can be identified directly with the **partition function** and the density f_* given in (2.4) that maximizes the entropy is to be identified with the density of the **Gibbs canonical ensemble**.

In deriving the density of the Gibbs canonical ensemble, it is implicit in the writing of the average $\langle \mathcal{O} \rangle$, given by equation (2.3), over the entire phase space that if the density (2.4) is to describe a state of thermodynamic equilibrium then the quantity $\mathcal{O}(x)$ must eventually be independent of time at long times. An even more restrictive requirement would be that $\mathcal{O}(x)$ is a constant of the motion. If $\mathcal{O}(x)$ is identified with the system energy U , then we are dealing with a system in which the energy is conserved. •

Example 2.3. As another illustration of the application of Theorem 2.2, consider the family of densities f with a given variance, *i.e.*

$$\sigma^2 = \int_{-\infty}^{\infty} x^2 f(x) dx.$$

Under this constraint, the maximal Boltzmann Gibbs entropy is attained when the density is Gaussian,

$$f_*(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2}.$$

This is quite easy to show, since for an arbitrary density f ,

$$\begin{aligned} H(f) &\leq - \int_{-\infty}^{\infty} f(x) \log \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} e^{-x^2/2\sigma^2} \right\} dx \\ &= \log \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} \right\} + \frac{1}{2\sigma^2} \int_{-\infty}^{\infty} x^2 f(x) dx \\ &= \frac{1}{2} - \log \left\{ \frac{1}{\sqrt{2\pi\sigma^2}} \right\} = H(f_*). \quad \bullet \end{aligned}$$

C. THE THERMODYNAMIC CONNECTION.

All of conventional equilibrium thermodynamics can be deduced from the density (2.4). Let us see how. It is a fundamental assumption of thermodynamics that

POSTULATE C. There exists a one to one correspondence between states of thermodynamic equilibrium and states of maximum entropy.

We add to this the following.

POSTULATE D. Given an observable $\mathcal{O}(x)$ and its average $\langle \mathcal{O} \rangle$, the density given by (2.4)-(2.6) maximizing the entropy with respect to \mathcal{O} corresponds to the density of the state of thermodynamic equilibrium attained physically.

If there is but one state of thermodynamic equilibrium that is attained regardless of the way in which the system is prepared then this is called a **globally stable equilibrium** and is associated with a globally stable state of maximal entropy (strong form of the Second Law). If, however, there are multiple states of thermodynamic equilibrium, each corresponding to a state of locally maximal entropy and dependent on the initial preparation of the system, then we say that these are **local or metastable states of equilibrium** (weak form of the Second Law).

Given these observations, it is natural to examine the consequences of associating the equilibrium thermodynamic entropy S_{TD}^* with the maximal Boltzmann Gibbs entropy H given by (2.7):

$$H(f_*) \leftrightarrow S_{TD}^*.$$

Since we have not specified units for H , a multiplicative constant c^{-1} may be necessary, *viz.*

$$H(f_*) = S_{TD}^*/c,$$

which implies from (2.7) that the equilibrium thermodynamic entropy is given by

$$S_{TD}^* = c \log Z + c \nu \langle \mathcal{O} \rangle$$

If, as before, we make the association of $\langle \mathcal{O} \rangle$ with the internal thermodynamic energy U ,

$$\langle \mathcal{O} \rangle = U,$$

we wish to then associate the parameter ν with some function of the temperature T . At this point, it should be noted that

$$\langle \mathcal{O} \rangle = -\frac{1}{Z} \frac{dZ}{d\nu}.$$

Taking the derivative of $\langle \mathcal{O} \rangle$ with respect to the parameter ν in this equation we have

$$\begin{aligned} \frac{d\langle \mathcal{O} \rangle}{d\nu} &= \frac{1}{Z^2} \left[\frac{dZ}{d\nu} \right]^2 - \frac{1}{Z} \left[\frac{d^2 Z}{d\nu^2} \right] \\ &= \langle \mathcal{O} \rangle^2 - \langle \mathcal{O}^2 \rangle. \end{aligned}$$

Remembering that the variance $D^2(\mathcal{O}|f_*)$ of a function \mathcal{O} with respect to a density f_* is simply given by

$$\begin{aligned} D^2(\mathcal{O}|f_*) &= \langle \mathcal{O}^2 \rangle - \langle \mathcal{O} \rangle^2 \\ &= \langle (\mathcal{O} - \langle \mathcal{O} \rangle)^2 \rangle \end{aligned}$$

and that the variance is by necessity non-negative, $D^2 \geq 0$, we immediately have that

$$\frac{d\langle \mathcal{O} \rangle}{d\nu} = -D^2(\mathcal{O}|f_*) \leq 0.$$

Therefore, if there is any connection between variations in the parameter ν and the average energy $\langle \mathcal{O} \rangle = U$, it must be an inverse one. Since our experience tells us that that temperature T and energy U are directly proportional to one another, this leads us to conclude that if the parameter ν and the temperature T are related to one another then it must be an inverse relationship.

Next in our investigation of the potential physical meaning of the parameter ν , consider two systems:

- (1) System A, operating in a phase space X_A , characterized by an energy functional $\mathcal{O}_A(x_a)$, average energy $\langle \mathcal{O}_A \rangle$, parameter ν_A ; and
- (2) System B, operating in a phase space X_B , characterized by an energy functional $\mathcal{O}_B(x_b)$, average energy $\langle \mathcal{O}_B \rangle$, and parameter ν_B .

By Theorem 2.2, the densities maximizing the entropy for systems A and B are, respectively,

$$f_{*A}(x_a) = \frac{1}{Z_A} e^{-\nu_A \mathcal{O}_A(x_a)} \quad \text{with} \quad Z_A = \int_{X_A} e^{-\nu_A \mathcal{O}_A(x_a)} dx_a, \quad (2.8)$$

and

$$f_{*B}(x_b) = \frac{1}{Z_B} e^{-\nu_B \mathcal{O}_B(x_b)} \quad \text{with} \quad Z_B = \int_{X_B} e^{-\nu_B \mathcal{O}_B(x_b)} dx_b. \quad (2.9)$$

We combine systems A and B into a third system C, operating on the product space $X_A \times X_B$, so the new system C has an energy functional $\mathcal{O}_C(x_a, x_b)$ and average energy $\langle \mathcal{O}_C \rangle$, and is characterized by a parameter ν_C . Again by Theorem 2.2 the density maximizing the entropy of the combined system C will be given by

$$f_{*C}(x_a, x_b) = \frac{1}{Z_C} e^{-\nu_C \mathcal{O}_C(x_a, x_b)} \quad (2.10)$$

with

$$Z_C = \int_{X_A \times X_B} e^{-\nu_C \mathcal{O}_C(x_a, x_b)} dx_a dx_b.$$

If systems A and B do not interact, then the density of the combined system C will be the product of the individual densities of systems A and B:

$$f_C(x_a, x_b) = f_A(x_a) f_B(x_b). \quad (2.11)$$

Furthermore, the energy of the combined system, \mathcal{O}_C , will be the sum of the separate energies of system A and system B :

$$\mathcal{O}_C(x_a, x_b) = \mathcal{O}_A(x_a) + \mathcal{O}_B(x_b) \quad \text{and} \quad \langle \mathcal{O}_C \rangle = \langle \mathcal{O}_A \rangle + \langle \mathcal{O}_B \rangle. \quad (2.12)$$

Remember from Theorem 2.2 that the $\langle \mathcal{O} \rangle$'s are nonnegative. Inserting equations (2.8) and (2.9) into the right hand side of (2.11), and (2.10) into the left hand side along with the relations (2.12) gives

$$\frac{1}{Z_C} e^{-\nu_C [\mathcal{O}_A(x_a) + \mathcal{O}_B(x_b)]} = \frac{1}{Z_A Z_B} e^{-\nu_A \mathcal{O}_A(x_a) - \nu_B \mathcal{O}_B(x_b)} \quad (2.13)$$

Now consider two possibilities. First, assume that the two systems A and B are characterized by the same parameter $\nu = \nu_A = \nu_B$. Then it is clear from (2.13) that $\nu_C = \nu$. If the parameter ν is a monotone function of temperature then this argument implies that combining two systems of the same temperature ($\nu_A = \nu_B$) results in a system of the same temperature.

Next, assume that $\nu_A < \nu_B$. Then, how can equation (2.13) be satisfied? Clearly, if the combined system C has a parameter ν_C such that

$$\nu_C \mathcal{O}_C(x_a, x_b) = \nu_A \mathcal{O}_A(x_a) + \nu_B \mathcal{O}_B(x_b),$$

then (2.13) will be satisfied. What is the value of the parameter ν_C ? It is easily obtained by multiplying the last relationship by $f_C = f_A f_B$ and integrating over the product space $X_C = X_A \times X_B$ to obtain

$$\nu_C \langle \mathcal{O}_C \rangle = \nu_A \langle \mathcal{O}_A \rangle + \nu_B \langle \mathcal{O}_B \rangle. \quad (2.14)$$

Furthermore, by writing (2.14) in the form

$$\nu_C = \nu_A r + \nu_B (1 - r),$$

where $0 < r = \frac{\langle \mathcal{O}_B \rangle}{\langle \mathcal{O}_A \rangle + \langle \mathcal{O}_B \rangle} < 1$, it is clear that $\nu_C < \nu_B$. Alternately, equation (2.14) can be rewritten in the form

$$\nu_C = \nu_A (1 - s) + \nu_B s,$$

where $0 < s = \frac{\langle \mathcal{O}_A \rangle}{\langle \mathcal{O}_A \rangle + \langle \mathcal{O}_B \rangle} < 1$, so $\nu_A < \nu_C$. Thus we have proved that when $\nu_A < \nu_B$ the parameter ν_C of the combined system is limited by

$$\nu_A < \nu_C < \nu_B.$$

If ν is interpreted as a monotone function of temperature this last result is in accord with our experience, since combining two systems of two different temperatures T_A and T_B will result in a combined system with a temperature T_C intermediate between T_A and T_B .

Thus, we conclude from these arguments that ν is a monotone function of the inverse temperature. If we take ν to be

$$\nu = \frac{1}{kT}$$

where k is Boltzmann's constant, then the entropy expression in (2.7) becomes

$$S_{TD}^* = c \log Z + cU/kT,$$

or

$$TS_{TD}^* = cT \log Z + (c/k)U. \quad (2.15)$$

If the constant c is taken to be identical with Boltzmann's constant, $c \equiv k$, then (2.15) immediately gives the **Gibb's function**

$$F = U - TS_{TD}^*, \quad (2.16)$$

the fundamental equation of equilibrium thermodynamics relating the **Helmholtz free energy**

$$F = -kT \log Z$$

to the internal energy U , temperature T , and equilibrium entropy S_{TD}^* .

Thus, by the use of Postulates A through D in conjunction with the identification of certain parameters and functions with corresponding quantities of thermodynamic interest, the result is the fundamental relationship on which all of equilibrium thermodynamics is based.

D. BOLTZMANN AND OTHER STATISTICS.

In addition to the relative ease with which the fundamental relationships of equilibrium thermodynamics can be deduced by a suitable identification of quantities in the density of the canonical ensemble, other results can be obtained by considering situations in which the energy functional is specified.

Continuous Energy Spectrum. First, consider the situation in which we have a system for which the energy functional is continuous and given by

$$\mathcal{O}(p) = \epsilon_0 + \frac{p^2}{2m},$$

where ϵ_0 is a zero point energy and p is the momentum, taken to be continuous. This might, for example, describe the situation in a one dimensional classical gas. The partition function is

$$Z = \sqrt{\frac{2\pi m}{\nu}} e^{-\nu\epsilon_0},$$

while the density maximizing the entropy is just

$$f_*(p) = \sqrt{\frac{\nu}{2\pi m}} e^{-\frac{\nu p^2}{2m}}, \quad (2.17)$$

and the parameter ν and the average energy $\langle \mathcal{O} \rangle$ are connected by the relation

$$\nu^{-1} = \langle \mathcal{O} \rangle - \epsilon_0$$

as before. Taking $\nu^{-1} = kT$ as we have argued for in the previous section, (2.17) takes the form

$$f_*(p) = \sqrt{\frac{1}{2\pi m kT}} e^{-\frac{p^2}{2m kT}},$$

which is the continuous **Maxwell-Boltzmann distribution** for particle momenta in one dimension, and $kT = \langle \mathcal{O} \rangle - \epsilon_0$.

This picture changes quite radically if the assumption concerning the continuity of the energy spectrum \mathcal{O} of the system is replaced by the assumption that it is discrete.

Discrete Two-level Energy Spectrum. As an example consider the situation in which the energy functional has only two values

$$\mathcal{O}(0) = \epsilon_0 \quad \text{or} \quad \mathcal{O}(1) = \epsilon_0 + \delta\epsilon,$$

where ϵ_0 and $\delta\epsilon$ are both constants with the dimensions of energy. ϵ_0 is to be thought of as some “ground state energy” $\mathcal{O}(0)$, while $\delta\epsilon$ is the value by which the energy can increment to its second level $\mathcal{O}(1)$. Now in searching for a density which maximizes the entropy we must interpret the integrals in equations (1.1), (2.3), and (2.6) as Stieltjes integrals from which we easily calculate that the partition function Z is given by

$$Z = e^{-\nu\epsilon_0} (1 + e^{-\nu\delta\epsilon}),$$

and thus the density maximizing the entropy is simply

$$f_*(0) = \frac{1}{1 + e^{-\nu\delta\epsilon}} \quad \text{and} \quad f_*(1) = \frac{e^{-\nu\delta\epsilon}}{1 + e^{-\nu\delta\epsilon}}.$$

Discrete Equally Spaced Multi-level Spectrum. Alternately, consider the situation in which the energy function can take on a number of discrete values of the form

$$\mathcal{O}(n) = \epsilon_0 + n\delta\epsilon \quad n = 0, 1, \dots, \quad (2.18)$$

where ϵ_0 and $\delta\epsilon$ are interpreted as before.

In this case the partition function Z is given by

$$Z = \frac{e^{-\nu\epsilon_0}}{1 - e^{-\nu\delta\epsilon}}, \quad (2.19)$$

and the density maximizing the entropy is

$$f_*(n) = [1 - e^{-\nu\delta\epsilon}] e^{-\nu n\delta\epsilon} \quad n = 0, 1, \dots. \quad (2.20)$$

General Discrete Multi-level Spectrum. Finally, we look at the situation in which the system energy may take any one of $(m + 1)$ discrete values,

$$\mathcal{O}(n) = \epsilon_0 + \epsilon_n, \quad n = 0, \dots, m$$

where m may be finite or not. Now the partition function is easily calculated to be

$$Z = e^{-\nu\epsilon_0} \sum_{i=0}^m e^{-\nu\epsilon_i},$$

and the density maximizing the Boltzmann Gibbs entropy is

$$f_*(n) = \frac{e^{-\nu\epsilon_n}}{\sum_{i=0}^m e^{-\nu\epsilon_i}}, \quad n = 0, \dots, m,$$

which is just the density of the **discrete Maxwell Boltzmann distribution**.

E. BLACKBODY RADIATION.

In the previous section when we considered the case where the energy had a discrete and equally spaced multi-level spectrum, had we allowed all values of $n \in R^+$ and not restricted ourselves to integer values of n in equation (2.18), the corresponding result would have been

$$f_*(n) = \nu\delta\epsilon e^{-\nu n\delta\epsilon},$$

which does not seem too different from (2.20). However, the differences become immediately apparent when the average energy $\langle \mathcal{O} \rangle$ is calculated in the discrete (integral n) case:

$$\begin{aligned} \langle \mathcal{O} \rangle &= \sum_{n=0}^{\infty} [\epsilon_0 + n\delta\epsilon] f_*(n) \\ &= \epsilon_0 + \frac{\delta\epsilon e^{-\nu\delta\epsilon}}{1 - e^{-\nu\delta\epsilon}}. \end{aligned} \quad (2.21)$$

If it is assumed that the energy functional in (2.18) is that of a system in which there is a strict relationship between the frequency of oscillation and the incremental energy $\delta\epsilon$ of the form

$$\delta\epsilon = \hbar\omega,$$

and that $\nu = 1/kT$ as we have argued for in Section C, then (2.21) takes the form

$$\langle \mathcal{O}(\omega, T) \rangle - \epsilon_0 = \hbar\omega \frac{e^{-\frac{\hbar\omega}{kT}}}{1 - e^{-\frac{\hbar\omega}{kT}}}. \quad (2.22)$$

This will be immediately recognized as the Planck formula for the average energy of a system of oscillators (relative to the ground state energy ϵ_0) at a temperature T and frequency ω . From this it is quite straightforward to derive the Planck formula for the spectrum of black body radiation $\epsilon(\omega, T)$ from the general relation

$$\epsilon(\omega, T) = [\langle \mathcal{O}(\omega, T) \rangle - \epsilon_0] \frac{\omega^2}{\pi^2 c^3}, \quad (2.23)$$

where c is the velocity of light. Substituting (2.22) into (2.23) immediately gives the **Planck blackbody radiation formula**

$$\epsilon(\omega, T) = \frac{\hbar}{\pi^2 c^3} \frac{\omega^3}{e^{\frac{\hbar\omega}{kT}} - 1}. \quad (2.24)$$

Note that had we used the result for the average energy of an ensemble with a continuous dependence on n in (2.18), then the result would have been

$$\epsilon(\omega, T) = \frac{kT}{\pi^2 c^3} \omega^2, \quad (2.25)$$

the **Rayleigh-Jeans radiation law** with its “ultraviolet catastrophe”. The same expression results from (2.24) in the high temperature limit with $\hbar\omega \ll kT$, while the low temperature limit with $\hbar\omega \gg kT$ gives the **Wien radiation law**

$$\epsilon(\omega, T) = \frac{\hbar}{\pi^2 c^3} \omega^3 e^{-\frac{\hbar\omega}{kT}}.$$

F. GENERAL ENTROPY MAXIMA.

It is quite easy to state and prove an obvious generalization of Theorem 2.2 applicable to systems in which there are multiple known averages $\langle \mathcal{O}_i \rangle$. This generalization is contained in:

Theorem 2.3. *Assume that a sequence of m non-negative measurable functions $\mathcal{O}_i(x)$, $i = 1, \dots, m$, and their averages $\langle \mathcal{O}_i \rangle$ over the entire space X are given. Then the maximum of the entropy $H(f)$ for all densities f , subject to the conditions*

$$\langle \mathcal{O}_i \rangle = \int_X \mathcal{O}_i(x) f(x) dx \quad (2.26)$$

occurs for the density

$$f_*(x) = \frac{1}{Z} \prod_{i=1}^m e^{-\nu_i \mathcal{O}_i(x)} \quad (2.27)$$

where

$$Z = \int_X \prod_{i=1}^m e^{-\nu_i \mathcal{O}_i(x)} dx, \quad (2.28)$$

and the ν_i 's are implicitly determined from

$$\langle \mathcal{O}_i \rangle = \frac{1}{Z} \int_X \mathcal{O}_i(x) e^{-\nu_i \mathcal{O}_i(x)} dx. \quad (2.29)$$

Proof. The demonstration is an extension of the proof of Theorem 2.2. \square

The density (2.27) maximizing the entropy is a generalization of the density of the grand canonical ensemble. If we know that a given system has a number of independent averages (2.26) of functions $\mathcal{O}_i(x)$, then the content of Theorem 2.3 can be used to construct the density that maximizes the entropy. This density can, in turn, be used to construct a generalized thermodynamics for that system. Grad (1952) and Jaynes (1957) have followed this procedure.

G. MAXIMAL ENTROPY PRINCIPLES.

As attempts to justify Postulate D on dynamical grounds increasingly met with failure, more and more authors tried to enshrine this hypothesis as a basic principle, often known as the **Maximal Entropy Principle**. Tolman (1938) seems to have been one of the first to espouse this point of view. He argued that since the techniques being used in thermodynamics were statistical in nature, one had to have some principle that would guide the selection of the proper density out of the unlimited number of possibilities. The Maximal Entropy Principle certainly offers one such guide. Jaynes (1957), Scalapino (1961), and Katz (1967) have written extensively on the use of the maximal entropy principle in reformulating classical and quantum statistical mechanics, and Lewis (1967) has tried to justify it on dynamical grounds.

It may appear that the use of the maximal entropy principle gives a great deal (equilibrium thermodynamics) for very little. Such is surely not the case. In actuality the hardest aspect of the understanding of thermodynamics is determining which systems, described by densities, will evolve toward equilibrium in such a way that the entropy is maximized.

H. SUMMARY.

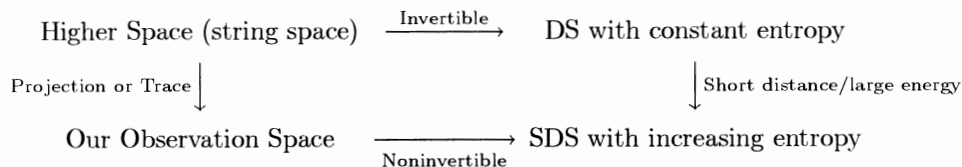
Based on the topics covered in this chapter it is clear that the central questions of what systems can be reasonably described by densities that approach a limit that maximizes the entropy rank as the most important ones that must be answered if we are to have any clear and comprehensive understanding of the foundations of thermodynamics since (Postulate D) we assume that the density maximizing the entropy characterizes the physically attained state of thermodynamic equilibrium. The treatment of these problems constitutes the remainder of this book.

21 OCTOBER, 1986: OXFORD
REVERSIBILITY

Though thermodynamics accounts for what we see in the real world, its impossible to derive thermodynamics from reversible (e.g. Hamiltonian) systems.

This fact has led to a tremendous wastage of effort as various individuals have tried to derive thermodynamics from the statistical mechanics of reversible systems, and specifically Hamiltonian systems. Two alternative points of view:

- (1) View Hamiltonian dynamics as an abstraction of, or approximation to, the dynamics of the real world. Works very well for large distances and/or small energies.
- (2) We perceive the phenomena described by thermodynamics but we are unable to perceive some coordinate.



The fact that \hbar shows up in the Sakur-Tetrode entropy just indicates the fundamental nature of the projection.

22 OCTOBER, 1986: OXFORD

A SET OF REMARKS

- (1) I think that the MEP can be viewed within the general context of variational principles (VP). Now other VP often are used to \implies equations of motion. Is it possible to use an extension of the MEP to obtain an H theorem? cf. Gerjuey et al. Rev. Mod. Phys. (1983), **55**, 729; R.M. Lewis "A unifying principle in statistical mechanics", J. Math. Phys. (1967), **8**, 1448-1459.]
- (2) Pauli exclusion principle $\implies \exists$ interactions between particles in spite of the fact that it was specifically excluded.
- (3) If have an AP transformation S then ACF will be periodic, in spite of the fact that entropy is at least constant or increasing.
- (4) I think it might be possible to model channel openings/closings as an AP process. How to calculate the distribution of open/closed times?
- (5) Action seems to play such a large role in, e.g., Feynman path integrals, and the Motz and Nelson derivations of the Schrodinger equation. How can I understand the intuitive interconnection between Lagrangians, Hamiltonians, and action. But note that action [as well as Hamiltonians and Lagrangians] concepts all come from classical equations of motion [i.e., all reversible].
- (6) In normalizing a density $\int f(y)dy = 1$ if have a d -dimensional mechanical system so $dy = dx dp$ then there must be a constant in f with dimensions \hbar^d (action raised to the d power). What is the connection of this with the Sakur-Tetrode entropy?

23 OCTOBER, 1986: OXFORD

REMARKS-QM

- (1) Suppose we have a SDS describing a "quantum" system. Suppose really does obey classical laws WRT radiation, i.e. only get radiation with acceleration. Then, how to understand radiation eg., from H atom. Works if and only if *electron isn't moving—I mean, is in a state of constant velocity—when in a stationary state*. In going from State 1 \rightarrow State 2, does accelerate and emits radiation (or emits it).
- (2) Maybe as AL suggests \exists a constant vacuum fluctuation giving rise to Brownian motion like movement of particle.
- (3) The reason that there has been such a failure of SM to \implies Thermodynamics based on Newtonian DS is that at the microscopic level these systems are not isolated from their environment.
 - a. At the macroscopic level, e.g., motion of planets, the isolated systems of Newtonian mechanics are a good approximation. But, at the microscopic level perhaps \exists *fluctuations that must be considered in examining the dynamics*. What could the origin of these fluctuations be?
 - a. Background energy radiated by other particles that are accelerated. This is the idea of stochastic electrodynamics [at least of Marshall].
 - b. Fluctuations of unknown origin, as in Nelson. This could be due, for example, to a trace operation though it is clear that \exists other possibilities.
- (4) Essential to concentrate on the experimental facts.
 - a. Spectra: Emission or absorption at discrete wavelengths.
 - b. Photoelectric effect: Dependence of electron emission on incident wavelength.

Note that both of the above situations can be viewed as ones in which \exists forcing of the system.

- c. Blackbody radiation: Distribution of energy radiated with frequency.
- d. Specific heats of solids: Related to blackbody radiation.

26 OCTOBER, 1986: EDINBURGH

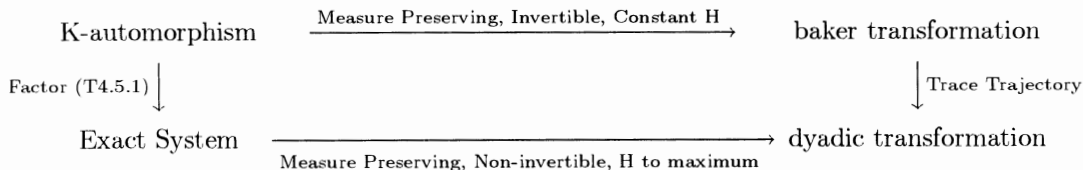
- (1) Marganeau and Murphy give a very good synopsis of Gibbs statistical mechanics and approach to thermodynamics.

Trouble is, of course, how to prove entropy \rightarrow maximum. Of course, for a Hamiltonian system this won't work. This is why ergodic hypothesis is introduced, but even that doesn't work.

- (2) Therefore, see that need an "exact hypothesis", or "AS" or "AP" hypothesis.
- (3) Is H constant \forall mixing transformations?
- (4) In our new AP paper [Stab + noise \implies AP] does entropy increase? [See work of Nick Provatas.]

4 NOVEMBER, 1986: OXFORD
FACTORS AND TRACES

- (1) K-automorphism, pp. 73-76



- (2) What is the connection between **trace** (D4.5.2) and **factor** (D7.2.2)? Trajectory of a factor is a special type of a trace.
- (3) Every exact transformation is a factor of a K-automorphism (T4.5.1). What about every asymptotically stable transformation? Probably every AS transformation is a factor of some generalization of a K-automorphism.
- (4) Given an exact S how can one construct a K automorphism $T \ni S$ is a factor of T ?

AL says: See Rochlin. If $S : X \rightarrow X$ then the corresponding T he constructs is on $X \times X \times \dots$ an infinite number of times.

- (5) From R4.1.4. Given $S : X \rightarrow X$ construct

$$T(x, y) = (S(x) + y, \beta x)$$

which is invertible and measure preserving.

If S is exact, when is T a K-automorphism?

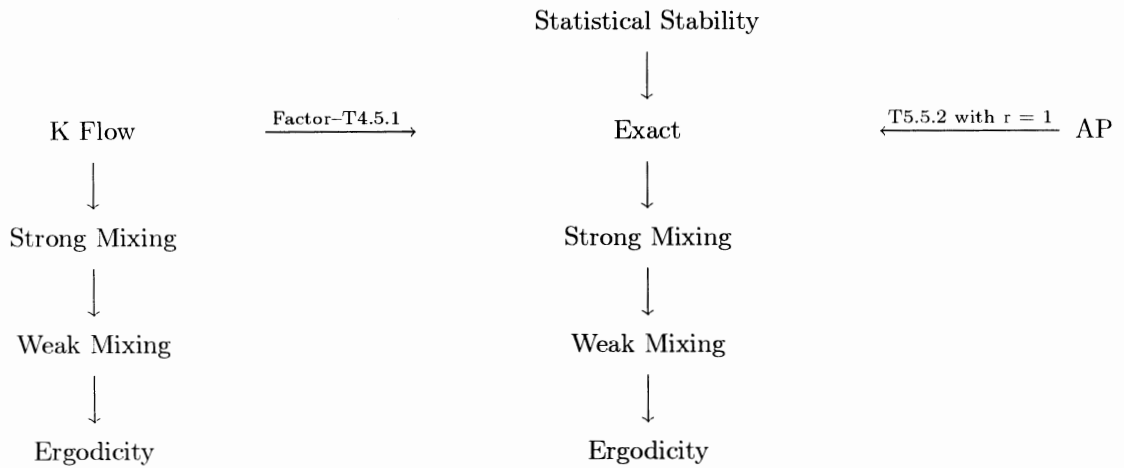
- (6) An intersecting and nonperiodic trajectory of a trace $\implies H$ is constant or increasing, i.e. $H(Pf) \geq H(f)$.

4 NOVEMBER, 1986: OXFORD
REVERSIBLE AND IRREVERSIBLE SYSTEMS

(1) Note the following connections.

DS-Reversible-Constant H

SDS-Irreversible-Const/Increasing H



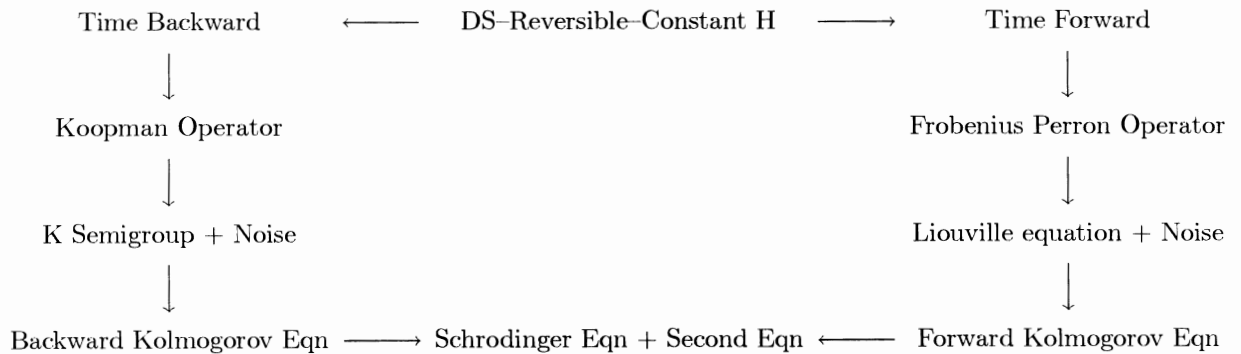
(2) Forward Kolmogorov equation (the Fokker Planck equation) is equivalent to

Semi-Group for Frobenius Perron Operator (Liouville equation) + Noise

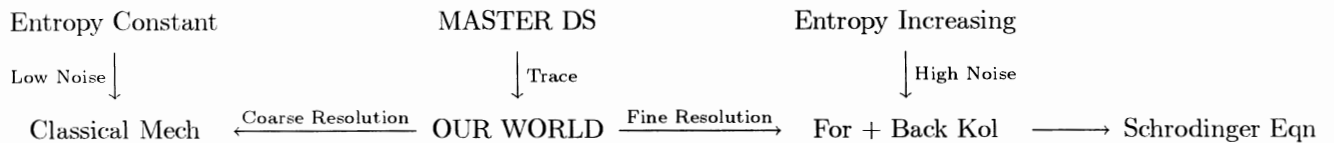
(3) Backward Kolmogorov equation is equivalent to

Semi-Group for Koopman Operator + Noise

(4) Nelsons approach to stochastic quantum mechanics:



(5) Where might the noise come from?



(6) Can have a system with $H \equiv$ constant and take away coordinate information to get increasing H . As an example need only consider the baker-dyadic example. This loss of information to give an increasing entropy is just the Ehrenfest coarse graining requirement.

Thus there seem to be two ways to get entropy to increase in a DS. Either

- a. Loss of information; or
- b. Addition of noise.

Do we live in a baker universe but only sense a dyadic section?

Generally,

$$\text{IRREVERSIBILITY} \implies \frac{dH}{dt} \geq 0.$$

When does

$$\text{IRREVERSIBILITY} \implies \frac{dH}{dt} > 0?$$

Who knows.

When does

$$\frac{dH}{dt} > 0 \implies \text{IRREVERSIBILITY?}$$

Always, since from pp262-264 if $\lim H$ or $\lim H_c \rightarrow 0$ then have exactness or asymptotic stability \implies irreversibility.

4 NOVEMBER, 1986: OXFORD
GENERALIZED BAKER, R-ADICS, AND NOISE

- (1) Consider the generalized baker transformation but only look at the x projection

$$S(x) = rx \pmod{1}.$$

If r = an integer, then $Pf_* = f_*$ has $f_* = 1$ as a unique solution, and S is exact. This also has a delta function ACF. r does not need to be an integer. See references in Keener file.

- (2) Alternately, another transformation

$$\tilde{S}(x) = [r - \sigma^2]x + \sigma^2\xi \pmod{1},$$

where ξ is an i.i.d. random variable uniformly distributed on $[0, 1]$, will have some other characteristics. What are they? AS I think.

With this situation could consider the low noise ($\sigma^2 \rightarrow 0$) and the high noise ($\sigma^2 \rightarrow r$) situations.

- (3) If you were collecting data but could only measure x you might come up with either (1) or (2) above as explanations (dynamics).
 (4) Alternative interpretation of (2) is

$$\tilde{T} = \begin{cases} \tilde{S}(x) & = [r - \sigma^2]x + \sigma^2\xi \pmod{1}, \\ U(\xi) & = p\xi \pmod{1} \text{ p an integer.} \end{cases}$$

- (5) Might r play the role of some universal constant? Maybe \exists two of them: one for x (k or kT) and one for y (\hbar or $\hbar\nu$).
 (6) Could you construct a thermodynamics for this type of system? Might be quite interesting.

4 NOVEMBER, 1986: OXFORD
LASOTA & TRAPLE, J. DIFF. EQN. (1986), **63**, 406-417

Consider

$$\frac{du}{dt} = g(u) + \xi(t)$$

or

$$\frac{du}{dt} = A(t)g(u) + \xi(t) \tag{2.1}$$

where $g(u)$ is continuous.

Idea is to take A and ξ as **traces of a measure preserving DS** $S_t : X \rightarrow X$ with $\mu(X) = 1$.

For a function f define:

- (1)

$$\text{Mean value} = Mf = \lim_{T \rightarrow \infty} \frac{1}{2T} \int_{-T}^T f(t) dt$$

- (2)

$$\text{Correlation function} = \Gamma(f(s)) = \lim_{T \rightarrow \infty} \frac{1}{2T} \int_{-T}^T f(t+s)f(t) dt$$

- (3)

$$\text{Covariance matrix} = Kf = \Gamma(f - Mf).$$

Definition. If Mf and $\Gamma(f(s))$ exist and $\Gamma(f(\cdot))$ is continuous, then f is stationary.

Definition. If f is stationary and $\lim_{s \rightarrow \infty} Kf = 0$ then f is pseudorandom. [This is the terminology of Bass.]

Assume that S_t is either ergodic or mixing

Proposition 5.1.

- (1) If S_t is ergodic then all traces are stationary.
- (2) If S_t is mixing then all traces are pseudorandom.

Corollary 5.1. If S_t is ergodic and A and ξ are traces, then the unique bounded solution of (2.1) is stationary. If S_t is mixing, then it is pseudorandom.

N.B. Arnold and Avez show that a transformation T is mixing if and only if $\text{ACF} \rightarrow 0$, i.e. is pseudorandom.

TRAPLE PREPRINT
DISCRETE PROCESSES WITH DYNAMICAL
AND SEMIDYNAMICAL PERTURBATIONS

Considers the discrete analog of (2.1), i.e.

$$u_{n+1} = A(n)g(u_n) + \xi_n$$

Has an exact correspondence to P5.1 and C5.1, namely with S continuous, invertible, and measure preserving on a normalized measure space

- (1) S ergodic $\implies \{u_n\}$ is stationary.
- (2) S mixing $\implies \{u_n\}$ is pseudorandom.

QUESTIONS.

- (1) What if S isn't invertible, i.e. if
 - a. S is measure preserving and exact, or
 - b. S is asymptotically stable.

Are the solutions of the DE or FDE also exact/AS?

- (2) What if S is statistically periodic. Does this \implies solutions are also?

- (3) What if only ξ is a trace. Not a problem if A is a constant since A constant is a trace.

If $A(t)$ is periodic, then take $\tilde{S} : C \rightarrow C$ to be rotation on a circle so $A(t) = \psi(\tilde{S}_t(z_0))$ and $S : X \rightarrow X$ so $\xi = \varphi(S_t(x_0))$. Then take $\hat{S}_t : X \times C \rightarrow X \times C$ so $\hat{S}(x, y) = (S_t(x_0), \tilde{S}_t(z_0))$ and the pair (A, ξ) is the trace of \hat{S}_t .

TURNING CONSTANT ENTROPY SYSTEM INTO INCREASING ENTROPY

Three ways to turn a system with constant entropy into a system with increasing entropy—all illustrated with the baker transformation.

- (1) Take a **trace** by throwing away all information on one coordinate, e.g. baker to dyadic.
- (2) **Coarse grain** by losing some information or precision, e.g. Andy Lasota's baker example.
- (3) Add **noise** from a heat bath.

13 JANUARY, 1987: BREMEN
MINIMAL ACTION AND ENTROPY

A curious fact (which I have seen elsewhere) is mentioned by Grössing [Phys. Lett. A (1981), 118,381] and should be understood. Comes from ideas of

- (1) L. de Broglie "La thermodynamique de la particule isolée", Gauthier-Villars, Paris, 1964; and
- (2) L. Brillouin "Tensors in mechanics and elasticity", Academic Press, New York, 1964.

Start with the Boltzmann formula for the relation between variation in action S and dissipation heat Q_0 [equivalent to energy $M_0 c^2$] of a periodic system with frequency $\nu = 1/\tau$:

$$\delta S = -\tau \delta Q_0 = -\tau \delta (M_0 c^2)$$

\implies

$$\nu \delta S = T \delta S_e$$

where S_e is the entropy of the system and T is the temperature of the heat bath.

Consider a particle with "internal heat" Q_0 [equivalent to a variational rest mass M_0] in contact with a *vacuum heat bath at temperature* $T \ni$

$$M_0 c^2 = h\nu = kT$$

This implies

$$\delta S = \delta S_e \frac{\hbar}{k}$$

so

$$\frac{\delta S}{\hbar} = \frac{\delta S_e}{k}$$

or

$$\boxed{\frac{S}{\hbar} = \frac{S_e}{k}}$$

In other words **on the natural trajectory (minimal action S corresponding to stationary states) of a particle the entropy is maximal!** This would seem to imply that **the Second Law of Thermodynamics is equivalent in some sense to a minimal action principle.**

Further note that

$$\frac{\delta S}{\hbar} = -\frac{\delta Q_0}{M_0 c^2}$$

so

$$\delta S_e = -\frac{k\delta Q_0}{M_0 c^2}.$$

However, with $S_e = k \ln P$ this gives in turn

$$P = P_0 e^{-\delta Q_0 / M_0 c^2} = P_0 e^{-\delta Q_0 / kT},$$

the Boltzmann formula.

20 JANUARY, 1987: BREMEN

BOSE EINSTEIN STATISTICS FOR DISTINGUISHABLE PARTICLES

From Tersoff and Bayer [Phys. Rev. Lett. (1983), **50**, 553-554]

Suppose we have N particles distributed among M states, $i = 1, \dots, M$. Assume that the probability of finding one particle in state i is w_i . Then a traditional combinatorial argument says that the probability of a given configuration $\{n_1, \dots, n_M\}$ is just

$$P\{n_i\} = N! \prod_{i=1}^M \frac{w_i^{n_i}}{n_i!} \quad \text{with} \quad \sum_i n_i = N. \quad (1)$$

If have the situation where all M state are equally likely (microcanonical ensemble), then $w_i = 1/M$ and

$$P\{n_i\} = \frac{1}{M^N} \frac{N!}{n_1! \dots n_M!}, \quad \sum_i n_i = N,$$

which just gives the traditional Maxwell Boltzmann statistics.

However, T and B argue that in the absence of this knowledge concerning the w_i , the most likely probability is obtained by averaging (1) over all possible configurations subject to $w_i \geq 0$ and $\sum_i w_i = 1$. Note that distinguishability of particles is to be retained. They claim that this procedure, viz.

$$\bar{P}\{n_i\} = \int_0^1 \dots \int_0^1 \frac{N!}{n_1! \dots n_M!} w_1^{n_1} \dots w_M^{n_M} dw_1 \dots dw_M \delta\left(1 - \sum_{i=1}^M w_i\right) \quad (2)$$

leads to Bose Einstein statistics, i.e.

$$\bar{P} = \frac{N!(M-1)!}{(N+M-1)!}.$$

To see how this result is obtained we must first remember that

$$\int_0^a x^m (a-x)^n dx = a^{(m+n+1)} \frac{m!n!}{(m+n+1)!} \quad \text{with } m, n \text{ integers.}$$

Then, using the δ -function allows us to write

$$w_M = 1 - \sum_{i=1}^{M-1} w_i \equiv a_{M-1} - w_{M-1}$$

where

$$a_{M-1} = 1 - \sum_{i=1}^{M-2} w_i.$$

This trick allows us to turn the M fold integral

$$\int_0^1 \cdots \int_0^1 w_1^{n_1} \cdots w_M^{n_M} dw_1 \cdots dw_M \delta\left(1 - \sum_{i=1}^M w_i\right)$$

into an $(M-1)$ fold integral:

$$= \int_0^1 dw_1 w_1^{n_1} \int_0^{1-w_1} dw_2 w_2^{n_2} \cdots \underbrace{\int_0^{a_{M-1}} dw_{M-1} w_{M-1}^{n_{M-1}} (a_{M-1} - w_{M-1})^{n_M}}_{I_{M-1}} \quad (4)$$

Therefore

$$I_{M-1} = a_{M-1}^{n_M + n_{M-1} + 1} \frac{n_M! n_{M-1}!}{(n_M + n_{M-1} + 1)!}$$

with $a_{M-1} = a_{M-2} - w_{M-2}$, and this implies that

$$\begin{aligned} I_{M-2} &= \int_0^{a_{M-2}} dw_{M-2} w_{M-2}^{n_{M-2}} \frac{n_M! n_{M-1}!}{(n_M + n_{M-1} + 1)!} \\ &= \frac{n_M! n_{M-1}! n_{M-2}!}{(n_M + n_{M-1} + n_{M-2} + 1)!} a_{M-2}^{n_M + n_{M-1} + n_{M-2} + 2}. \end{aligned}$$

Thus after the final $(M-1)^{st}$ integration we have that (4) is in fact equal to

$$I_1 = \frac{\prod_{i=1}^M n_i!}{(N + M - 1)!}.$$

But the sequence of the $(M-1)$ integrations was totally arbitrary, save for the restrictions on the w_i , and there were therefore $(M-1)!$ ways of performing them. Each way will, moreover, give precisely the same value of I_1 . Thus we are left with the final result that the average (2) is indeed given by

$$\begin{aligned} \bar{P}\{n_i\} &= \frac{N!}{\prod_{i=1}^M n_i!} \frac{\prod_{i=1}^M n_i!}{(N + M - 1)!} (M-1)! \\ &= \frac{N!(M-1)!}{(N + M - 1)!} \end{aligned}$$

There are two important points here:

- (1) The statistics that a given type of particle obeys is not a criterion on which one may decide the question of distinguishability; and
- (2) Totally distinguishable particles may obey Bose Einstein statistics. [Note: Restricting n_i to 0 or 1 \implies Fermi Dirac statistics, again with distinguishable particles. See Petroni and Viger, Phys. Lett. (1984), **101A**, 4-6]

LASOTA MIXING
19 MARCH, 1987: OBERWÖLFACH

Let X be a sigma finite measure space, and $S : X \rightarrow X$ a dynamics that is not necessarily measure preserving.

Definition LM1. We say that S is **Lasota Mixing 1** if and only if $\forall A, B, C \subset X$ with $\mu(A), \mu(B), \mu(C)$ nonzero and finite we have

$$\lim_{n \rightarrow \infty} \frac{\mu(S^{-n}(C) \cap A)}{\mu(S^{-n}(C) \cap B)} \rightarrow \frac{\mu(A)}{\mu(B)}. \quad (1)$$

OBSERVATIONS ABOUT LM1.

- (1) This definition reduces to the normal definition of mixing if S preserves the measure μ . To see this consider $B = X$ and $\mu(X) = 1$ so

$$\begin{aligned} \mu(S^{-n}(C) \cap B) &= \mu(S^{-n}(C) \cap X) \\ &= \mu(S^{-n}(C)) \\ &= \mu(C), \end{aligned}$$

where the last two lines follow from the assumption that μ is preserved. Therefore we have

$$\lim_{n \rightarrow \infty} \mu(S^{-n}(C) \cap A) = \mu(A)\mu(C).$$

- (2) In equation (1) the left hand side may not be defined for small n , i.e. n must be sufficiently large to permit adequate spreading. This does not, however, matter for the limit.
 (3) As an example of Lasota Mixing 1, we might consider the baker transformation in which you have compression by a factor of 4 but only stretch by a factor of 2:

$$T(x, y) = \begin{cases} 2x, \frac{1}{4}y & x \in [0, \frac{1}{2}] \\ 2x - 1, \frac{1}{4}y + \frac{1}{2} & x \in (\frac{1}{2}, 1] \end{cases}$$

- (4) The definition of Lasota Mixing 1 is good for situations in which the contraction (or expansion) of a set by iteration is *independent of the set* (or its location).

In thinking about a second (and more general) definition of Lasota Mixing, let X be a sigma finite measure space, and $S : X \rightarrow X$ a dynamics that is not necessarily measure preserving.

Definition LM2. We say that S is **Lasota Mixing 2** if and only if $\forall A, B, C \subset X$ with $\mu(A), \mu(B), \mu(C)$ nonzero and finite \exists a finite $\lambda > 0$, independent of C , \ni

$$\lim_{n \rightarrow \infty} \frac{\mu(S^{-n}(C) \cap A)}{\mu(S^{-n}(C) \cap B)} \rightarrow \lambda \quad (2)$$

In general, λ depends on A and B .

OBSERVATIONS ABOUT LM2.

Theorem. If $\mu(X) = 1$ and S is measure preserving, then LM2 is equivalent to normal (Strong or Hopf) mixing.

Proof. Since B is arbitrary, take $B = X$. then we have

$$\mu(X \cap S^{-n}(C)) = \mu(S^{-n}(C)) = \mu(C)$$

since S is measure preserving. Thus from (2) we have

$$\lim_{n \rightarrow \infty} \mu(S^{-n}(C) \cap A) = \lambda\mu(C)$$

since λ only depends on A . This, in turn, implies that

$$\lim_{n \rightarrow \infty} \mu(S^{-n}(X \setminus C) \cap A) = \lambda\mu(X \setminus C)$$

since λ is independent of C . But we can rewrite the left hand side of this relation as

$$\begin{aligned}\mu(S^{-n}(X \setminus C) \cap A) &= \mu((X \setminus S^{-n}(C)) \cap A) \\ &= \mu(A \setminus S^{-n}(C)) \\ &= \mu(A) - \mu(A \cap S^{-n}(C)) \\ &\rightarrow \mu(A) - \lambda\mu(C)\end{aligned}$$

so we have

$$\begin{aligned}\mu(A) - \lambda\mu(C) &= \lambda\mu(X \setminus C) \\ &= \lambda[\mu(X) - \mu(C)] \\ &= \lambda[1 - \mu(C)].\end{aligned}$$

This implies that $\lambda = \mu(A)$ and thus

$$\lim_{n \rightarrow \infty} \mu(S^{-n}(C) \cap A) = \mu(A)\mu(C)$$

Theorem: 15 June, 1987: Brissac. *If S is LM2, then S is ergodic.*

Proof. Assume C is an invariant set so

$$C = S^{-1}(C) \quad \implies \quad C = S^{-n}(C).$$

From the definition of LM2 we have

$$\frac{\mu(A \cap C)}{\mu(B \cap C)} = \lambda$$

We want to show that λ independent of $C \implies C \subset X$ is trivial.

a. If $C = X$ then λ is independent of C since

$$\lambda = \frac{\mu(A)}{\mu(B)}.$$

b. A is arbitrary so set $A = X \setminus C \implies$

$$\mu(A \cap C) = 0 \tag{3}$$

But

$$\mu(A \cap C) = \lambda\mu(B \cap C)$$

so with (3) and $\lambda > 0$ (definition of LM2), we must have $\mu(B \cap C) = 0$. Since $\mu(B) > 0$ by assumption, this $\implies \mu(C) = 0$.

Therefore, all invariant subsets are trivial and ergodicity is proved.

Theorem. *S ergodic with stationary density f_* is LM2 \iff*

$$\lim_{n \rightarrow \infty} \langle P^n f, g \rangle = \langle f, 1 \rangle \langle f_*, g \rangle \quad f \in L^1, g \in L^\infty$$

The proof is as in Lasota and Mackey with $f_* = 1$.

Theorem. *S is LM2 $\iff \{P^n f\}$ is weakly convergent to f_* $\forall f \in \mathcal{D}$.*

16 JUNE, 1987: BRISSAC
CORRELATIONS AND LASOTA MIXING

See "Time's Arrow", Chapter 5 (Mixing), Section C (The Decay of Correlations) for the relevant computations reprinted below.

To understand the connection between mixing and the decay of correlations requires the introduction of a few concepts. If we have a time series $x(t)$ [either discrete or continuous], and two bounded integrable functions $\sigma, \eta : X \rightarrow R$, then the **correlation** of σ with η is defined as

$$R_{\sigma, \eta}(\tau) = \lim_{T \rightarrow \infty} \frac{1}{T} \sum_{t=0}^{T-1} \sigma(x(t+\tau))\eta(x(t))$$

in the discrete time case, or

$$R_{\sigma,\eta}(\tau) = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \sigma(x(t+\tau))\eta(x(t)) dt$$

in the continuous case. The **average** of the function σ is just

$$\langle \sigma \rangle = \lim_{T \rightarrow \infty} \frac{1}{T} \sum_{t=0}^{T-1} \sigma(x(t)),$$

or

$$\langle \sigma \rangle = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T \sigma(x(t)) dt,$$

so it is clear that

- (1) $R_{\sigma,\eta}(0) = \langle \sigma \eta \rangle$; and
- (2) $R_{\sigma^2}(0)R_{\eta^2}(0) \geq R_{\sigma,\eta}(\tau)$. This follows directly by writing out the expression $\langle [\alpha\sigma(t) + \beta\eta(t+\tau)]^2 \rangle$ for real and nonzero α and β , and noting that it must be nonnegative.

The **covariance** of σ with η , $C_{\sigma,\eta}(\tau)$, is defined by

$$C_{\sigma,\eta}(\tau) = R_{\sigma,\eta}(\tau) - \langle \sigma \rangle \langle \eta \rangle,$$

while the **normalized covariance** $\rho_{\sigma,\eta}(\tau)$ is

$$\rho_{\sigma,\eta}(\tau) = \frac{R_{\sigma,\eta}(\tau) - \langle \sigma \rangle \langle \eta \rangle}{\langle \sigma \eta \rangle - \langle \sigma \rangle \langle \eta \rangle}.$$

Clearly, $\rho_{\sigma,\eta}(0) = 1$.

Now assume we have an ergodic transformation S_t with consequent unique stationary density f_* , operating in a finite normalized phase space X , and that S_t is generating the sequence of values $\{x(t)\}$. Then the correlation of σ with η can be written in both the discrete and continuous time case as

$$R_{\sigma,\eta}(\tau) = \int_X \sigma(S_\tau(x))\eta(x)f_*(x) dx \quad (5.7)$$

by use of the extension of the Birkhoff Ergodic Theorem 4.6. Using the definition of the Koopman operator, along with the adjointness of the Frobenius-Perron and Koopman operators, equation (5.7) can be rewritten in the form

$$R_{\sigma,\eta}(\tau) = \langle \eta f_*, U^\tau \sigma \rangle = \langle P^\tau(\eta f_*), \sigma \rangle. \quad (5.8)$$

Writing the defining relation for mixing transformations as in the proof of Theorem 5.1, it is clear that for general functions η and σ we have

$$\lim_{t \rightarrow \infty} \langle P^t(\eta f_*), \sigma \rangle = \langle \eta f_*, 1 \rangle \langle f_*, \sigma \rangle,$$

so (5.8) yields

$$\lim_{\tau \rightarrow \infty} R_{\sigma,\eta}(\tau) = \langle \eta \rangle \langle \sigma \rangle$$

when S_t is mixing. Thus we have the following result connecting mixing with the limiting behaviour of the normalized covariance. Namely,

Theorem 5.3. S_t is f_* mixing if and only if

$$\lim_{\tau \rightarrow \infty} \rho_{\sigma,\eta}(\tau) = 0.$$

16 JUNE, 1987: BRISSAC

Both Krylov and Ma emphasize decay of correlations to zero in a finite time as being important for the approach of the entropy to its maximum. Many exact transformations have this property, so we have the following conjectures.

Conjecture 1. $S : X \rightarrow X$ measure preserving (is it necessary that measure be finite). S is exact if and only if \exists finite $\tau_0 > 0 \ni$

$$\rho_{f,g}(\tau) = 0 \quad \forall \tau > \tau_0.$$

Corollary 1. \exists finite $n_0(f) > 0 \ni$

$$H(P^n f) = 0 \quad \forall n > n_0(f).$$

Conjecture 2. $S : X \rightarrow X$ ergodic with stationary density f_* . S is asymptotically stable if and only if \exists finite $\tau_0 > 0 \ni$

$$R_{f,g}(\tau) = \langle f, 1 \rangle \langle f_*, g \rangle \quad f \in L^1, g \in L^\infty$$

$$\forall \tau > \tau_0.$$

Corollary 2. \exists finite $n_0(f) > 0 \ni$

$$H(P^n f | f_*) = 0 \quad \forall n > n_0(f).$$

2 JULY, 1987: BRISSAC

WEAK LASOTA MIXING

In the normal definition of weak mixing we have $S : X \rightarrow X$ on a normalized measure space, S measure preserving $\iff f_* = 1$ is the only stationary density. Then S is **weak mixing** if and only if

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=0}^{n-1} |\mu(A \cap S^{-k}(B)) - \mu(A)\mu(B)| = 0 \quad A, B \in \mathcal{A}.$$

An obvious extension to a non measure preserving S is given by

Definition. S is **Lasota Weak Mixing** if $\forall A, B, C \subset \mathcal{A} \ni$ finite positive λ , independent of C , \ni

$$\lim_{n \rightarrow \infty} \frac{1}{n} \sum_{k=0}^{n-1} \left| \frac{\mu(A \cap S^{-k}(C))}{\mu(B \cap S^{-k}(C))} - \lambda \right| = 0 \quad \forall A, B \subset \mathcal{A}.$$

GENERALIZATIONS OF K-AUTOMORPHISM

In the normal case we define K-automorphism in the following way. We have $S^n(\mathcal{A}) = \{S^n(A) : A \subset \mathcal{A}\}$. (X, \mathcal{A}, μ) is normalized and $S : X \rightarrow X$ is invertible and $\ni S$ and S^{-1} are measurable and measure preserving. S is a K automorphism is \ni a sigma algebra $\mathcal{A}_0 \subset \mathcal{A} \ni$

- (1) $S^{-1}(\mathcal{A}_0) \subset \mathcal{A}_0$;
- (2) The sigma algebra $\bigcap_{n=0}^{\infty} S^{-n}(\mathcal{A}_0)$ is trivial (only consists of sets of measure 0 or 1); and
- (3) The smallest sigma algebra containing $\bigcup_{n=0}^{\infty} S^{-n}(\mathcal{A}_0)$ is \mathcal{A} .

How to generalize this definition to non measure preserving S so that the new property \iff Lasota Mixing? \ni two questions here:

- (1) Generalize K automorphism definition to non measure preserving S . **Hint:** Look at the proof that the baker transformation is a K automorphism (E4.5.1, pp 74-5) for clue of how to generalize.
- (2) Show that the generalization \iff Lasota Mixing. **Hint:** Look at proof of Theorem 4.5.2 (every K auto is mixing) for the clue. See also Walters (1982) **An Introduction to Ergodic Theory**, Springer; and Parry (1981) **Topics in Ergodic Theory**, Cambridge University Press.

4 JULY, 1987: MONTREAL
 VARIOUS STATEMENTS OF THE LAWS OF THERMODYNAMICS
 BY THOMPSON, MA, AND BUCHDAHL

Zeroth Law. All three are in agreement. If A is in equilibrium with B and B is likewise in agreement with C , then A is in equilibrium with C .

First Law. Q is heat, W is work, and U is internal temperature. Applies to adiabatic processes in thermally isolated systems.

- (1) Thompson and Ma say that in an adiabatic transformation from $1 \rightarrow 2$, $\Delta W_{12} = -\Delta U_{12}$ and for any such process $Q = \Delta W + \Delta U$.
- (2) Buchdahl says that the amount of work W done in an adiabatic transition is solely dependent on the initial and final states $\implies \Delta W + \Delta U = 0$, while in a nonadiabatic transition $Q = \Delta W + \Delta U$.

Second Law.

- (1) Thompson and Ma say that for reversible systems \exists an absolute temperature scale $\ni \delta Q/T$ is an exact differential of a quantity S called entropy, while for irreversible changes in a thermally isolated system S increases.
- (2) Buchdahl says that \exists an ordering of states reflected in the entropy function $S \ni S''$ is adiabatically inaccessible from $S' \iff S'' < S'$.

Third Law. Entropy goes to zero as $T \rightarrow 0$. Ma points out that this plus

$$S(T) = \int_0^T \frac{C}{T'} dT',$$

where

$$C(T') = \frac{dQ}{dT}$$

is the heat capacity, was the basis of the work of Sakkur and Tetrode.

21 JULY, 1987: MONTREAL
 FINITE TIME EXACTNESS

Seems to me that it might be worthwhile to define a new type of chaotic behaviour, a variation of exactness or asymptotic stability [i.e. a special case], in which we have strong convergence of $\{P^n f\}$ to f_* after a finite number of steps:

$$\|P^n f - f_*\| = 0 \quad \forall \quad n \geq n_0(f).$$

- (1) Probably only works for a finite measure space.
- (2) Example is the dyadic transformation. Pick any set $A \subset [0, 1]$ of nonzero measure $\mu(A) > 0$. Then $\mu(S^n(A)) = 1$ after a finite n .
- (3) This is related to Ma's conception that the origin of the Second Law is the decay of correlations in a finite number of steps. Remember that get decay of correlations to zero after an infinite time with mixing. [Question: 13 March, 1995—couldn't this decay also occur with mixing in a finite time for the baker transformation?].
- (4) Is there any connection between the "thermodynamic limit" and the finiteness or non-finiteness of the limiting value of n ?
- (5) Wrote Andy Lasota with these ideas today.

23 JULY, 1987: ST. GABRIEL
 COARSE GRAINING AND ASYMPTOTIC PERIODICITY

If you coarse grain an AP system, can you cause the entropy to converge to zero rather than being periodic?

23 JULY, 1987: ST. GABRIEL
RANDOM THOUGHTS

- (1) In an isolated system if it is reversible then entropy is constant, but if it is irreversible then entropy may increase. However, in a nonisolated system (for example, a system with added noise) then entropy may increase regardless of whether original system was reversible or not. QUESTION: In a nonisolated system, if we consider [System + Perturbation] then is the entropy of the whole constant?
- (2) Is it ever possible that H as opposed to H_c might be periodic?
- (3) A system with a nonuniform f_* may have an H (not H_c) that decreases. This was the reason to introduce the conditional entropy in the first place. QUESTION: How is this important for the development of structure in biology-chemistry-physics? How is it related to the development of structure and/or order?
- (4) Gibbs and others consider ensembles in Γ space ($6N$ dimensional) but we (LM) consider them in μ space ($6D$). Whats the connection?
- (5) Clarify the connection between concepts of ergodicity, quasiergodicity, metric transitive and metric indecomposability in the statistical mechanics literature and our approach.
- (6) AP systems and development of order (eg. BZ reaction). AP could mimic the periodicity seen in the BZ reaction. Start with uniform concentration (hi entropy, maximal disorder) and go to spontaneous periodic behaviour in space/time (low entropy, ordered). Is it better to use H rather than H_c ?

CONJECTURE BY ANDY ABOUT TRACE PERTURBATION
8 APRIL, 1988: LUBLIN

Suppose we have two transformations:

$$x_{n+1} = S(x_n) \quad n = 0, 1, \dots$$

and

$$\xi_{t+1} = T(\xi_t) \quad t = 0, 1, \dots$$

Let T be statistically stable, and examine the perturbed system

$$x_{n+1} = S(x_n) + \epsilon \xi_{kn} \tag{*}$$

[Alternatively, one could take $\xi_{t+1} = T^k \xi_t$ and $x_{n+1} = S(x_n) + \epsilon \xi_n$.

Andy Lasota's Conjecture. If k is sufficiently large, then the eventual behaviour of the f_n generated by (*) will be asymptotically periodic.

- (1) Note that what we are doing in (*) is perturbing S with every k^{th} iterate of T .
- (2) Try this numerically with S a Keener map, and T a quadratic map.
- (3) Does it also work if T is just exact, like a tent or dyadic map? Probably.

FROBENIUS PERRON OPERATOR AND DDE'S
9 APRIL, 1988: LUBLIN

In a DDE one must specify an initial function on the interval $[-\tau, 0]$. Thus the DDE is really mapping functions into functions in some function space. this is the primary problem in defining a Frobenius Perron operator since it is totally unclear what *measure* should be used in this space of functions, i.e., which is the most **natural** measure.

H THEOREMS FROM THE FOKKER PLANCK EQUATION
9 APRIL, 1988: LUBLIN

Horstiemke and Lefever (pp. 112-113) talk about a Fokker Planck equation (in one dimension) with an equilibrium solution f_* supported on $[a, b]$. They then go on to define a functional

$$\phi(t) = \int_a^b f(x, t) \log \left[\frac{f(x, t)}{f_*(x)} \right] dx$$

which is clearly the negative of the conditional entropy $H(f|f_*)$. It is easy to show that $\phi(t) \geq 0$ with $\phi(t) = 0 \iff f = f_*$. They point out that if one can show that $\dot{\phi}(t) \leq 0$ with $\dot{\phi}(t) = 0 \iff f = f_*$, then ϕ is a Liapunov function and f_* is globally asymptotically stable.

They go through an integration by parts of the Fokker Planck equation to claim that they have done just this, i.e. show $\dot{\phi}(t) \leq 0$ with $\dot{\phi}(t) = 0 \iff f = f_*$. However, Andy says that the proof is incomplete because \exists examples such that the distance between f and f_* is ϵ positive at $t \rightarrow \infty$, that is $f \rightarrow f_*$ more slowly than $t \rightarrow \infty$.

Riskin (**The Fokker Planck Equation**) has a similar proof according to AL, but he allows his Fokker Planck equation to have time dependent coefficients and AL says that in this case the proof is simply wrong. He offers a counter example of a Fokker Planck like equation with time dependent coefficients in which the proof does not hold.

Counter Example. Consider

$$u_T = u_{xx} \quad \text{with} \quad u_x(0, t) = u_x(1, t) = 0.$$

Make the time transformation

$$T = \frac{t}{1+t},$$

so for $t \in [0, \infty]$ we have $T \in [0, 1]$. Now with

$$u_T = u_t \frac{dt}{dT} = (1+t)^2 u_t,$$

the transformed PDE becomes

$$u_t = \frac{1}{(1+t)^2} u_{xx} \quad x, t \in [0, 1] \times [0, 1]$$

a PDE with a time dependent diffusion coefficient.

If you solve the original equation in a Fourier series then would have

$$u \simeq \sum_n a_n e^{-n^2 T^2} \cos nx \rightarrow a_0 \quad \text{with} \quad T \rightarrow \infty.$$

Make the change of variables to get the solution in the new variable

$$u \simeq \sum_n a_n e^{-n^2 \left(\frac{1}{1+t}\right)^2} \cos nx \rightarrow \sum_n a_n e^{-n^2} \cos nx \quad \text{with} \quad t \rightarrow \infty.$$

But, as $t \rightarrow \infty$ we have $T \rightarrow 1$ and the system with t dependent coefficient for sure doesn't go to its maximal entropy state!

TRACE PERTURBATION AGAIN (SEE 8/4/88)

9 APRIL, 1988: LUBLIN

There are some problems with this whole idea. Consider the following:

- (1) If we have

$$x_{n+1} = S(x_n) + \xi_n$$

where the ξ_n are i.i.d. random variables, then given a density f_n of the x_n we have no trouble constructing an operator P to give f_{n+1} through $f_{n+1} = P f_n$. This is so because of the assumed independence of the ξ_n .

- (2) However, if we have

$$\begin{aligned} x_{n+1} &= S(x_n) + \epsilon y_n \\ y_{n+1} &= T^k(y_n) \end{aligned}$$

with $k \geq 1$, then it is not possible to calculate f_{n+1} given f_n in the same way as in the previous remark. The problem lies in the fact that

$$x_n \quad \text{depends on} \quad y_0, \dots, y_{n-1}$$

and

$$y_n \quad \text{depends on} \quad y_0, \dots, y_{n-1}$$

which implies that they are not independent and therefore we do not have available the tools that we had at our disposal in 1.

- (3) One possible way out of this quandary might be to obtain an operator P governing the two dimensional density $f(x, y)$ so

$$f_{n+1}(x, y) = P f_n(x, y)$$

and then to look at the marginal density

$$f_{n+1}(x) =: \int_Y f_{n+1}(x, y) dy.$$

- (4) However, this introduces another problem, illustrated by the special case of a transformation S such that $S(x) \equiv 0 \quad \forall x$. Then our system becomes

$$\begin{aligned} x_{n+1} &= y_n \\ y_{n+1} &= T^k(y_n). \end{aligned}$$

Now (x_{n+1}, y_{n+1}) are both functions of the same variable (y_n) and therefore the density $f_{n+1}(x, y)$ becomes degenerate \implies no way to calculate the marginal density $f_{n+1}(x)$! Note that this will occur for any $S \ni |S'| < 1 \quad \forall X$ (as in the Keener map).

- (5) Discuss this with Traple in Krakow.

POINCARÉ RECURRENCE AND ROUGH DENSITIES
9 APRIL, 1988: LUBLIN

- (1) We know that for a mathematical density the Poincaré recurrence theorem implies absolutely nothing about the behaviour of the density evolution. But, for a real (rough) density the situation is much different. Consider the following.
- (2) Suppose we have a trajectory evolving under the action of $x_{n+1} = S(x_n)$, and we pick an initial point x_0 in a set A with $\mu(A) = \epsilon$. Then if S is at least mixing, then we must wait on average a time

$$T = \left\lceil \frac{1}{\epsilon} \right\rceil,$$

where $\lceil \cdot \rceil$ denotes the integer value function, such that $x_T \in A$ and $x_j \notin A \quad \forall j = 1, \dots, T-1$. For example, if $\epsilon = 1/10$ then $T \simeq 10$.

- (3) Pick two initial points $x_0 \in A$ and $y_0 \in B$ with $\mu(A) = \mu(B) = \epsilon$. Let each trajectory evolve under the action of S , and consider this in a two dimensional space such that

$$(x_{n+1}, y_{n+1}) = (S(x_n), S(y_n)).$$

If S is mixing, then with $z_{n+1} = (x_{n+1}, y_{n+1}) = S_2(z_n)$, S_2 is at least ergodic. [For a proof see Peter Walters, **Ergodic Theory: Introductory Lectures**, Lecture Notes in Mathematics, volume 458, 1975; ISBN 0-387-07163-6. There he proves in Theorem 1.10, page 44, that if T is measure preserving and $\mu(X) = 1$ then

$$T \text{ weakly mixing} \iff T \times T \text{ weakly mixing} \iff T \times T \text{ ergodic.}]$$

Now we must wait a time

$$T \simeq \left\lceil \frac{1}{\epsilon^2} \right\rceil$$

on average for $(x_T, y_T) \in A \times B$.

- (4) Extending this argument to N initial points we must wait an average time

$$T \simeq \left\lceil \frac{1}{\epsilon^N} \right\rceil$$

for the recurrence of the initial (rough) density. This of course presupposes that $\epsilon \leq 1/N$.

Step 3. Define the *product partition* $A \vee B$ of two partitions

$$(A) = A_1, \dots, A_n \quad \text{and} \quad (B) = B_1, \dots, B_n$$

by all possible intersections

$$A_i \cap B_j \quad i = 1, \dots, n, \quad j = 1, \dots, n$$

that have positive measure.

Step 4. Define the KS entropy of the partition A by

$$h(A) = \sum_{i=1}^n \eta(m(A_i))$$

where

$$\eta(x) = \begin{cases} -x \log x & x > 0 \\ 0 & x = 0 \end{cases}$$

Remark 3. $h(A)$ is totally unchanged by the addition or subtraction of sets of measure zero to the partition.

Remark 4. There is only a vague similarity between the KS entropy $h(A)$ and my coarse grained Boltzmann Gibbs entropy.

Step 5. From a partition $(A) = (A_1, \dots, A_n)$ construct the partition

$$A \vee T^{-1}(A) \vee \dots \vee T^{-k}(A).$$

Then the entropy of the transformation T with respect to the partition A is defined as

$$h(A, T) = \lim_{k \rightarrow \infty} \frac{1}{k} h(A \vee T^{-1}(A) \vee \dots \vee T^{-k}(A)).$$

Step 6. Define the KS entropy of T by

$$h(T) = \sup_{(A)} h(A, T)$$

where the supremum is taken over all possible partitions A .

Remark 5. As it stands, this is clearly impossible because how can you calculate over all possible partitions A ? This is circumvented by the following

We say that a partition A is a *generator* if A is the smallest sigma algebra containing all of the sets $A, T^{-1}(A)$, etc. Example: $[0, \frac{1}{2}]$, $(\frac{1}{2}, 1]$ is the generator for the tent map and the dyadic map.

Theorem. If A is a generator, then $h(T) = h(A, T)$.

Remark 6. This theorem makes the calculation of the KS entropy possible.

Remark 7. If T is invertible, then can also calculate $h(T)$ by using

$$A \vee T(A) \vee \dots \vee T^k(A).$$

Remark 8. The KS entropy measures the speed of mixing in some sense.

Example. Lets calculate the KS entropy of the tent map with $a = 2$. Take $A = [0, \frac{1}{2}]$, $(\frac{1}{2}, 1]$. Then

$$A \vee T^{-1}(A) = [0, \frac{1}{4}], (\frac{1}{4}, \frac{1}{2}], (\frac{1}{2}, \frac{3}{4}], (\frac{3}{4}, 1]$$

so

$$h(A \vee T^{-1}(A)) = -\frac{1}{4} \sum_{i=1}^4 \log \left(\frac{1}{4} \right) = \log 2^2.$$

By induction we find that

$$h(T) = \lim_{k \rightarrow \infty} \frac{1}{k} \log 2^{k+1} = \log 2.$$

POSSIBILITY OF AP IN CT SYSTEMS: DISCUSSION WITH AL AND RR
14 APRIL, 1988: KATOWICE

RR thins that in a CT system, you will approach a fixed density without perturbations of coefficients. AL agrees, and their argument is as follows.

In a DT system that is AP, we have

$$P^n f(x) = \sum_i \lambda_i(f) g_i(x)$$

and if extend this to a CT system

$$P^t f(x) = P^n(P^\theta f(x)) = \sum_i \lambda_i(P^\theta f) g_i(x)$$

since $\forall t \in R \exists n \in N$ and $\theta \in [0, 1] \ni t = n + \theta$. But, in DT we have a constant permutation that can't exist in CT. Reason is that in DT the g_i 's are orthogonal (disjoint support) \implies there can't be continuous movement of densities with associated coefficients \implies there is no permutation of coefficients and therefore no permutation of densities.

Conjecture. If there are no invariant sets (i.e. P is ergodic then in CT asymptotic periodicity is equivalent to asymptotic stability.

Rudnicki has a student working on this for his thesis.

PERTURBATION OF MAPS
DISCUSSION WITH J. TRAPLE AND A. LASOTA
17 APRIL, 1988: KRAKOW

- (1) We considered (see Oberwölfach notes) the perturbation of a map by the parabola

$$\begin{aligned} x_{n+1} &= \lambda x_n + \beta y_n & |\lambda| < 1 \\ y_{n+1} &= 4y_n(1 - y_n). \end{aligned}$$

- (2) Traple [JMAA (1988), **129**, 118-130] in his Theorem 5.1 (page 129) says that if perturb a system with another system \sum that is *mixing*, then solution of perturbed system is *pseudo random* in the sense of Bass which means that $\lim_{\tau \rightarrow \infty} (\text{covariance function}) = 0$.
- (3) If define a *random solution* as one in which the covariance = 0 $\forall \tau$ except for $\tau = 0$, then I conjecture that if \sum is asymptotically stable then the solution of the original (perturbed) equation is random.

Three additional points from conversation between Krakow and Lublin with AL:

- (1) Stochastic perturbation of a map with ξ_n that have no density gives a fractal attractor.
- (2) Perturbation of a system by a semi-dynamical system (e.g as above) may also give a fractal attractor. But, it also may have a density.
- (3) Perturbation of a system by ξ_n distributed with a density will produce asymptotic periodicity as in our Physica D paper.

THOUGHTS PLUS ANDRE/ZENG COMMENTS
13 MAY, 1988: GUELPH

- (1) We can have a large system with constant entropy, and by taking a trace WRT dynamic variables we get a situation with increasing entropy.
- (2) Question: Is it possible to do the same thing by using only some subset A of the entire phase space X , $A \subset X$? For example, we might have a universe with constant entropy while \exists an increasing entropy in some subset.
- (3) It would seem that this is impossible if $H(P^t f|f_*) \geq 0$, cuz if $H_{tot} = \text{const}$ while $H_A(P^t f|f_*) \uparrow$, then this \implies that need $H_{X \setminus A}(P^t f|f_*) \downarrow$.
- (4) AL: Conceptually not the way physicists think. Why define conditional entropy—requires an example or a sentence.
- (5) Z: Need more physical examples and comparison with physical systems.
- (6) Z: Connection between reversible and irreversible Markov operators and reversible and irreversible systems is unclear.

- item AL/Z: Clarify the connection between Boltzmann, Gibbs, and my approach.
- (7) AL: Need examples of how Markov operators make the density evolve. Give examples from physics of evolution equations for densities, e.g. the Liouville equation, Fokker-Planck equation, heat equation, Schrodinger equation. Maybe use the heat equation to show pictures of evolution of the density.
 - (8) Make clear the difference between reversible and irreversible systems.
 - (9) Make clear the distinction between **time reversal invariance** ($t \rightarrow -t$ and equations don't change form), **time shift invariance** ($\exists \tau \ni x(t) = x(t + \tau) \implies x$ is constant or periodic), and **time translation invariance** ($x(t) = x(t + \tau) \forall \tau \implies x$ is constant).
 - (10) First Hopf bifurcation breaks the symmetry of the time translation invariance. Higher order (secondary) bifurcations break time shift invariance.
 - (11) AL: See Reichl for scaling arguments and phase transitions.
 - (12) Z: Add section to illustrate classical work of Boltzmann on approach of system to equilibrium.
 - (13) Z: How do you connect evolution of density to evolution of a thermodynamic system
 - (14) Z: Add a discussion of nonequilibrium thermodynamics, and relate it to the present work [Onsager, de Groot, Mazur, Lewis].
 - (15) AL: Add more examples of continuous time systems.
 - (16) Z/AL: Every time a theorem is proved, connect the consequences with the physics. Before theorem tell what going to prove. State theorem as physically as possible. Make proofs as transparent as possible.
 - (17) AL: Add the Gibbs mixing paradox.
 - (18) Z: Make the distinction between extensive and intensive variables.
 - (19) Z: Suggests I look at Renyi on information theory.
 - (20) Z: Dissipation in a dynamical sense corresponds to an attractor with dimension contraction relative to the initial dimension. This is **not** the same as thermodynamic dissipation which we usually associate with loss of energy.
 - (21) LG: Connection between equilibrium and non-equilibrium physics.
 - (22) Question: Is it possible to use the Hille-Yoshida theorem $\frac{du}{dt} = Mu$ to derive a general expression for \dot{H} and nonequilibrium thermodynamics and irreversible thermodynamics? See Lewis.
 - (23) Question: Add superadditive entropy with Loskot paper?

DENSITY DEPENDENT DYNAMICS
28 OCTOBER, 1988: KATOWICE

- (1) In discussion with Andy we realized that if you have a continuous time density dependent dynamics (e.g. the Bohm equations obtained from the Schrodinger equation) then would have

$$\frac{dx_i}{dt} = F_i(x, u) \quad i = 1, \dots, d$$

and the evolution of the density $u(t, x)$ is just governed by the equation

$$\frac{\partial u}{\partial t} + \sum_i \frac{\partial}{\partial x_i} (u F_i) = 0.$$

There are some existence and uniqueness results for such nonlinear equations, but probably not much in terms of stability results.

- (2) For density dependent discrete time dynamics (maps) the situation is much harder since we haven't an explicit form that allows us to calculate the Frobenius Perron operator. Andy thinks the best hope is to pick a map that we know a lot about (preferably onto) and then make the coefficients density dependent. Hopefully it might even have some biological application!
- (3) As an example we might pick a modified hat map $x_{n+1} = S(x_n)$ with

$$S(x) = \begin{cases} x \left\{ \alpha + \frac{\beta}{2x} \int_0^{2x} f(x) dx \right\} & x \in [0, \frac{1}{2}] \\ (1-x) \left\{ \gamma + \frac{\delta}{2(1-x)} \int_{2x-1}^1 f(x) dx \right\} & x \in (\frac{1}{2}, 1] \end{cases}$$

with $\alpha + \beta = 2$, $\gamma + \delta = 2$, and f is the density.

- (4) A quick check shows that $S(0) = S(1) = 0$ and $S(\frac{1}{2}) = 1$ If you start with $f_0(x) = 1$ than you get the old hat map back.
- (5) Hopefully, if start with $f_0(x)$ that doesn't differ from $f_* = 1$ too much (in C^1 topology), then can prove that $f_n \rightarrow f_*$, an analog of local stability in differential equations.
- (6) Another possibility might be a hat map with

$$a(f) = 1 + \int_{\Delta} f(x) dx \quad \Delta \subset [0, 1]$$

- (7) Or the random map

$$x_{i+1} = \begin{cases} S_1(x) & p(f) = \int_{\Delta} f(x) dx \\ S_2(x) & 1 - p(f) \end{cases}$$

SCHWARZCHILD (PRISONER) THEOREM
1 NOVEMBER, 1988: KATOWICE

Theorem. Let (X, Σ, μ) be a finite measure space, $S_t : X \rightarrow X$, $t \in \mathbb{R}$ (so S is invertible), and μ an invariant measure. Further let $A \subset X$ and define

$$A_- = \{x \in X : S_{-t}(x) \in A \forall t \in (-\infty, 0]\}$$

(the set of all trajectories from $-\infty$ to 0) and

$$A_+ = \{x \in X : S_t(x) \in A \forall t \in (0, \infty)\}.$$

Then if a trajectory was in A_- it will always be in A_+ and vice versa.

Proof. We have

$$A_- = \bigcap_{t \geq 0} S_t(A) \quad \text{and} \quad A_+ = \bigcap_{t \leq 0} S_t(A)$$

since $y \in S_t(A) \iff S_{-t}(y) \in A$.

Further, since μ is an invariant measure we have

$$\mu(A_+) = \mu(S_{-t}(A_+)).$$

Now

$$\begin{aligned} S_{-t}(A_+) &= S_{-t}(\bigcap_{\tau \geq 0} S_{\tau}(A)) \\ &= \bigcap_{\tau \geq 0} S_{\tau-t}(A) \\ &= \bigcap_{u \geq -t} S_u(A) \end{aligned}$$

so

$$\mu(A_+) = \mu(S_{-t}(A_+)) = \mu(\bigcap_{u \geq -t} S_u(A))$$

and

$$\begin{aligned} \lim_{t \rightarrow \infty} \mu(A_+) &= \mu(\bigcap_{t > 0} \bigcap_{u \geq -t} S_u(A)) \\ &= \mu(\bigcap_{u = -\infty}^{\infty} S_u(A)) \\ &= \mu(A_+ \cap A_-) \end{aligned}$$

In a completely analogous fashion

$$\lim_{t \rightarrow \infty} \mu(A_-) = \mu(A_+ \cap A_-).$$

Now

$$\begin{aligned} A_+ \setminus A_- &= \text{trajectories in } A_+ \text{ that didn't come from } A_- \\ &\subset A_+ \setminus (A_+ \cap A_-) \end{aligned}$$

and

$$A_- \setminus A_+ = \text{trajectories in } A_- \text{ that didn't go to } A_+ \\ \subset A_- \setminus (A_+ \cap A_-).$$

Therefore

$$\mu(A_+ \setminus A_-) \leq \mu(A_+ \setminus (A_+ \cap A_-)) \\ = \mu(A_+) - \mu(A_+ \cap A_-) = 0$$

and

$$\mu(A_- \setminus A_+) \leq \mu(A_- \setminus (A_+ \cap A_-)) \\ = \mu(A_-) - \mu(A_+ \cap A_-) = 0$$

so

$$\mu(A_+ \setminus A_-) = \mu(A_- \setminus A_+) = 0.$$

Define

$$A \div B = (A \setminus B) \cup (B \setminus A)$$

so

$$\mu(A_+ \div A_-) = 0. \quad \square$$

PERTURBATION OF DISCRETE TIME SYSTEM WITH ANOTHER
DISCUSSION WITH J. TRAPLE
3 NOVEMBER, 1988: KRAKOW

In thinking about how we might start to look at the perturbation of a discrete time system by another, one possibility is to consider

$$u_{i+1}^k = S(u_i^k) + \varphi(T^{ki}(x_0)) \quad k = 1, 2, \dots$$

For example, with $S(x) = ax$, $|a| < 1$, and $k = 1$ we have

$$u_{i+1}^1 = \lambda(T^i(x_0))$$

where

$$\lambda(w) = \sum_{m=-\infty}^{\infty} a^{-m} \varphi(T^{m-1}(w)).$$

We could, for example, pick T to be the ubiquitous parabola $t(x) = 4x(1-x)$.

COARSE GRAINED ENTROPY
DISCUSSION WITH R. RUDNICKI
10 NOVEMBER, 1988: KATOWICE

Its certainly true that for an invertible system

$$H(P^t f|f_*) = H(f|f_*) = \text{constant} \quad \forall t$$

Suppose our invertible system is mixing. Then if n is the index of the partition (the number of units) it is also the case that

$$\lim_{t \rightarrow \infty} H_n^{CG}(P^t f|f_*) = 0.$$

But, we should also expect that

$$\lim_{n \rightarrow \infty} H_n^{CG}(P^t f|f_*) \rightarrow H * P^t f|f_*$$

This seems like a real paradox!

A partial (?) explanation. Let

$$g(t) = H(P^t f|f_*) = \text{constant}$$

and

$$g_n(t) = H_n^{CG}(P^t f|f_*).$$

Then $\forall t < \infty$

$$0 \geq g_1 > g_2 > \dots > g(t) = \text{constant}.$$

Thus the g_n , though increasing to 0 as $n \rightarrow \infty$, approach a constant limiting function $g(t)$. [I don't think this is any explanation at all.]

SUPER ADDITIVE ENTROPIES
DISCUSSION WITH RUDNICKI AND LOSKOT
11 NOVEMBER, 1988: KATOWICE

Their paper was rejected by J. lebowitz (Comm. Math. Phys.) since results had been previously obtained by Csiszar, I. (1967). "Information type measures of the differences of probability distributions and indirect observations", *Studia Sci. Math. Hungaria* **2**, 299-318.

ibid. "On topological properties of f divergences" pp 329-339.

Rudnicki and Loskot proved that for any concave function η

$$\lim_{n \rightarrow \infty} H_\eta(f_n|g_n) = \eta(1) \implies \lim_{n \rightarrow \infty} \|f_n - g_n\|_{L^1} = 0.$$

The converse can also be proved if \exists conditions on η . They say that

(1) η concave and continuous in R^+ ; and/or

(2) η is *strictly* concave at 1 which means that η can't be linear in a neighborhood of 1

are sufficient.

COARSE GRAINED ENTROPY—SOME THOUGHTS
12 NOVEMBER, 1988: KATOWICE

- (1) Though we know that for mixing systems $H_n^{CG}(P^t f|f_*) \rightarrow 0$ eventually, how many fluctuations can it have along the way. How severe can they be?
- (2) Perhaps the number and severity of the fluctuations in the entropy in its travels to 0 depend on n .
- (3) to address these two points it would be most interesting to examine the effects of changing the coarse graining index n on the evolution of the entropy of a model mixing system [start with the baker transformation of course]. (a). Could uniformly coarse grain throughout the phase space [i.e. CG with respect to x and y equally]; (b). Alternately could CG in either x or y .
- (4) If have a CG mixing system with initial entropy $H(f|f_*)$ and find, for example that

$$H(f|f_*) > H(Pf|f_*) > H(P^2 f|f_*)$$

and then

$$H(P^2 f|f_*) < H(P^3 f|f_*) < \dots < 0$$

then is this some crude example of the development and then aging and destruction (death) of a biological organism?

DISCUSSION WITH ANDY CONCERNING ENTROPY
12 NOVEMBER, 1988: KATOWICE

See background notes from Oxford, Fall, 1986!

Suppose we have a finite number (though large) of particles and we are able to continuously measure and plot the entropy of this collection.

Though the Poincaré recurrence time is of the order of

$$\tau_P \simeq \mathcal{O}(10^{10^{23}}),$$

if one was able to observe this system for a time t **many** order of magnitude larger than τ_P the graph of the entropy might look like

Andy says that if perturb the system to an entropy level $-c$, then \exists no reason to expect that the subsequent

entropy will increase or decrease as \exists bipolar possibilities for each such $-c$ if you can observe the system (universe) for an infinitely long time.

Question 1. Seems to me that if, at a time t you are at an entropy level of $h(t)$, then perturbing to a level of $-c$ you will get an unambiguous increase of decrease in H **depending on the state you were in at time t** , i.e. on the density $f(x, t)$.

AL's idea—which I don't understand.

Consider τ_P^{-1} as something of a probability of a fluctuation in entropy to increased values per unit time. Then he claims that, with probability

$$1 - \frac{1}{\tau_P}$$

if you change (perturb) the entropy to a value $-c$ then you will be at the minimum of a fluctuation!

The consequences of this are two fold and, if true, amazing.

- (1) Following a perturbation to a smaller entropy value, the subsequent entropy evolution will always appear to be increasing.
- (2) If the direction of time were suddenly reversed and entropy was the only indicator of the “arrow of time”, then one would be unable to detect this time reversal!

Question 2. How can this assertion be proved? Does it require any assumption(s) concerning the nature of the dynamics responsible for generating the evolution of the entropy? Can it possibly be independent of the dynamics?

19 NOVEMBER, 1991

QUANTUM MECHANICS AND HIDDEN VARIABLES

When I was a student, I was very disturbed by quantum mechanics. Even more disturbing to me was the fact that neither my professor nor the other students seemed to have any difficulty with it. I later learned that I was not alone.

Almost from its very inception, the formalism and interpretation of quantum mechanics spawned a number of attempts to find alternative formulations that had interpretations more in accord with the notions of reality that physicists were accustomed to from their study of macroscopic behaviour (see Jammer [1989, **The Conceptual Development of Quantum Mechanics**, AIP; and 1974, **The Philosophy of Quantum Mechanics**, Wiley] for an excellent account of the history of this subject). Some of these came wearing the clothes of so called “hidden variables” theories.¹ These are interesting because of their connection with the operation of taking a trace of a dynamical system, and because they illustrate that taking a trace of a reversible system may not automatically lead to entropy evolution as time changes.

A few years ago I happened to read two papers written by the physicist David Bohm [Physical Review (1952a,b), **85**, 166-193] that excited me because they provided a simple example of a hidden variables theory that was completely consistent with the predictions of quantum mechanics. In my opinion, the original work of Bohm is one of the most interesting of the existing hidden variables theories (there are many) because of its simplicity, and because it was the first widely known² clear counter example that led to the discovery of the inapplicability of the famous “proof” by von Neumann (1932) that hidden variable representations of quantum mechanics were impossible.

Following Bohm³, we consider the non-relativistic Schrödinger equation for a single particle with position x and mass m moving in a potential $V(x)$ (the argument carries through for many particle systems)

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi. \quad (1)$$

Bohm postulated that the wave function ψ is an objectively real quantity that is to be thought of as a field, satisfying a field equation (1) just like the electromagnetic field satisfies Maxwell's equations. Since ψ is generally complex, we let the amplitude of ψ be \sqrt{f} and its phase be \mathcal{S} (both f and \mathcal{S} are real quantities) so

$$\psi = \sqrt{f} e^{i\mathcal{S}/\hbar}, \quad (2)$$

¹To my knowledge, the most penetrating analysis of hidden variable theories is by Belinfante (1973), **A Survey of Hidden-Variables Theories**, Pergamon Press, Oxford.

²de Broglie's “pilot wave” hypothesis in his 1927 thesis is mathematically identical with Bohm's theory, though with differing interpretations on various points.

³Bohm's hidden variable theory is what Belinfante calls a hidden variable theory of the first kind, i.e., those in which deviations from the predictions of quantum mechanics will only occur in a non-equilibrium situation, whereas von Neumann's “proof” only applies to hidden variable theories of the zeroth kind.

with $\psi^* = \sqrt{f}e^{-i\mathcal{S}/\hbar}$ and $\psi\psi^* = f$.

It is a simple series of calculations to show that f and \mathcal{S} satisfy the pair of coupled partial differential equations

$$\frac{\partial f}{\partial t} + \nabla \cdot \left(f \frac{\nabla \mathcal{S}}{m} \right) = 0 \quad (3)$$

and

$$\frac{\partial \mathcal{S}}{\partial t} + \frac{(\nabla \mathcal{S})^2}{2m} + V(x) + V_Q(x, f) = 0, \quad (4)$$

where

$$V_Q = -\frac{\hbar^2}{2m} \frac{\nabla^2(\sqrt{f})}{\sqrt{f}}. \quad (5)$$

How should we interpret this rewriting of the Schrödinger equation? Bohm reasoned as follows. \mathcal{S} is the solution of equation (4), and in the “classical” limit of $\hbar \rightarrow 0$ this equation is precisely the Hamilton-Jacobi equation for a particle moving in a potential V . If one considers a large number of particles moving according to (4), then from classical mechanics $\nabla \mathcal{S}/m$ is the velocity $v(x)$ of a particle at the point x . When $\hbar \neq 0$, Bohm interpreted (4) as the Hamilton-Jacobi equation for a single particle moving in a combined potential consisting of the classical potential V plus a quantum potential V_Q given by (5).

Bohm took the classical results as a justification for identifying the velocity v with $\nabla \mathcal{S}$ through the relation

$$v = \frac{\nabla \mathcal{S}}{m}, \quad (6)$$

thereby explicitly assuming that even in a quantum mechanical situation particles are real objects (not manifestations of wave functions that collapse upon measurement) and we can attach objective meaning to both particle position x and the wave function ψ .

With (6), equations (3) and (4) can be rewritten in the form

$$\frac{\partial f}{\partial t} + \nabla \cdot (fv) = 0 \quad (7)$$

and

$$\frac{\partial \mathcal{S}}{\partial t} + \frac{1}{2}mv^2 + V(x) + V_Q(x, f) = 0. \quad (8)$$

Mathematically, $f = \psi\psi^*$ is a density since $f \geq 0$ and $\int \psi\psi^* dx = \int f dx = 1$. The fact that (7) is of the form of a classical conservation, or continuity, equation for the density, much like the Liouville equation, was used by Bohm to motivate his final major assumption that $f = \psi\psi^*$ is a physical probability density of an ensemble of particles. Precisely the same point of view was taken by Schrödinger [1978, **Wave Mechanics**, Chelsea Pub. Co., New York] in his original development of the Schrödinger equation.

It is worth noting here that if, in analogy with the classical situation, we set

$$\mathcal{H} = \frac{1}{2}mv^2 + V + V_Q \quad (9)$$

then (8) is equivalent to

$$\frac{\partial \mathcal{S}}{\partial t} = -\mathcal{H} \quad (10)$$

or to

$$\begin{aligned} \frac{dx}{dt} &= v = \frac{1}{m} \frac{\partial \mathcal{H}}{\partial v} \\ m \frac{dv}{dt} &= \frac{d}{dt} \nabla \mathcal{S} = -\nabla \mathcal{H}. \end{aligned} \quad (11)$$

Noting further that

$$\frac{d}{dt} \left(\frac{1}{2}mv^2 \right) = -v \cdot \nabla \mathcal{H} = -\frac{d}{dt} (V + V_Q),$$

we have

$$\mathcal{H} = \frac{1}{2}mv^2 + V + V_Q = \text{constant}, \quad (12)$$

so \mathcal{H} plays the role of a conserved energy for the system.

Equations (11) are clearly reversible (and even of Hamiltonian form), so from the results of Mackey [1991, **Time's Arrow: The Origins of Thermodynamic Behavior**, Springer-Verlag, New York], if we identify $f(t, x) = P^t f(x)$ then it is clear that the conditional entropy H_c satisfies

$$H_c(P^t f|f_*) \equiv H_c(f|f_*)$$

for all initial densities. That there is no entropy evolution in quantum systems described by the Schrödinger equation is well known, and has been proved by Wehrl [Reviews of Modern Physics (1978), **50**, 221-260] using different techniques.

It is perhaps unfortunate that Bohm's work has acquired the label of a hidden variable theory. Since he is attaching objective significance to both particle position and the wave function, what are the "hidden variables" in Bohm's reinterpretation of quantum mechanics? It seems that there are two. First, the Schrödinger equation only deals with particle position x as the velocity v does not enter. Secondly, and more importantly, is the appearance of the quantum potential V_Q in Bohm's interpretation. Since equations (7) and (8) differ from their classical counterparts only in the appearance of V_Q , any attempt to deduce quantum mechanics from some more comprehensive theory must explain the origin of the quantum potential. We will return to this point in Chapter 11 when we discuss Nelson's derivation of the Schrödinger equation.

The quantum potential V_Q is a strange bird for at least two reasons.

- (1) V_Q is quite different from any form of potential function we are accustomed to in classical physics because of its dependence on the probability density function $f(t, x)$ at all points in configuration space, and its lack of explicit diminution as the distance between a point and a particle increases. The former is the origin of the "nonlocal" nature of quantum mechanics, with its apparent conflict with relativistic theory, though Bohm and Hiley (1984) have argued that this conflict is more apparent than real.
- (2) The second peculiar aspect of the quantum potential V_Q arises through the way in which it depends on the probability density function u , viz.

$$V_Q \sim \frac{\nabla^2(\sqrt{f})}{\sqrt{f}}.$$

From this it is clear that the quantum potential at a particular point in space is independent of the magnitude of the probability density function at that point, depending only on the shape of f .

26 JANUARY, 1994

THE BOHR TREATMENT OF ATOMIC SPECTRA

These notes summarize the treatment followed by N. Bohr¹⁻⁴ in his explanation of the emission and absorption spectra of various elements. This work was later summarized by Bohr in yet a fifth paper⁵.

The impetus for Bohr's work was the observation, by 1913 quite well established, that the spectra of atomic hydrogen can be very accurately described by the formula

$$\bar{\nu} = R_\infty \left\{ \frac{1}{n'^2} - \frac{1}{n^2} \right\} \quad n' < n \quad \text{with both being positive integers}, \quad (1)$$

wherein $\bar{\nu}$ (in units of mt^{-1}) is the wavenumber [related to the frequency ν (sec^{-1}) by $\nu = c\bar{\nu}$, where c is the speed of light], and R_∞ is the *Rydberg constant* appropriate for hydrogen. When $n' = 1$, equation (1) describes the *Lyman* series in the ultraviolet region (discovered in 1906); for $n' = 2$ it describes the visible *Balmer* series first described in 1885; with $n' = 3$ one recovers a good description of the infrared *Paschen* series of 1908. $n' = 4$ corresponds to the 1922 *Brackett* series (also infrared); and $n' = 5$ gives the far infrared *Pfund* series.

¹N. Bohr, "On the constitution of atoms and molecules", Phil. Mag. (1913), **26**, 1-25.

²N. Bohr, "On the constitution of atoms and molecules: II. Systems containing only a single nucleus", Phil. Mag. (1913), **26**, 476-502.

³N. Bohr, "On the constitution of atoms and molecules: III. Systems containing several nuclei", Phil. Mag. (1913), **26**, 857-875.

⁴N. Bohr, "On the effect of electric and magnetic fields on spectral lines", Phil. Mag. (1914), **27**, 506-524.

⁵N. Bohr, "On the quantum theory of radiation and the structure of the atom", Phil. Mag. (1915) **30**, 394-415.

In trying to understand the phenomenology described by equation (1), Bohr used a mixture of classical physics, and what we now call the “old” quantum mechanics. Let us first examine the classical portion of his treatment.

For an electron-proton system, where the proton is fixed (infinitely massive) and the electron has finite mass m_e , from Newton’s laws $m_e a = F$, where a is the acceleration and F is the force, for circular motion we obtain

$$m_e \frac{v^2}{r} = \frac{|A|}{r^2}, \quad (2)$$

where r is the radius of the orbit, v is the electron velocity, and the constant A is given by

$$A = -\frac{e^2}{4\pi\epsilon_0} = -\frac{e^2 c^2}{10^7}. \quad (3)$$

(e is the electronic charge and c is the velocity of light.)

Since, in a circular orbit, $v = r\omega$, where ω is the angular frequency, equation (2) can also be written in form

$$m_e r \omega^2 = \frac{|A|}{r^2}, \quad (4)$$

If E is the total energy of the electron, then it is made up of the sum of the kinetic and potential energy:

$$E = E_{kin} + E_{pot} \quad (5)$$

where the kinetic energy is defined in a usual fashion

$$E_{kin} = \frac{1}{2} m_e v^2. \quad (6)$$

From the customary definition of the potential energy,

$$E_{pot} = -\int_r^\infty \frac{|A|}{r'} dr' = -\frac{|A|}{r}. \quad (7)$$

This potential energy corresponds to the work required to remove the electron from position r to ∞ , and the point at which the potential energy goes to zero must correspond to the ionization potential for the electron-proton pair. Thus, we can write the total energy of equation (4) as

$$E = \frac{1}{2} m_e v^2 + \frac{A}{2r} = \frac{1}{2} m_e v^2 - \frac{|A|}{2r} = \frac{A}{2r} = -\frac{|A|}{2r}, \quad (8)$$

where we have used (2) to arrive at the final result. Alternately, we can solve (4) for r :

$$r = \left(\frac{|A|}{m_e \omega^2} \right)^{\frac{1}{3}}, \quad (9)$$

to give

$$E = -\frac{|A|^{\frac{2}{3}}}{2} (m_e \omega^2)^{\frac{1}{3}}. \quad (10)$$

So far, the treatment is entirely classical, and equations (9) and (10) point out the inadequacy of any classical treatment to explain the spectral phenomena described by (1). Namely, from equation (9) in a classical situation all energies are allowed as well as all radii. However, since the electron is moving in a circular orbit, it is under constant acceleration, and consequently should be radiating electromagnetic waves at a frequency equivalent to its orbital frequency, i.e.

$$\nu = \frac{\omega}{2\pi}. \quad (11)$$

Consequently the electron should lose energy in a continuous fashion and eventually spiral into the nucleus. All of this is quite elementary, and simply a summary of the well known classical paradox with respect to the observed discrete spectrum of radiation described by equation (1).

Faced with this impasse from classical theory, Bohr made the following postulates:

- (1) Although the classical equations of motion (as sketched out above for circular orbits) are valid for an electron in an atom, only certain orbits (denoted by the index $n = 1, 2, \dots$) are allowed, and in these orbits the electron has a fixed binding energy E_n .
- (2) In these allowed orbits (which can be thought of as corresponding to *stationary states*) there is no emission of radiation even though this would be expected on the basis of classical electromagnetic theory.
- (3) An electron going from a stationary state of binding energy E_n (remember that on a classical basis that the binding energy is negative) at radius r_n to a second stationary state with a binding energy $E_{n'} < E_n$ at a smaller radius $r_{n'}$ will radiate electromagnetic waves at a frequency ν proportional to the difference in the binding energies in the two orbits.

$$E_n - E_{n'} \propto \nu.$$

Bohr assumed the constant of proportionality is Planck's constant h :

$$E_n - E_{n'} = h\nu = hc\bar{\nu}. \quad (12)$$

The adsorption of energy would be described by the reverse process. Through a comparison of equations (1) and (12), Bohr then concluded that the energies in the stationary states must have the form

$$E_n = -\frac{R_\infty hc}{n^2}. \quad (13)$$

- (4) Things in the Bohr papers now become a bit clouded, but the fourth postulate essentially utilizes a primitive form of what he later enunciated as the *correspondence principle*. Bohr argued that in the situation that we are observing a transition from a state $n - \delta$ to n , and n is large relative to δ , we should identify ν with the classical orbital frequency $\omega/2\pi$. In such a circumstance, from equation (1) and the relation between wavenumber and frequency we have

$$\begin{aligned} \nu &= R_\infty c \left[\frac{1}{(n - \delta)^2} - \frac{1}{n^2} \right] \\ &= \frac{R_\infty c}{n^2} \left[\frac{1}{[1 - \delta/n]^2} - 1 \right] \\ &\simeq \frac{2R_\infty c\delta}{n^3}. \end{aligned} \quad (14)$$

Thus, in going from the $n - 1$ to n level with n large, we have that

$$\nu \simeq \frac{2R_\infty c}{n^3}. \quad (15)$$

Now setting $\omega = 2\pi\nu$, with ν given by (15), in equation (10), along with equation (13), we immediately obtain an expression for the Rydberg constant, namely

$$R_\infty = \frac{m_e e^4}{8\epsilon_0^2 h^3 c}. \quad (16)$$

Equation (16) was Bohr's main result, and with the value of h estimated from black body radiation and experiments on the photoelectric effect, and the other constants, he was able to obtain a numerical value for the Rydberg constant consistent with spectroscopic measurements.

With these relations, we can put some more flesh on the character of these stationary orbits assumed by Bohr. From equation (13) we can write the energy of the n^{th} stationary state as

$$E_n = -\frac{|A|}{2r_n}, \quad (17)$$

or

$$\boxed{E_n = \frac{E_1}{n^2}} \quad (18)$$

wherein

$$E_1 = -\frac{m_e |A|^2}{2 \hbar^2}, \quad (19)$$

and we use the now customary notation $\hbar = h/2\pi$. Using the expression for the energy in equation (8) we can solve for r_n to give

$$r_n = \frac{n^2 \hbar^2}{m_e |A|}, \quad (20)$$

or

$$\boxed{r_n = n^2 r_1} \quad (21)$$

with

$$r_1 = \frac{\hbar^2}{m_e |A|}. \quad (22)$$

Equation (4) now yields

$$\begin{aligned} \omega_n &= \left(\frac{n\hbar}{m_e} \right) \left(\frac{m_e |A|}{n^2 \hbar^2} \right)^2 \\ &= m_e \frac{|A|^2}{(n\hbar)^3}, \end{aligned} \quad (23)$$

or

$$\boxed{\omega_n = \frac{\omega_1}{n^3}} \quad (24)$$

where

$$\omega_1 = m_e \frac{|A|^2}{\hbar^3}. \quad (25)$$

Since the period T_n is just $T_n = 1/f_n$ and $f_n = 2\pi\omega_n$ it is immediate from (24) that

$$\boxed{T_n = n^3 T_1}, \quad (26)$$

with $T_1 = 1/2\pi\omega_1$. The time required for the propagation of effects from electron to proton (the *delay*) is just $\tau = r/c$, so from the above relations we find

$$\tau_n = \frac{n^2 \hbar^2}{m_e c |A|} \quad (27)$$

or more simply

$$\boxed{\tau_n = n^2 \tau_1}, \quad (28)$$

with

$$\tau_1 = \frac{\hbar^2}{m_e c |A|}. \quad (29)$$

From equation (2) in conjunction with (21), we may write v_n as

$$v_n = \frac{|A|}{n\hbar}, \quad (30)$$

or

$$\boxed{v_n = \frac{v_1}{n}} \quad (31)$$

with

$$v_1 = \frac{|A|}{\hbar}. \quad (32)$$

In a circular orbit, the angular momentum is

$$p = m_e v r,$$

which means that

$$m_e v_n r_n = n \hbar \quad (33)$$

so as a consequence of this entire treatment the angular momentum also ends up being quantized. Many authors incorrectly present the Bohr treatment as if quantized angular momentum was one of his postulates, but this is not the case.

Having all of these relations, its instructive to see what the numbers really look like. Taking the best available modern determinations we use (unless otherwise noted, these values are taken from⁶):

- (1) speed of light $c = 2.99792458 \times 10^8 \text{ ms}^{-1}$;
- (2) $\epsilon_0 = 10^7/4\pi c^2 \text{ Fm}^{-1}$;
- (3) electronic charge $e = 1.60217733 \times 10^{-19} \text{ C}$
or⁷
 $e = 1.60217670 \times 10^{-19} \text{ C}$;
- (4) electron mass $m_e = 9.1093897 \times 10^{-31} \text{ kg}$;
- (5) $h = 6.6260755 \times 10^{-34} \text{ Js} \implies \hbar = 1.054573 \times 10^{-34} \text{ Js}$
or⁷
 $h = 6.6260704 \times 10^{-34} \text{ Js} \implies \hbar = 1.054572 \times 10^{-34} \text{ Js}$;
- (6) $R_\infty = 1.0973731534 \times 10^7 \text{ m}^{-1}$
or⁸
 $R_\infty = 1.097373156830 \times 10^7 \text{ m}^{-1}$
or⁹
 $R_\infty = 1.097373156841 \times 10^7 \text{ m}^{-1}$

we first find that **calculating** h from equation (16) using the CODATA⁶ values, especially for R_∞ , that the precise value quoted in the CODATA figures results. Namely,

$$h = 6.6260755 \times 10^{-34} \text{ Js},$$

which is a bit suspicious since in the CODATA report they make no mention of how their best figure for h was arrived at. Going further we rather easily find, using the 1986 CODATA values, that

- (1) Energy in the first Bohr orbit is $E_1 = -2.1798741 \times 10^{-18} \text{ J}$;
- (2) Radius in the first Bohr orbit is $r_1 = 5.29177249 \times 10^{-11} \text{ m}$;
- (3) Angular frequency in the first Bohr orbit is $\omega_1 = 4.13413732 \times 10^{16} \text{ s}^{-1}$;
- (4) Period in the first Bohr orbit is $T_1 = 1.51982989 \times 10^{-16} \text{ s}$;
- (5) Delay to the first Bohr orbit is $\tau_1 = 1.7651453 \times 10^{-19} \text{ s}$;
- (6) Velocity in the first Bohr orbit is $v_1 = 2.18769141 \times 10^6 \text{ ms}^{-1}$;
- (7) Frequency in the first Bohr orbit is $f_1 = 6.57968374 \times 10^{15} \text{ sec}^{-1}$;
- (8) Ratio of the period to the delay in the first Bohr orbit is

$$\frac{T_1}{\tau_1} = 2\pi \times 137.03590744504,$$

where $137. \dots$ is the “fine structure constant”. This last relation can be written in the alternate form

$$\frac{1}{\omega_1 \tau_1} = 137.03590744504.$$

Interestingly, this is not the same value as given in the CODATA report⁶, namely

$$\alpha^{-1} = 137.0359895,$$

nor does it match the recent value⁷ determined from measurements on the quantized Hall effect and the Josephson junction carried out at the NBS:

$$\alpha^{-1} = 137.0359940.$$

⁶E.R. Cohen & B.N. Taylor, “The 1986 adjustment of the fundamental physical constants”, Rev. Mod. Phys. (1987) **59**, 1121-1148.

⁷M.E. Cage, R.F. Dziuba, R.E. Elmquist, B.F. Field, G.R. Jones, P.T. Olsen, W.D. Phillips, J.Q. Shields, R.L. Steiner, B.N Taylor & E.R. Williams, “NBS determination of the fine-structure constant and of the quantized Hall resistance and Josephson frequency to voltage quotient in SI units”, IEEE Trans. Instru. Meas. (1989), **38**, 284-289.

⁸F. Nez, M.D. Plummer, S. Bourzeix, L. Julien, F. Biraben, R. Felder, O. Acef, J.J. Aondy, P. Laurent, A. Clairon & M. Abed, “Precise frequency measurement of the 2S–8S/8D transitions in atomic hydrogen: New determination of the Rydberg constant”, Phys. Rev. Lett. (1992) **69**, 2326-2329.

⁹T. Andreae, W. König, R. Wynands, D. Leibfried, F. Schmidt-Kaler, C. Zimmerman & D. Meschede, “Absolute frequency measurement of the hydrogen 1S–2S transition and a new value of the Rydberg constant”, Phys. Rev. Lett. (1992) **69**, 1923-1926.

A simpler route to the Bohr results.

It is interesting that a much simpler and more transparent way is available to derive the essence of the Bohr results. It is the following.

First, we have equation (4), which I repeat for ease of exposition:

$$m_e r \omega^2 = \frac{|A|}{r^2}. \quad (4)$$

Furthermore, for circular planar motion the angular momentum of the electron is constant, so

$$m_e \omega r^2 = C, \quad (34)$$

where C is an unknown quantity to be determined. Solving (4) and (34) for the pair (r, ω) gives

$$r = \frac{C^2}{m_e |A|} \quad (35)$$

and

$$\omega = \frac{m_e |A|^2}{C^3} \quad (36)$$

respectively. If we also adopt the Bohr approximation derived from the Rydberg equation:

$$\nu \simeq \frac{2R_\infty c \delta}{n^3}, \quad (14)$$

and assume

$$\omega = 2\pi\nu \simeq \frac{4\pi R_\infty c \delta}{n^3}, \quad (37)$$

then in conjunction with (36) we have after a bit of algebra the result

$$\left(\frac{2\pi C}{n}\right)^3 = \frac{m_e e^4}{8R_\infty \epsilon_0^2}. \quad (38)$$

The right hand side of equation (38) is numerically equal to the value of the Planck constant raised to the third power:

$$\left(\frac{2\pi C}{n}\right)^3 = \frac{m_e e^4}{8R_\infty \epsilon_0^2} = h^3. \quad (39)$$

Consequently, we must have

$$C_n = n \frac{h}{2\pi} = n\hbar, \quad (40)$$

so

$$r_n = \frac{n^2 \hbar^2}{m_e |A|} \quad (41)$$

and

$$\omega_n = \frac{m_e |A|^2}{n^3 \hbar^3} \quad (42)$$

respectively.

Finally, we note that from equation (7), we can write

$$E_n = -\frac{m_e A^2}{2n^2 \hbar^2}, \quad (43)$$

so

$$E_n - E_m = \frac{m_e A^2}{2\hbar^2} \left[\frac{1}{m^2} - \frac{1}{n^2} \right] = \hbar R_\infty c = \left[\frac{1}{m^2} - \frac{1}{n^2} \right] = \hbar R_\infty c = \hbar\nu. \quad (44)$$

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COLLAPSE OF THE WAVE FUNCTION

In the Copenhagen interpretation of QM, as enunciated by Bohr, one of the major issues is the so called measurement problem. In this, it is stated that once any measurement is made on a QM system then the associated wave function "collapses" to a delta function. Lets examine this proposition via an analogy.

Consider a dynamical system (or SDS) T , and the associated evolution of densities f via the FP operator. Assume that T is such that we at least have a stationary density f_* . Now, if we were to make a measurement of the position (or whatever variable is evolving under the action of T) at a given time can we assert that the stationary density f_* collapses at the instant of measurement? Of course not— f_* is an independent entity as associated with the evolution of an ensemble, and the existence or not of f_* is completely independent of any measurements that we make on the system.

I think that through this analogy we can immediately see the foolishness of this notion that the wave function collapses.