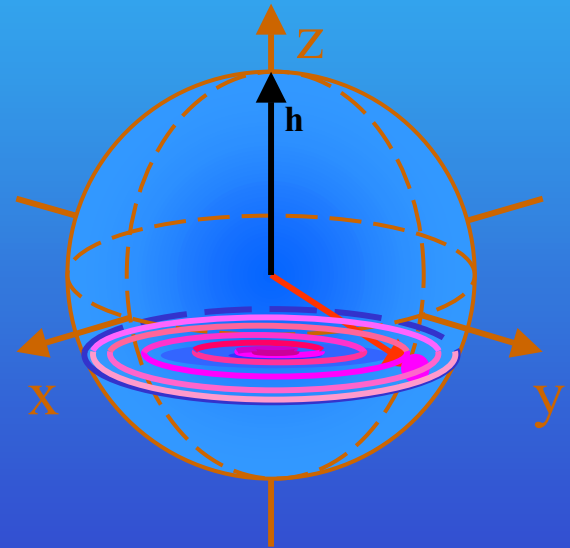
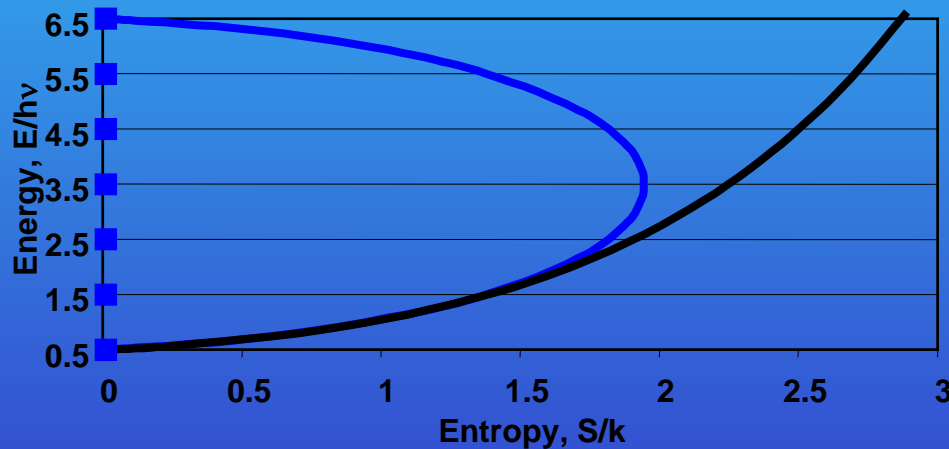


Mechanics and **Thermodynamics** fundamentally **united** by
density operators with an **ontic status** obeying a locally
maximum entropy production dynamics. But at what price?

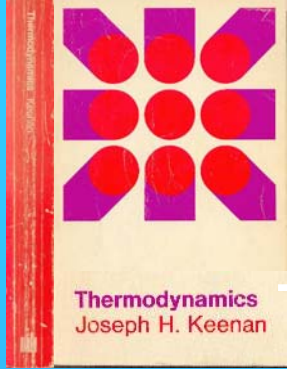
Gian Paolo Beretta
Università di Brescia, Italy



G.P. Beretta, **PIAF '09 "New Perspectives on the Quantum State"**, Perimeter Institute, Sept.27-Oct.2, 2009

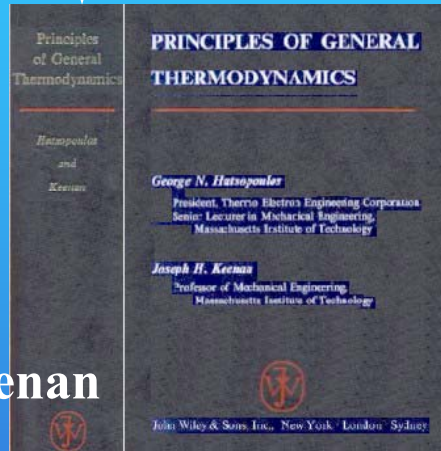
References available at: www.quantumthermodynamics.org

The Keenan school of Thermodynamics from engineering, to physics, to mathematical-physics, and back!



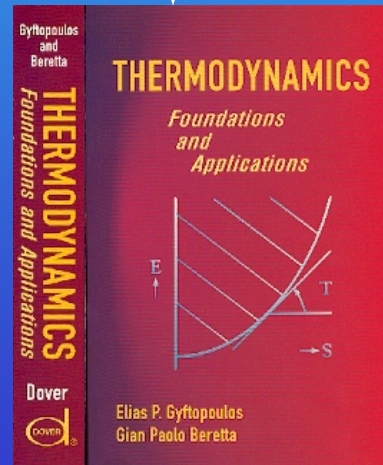
Keenan

MIT press 1941



Hatsopoulos-Keenan

Wiley 1965



Gyftopoulos-Beretta

Macmillan 1991

(Dover 2005)

Recent Symposium
AIP 2008



G.P. Beretta, **PIAF '09 "New Perspectives on the Quantum State"**, Perimeter Institute, Sept.27-Oct.2, 2009

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Outline

- 1) Concept of individual state and an unambiguous representation of preparations, not based on the (von Neumann) density operator
- 2) An ansatz (1976) allows to embed Thermodynamics into Quantum Theory
 - Ontic status of density operators and microscopic entropy
- 3) Geometrical construction (1981) of a 'maximal entropy generation' dynamics
 - Ontic and microscopic status to the second law and to irreversibility
- 4) The price to pay, due to nonlinearity of the dynamical law



Part I

- 1) Concept of individual state and an unambiguous representation of preparations, not based on the (von Neumann) density operator
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Part I

- 1) Concept of individual state and an unambiguous representation of preparations, not based on the (von Neumann) density operator

In 1970's language:

On the distinction between quantal and nonquantal uncertainties...

In today's language:

On the operational/instrumental distinction between ontic and epistemic probabilities...

In 1930's language:

On the unambiguous mathematical representation of measurement statistics from homogeneous and heterogeneous ensembles

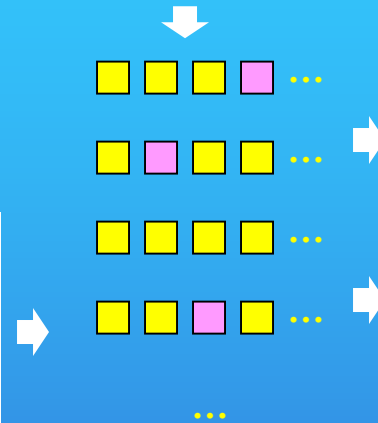


“Tomography” of a preparation (or ensemble) at time t

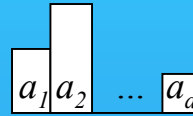
Park and Band, FoundPhys,
1, 133 (1970); 1, 211 (1971);
1, 339 (1971)

Ensemble \mathcal{E}_Π
of identical systems all
prepared by Π at time t

Statistics of
measurement outcomes
(all at time t)

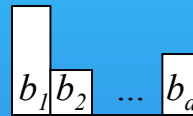


Measurement
procedure A



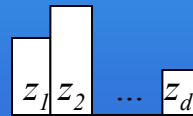
$$p_{a_j} = \langle Q_{a_j} \rangle = \lim_{N_A \rightarrow \infty} N_{a_j} / N_A$$

Measurement
procedure B



$$p_{b_j} = \langle Q_{b_j} \rangle = \lim_{N_B \rightarrow \infty} N_{b_j} / N_B$$

Measurement
procedure Z



$$p_{z_j} = \langle Q_{z_j} \rangle = \lim_{N_Z \rightarrow \infty} N_{z_j} / N_Z$$

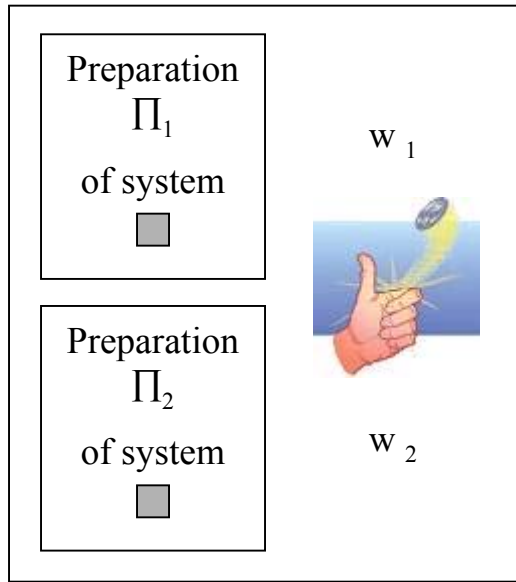
If A, B, \dots, Z are all the *conceivable* measurements, then preparation Π (and hence ensemble \mathcal{E}_Π) is completely characterized (at time t) by the set of numbers (*tomography* at time t):

$$\langle \Pi \rangle = \langle \mathcal{E}_\Pi \rangle = \{p_{a_1}, \dots, p_{a_d}, p_{b_1}, \dots, p_{b_d}, \dots, p_{z_1}, \dots, p_{z_d}\}$$



Statistical mixing of preparations (or ensembles)

Preparation Π



For any observable A , the mean (at time t) is

$$\langle A \rangle_{\Pi} = w_1 \langle A \rangle_{\Pi_1} + w_2 \langle A \rangle_{\Pi_2}$$

and, therefore, the tomography is

$$\langle \Pi \rangle = w_1 \langle \Pi_1 \rangle + w_2 \langle \Pi_2 \rangle$$

Homogeneous vs Heterogeneous preparations (or ensembles)

Given a preparation Π , we may look for *all conceivable decompositions*. A preparation is *homogeneous* (von Neumann), denoted Π^o , iff there is no conceivable way to obtain the same tomography from a nontrivial statistical mixture of two *different* preparations (different means *with different tomography*), i.e.,

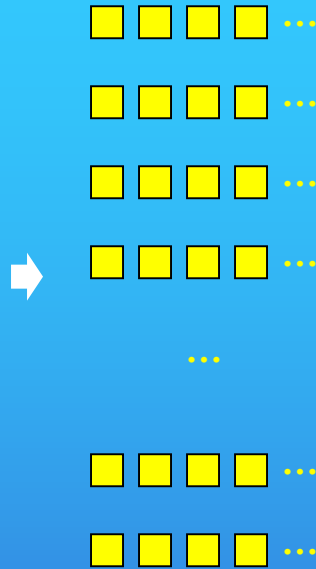
iff $\langle \Pi \rangle = w_1 \langle \Pi_1 \rangle + w_2 \langle \Pi_2 \rangle$ with $w_1, w_2 > 0$ implies $\langle \Pi_1 \rangle = \langle \Pi_2 \rangle$



Homogeneous preparations (or ensembles) and “states”


Von Neumann, book, engl.transl.1932

Preparation
 Π^o
of system



For a homogeneous preparation, Π^o , no subdivision into different subensembles is conceivable.

Therefore, its tomography $\langle \Pi^o \rangle$ at time t can be safely viewed as an intrinsic individual feature of each and every member of the ensemble: *the “ontic” individual state.*

Each system “is in state” 

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J.L. Park, AmJPhys., 36, 211 (1968) - "Nature of quantum states"

Preparation
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...



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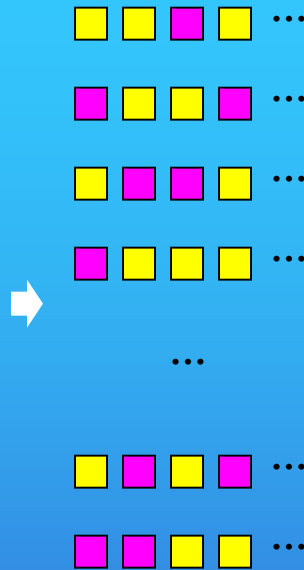
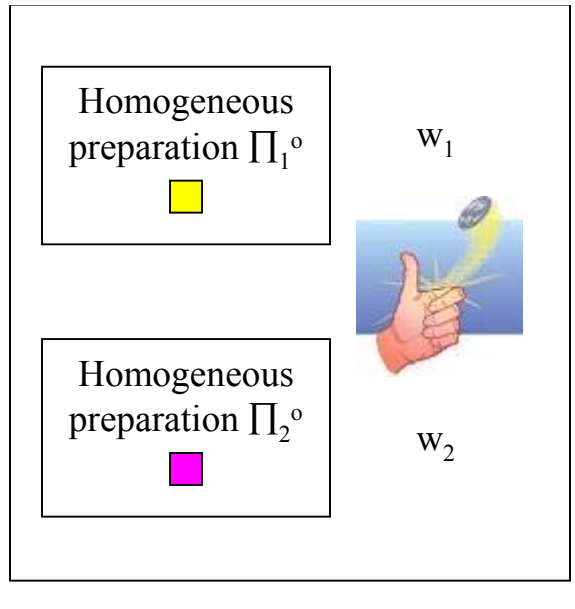
Each system “is in state” 

However, this view is unambiguous only if (the tomography of) every heterogeneous preparation (ensemble) admits a **unique decomposition** into homogeneous components. Otherwise:

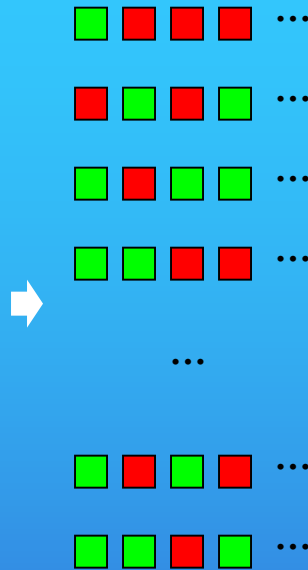
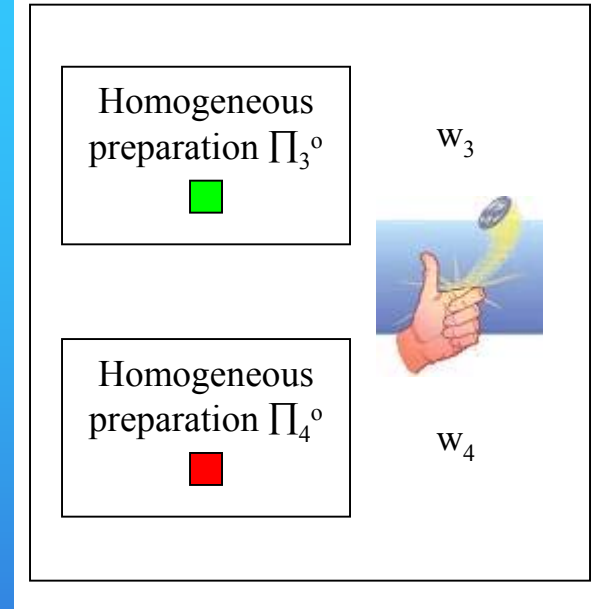


Homogeneous preparations (or ensembles) and “states”

$$\langle \Pi \rangle = w_1 \langle \Pi_1^o \rangle + w_2 \langle \Pi_2^o \rangle$$



$$\langle \Pi \rangle = w_3 \langle \Pi_3^o \rangle + w_4 \langle \Pi_4^o \rangle$$



“State is either  or  ”

Contradiction !

“State is either  or  ”

Schrödinger, PCPS, 32, 446 (1936)

quant-ph/0509116

Park&Band, FoundPhys, 6, 157 (1976)

ModPhysLettA, 21, 2799 (2006)

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Conditions for a mathematical representation compatible with the notion of individual state

For a theory to be compatible with the notion of individual state of a system, it must represent preparations, i.e., their tomography, by elements $\{\mu\}$ of a set such that:

- to **every preparation** Π and each instant of time t there corresponds a **unique element** $\mu(t)$ which determines its tomography at time t , i.e.,

$$\langle \Pi \rangle_t = f[\mu(t)]$$

with f an invertible (multivalued) functional;

- if preparation Π is the **statistical composition** (with weights w_1, w_2) of two preparations Π_1, Π_2 then

$$f(\mu) = w_1 f(\mu_1) + w_2 f(\mu_2) ;$$

- to **every homogeneous preparation** Π^o there corresponds a **unique indecomposable element** μ^o which admits no nontrivial weighted decomposition into different elements, i.e., such that $f(\mu^o) = w f(\mu_1) + (1 - w) f(\mu_2)$ with $0 < w < 1$ implies $\mu_1 = \mu_2 = \mu^o$;

PhD Thesis (1981), quant-ph/0509116

- every element μ admits a **unique decomposition into a weighted sum of indecomposable elements**, i.e., if the set is discrete

$$f(\mu) = \sum_j w_j(\mu) f(\mu_j^o) \quad \sum_j w_j = 1, w_j \geq 0 \quad (1)$$

or, if the set is continuous,

$$f(\mu) = \int_{\mathcal{P}} w(\mu, \alpha) f(\mu_\alpha^o) d\alpha \quad \int_{\mathcal{P}} w(\mu, \alpha) d\alpha = 1$$

where α denotes a set of continuous parameters which over the range \mathcal{P} span all the homogeneous preparations μ_α^o , and $w(\mu, \alpha)$ is some epistemic **probability density distribution** over this set with respect to the uniform measure.



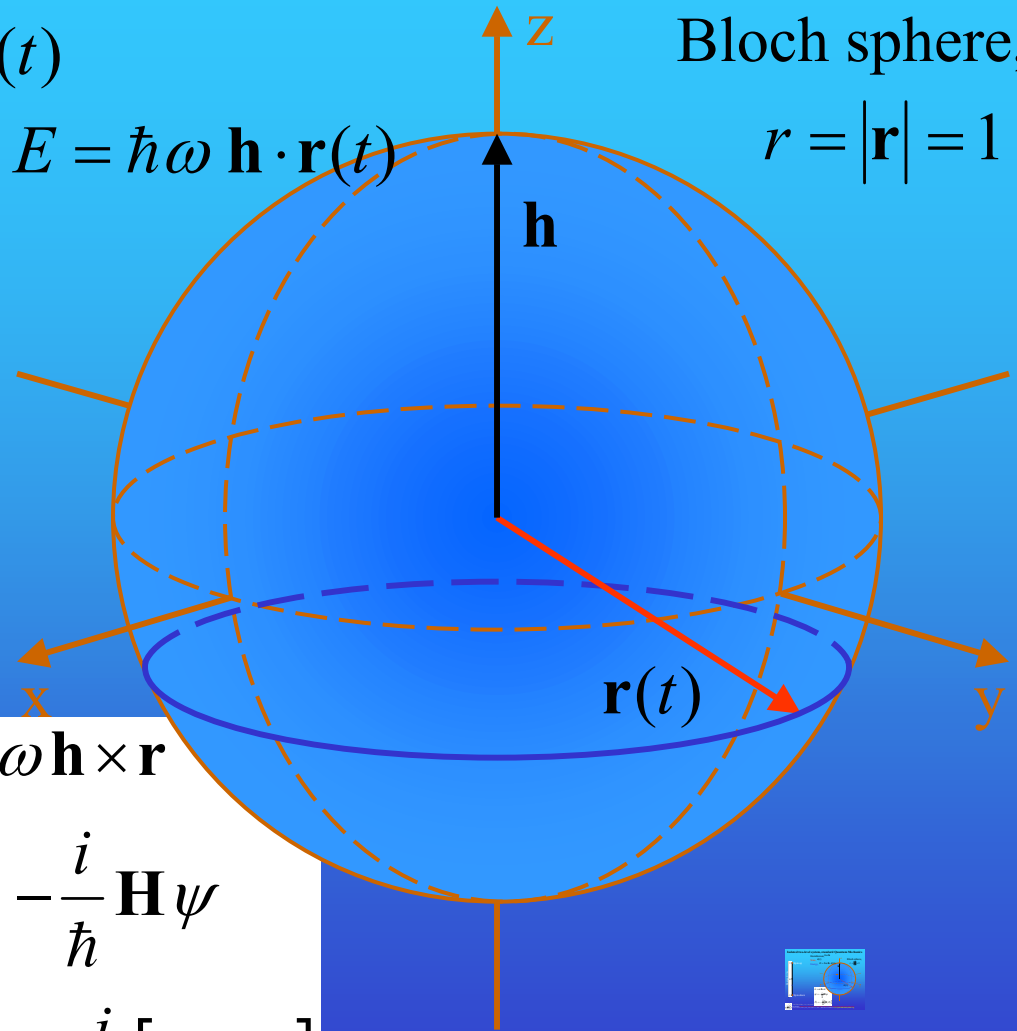
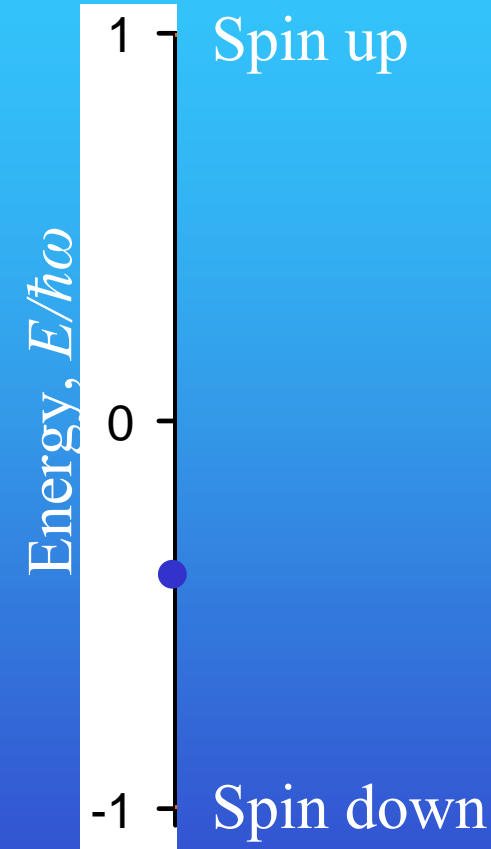
Isolated and uncorrelated 2-level particle

Hamiltonian, $\hbar\omega \mathbf{h}$

State, $\mathbf{r}(t)$

Energy, $E = \hbar\omega \mathbf{h} \cdot \mathbf{r}(t)$

Bloch sphere, $r = |\mathbf{r}| = 1$



$$\dot{\mathbf{r}} = \omega \mathbf{h} \times \mathbf{r}$$

$$\dot{\psi} = -\frac{i}{\hbar} \mathbf{H} \psi$$

$$\dot{P}_{\psi} = -\frac{i}{\hbar} [\mathbf{H}, P_{\psi}]$$



The von Neumann representation of heterogeneous preparations via density operators is incompatible with the notion of individual state

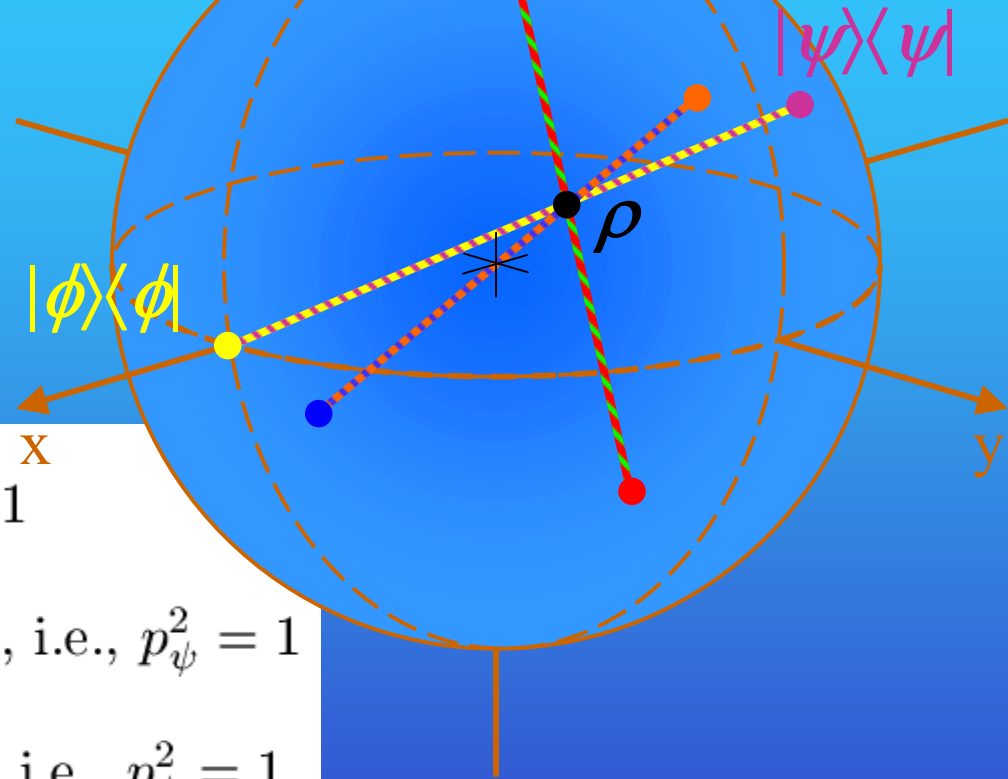
Schrödinger, PCPS, 32, 446 (1936)

ParkBand-FoundPhys-6-157-1976

many others later

quant-ph/0509116

ModPhysLettA-21-2799-2006



$$\rho = \frac{1}{2}(I + \underline{r}_\rho \cdot \underline{\sigma}) \quad \text{mixed if } r_\rho^2 < 1$$

$$P_\psi = |\psi\rangle\langle\psi| = \frac{1}{2}(I + \underline{p}_\psi \cdot \underline{\sigma}) \quad \text{pure, i.e., } p_\psi^2 = 1$$

$$P_\phi = |\phi\rangle\langle\phi| = \frac{1}{2}(I + \underline{p}_\phi \cdot \underline{\sigma}) \quad \text{pure, i.e., } p_\phi^2 = 1$$

$$\rho = w_\psi P_\psi + w_\phi P_\phi \quad \text{i.e., } \underline{r}_\rho = w_\psi \underline{p}_\psi + w_\phi \underline{p}_\phi$$



A representation of heterogeneous preparations via probability density distributions over the set of possible ontic states

Representation of a generic preparation

$$w(\mu, \alpha) \quad \text{with} \quad \int_{\mathcal{P}} w(\mu, \alpha) d\alpha = 1$$

for a qubit, $\alpha = \theta, \phi$ (spherical coordinates on the Bloch sphere):

$$\alpha \Rightarrow |\psi_\alpha\rangle\langle\psi_\alpha| \quad |\psi\rangle \Rightarrow \alpha_{|\psi\rangle}$$

Representation of a **homogeneous preparation**

$$w(\mu_{|\psi\rangle}^o, \alpha) = \delta(\alpha - \alpha_{|\psi\rangle})$$

Notice: only for **linear observables**,

$$f_L(\mu_{|\psi\rangle}^o) = \text{Tr}(L|\psi\rangle\langle\psi|)$$

$$\begin{aligned} f_L(\mu) &= \int_{\mathcal{P}} w(\mu, \alpha) f_L(\mu_\alpha^o) d\alpha \\ &= \int_{\mathcal{P}} w(\mu, \alpha) \text{Tr}(L|\psi_\alpha\rangle\langle\psi_\alpha|) d\alpha \\ &= \text{Tr} \left(L \int_{\mathcal{P}} w(\mu, \alpha) |\psi_\alpha\rangle\langle\psi_\alpha| d\alpha \right) \\ &= \text{Tr}(LW) \quad \text{with} \quad W = \int_{\mathcal{P}} w(\mu, \alpha) |\psi_\alpha\rangle\langle\psi_\alpha| d\alpha \end{aligned}$$

So, we see that knowing W fixes the linear observables, but **the linear observables are insufficient** to determine the preparation $w(\mu, \alpha)$.



Is this a fundamental indication (theorem) there must exist some measurable observables which need to be represented by **nonlinear** functionals of $|\psi\rangle\langle\psi|$?

Part II

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The need to represent some measurable observables by nonlinear functionals comes from thermodynamics (at least in our engineering "very ontic" view!)

- Adiabatic availability of nonequilibrium states
- Entropy
- Spontaneous relaxation towards equilibrium



A physical ansatz (departs drastically from Stat.Mech.) sufficient to **unite Mechanics and Thermodynamics**

- The density matrix ρ , even if non-pure, represents a real ontological object, the actual state of the world (system, single particle, even if unentangled).
- ρ is **not** understood as needed to represent an epistemic ignorance of which particular pure state the world is 'really' in. The 'real' state is ρ .
- The ontic status attributed to the density matrix also legitimates treating the entropy $-\mathbf{k}_B \text{Tr } \rho \ln \rho$ as an ontic physical quantity, like energy or mass.
- $-\mathbf{k}_B \text{Tr } \rho \ln \rho$ is **not** understood as measuring how broad is an epistemic probability distribution.

GN Hatsopoulos and
EP Gyftopoulos,
Found.Phys., Vol. 6,
15, 127, 439, 561 (1976)



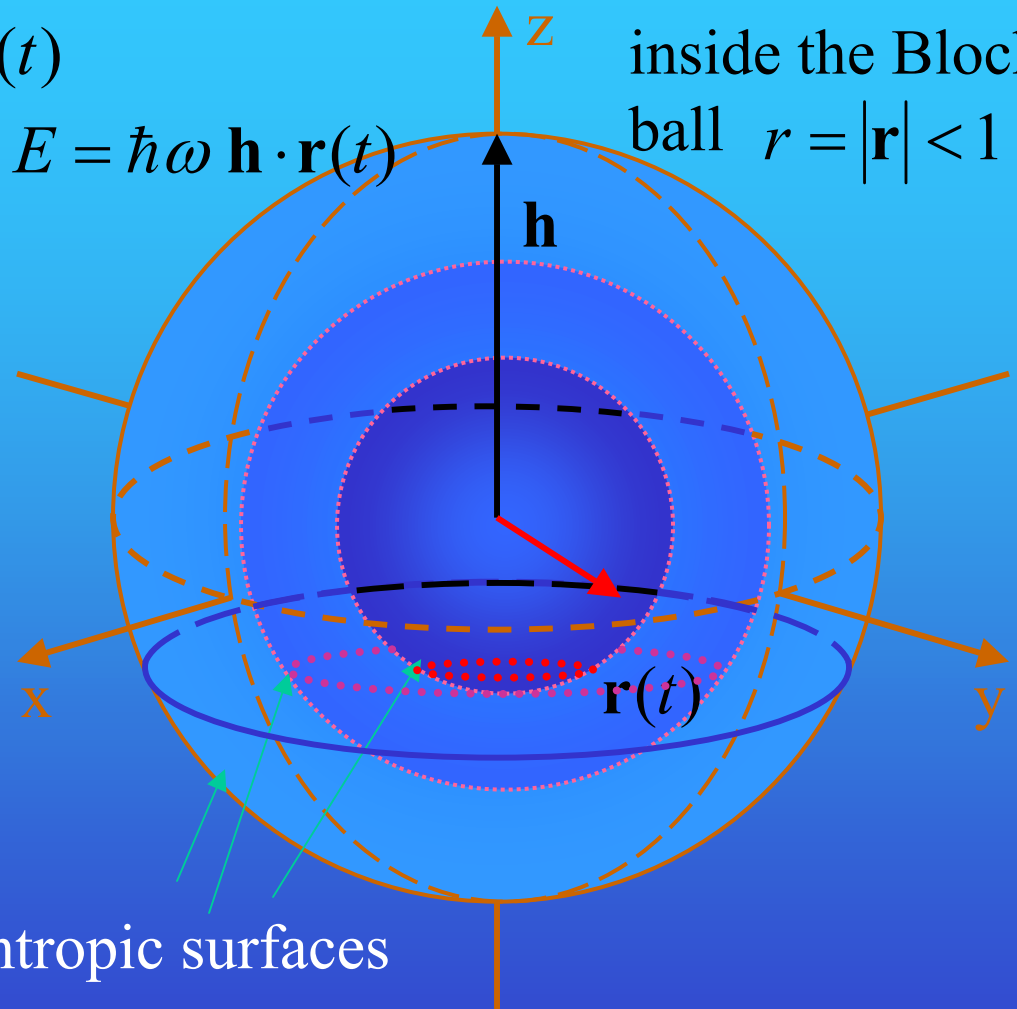
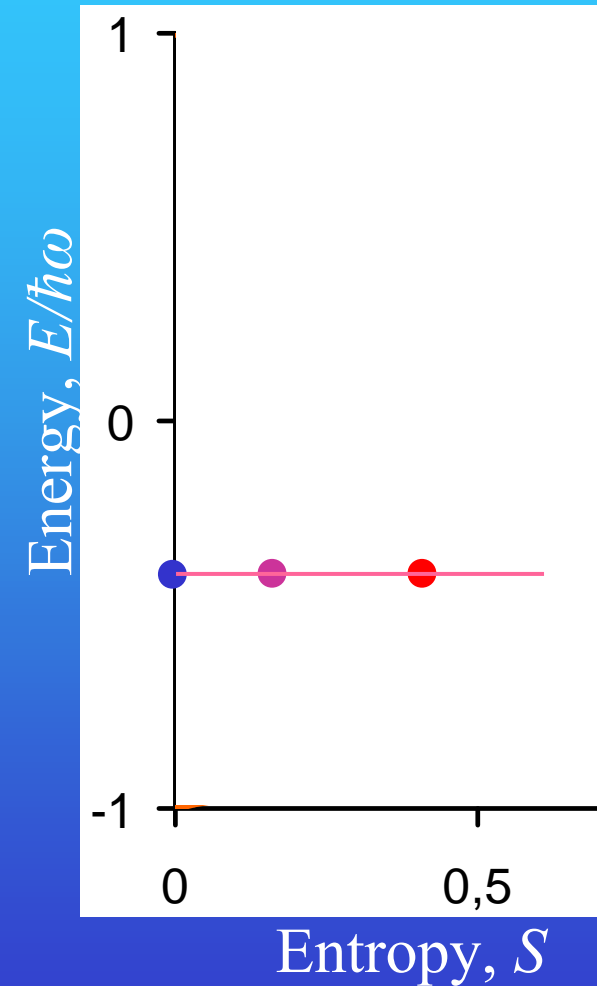
Isolated and uncorrelated 2-level particle

Hamiltonian, $\hbar\omega \mathbf{h}$

State, $\mathbf{r}(t)$

Energy, $E = \hbar\omega \mathbf{h} \cdot \mathbf{r}(t)$

Ontic states also
inside the Bloch
ball $r = |\mathbf{r}| < 1$



Isoentropic surfaces

$$S = -k_B \left(\frac{1+r}{2} \ln \frac{1+r}{2} + \frac{1-r}{2} \ln \frac{1-r}{2} \right)$$



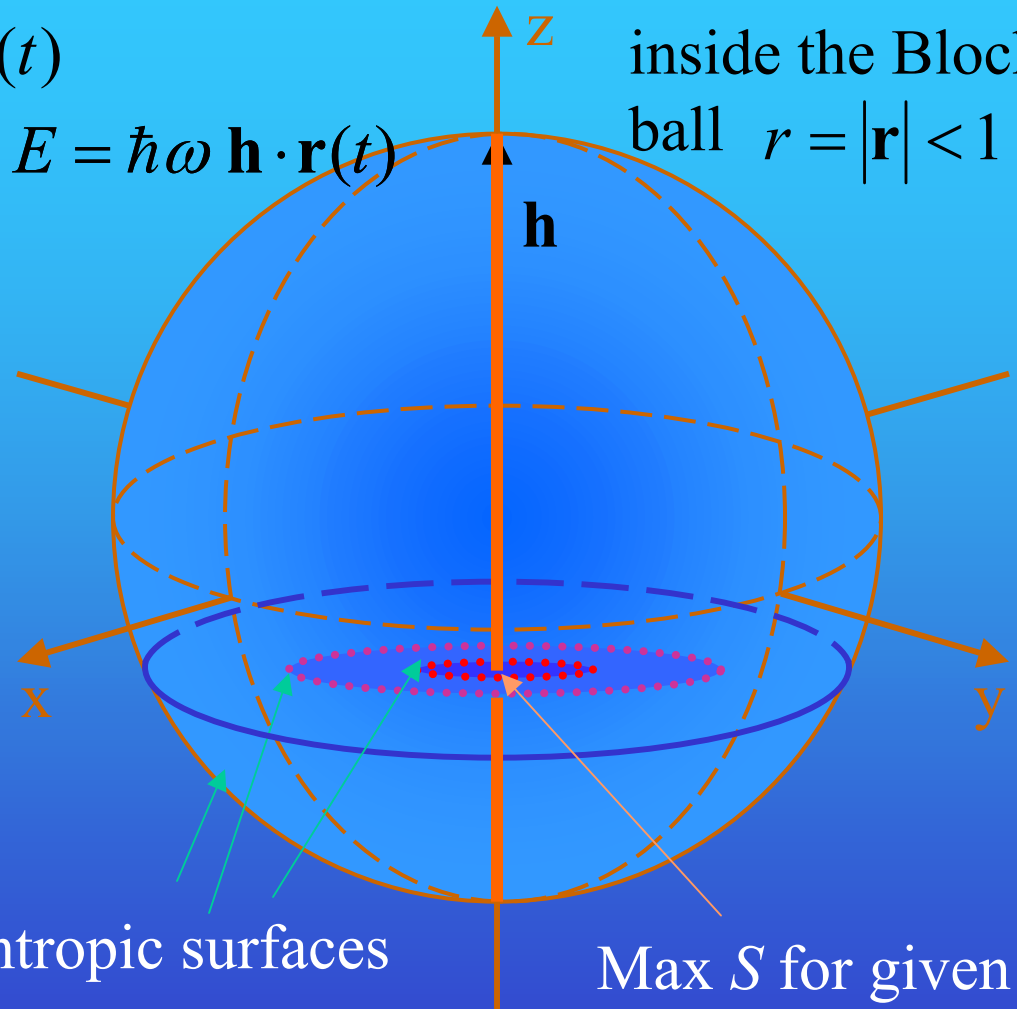
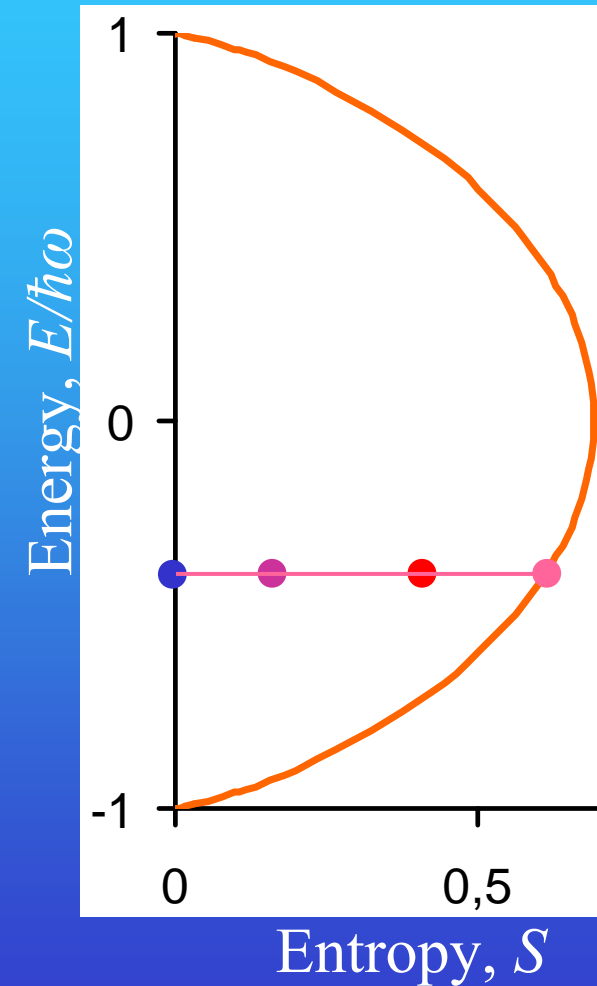
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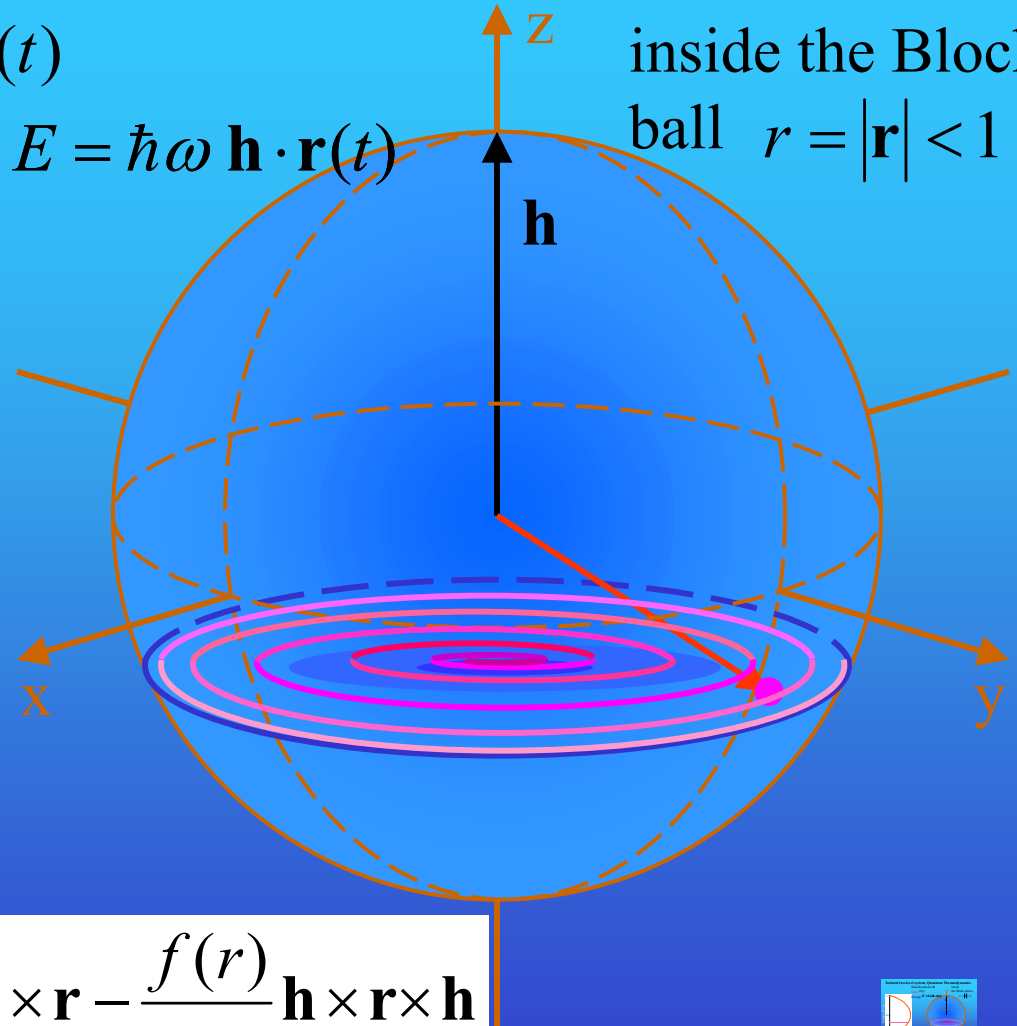
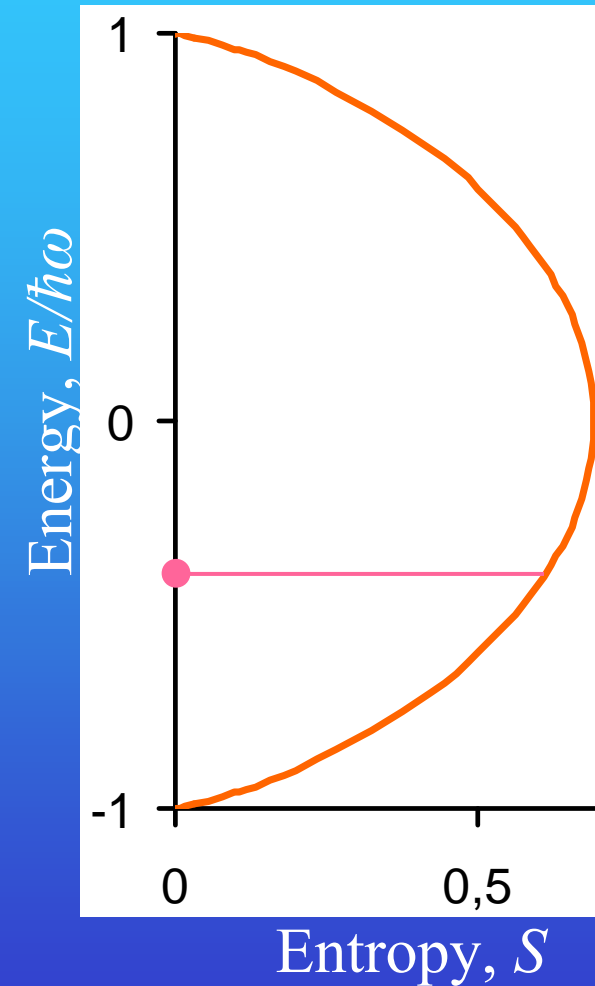
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Ontic states also
inside the Bloch
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$$\dot{\mathbf{r}} = \omega \mathbf{h} \times \mathbf{r} - \frac{f(r)}{\tau} \mathbf{h} \times \mathbf{r} \times \mathbf{h}$$

$$S \neq 0$$

Int.J.Theor.Phys., 24, 119 (1985)

G.P. Beretta, **PIAF '09 "New Perspectives on the Quantum State"**, Perimeter Institute, Sept.27-Oct.2, 2009

References available at: www.quantumthermodynamics.org



Isolated and uncorrelated 2-level particle

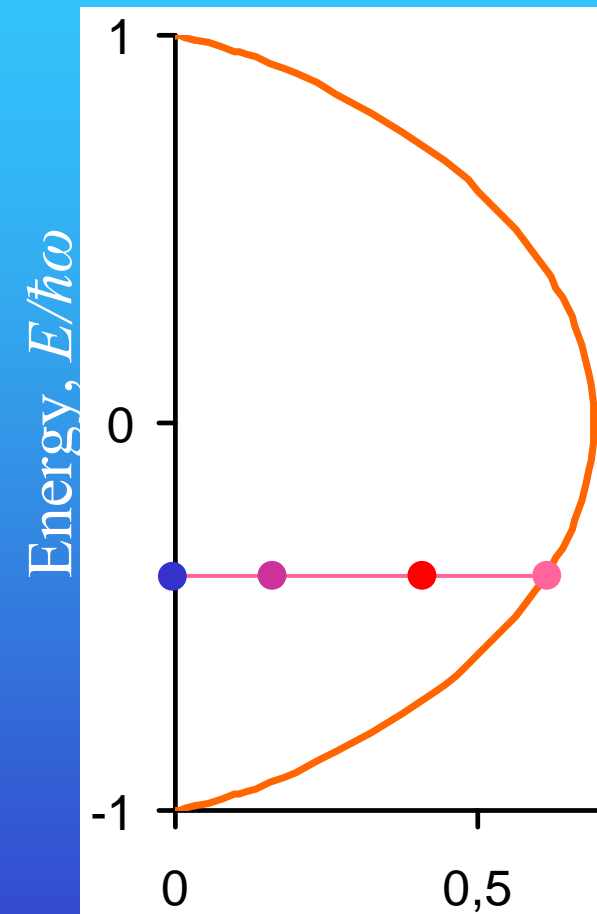
Hamiltonian, $\hbar\omega \mathbf{h}$

On the surface of
the Bloch sphere,

State, $\mathbf{r}(t)$

Energy, $E = \hbar\omega \mathbf{h} \cdot \mathbf{r}(t)$

$$r = |\mathbf{r}| = 1$$

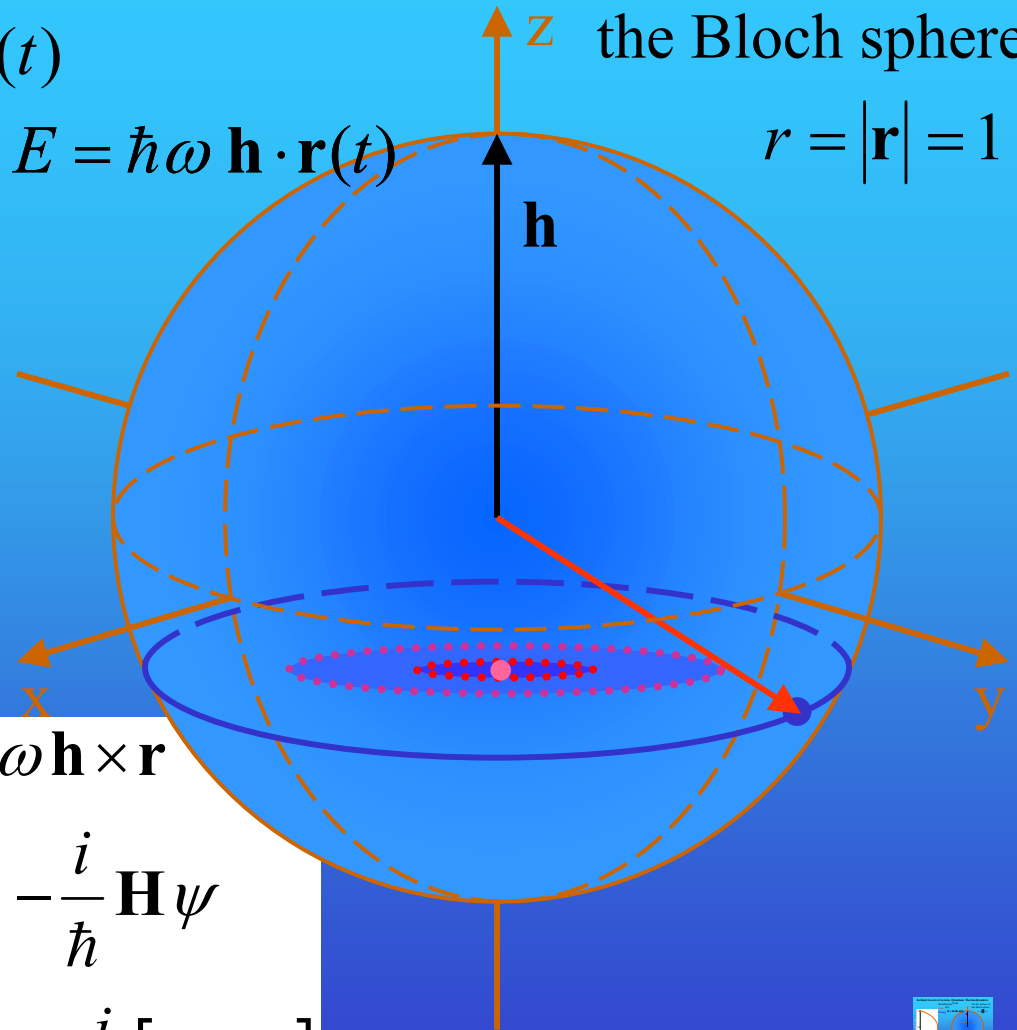


Entropy, S

$$\dot{\mathbf{r}} = \omega \mathbf{h} \times \mathbf{r}$$

$$\dot{\psi} = -\frac{i}{\hbar} \mathbf{H} \psi$$

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$$S = 0$$

Int.J.Theor.Phys., 24, 119 (1985)

G.P. Beretta, PIAF '09 "New Perspectives on the Quantum State", Perimeter Institute, Sept.27-Oct.2, 2009

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Ontic interpretation of the eigenvalues of ρ

Isolated and uncorrelated N-level particle

Energy levels e_j $j = 1, 2, \dots, N$ (eigenvalues of \mathbf{H})

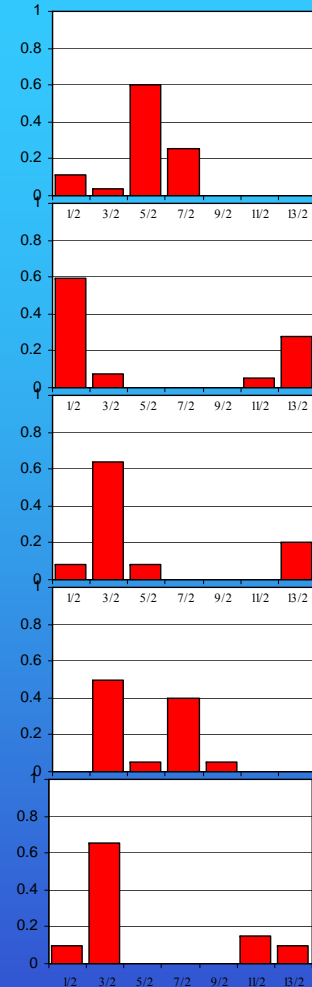
$$E = \sum_j p_j e_j \quad \text{energy (assuming } \rho \mathbf{H} = \mathbf{H} \rho \text{)}$$

The eigenvalues p_j of the density operator ρ

usually interpreted as "probabilities"

can be physically thought as measuring the degree of involvement of level e_j in sharing the energy load

$S = -k_B \sum_j p_j \ln p_j$ entropy measures the global degree of sharing the energy load among levels



Example, $N=7$, different distributions with same E and S



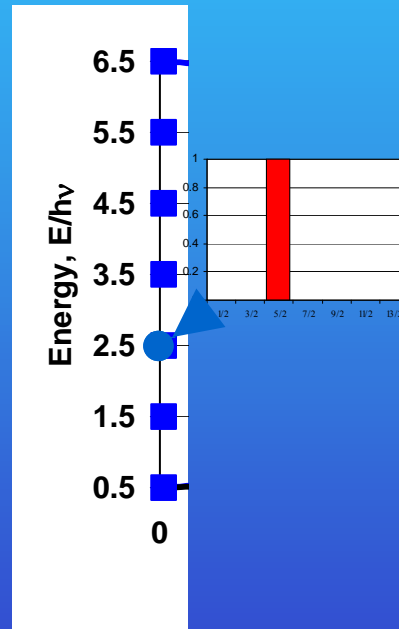
Giving an "ontic" status to entropy and the Second Law

p_j eigenvalues of ρ (for simplicity, assume $\rho H = H\rho$)

$E = \sum_j p_j e_j$ energy

$S = -k_B \sum_j p_j \ln p_j$ entropy : global degree of sharing

In Quantum Mechanics, an isolated and uncorrelated particle is always thought as being in a pure state. If $\rho H = H\rho$, this means that only one energy level carries the energy



Giving an "ontic" status to entropy and the Second Law

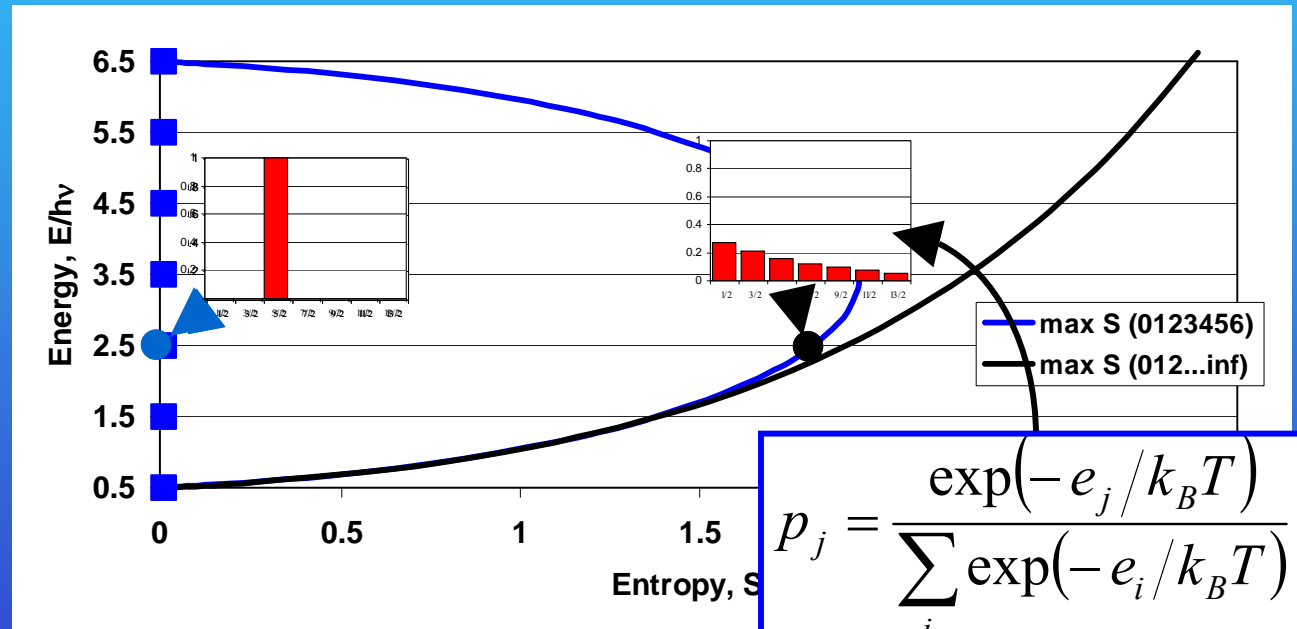
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In equilibrium **Quantum Thermodynamics**, the only stable distribution for the given E , is that which maximizes S

In **Quantum Mechanics**, an isolated and uncorrelated particle is always thought as being in a pure state. If $\rho H = H\rho$, this means that only one energy level carries the energy



$$p_j = \frac{\exp(-e_j/k_B T)}{\sum_i \exp(-e_i/k_B T)}$$

canonical distribution



Giving an "ontic" status to entropy and the Second Law

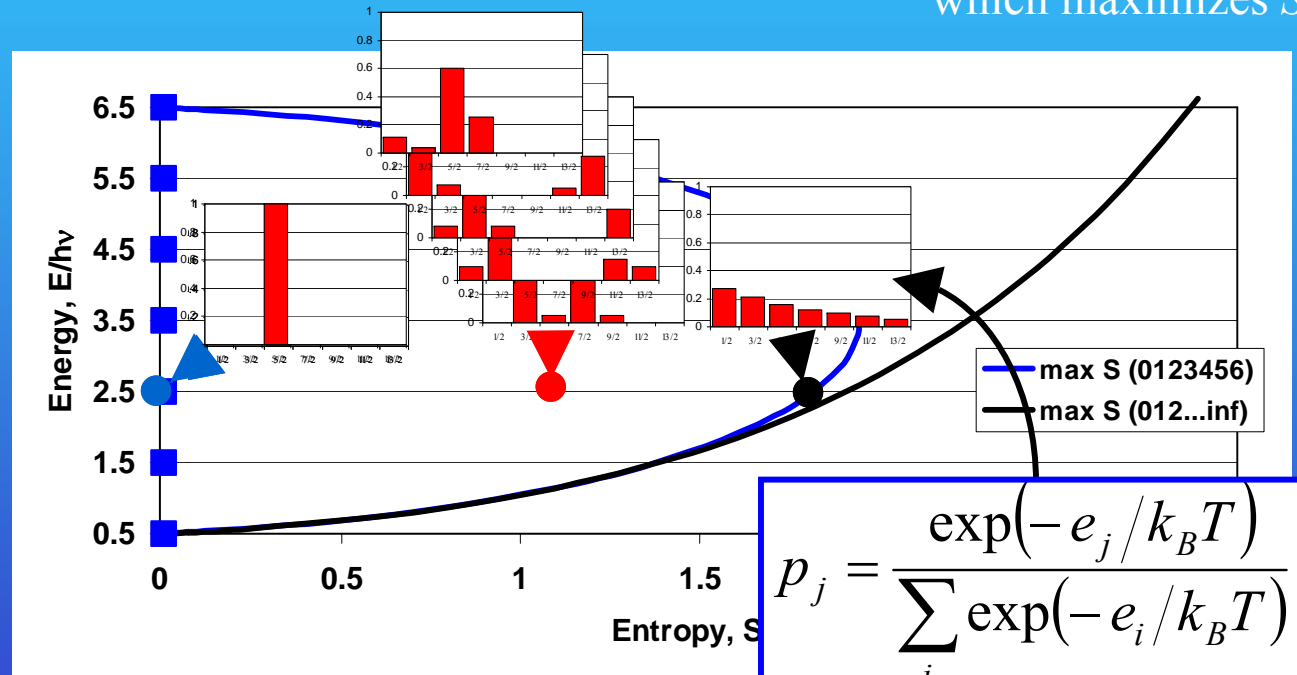
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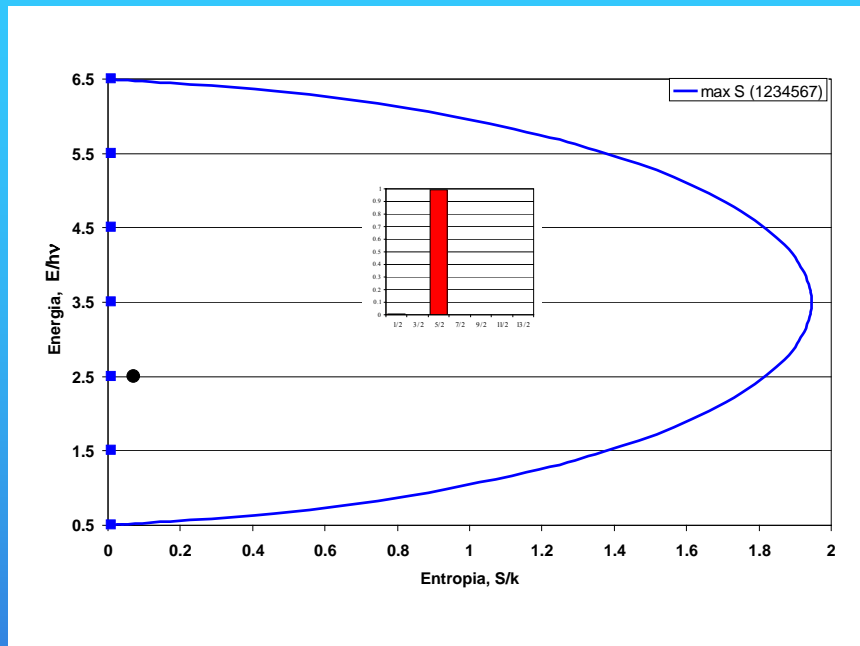
All other distributions with the given E , cannot be stable equilibrium

$$p_j = \frac{\exp(-e_j/k_B T)}{\sum_i \exp(-e_i/k_B T)}$$

canonical distribution

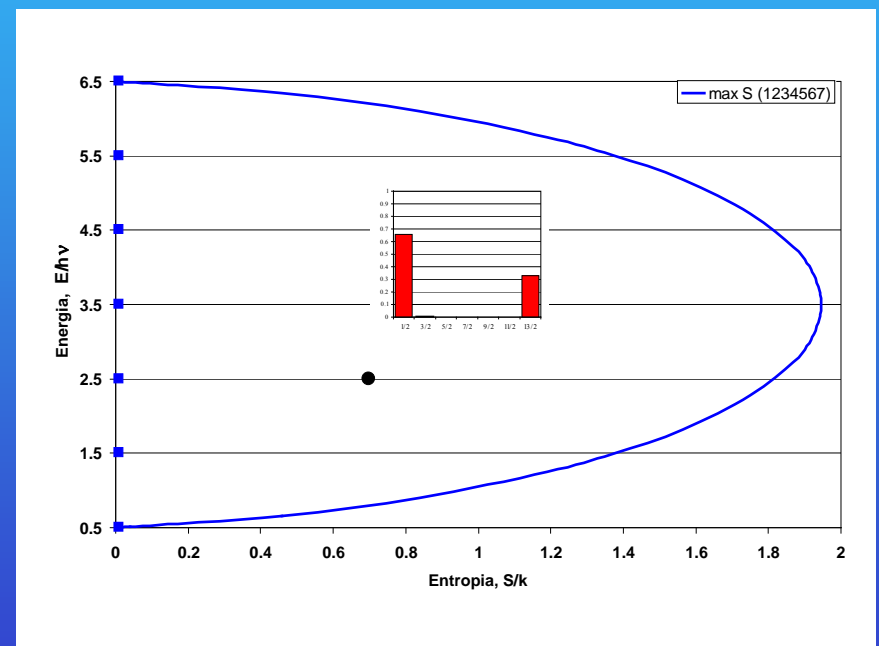


Giving an "ontic" status to irreversibility

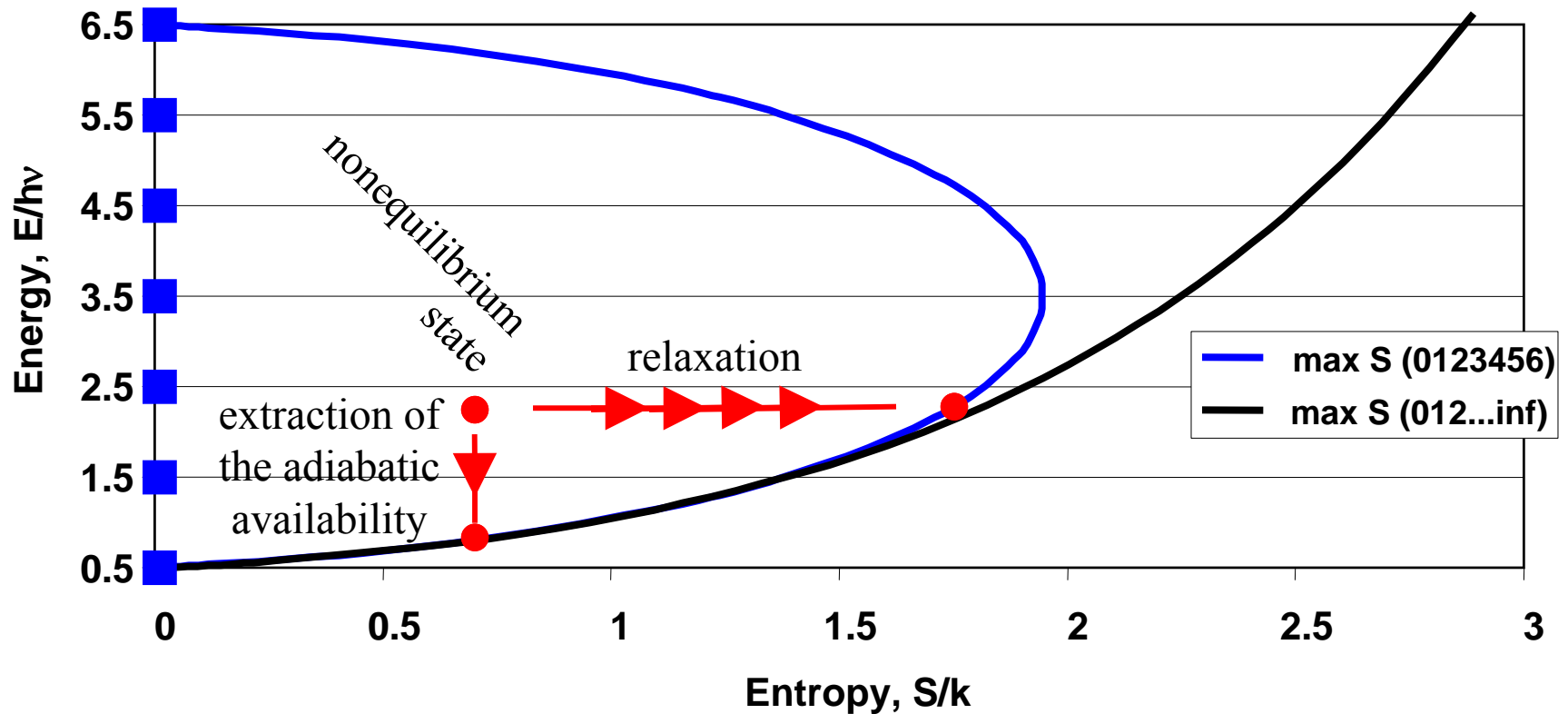


In Quantum Thermodynamics, irreversible time evolution, for $\rho H = H \rho$, can be interpreted as the internal **redistribution of energy** among all the eigenmodes of energy storage that are accessible to the particle

How to construct an equation of motion for ρ which has the canonical equilibrium distribution as the only stable equilibrium one for each given value of E ?



Unitary dynamics cannot describe relaxation to equilibrium, nor extraction of the adiabatic availability

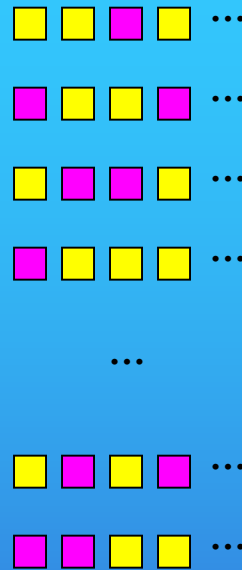
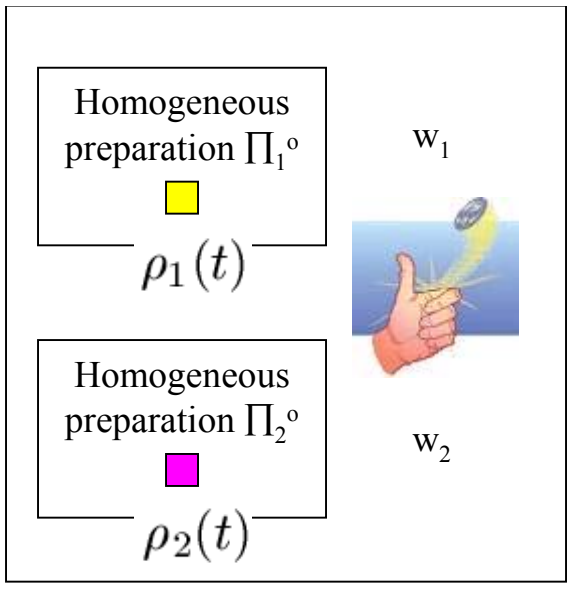


... because the eigenvalues of the density operator change with time in these processes.



No need for linearity of the dynamical law

$$\langle \Pi \rangle = w_1 \langle \Pi_1^o \rangle + w_2 \langle \Pi_2^o \rangle$$



The density operator

$$w_1 \rho_1(t) + w_2 \rho_2(t)$$

does **not** represent the heterogeneous preparation

$$\langle \Pi \rangle_t = w_1 \langle \Pi_1^o \rangle_t + w_2 \langle \Pi_2^o \rangle_t$$

The description must be such that

$$\frac{d\langle \Pi \rangle_t}{dt} = w_1 \frac{d\langle \Pi_1^o \rangle_t}{dt} + w_2 \frac{d\langle \Pi_2^o \rangle_t}{dt}$$

“State at time t is either  or  ”

Linearity is instead required by the (von Neumann) epistemic view...



Part III

- 1) Concept of individual state and an unambiguous representation of preparations, not based on the (von Neumann) density operator
- 2) An ansatz (1976) allows to embed Thermodynamics into Quantum Theory
 - Ontic status of density operators and microscopic entropy
- 3) Geometrical construction (1981) of a 'maximal entropy generation' dynamics
 - Ontic and microscopic status to the second law and to irreversibility
- 4) The price to pay, due to nonlinearity of the dynamical law

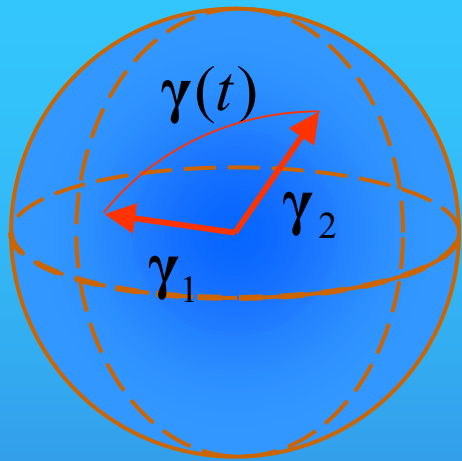


Part III

- 1) Concept of individual state and an unambiguous representation of preparations, not based on the (von Neumann) density operator
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- 3) Geometrical construction (1981) of a 'maximal entropy generation' dynamics
 - Ontic and microscopic status to the second law and to irreversibility
 - "Design of the equation" using square-root density operator



Steepest-entropy-ascent: why square-root probabilities



In probability space, the Fisher-Rao metric provides a unique natural distance between probability distributions. For a one-parameter family of discrete distributions, $\mathbf{p}(t) = \{p_i(t)\}$, where t is a parameter, the distance between distributions $\mathbf{p}(t + dt)$ and $\mathbf{p}(t)$ is

$$d\ell = \sqrt{\sum_i p_i \left(\frac{d \ln p_i}{dt} \right)^2} dt = 2 \sqrt{\sum_i \left(\frac{d \sqrt{p_i}}{dt} \right)^2} dt$$

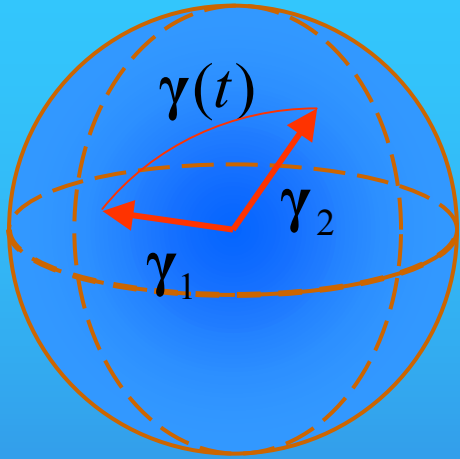
Therefore, square-root probabilities $\gamma_i = \sqrt{p_i}$ are more natural variables:

- the space becomes the unit sphere, $\boldsymbol{\gamma} \cdot \boldsymbol{\gamma} = 1$ ($\sum_i p_i = 1$);
- the Fisher-Rao metric simplifies to $d\ell = 2\sqrt{\dot{\boldsymbol{\gamma}} \cdot \dot{\boldsymbol{\gamma}}} dt$;
- the distance between any two distributions is the angle $d(\boldsymbol{\gamma}_1, \boldsymbol{\gamma}_2) = \cos^{-1}(\boldsymbol{\gamma}_1 \cdot \boldsymbol{\gamma}_2)$

Wootters,
Phys.Rev.D, 23, 357 (1981)



Steepest-entropy-ascent: **square root of density operator**



In the space of linear operators on \mathcal{H} , let

$$X \cdot Y = \text{Tr}(X^\dagger Y + Y^\dagger X)/2$$

be the *real* scalar product. Then,

$$\begin{aligned} \gamma &= U\sqrt{\rho} & U^\dagger &= U^{-1} & \rho &= \gamma^\dagger \gamma \\ 1 &= \text{Tr}\rho = \gamma \cdot \gamma \end{aligned}$$

Ph.D.thesis, MIT (1981)

(now at quant-ph/0509116)

Nuovo Cimento B, 82, 169 (1984)

Nuovo Cimento B, 87, 77 (1985)

NatoAsi LecNotes, 278, 441 (1986)

quant-ph-0112046

Gheorghiu-Svirschevski,

Phys.Rev.A, 022105 (2001)

quant-ph-0907.1977

For a one-parameter family $\gamma(t)$ (H time independent),

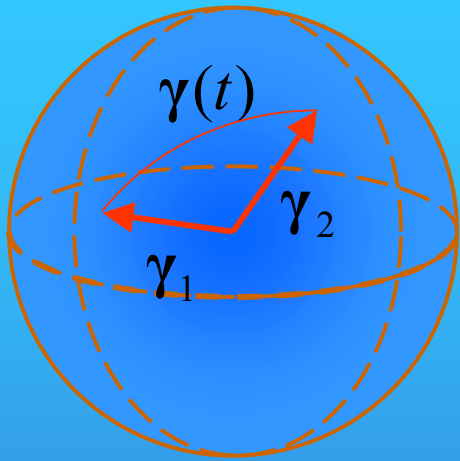
$$d\ell = 2\sqrt{\dot{\gamma} \cdot \dot{\gamma}} dt \quad 1/\tau = d\ell/dt \quad \tau = 1 / 2\sqrt{\dot{\gamma} \cdot \dot{\gamma}}$$



G.P. Beretta, **PIAF '09 "New Perspectives on the Quantum State"**, Perimeter Institute, Sept.27-Oct.2, 2009

References available at: www.quantumthermodynamics.org

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$$X \cdot Y = \text{Tr}(X^\dagger Y + Y^\dagger X)/2$$

be the *real* scalar product. Then,

$$\gamma = U\sqrt{\rho} \quad U^\dagger = U^{-1} \quad \rho = \gamma^\dagger \gamma$$

$$1 = \text{Tr}\rho = \gamma \cdot \gamma$$

$$\langle H \rangle = \text{Tr}\rho H = \gamma \cdot H'/2 \quad \text{where } H' = 2\gamma H$$

$$\langle S \rangle = -k_B \text{Tr}\rho \ln \rho = \gamma \cdot S'/2 \quad \text{where } S' = -4k_B \gamma \ln \gamma$$

For a one-parameter family $\gamma(t)$ (H time independent),

$$d\ell = 2\sqrt{\dot{\gamma} \cdot \dot{\gamma}} dt \quad 1/\tau = d\ell/dt \quad \tau = 1 / 2\sqrt{\dot{\gamma} \cdot \dot{\gamma}}$$

$$\dot{\rho} = \dot{\gamma}^\dagger \gamma + \gamma^\dagger \dot{\gamma}$$

$$\text{Tr}\dot{\rho}/2 = \dot{\gamma} \cdot \gamma = 0 \quad \text{preserve normalization}$$

$$d\langle H \rangle/dt = \dot{\gamma} \cdot H' = 0 \quad \text{conserve energy (isolated particle)}$$

$$d\langle S \rangle/dt = \dot{\gamma} \cdot S'$$

Ph.D.thesis, MIT (1981)

(now at quant-ph/0509116)

Nuovo Cimento B, 82, 169 (1984)

Nuovo Cimento B, 87, 77 (1985)

NatoAsi LecNotes, 278, 441 (1986)

quant-ph-0112046

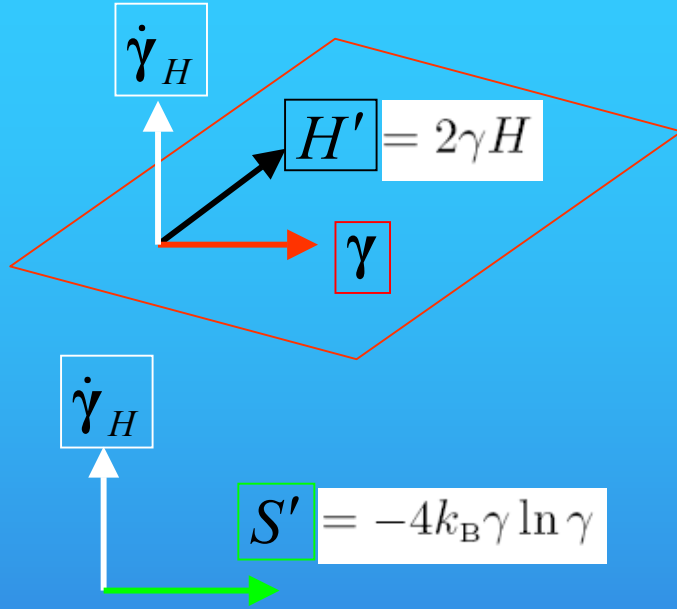
Gheorghiu-Svirschevski,

Phys.Rev.A, 022105 (2001)

quant-ph-0907.1977



Hamiltonian dynamics: **Schroedinger-von Neumann eq.**



$$\dot{\gamma}_H = i\gamma\Delta H/\hbar \quad \Rightarrow \quad \dot{\rho}_H = -i[H, \rho]/\hbar$$

$$\Delta H = H - \langle H \rangle I.$$

quant-ph/0509116

quant-ph/0511091

quant-ph/0612215

Phys.Rev.E, 73, 026113 (2006)

Entropy, 10, 160 (2008)

Rep.Math.Phys. (2009)

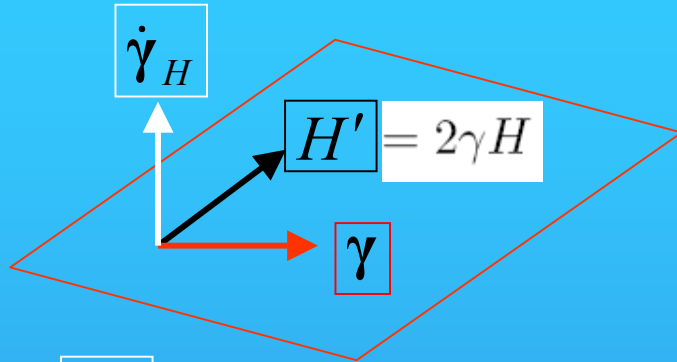
quant-ph/0907.1977



G.P. Beretta, **PIAF '09 "New Perspectives on the Quantum State"**, Perimeter Institute, Sept.27-Oct.2, 2009

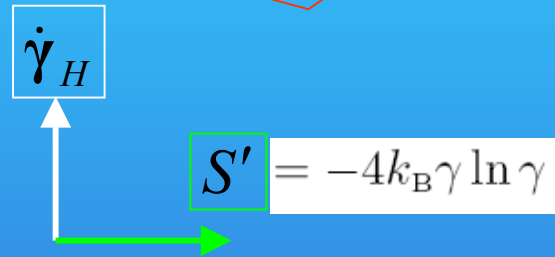
References available at: www.quantumthermodynamics.org

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$$\dot{\gamma}_H = i\gamma\Delta H/\hbar \Rightarrow \dot{\rho}_H = -i[H, \rho]/\hbar$$

$$\Delta H = H - \langle H \rangle I.$$



Note: since $\gamma\Delta H \cdot \gamma\Delta H = \text{Tr}\rho(\Delta H)^2 = \langle \Delta H \Delta H \rangle$ and

$$\dot{\gamma}_H \cdot \dot{\gamma}_H = \langle \Delta H \Delta H \rangle / \hbar^2$$

the Fischer-Rao metric is

$$d\ell = 2\sqrt{\dot{\gamma}_H \cdot \dot{\gamma}_H} dt = dt/\tau_H$$

which defines the intrinsic Hamiltonian time τ_H such that

$$\langle \Delta H \Delta H \rangle \tau_H^2 = \hbar^2/4$$

Exact time-energy uncertainty relation

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quant-ph/0509116

quant-ph/0511091

quant-ph/0612215

Phys.Rev.E, 73, 026113 (2006)

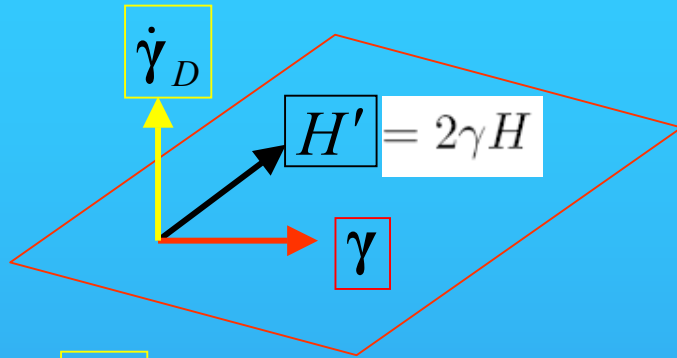
Entropy, 10, 160 (2008)

Rep.Math.Phys. (2009)

quant-ph/0907.1977

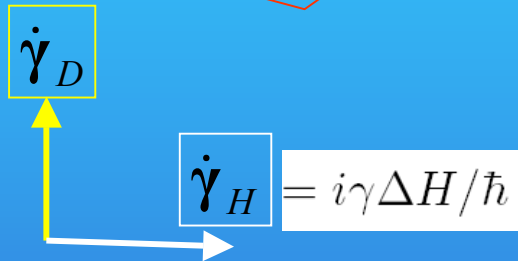


Steepest-entropy-ascent: **non-Hamiltonian contribution**



$$\dot{\gamma}_H = i\gamma\Delta H/\hbar \quad \Rightarrow \quad \dot{\rho}_H = -i[H, \rho]/\hbar$$

$$\Delta H = H - \langle H \rangle I.$$



Instead, let us assume

$$\dot{\gamma} = \dot{\gamma}_H + \dot{\gamma}_D$$

with $\dot{\gamma}_D$ in the direction of steepest entropy ascent compatible with the constraints

$$\dot{\gamma}_D \cdot \gamma = 0 \quad (\text{conservation of } \text{Tr} \rho = 1)$$

$$\dot{\gamma}_D \cdot H' = 0 \quad (\text{conservation of } \langle H \rangle)$$

As a result $\dot{\gamma}_D$ will also be orthogonal to $\dot{\gamma}_H$.

quant-ph/0509116

quant-ph/0511091

quant-ph/0612215

Phys.Rev.E, 73, 026113 (2006)

Entropy, 10, 160 (2008)

Rep.Math.Phys. (2009)

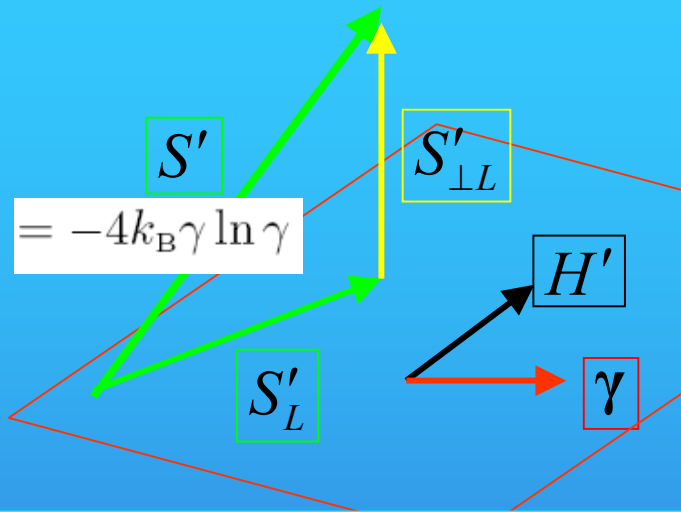
quant-ph/0907.1977



G.P. Beretta, **PIAF '09 "New Perspectives on the Quantum State"**, Perimeter Institute, Sept.27-Oct.2, 2009

References available at: www.quantumthermodynamics.org

Steepest-entropy-ascent: finding the “direction”



Let $L(\gamma, H')$ be the real linear span of “vectors” γ and H' . Denote by S'_L the orthogonal projection of the “entropy gradient vector” S' onto L , and by $S'_{\perp L}$ its orthogonal complement, so that

$$S' = S'_L + S'_{\perp L}$$

If γ and H' are linearly independent, we may write

$$d\langle S \rangle / dt = d(-k_B \text{Tr} \rho \ln \rho) / dt = \dot{\gamma} \cdot S'$$

$$S'_{\perp L(\gamma, H')} = \frac{\begin{vmatrix} S' & \gamma & H' \\ S' \cdot \gamma & \gamma \cdot \gamma & H' \cdot \gamma \\ S' \cdot H' & \gamma \cdot H' & H' \cdot H' \end{vmatrix}}{\begin{vmatrix} \gamma \cdot \gamma & \gamma \cdot H' \\ \gamma \cdot H' & H' \cdot H' \end{vmatrix}}$$

quant-ph/0509116

quant-ph/0511091

quant-ph/0612215

Phys.Rev.E, 73, 026113 (2006)

Entropy, 10, 160 (2008)

Rep.Math.Phys. (2009)

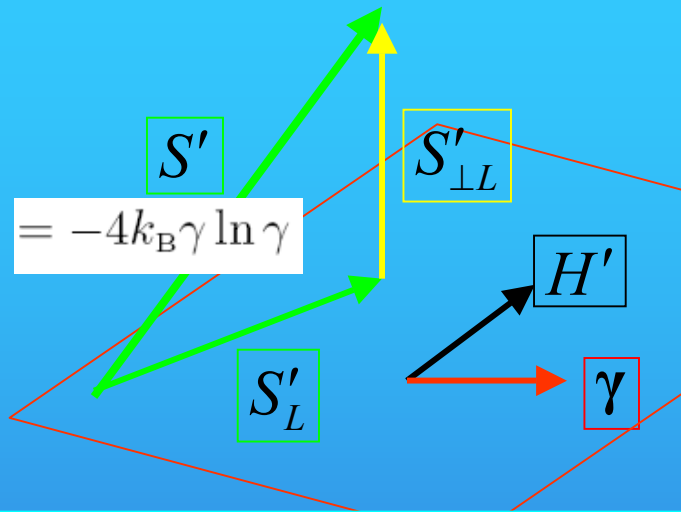
quant-ph/0907.1977



G.P. Beretta, **PIAF '09 "New Perspectives on the Quantum State"**, Perimeter Institute, Sept.27-Oct.2, 2009

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quant-ph/0509116

quant-ph/0511091

quant-ph/0612215

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quant-ph/0907.1977



G.P. Beretta, PIAF '09 “New Perspectives on

ct.2, 2009

References available at: www.quantumthermodynamics.org

$$\dot{\gamma}_D = \frac{1}{4k_B \tau} S'_{\perp L(\gamma, H')}$$

Steepest-entropy-ascent: **dynamical law** (single isolated particle)

Trajectories will be
geodesics in the
constant energy
surface in square-
root density
operator space

The equation of motion for γ is therefore

$$\dot{\gamma} = \frac{i}{\hbar} \gamma \Delta H + \frac{1}{4k_B \tau} S'_{\perp L(\gamma, H')}$$

$$\dot{\gamma} = \dot{\gamma}_H + \dot{\gamma}_D$$

$$\dot{\gamma}_H = i \gamma \Delta H / \hbar$$

$$\dot{\gamma}_D = \frac{1}{4k_B \tau} S'_{\perp L(\gamma, H')}$$

quant-ph/0509116

quant-ph/0511091

quant-ph/0612215

Phys.Rev.E, 73, 026113 (2006)

Entropy, 10, 160 (2008)

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quant-ph/0907.1977



G.P. Beretta, **PIAF '09 "New Perspectives on**

ct.2, 2009

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$$\dot{\gamma} = \frac{i}{\hbar} \gamma \Delta H + \frac{1}{4k_B \tau} S' \perp L(\gamma, H')$$

or, equivalently, for the density operator

$$\dot{\rho} = -\frac{i}{\hbar} [H, \rho] + \frac{1}{2k_B \tau} \{\Delta M, \rho\}$$

quant-ph/0509116

quant-ph/0511091

quant-ph/0612215

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G.P. Beretta, **PIAF '09 "New Perspectives on the Quantum State"**, Perimeter Institute, Sept.27-Oct.2, 2009

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$$\dot{\rho} = -\frac{i}{\hbar} [H, \rho] + \frac{1}{2k_B \tau} \{\Delta M, \rho\}$$

where M (“non-equilibrium Massieu operator”) is

$$M = S - \frac{H}{\theta} \quad \theta = \frac{\langle \Delta H \Delta H \rangle}{\langle \Delta S \Delta H \rangle}$$

where $S = -k_B \ln(\rho + P_{\text{Ker } \rho})$ and

$$\langle \Delta F \Delta G \rangle = \text{Tr}(\rho \{\Delta F, \Delta G\})/2$$

The nonlinear functional θ may be interpreted as a kind of *nonequilibrium temperature*.

quant-ph/0509116

quant-ph/0511091

quant-ph/0612215

Phys.Rev.E, 73, 026113 (2006)

Entropy, 10, 160 (2008)

Rep.Math.Phys. (2009)

quant-ph/0907.1977



Steepest-entropy-ascent: dynamical law (single isolated particle)

τ = “intrinsic time”
characteristic of the
relaxation and
spontaneous
internal
redistribution
(functional of ρ)

The equation of motion for γ is therefore

$$\dot{\gamma} = \frac{i}{\hbar} \gamma \Delta H + \frac{1}{4k_B \tau} S'_{\perp L(\gamma, H')}$$

or, equivalently, for the density operator

$$\dot{\rho} = -\frac{i}{\hbar} [H, \rho] + \frac{1}{2k_B \tau} \{\Delta M, \rho\}$$

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quant-ph/0509116

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Phys.Rev.E, 73, 026113 (2006)

Entropy, 10, 160 (2008)

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quant-ph/0907.1977



Part III

- 1) Concept of individual state and an unambiguous representation of preparations, not based on the (von Neumann) density operator
- 2) An ansatz (1976) allows to embed Thermodynamics into Quantum Theory
 - Ontic status of density operators and microscopic entropy
- 3) Geometrical construction (1981) of a 'maximal entropy generation' dynamics
 - Ontic and microscopic status to the second law and to irreversibility
- Main features of this largely irreversible nonlinear quantum dynamics



Steepest-entropy-ascent: **rate of entropy increase**

$$\dot{\rho} = -\frac{i}{\hbar}[H, \rho] + \frac{1}{2k_B\tau}\{\Delta M, \rho\}$$

where

$$M = S - \frac{H}{\theta} \quad S = -k_B \ln(\rho + P_{\text{Ker } \rho}) \quad \theta = \frac{\langle \Delta H \Delta H \rangle}{\langle \Delta S \Delta H \rangle}$$

The rate of entropy generation is (nonnegative)

$$\begin{aligned} \frac{d\langle S \rangle}{dt} &= \frac{d(-k_B \text{Tr} \rho \ln \rho)}{dt} = \dot{\gamma} \cdot S' = \frac{1}{k_B\tau} \langle \Delta M \Delta M \rangle \\ &= \frac{1}{k_B\tau} \left(\langle \Delta S \Delta S \rangle - \frac{\langle \Delta H \Delta H \rangle}{\theta^2} \right) \\ &= \frac{1}{4k_B\tau} S'_{\perp L} \cdot S'_{\perp L} = 4k_B\tau \dot{\gamma}_D \cdot \dot{\gamma}_D \end{aligned}$$

quant-ph/0509116
quant-ph/0511091
quant-ph/0612215
Phys.Rev.E, 73, 026113
Entropy, 10, 160 (2008)
Rep.Math.Phys. (2009)
quant-ph/0907.1977



Steepest-entropy-ascent: **simple form when $[H,\rho]=0$**

Ph.D.thesis, MIT (1981), quant-ph/0509116

Nuovo Cimento B, 82, 169 (1984); 87, 77 (1985)

NATO-ASI Lecture Notes, 278, 441 (1986)

Phys.Rev.E, 73, 026113 (2006)

Smooth, constant energy,
spontaneous internal redistribution
of the eigenvalues p_j of ρ , which can be
interpreted as degree of
“energy sharing involvement”
of the active levels e_j (active means $p_j > 0$).

$$\frac{dp_j}{dt} = -\frac{1}{\tau} \frac{\begin{vmatrix} p_j \ln p_j & p_j & e_j p_j \\ \sum p_i \ln p_i & 1 & \sum e_i p_i \\ \sum e_i p_i \ln p_i & \sum e_i p_i & \sum e_i^2 p_i \end{vmatrix}}{\begin{vmatrix} 1 & \sum e_i p_i \\ \sum e_i p_i & \sum e_i^2 p_i \end{vmatrix}}$$

$$\frac{dS}{dt} = \frac{k}{\tau} \frac{\begin{vmatrix} \sum p_i (\ln p_i)^2 & \sum p_i \ln p_i & \sum e_i p_i \ln p_i \\ \sum p_i \ln p_i & 1 & \sum e_i p_i \\ \sum e_i p_i \ln p_i & \sum e_i p_i & \sum e_i^2 p_i \end{vmatrix}}{\begin{vmatrix} 1 & \sum e_i p_i \\ \sum e_i p_i & \sum e_i^2 p_i \end{vmatrix}} \geq 0$$



Existence and uniqueness of solutions $\rho(t)$ for any $\rho(0)$

Theorems about “good behavior” as a dynamical equation:

- The nonlinear term $\rho \ln \rho$ is not Cauchy-Lipschitz, but it satisfies the first Osgood condition

$$|y_1 \ln y_1 - y_2 \ln y_2| < K |y_1 - y_2| \ln \frac{1}{|y_1 - y_2|}$$

and so, despite the logarithmic singularity of $y \ln y$ at $y = 0$, the solution is unique.

- Any initially zero eigenvalue of ρ remains zero at all times.
- Hence, because of uniqueness, no initially positive eigenvalue of ρ can ever become zero (or negative): the nonnegativity of ρ is preserved.
- The above holds both forward and backwards in time!



Nuovo Cimento B, 82, 169 (1984); 87, 77 (1985)

G.P. Beretta, **PIAF '09 "New Perspectives on the Quantum State"**, Perimeter Institute, Sept.27-Oct.2, 2009

References available at: www.quantumthermodynamics.org

Existence and uniqueness of solutions $\rho(t)$ for any $\rho(0)$

Dynamical group, not
just a semigroup !

The inverse map exists

Mathematical
reversibility

A *dynamical system* on a metric space (\mathcal{G}, d) is a mapping $u : \mathbb{R}^+ \times \mathcal{G} \longrightarrow \mathcal{G}$ such that, for all t, s in \mathbb{R}^+ and all γ in \mathcal{G} :

- $u(\cdot, \gamma) : \mathbb{R}^+ \longrightarrow \mathcal{G}$ is continuous;
- $u(t, \cdot) : \mathcal{G} \longrightarrow \mathcal{G}$ is continuous;
- $u(0, \gamma) = \gamma$;
- $u(t + s, \gamma) = u(t, u(s, \gamma))$.

The dynamical system is determined by a one-parameter *semigroup* $\Lambda(t) : \mathcal{G} \longrightarrow \mathcal{G}$ such that, for all t in \mathbb{R}^+ and all γ in \mathcal{G} :

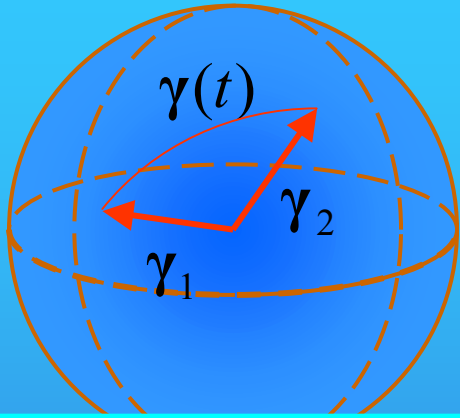
- $\Lambda(t)\gamma = u(t, \gamma)$;
- therefore, $\Lambda(t)\Lambda(s) = \Lambda(t + s)$.

If the inverse map $\Lambda(t)^{-1}$ exists, the dynamical map can be extended to a *group* by

- $\Lambda(-t) = \Lambda(t)^{-1}$.



Entropy increase, metric, and time-entropy uncertainty



$$M = S - \frac{H}{\theta} \quad \theta = \frac{\langle \Delta H \Delta H \rangle}{\langle \Delta S \Delta H \rangle}$$

Going back to the Fisher-Rao metric, when $[H, \rho] = 0$,

$$\begin{aligned} d\ell &= 2\sqrt{\dot{\gamma}_D \cdot \dot{\gamma}_D} dt = dt/\tau_D \\ &= \sqrt{\frac{1}{k_B\tau} \frac{d\langle S \rangle}{dt}} dt \\ &= \frac{1}{2k_B\tau} \frac{d\langle S \rangle}{d\ell} dt \\ &= \frac{\sqrt{\langle \Delta M \Delta M \rangle}}{k_B\tau} dt \\ &= \frac{1}{k_B\tau} \sqrt{\langle \Delta S \Delta S \rangle - \frac{\langle \Delta H \Delta H \rangle}{\theta^2}} dt \end{aligned}$$

which defines also the intrinsic dissipative time τ_D such that

$$\langle \Delta S \Delta S \rangle \tau_D^2 \geq \langle \Delta M \Delta M \rangle \tau_D^2 = (k_B\tau)^2$$

(a general time-entropy uncertainty relation).

quant-ph/0509116

quant-ph/0511091

quant-ph/0612215

Phys.Rev.E, 73, 026113 (2006)

Entropy, 10, 160 (2008)

Rep.Math.Phys. (2009)

quant-ph/0907.1977



G.P. Beretta, **PIAF '09 "New Perspectives on the Quantum State"**, Perimeter Institute, Sept.27-Oct.2, 2009

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Steepest-entropy-ascent: **Onsager reciprocity everywhere**

Any nonequilibrium ρ can be written as

$$\rho = \frac{B \exp(-\sum_j f_j X_j) B}{\text{Tr} B \exp(-\sum_j f_j X_j)}$$

where the set $\{I, X_j\}$ spans the real space of hermitian operators on (\mathcal{H}) , and $B = B^\dagger$. Hence,

$$\begin{aligned}\langle X_j \rangle &= \text{Tr}(\rho X_j) \\ \langle S \rangle &= k_B f_0 + k_B \sum_j f_j \langle X_j \rangle \\ \text{where } k_B f_j &= \left. \frac{\partial \langle S \rangle}{\partial \langle X_j \rangle} \right|_{\langle X_{i \neq j} \rangle}\end{aligned}$$

may be interpreted as a “generalized affinity” or force, and

$$\langle \dot{X}_j \rangle_D = \dot{\gamma}_D \cdot X'_j \quad \text{with } X'_j = 2\gamma X_j$$

is the “dissipative part” of rate of change of $\langle X_j \rangle$. We find

$$\langle \dot{X}_i \rangle_D = \sum_j f_j L_{ij}(\rho)$$

Found.Phys., 17, 365 (1987)

quant-ph-0112046

Rep.Math.Phys. (2009)

quant-ph/0907.1977



G.P. Beretta, **PIAF '09 "N**

Steepest-entropy-ascent: Onsager reciprocity everywhere

For all states, however far from stable equilibrium,

$$\langle \dot{X}_i \rangle_D = \sum_j f_j L_{ij}(\rho)$$

where the coefficients (*nonlinear* in ρ) form a symmetric, non-negative definite Gram matrix $[\{L_{ij}(\rho)\}]$,

$$L_{ij}(\rho) = \frac{1}{\tau(\rho)} \frac{\begin{vmatrix} \langle \Delta X_i \Delta X_j \rangle & \langle \Delta H \Delta X_j \rangle \\ \langle \Delta X_i \Delta H \rangle & \langle \Delta H \Delta H \rangle \end{vmatrix}}{\langle \Delta H \Delta H \rangle} = L_{ji}(\rho)$$

Entropy generation a quadratic form of the affinities

$$\frac{d\langle S \rangle}{dt} = k_B \sum_i \sum_j f_i f_j L_{ij}(\rho)$$

If $[\{L_{ij}(\rho)\}]$ is positive definite,

$$f_j = \sum_i L_{ij}^{-1}(\rho) \langle \dot{X}_i \rangle_D$$

Entropy generation a quadratic form of the affinities
quadratic form of the dissipative rates

$$\frac{d\langle S \rangle}{dt} = k_B \sum_i \sum_j L_{ij}^{-1}(\rho) \langle \dot{X}_i \rangle_D \langle \dot{X}_j \rangle_D$$

Linear interrelations
between rates and
affinities.

But the L_{ij} 's are
nonlinear
functionals of ρ

Found.Phys., 17, 365 (1987)

quant-ph-0112046

Rep.Math.Phys. (2009)

quant-ph/0907.1977



G.P. Beretta, PIAF '09 "New Perspectives

Refer

Part III

- 1) Concept of individual state and an unambiguous representation of preparations, not based on the (von Neumann) density operator
- 2) An ansatz (1976) allows to embed Thermodynamics into Quantum Theory
 - Ontic status of density operators and microscopic entropy
- 3) Geometrical construction (1981) of a 'maximal entropy generation' dynamics
 - Ontic and microscopic status to the second law and to irreversibility
 - Reduces to the Schroedinger equation for pure density operators
 - The theory is a generalization of Quantum Mechanics which does not contradict it in any way
 - The second law as a theorem about the stability of the equilibrium states



Steepest-entropy-ascent: **equilibrium states, limit cycles..**

..and the Second Law as a theorem!

The rate of entropy generation is zero (and the evolution is Schrödinger–von Neumann) iff $\gamma_D = 0$, i.e., when S' lies in $L(\gamma, H')$. Then,

$$\rho = \frac{B \exp(-H/k_B T) B}{\text{Tr}[B \exp(-H/k_B T) B]} \quad \text{for some } B = B^2$$

where $T = \theta = \sqrt{\langle \Delta H \Delta H \rangle / \langle \Delta S \Delta S \rangle}$.

These nondissipative states are

- equilibrium states if $[B, H] = 0$;
- mixed limit cycles if $[B, H] \neq 0$ and $\text{Tr} B > 1$, then $B(t) = U(t)B(0)U^{-1}(t)$;
- pure limit cycles if $[B, H] \neq 0$ and $\text{Tr} B = 1$ (the usual Schrödinger dynamics of standard QM), then $\rho(t) = U(t)\rho(0)U^{-1}(t)$.

The only equilibrium states dynamically *stable* (according to Lyapunov) are those with $B = I$. All the other are unstable. This is the Hatsopoulos-Keenan statement of the Second Law: *for each given value of the mean energy $\langle E \rangle$ there is one and only one stable equilibrium state.*

quant-ph-0112046

quant-ph-0612215

quant-ph-0511091

Phys.Rev.E, 73, 026113 (2006)



G.P. Beretta, PIAF '09 "New

009

rg

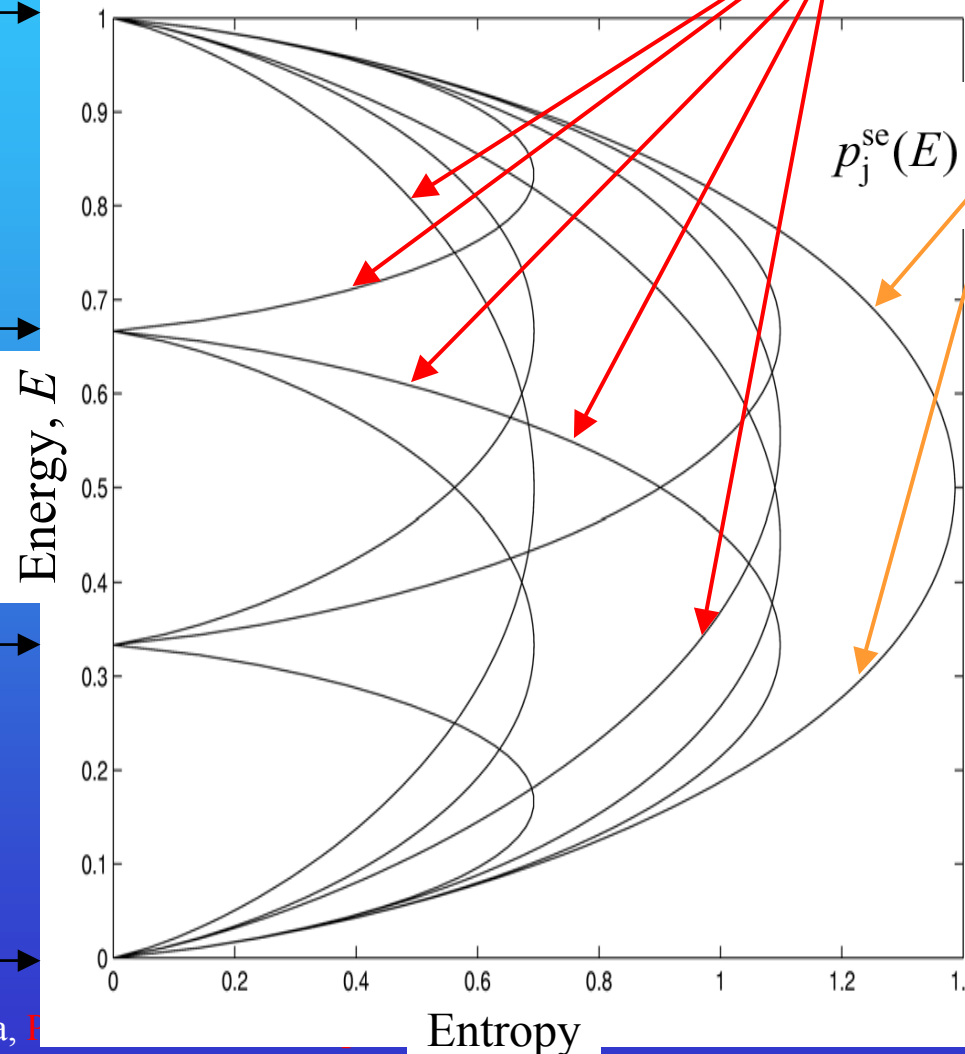
Equilibrium states for a 4-level isolated particle

Phys.Rev.E, 73, 026113 (2006)

$$p_j^{\text{pe}}(E, \delta) = \frac{\delta_j \exp(-\beta^{\text{pe}}(E, \delta) e_j)}{\sum_{i=1}^N \delta_i \exp(-\beta^{\text{pe}}(E, \delta) e_i)}$$

lowest entropy and unstable equilibrium states

$e_4 = 1$ →
 $e_3 = 2/3$ →
 $e_2 = 1/3$ →
 $e_1 = 0$ →



$$p_j^{\text{se}}(E) = \frac{\exp(-e_j/kT(E))}{\sum_{i=1}^N \exp(-e_i/kT(E))}$$

(canonical distribution)
stable equilibrium states



G.P. Beretta, I

er Institute, Sept.27-Oct.2, 2009

References available at: www.quantumthermodynamics.org

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- Dynamical group, not a semi-group

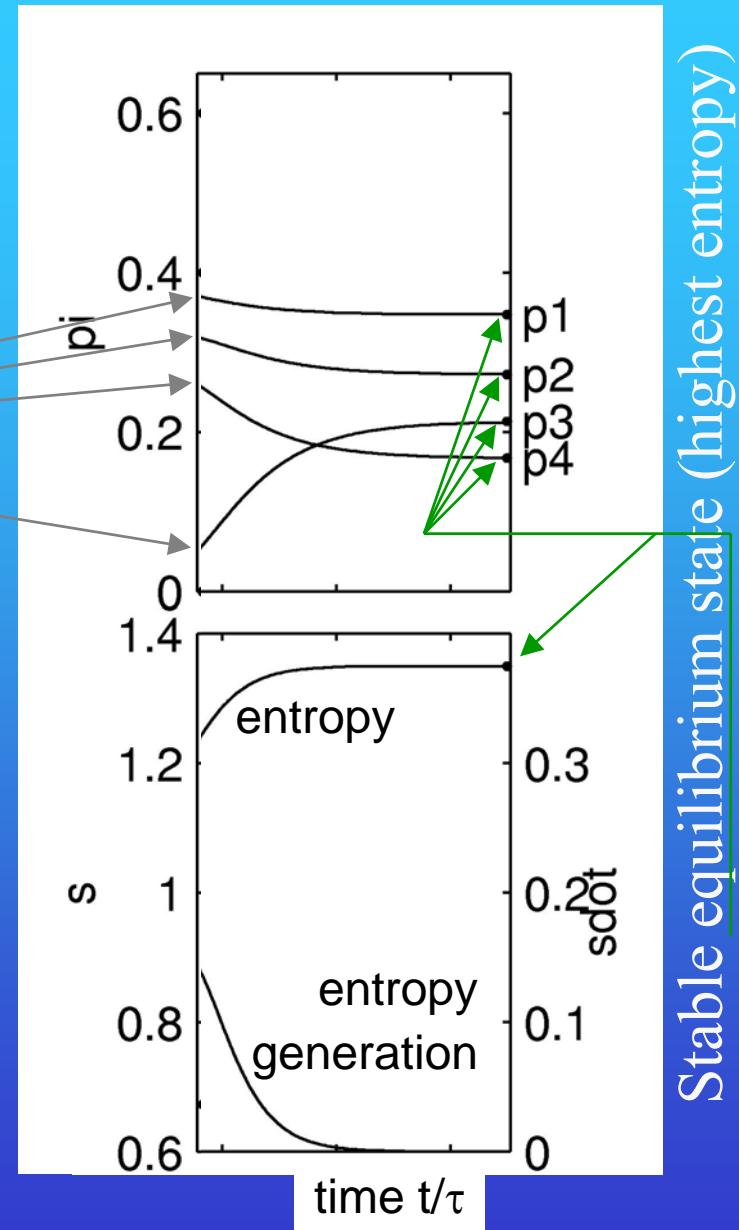


Relaxation to equilibrium for a 4-level isolated particle

$$N = 4$$

$$[H, \rho] = 0$$

An arbitrary initial distribution (state)



Phys.Rev.E, 73, 026113 (2006)

G.P. Beretta, **PIAF '09 "New Perspectives on the Quantum State"**, Perimeter Institute, Sept.27-Oct.2, 2009

References available at: www.quantumthermodynamics.org



Relaxation to equilibrium for a 4-level isolated particle

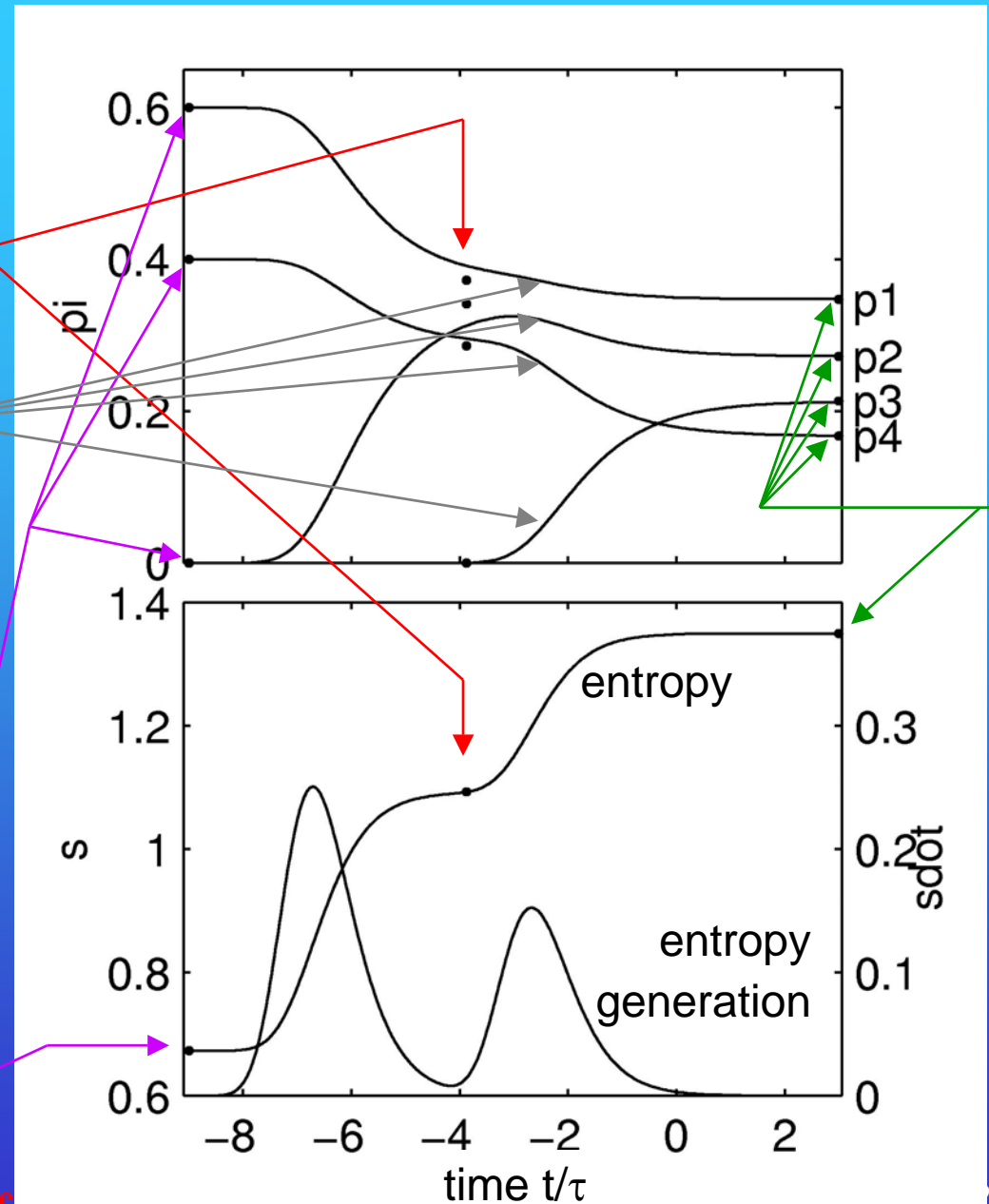
The trajectory passes very close to an unstable equilibrium state

An arbitrary initial distribution (state)

Strong causality:

given any initial state the trajectory is unique and defined for $-\infty < t < +\infty$

We can trace back the lowest entropy 'ancestral' state



Stable equilibrium state (highest entropy)



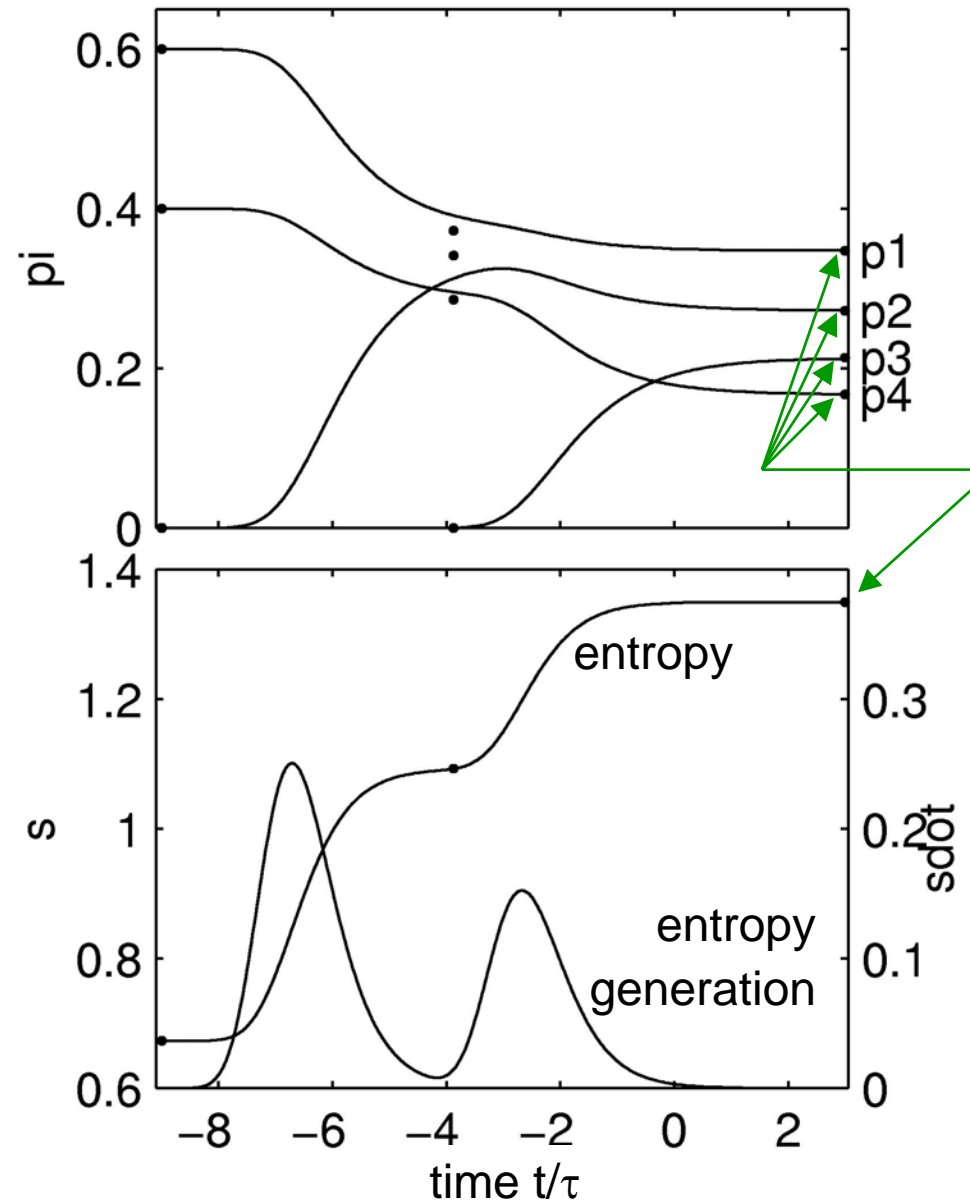
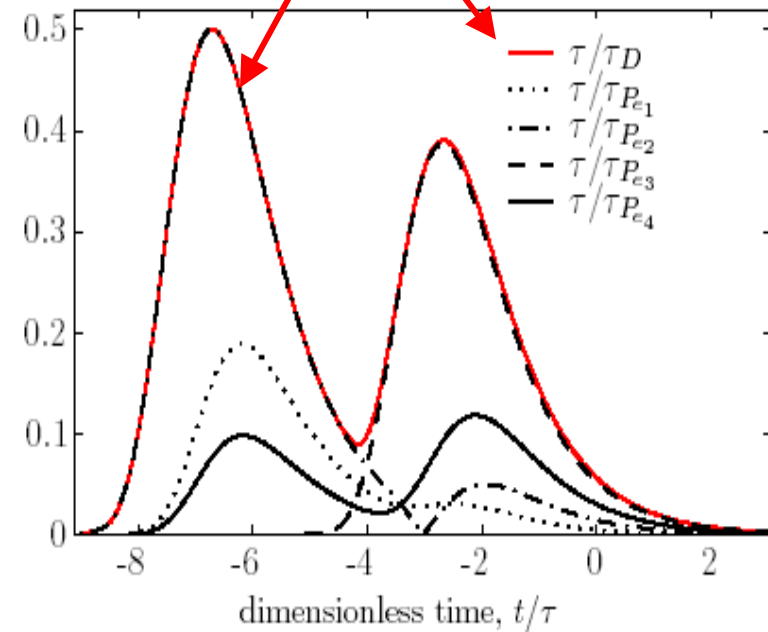
Phys.Rev.E, 73, 026113 (2006)

G.P. Beretta, PIAF '09 "New Perspectives"

References available at: www.quantumtheory.manchester.ac.uk

Relaxation to equilibrium for a 4-level isolated particle

time-entropy
uncertainty
bound



Stable equilibrium state (highest entropy)

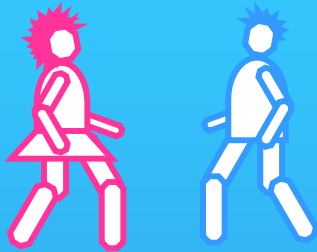
Part IV

- 1) Concept of individual state and an unambiguous representation of preparations, not based on the (von Neumann) density operator
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- 4) The price to pay, due to nonlinearity of the dynamical law
 - Structure of the nonlinear dynamical law for composite systems
 - Locality and separability



No free lunch!* Dealing with composite systems

(*Except at PI)



A = Alice

B = Bob

In linear dynamics, the equation of motion remains

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho]$$

and the structure of the Hamiltonian

$$H = H_A \otimes I_B + I_A \otimes H_B + V_{AB}$$

generates the proper unitary time evolution.

In our nonlinear dynamics, the “proper” time evolution obtains only if the structure of the system is embedded explicitly also in the dynamical equation itself:

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] + \frac{1}{2k_B\tau_A}\{(\Delta M)^A, \rho_A\} \otimes \rho_B + \frac{1}{2k_B\tau_B}\rho_A \otimes \{(\Delta M)^B, \rho_B\}$$

Simply taking

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] + \frac{1}{2k_B\tau}\{\Delta M, \rho\}$$

would entail unphysical results such as superluminal energy exchange even in the absence of interactions!

Nuovo Cimento B, 87, 77 (1985)

quant-ph-0112046

Rep.Math.Phys. (2009)



G.P. Beretta, PI

Steepest-locally-perceived-entropy-ascent

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] + \frac{1}{2k_B\tau_A}\{(\Delta M)^A, \rho_A\} \otimes \rho_B + \frac{1}{2k_B\tau_B}\rho_A \otimes \{(\Delta M)^B, \rho_B\}$$

where τ_A, τ_B are local characteristic times; for $J = A, B$

$$(\Delta M)^J = (\Delta S)^J - (\Delta H)^J / \theta_J$$

$$\theta_J = \langle (\Delta H)^J (\Delta H)^J \rangle / \langle (\Delta S)^J (\Delta H)^J \rangle$$

The following "locally perceived" energy and entropy operators, will determine the "steepest locally perceived entropy ascent" dynamics

$$(\Delta H)^A = \text{Tr}_B[(I_A \otimes \rho_B)\Delta H]$$

$$(\Delta H)^B = \text{Tr}_A[(\rho_A \otimes I_B)\Delta H]$$

$$(\Delta S)^A = \text{Tr}_B[(I_A \otimes \rho_B)\Delta S]$$

$$(\Delta S)^B = \text{Tr}_A[(\rho_A \otimes I_B)\Delta S]$$

Each local dissipative term separately "conserves" the overall system's mean energy $\langle H \rangle = \text{Tr}(\rho H)$. Each subsystem's contribution to the overall system's rate of entropy change is nonnegative definite

$$\frac{d\langle S \rangle}{dt} = \frac{1}{k_B\tau_A} \langle (\Delta M)^A (\Delta M)^A \rangle + \frac{1}{k_B\tau_B} \langle (\Delta M)^B (\Delta M)^B \rangle$$



Steepest-locally-perceived-entropy-ascent

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] + \frac{1}{2k_B\tau_A}\{(\Delta M)^A, \rho_A\} \otimes \rho_B + \frac{1}{2k_B\tau_B}\rho_A \otimes \{(\Delta M)^B, \rho_B\}$$

where τ_A, τ_B are local characteristic times; for $J = A, B$

$$(\Delta M)^J = (\Delta S)^J - (\Delta H)^J / \theta_J$$

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The following "locally perceived" energy and entropy operators, will determine the "steepest locally perceived entropy ascent" dynamics

$$(\Delta H)^A = \text{Tr}_B[(I_A \otimes \rho_B) \Delta H]$$

$$(\Delta H)^B = \text{Tr}_A[(\rho_A \otimes I_B) \Delta H]$$

$$(\Delta S)^A = \text{Tr}_B[(I_A \otimes \rho_B) \Delta S]$$

$$(\Delta S)^B = \text{Tr}_A[(\rho_A \otimes I_B) \Delta S]$$

if $\rho \neq \rho_A \otimes \rho_B$

does not imply

$$\frac{d\rho_A}{dt} = f(\rho_A)$$

Each local dissipative term separately "conserves" the overall system's mean energy $\langle H \rangle = \text{Tr}(\rho H)$. Each subsystem's contribution to the overall system's rate of entropy change is nonnegative definite

$$\frac{d\langle S \rangle}{dt} = \frac{1}{k_B\tau_A} \langle (\Delta M)^A (\Delta M)^A \rangle + \frac{1}{k_B\tau_B} \langle (\Delta M)^B (\Delta M)^B \rangle$$



Conclusions

- 1) Concept of individual state and an unambiguous representation of preparations, not based on the (von Neumann) density operator
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- 4) The price to pay, due to nonlinearity of the dynamical law
 - Rediscoveries
 - Epilogue
 - Measurable effects?
 - Summary



Steepest entropy ascent: “rediscoveries” (15 years later)

- In 2001, S. Gheorghiu-Svirschevski [Phys.Rev.A, 63, 022105-054102 (2001)] re-derived our equation from the variational principle

$$\max \frac{d\langle S \rangle}{dt} \quad \text{subject to} \quad \frac{d\langle H \rangle}{dt} = 0, \quad \frac{d\text{Tr}\rho}{dt} = 0 \quad \text{and} \quad \dot{\gamma}_D \cdot \dot{\gamma}_D = c^2$$

where c^2 is some real functional. Introducing Lagrange multipliers

$$L = \dot{\gamma}_D \cdot S' - \lambda_1 \dot{\gamma}_D \cdot \gamma - \lambda_H \dot{\gamma}_D \cdot H' - \lambda_\tau \dot{\gamma}_D \cdot \dot{\gamma}_D$$

Maximizing yields exactly our dynamics equation.

- In 2001, A. Caticha [AIP Conf.Proc., 568, 72 (2001)] formally rederives steepest entropy ascent dynamical equations, in the case of a continuous (non quantum) probability distribution.
- In 2002, M. Lemanska and Z. Jaeger [Physica D, 170, 72 (2002)] attempt a similar approach, without changing variables to square-root probabilities. As a result, their equation diverges when some probability is zero.

Unfortunately, none of them acknowledged our work, except Gheorghiu-Svirschevski in an addendum.



NATURE VOL. 316 4 JULY 1985

Uniting mechanics and statistics

An adventurous scheme which seeks to incorporate thermodynamics into the quantum laws of motion may end arguments about the arrow of time — but only if it works.

NEWS & VIEWS

NEWS AND VIEWS

Uniting mechanics and statistics

An adventurous scheme which seeks to incorporate thermodynamics into the quantum laws of motion may end arguments about the arrow of time — but only if it works.

The logical relationship between the laws of mechanics and those of thermodynamics deserves more attention than it usually receives. Thermodynamics and statistical mechanics are ways of describing the behaviour of macroscopic systems made from components whose behaviour is determined by the laws of mechanics, classically those of Newton (as amended), but otherwise the equations of motion of quantum mechanics. Where the first law of thermodynamics is concerned, there is no difficulty. In both classical and quantum mechanics, total energy is a constant of the motion and is thus always conserved, at least in a closed system.

The difficulty arises chiefly with the second law of thermodynamics, and not only because there is such a variety of ways in which this principle can be defined. But now a group of three theoreticians has put forward an intriguing way in which the laws of quantum mechanics may be modified so as to incorporate the second law from what appears to be the outset (Beretta, G. F., Gyngö, P. & Parisi, L., *J. Non-Equilibrium Thermodynamics* 8, 77-97, 1985). Whether the modification proposed is sufficient, only time will tell, but the objective seems well worth the trouble Beretta *et al.* have taken.

The difficulty is well illustrated by the way in which some kind of correspondence is established between the mechanical behaviour of a system and its thermodynamic properties. For more than a century, people have been brooding on the paradox that while the laws of classical (and, for that matter, quantum) mechanics are symmetrical with respect to time inversion, the second law selects from all possible trajectories of motion only those corresponding to a continual increase of the entropy. The arrow of time is conjured like a rabbit from a hat.

The definition of entropy in terms of the mechanical properties of the constituents of a system is similarly clouded. The classical model in Boltzmann's *H*-theorem (1872), which shows that the rate of change with time of a certain mathematical construct from the probability distribution of single particles in phase space will always be zero or negative. So Boltzmann argued, his quantity *H* is admirably suited to be the negative of what is known in thermodynamics as entropy. This is an argument by analogy, but none the worse for that — if it works.

Since Boltzmann's time, there has

accumulated a rich literature on the implied paradox of the conflict between the irreversibility of macroscopic processes and the reversibility (in time) of the laws of mechanics and thus of microscopic processes. Indeed, the argument was begun by Loschmidt in 1876, but now even elementary textbooks of thermodynamics reckon to give some kind of account of it.

The standard explanation is that the apparent paradox is not a paradox at all, but a confusion about time-scales. Any measure of entropy, that derived from Boltzmann's *H* or otherwise, will fluctuate (and so decrease as well as increase on a short timescale), which is not inconsistent with the notion that the average value of the entropy should increase steadily over long periods of time (or remain unchanged when the system is in equilibrium).

Much the same is said of the recurrence paradox, based on the observation due to Poincaré that the point in phase space (momentum as well as position) representing the state of a classical system will return to more or less the same place after a sufficient length of time. On the face of things, that means that non-equilibrium states of a system will repeatedly recur.

The standard resolution of this paradox is the observation that, for any realistic system, the interval of time between recurrences will be huge, much greater than, say, the age of the Universe. Again there is nothing wrong with these arguments, but they are far from being rigorous.

So why not take the bull by the horns, and build irreversibility into the laws of mechanics? That is the point from which Beretta *et al.* start. Properly, they acknowledge that they are not the first to treat this path. They work with quantum statistical mechanics, where the formalism is easier. They start from the equation of motion for the operator representing the state of a physical system, say \mathbf{m} , which is, in operator language, $d\mathbf{m}/dt = -i[\mathbf{H}, \mathbf{m}]$, where \mathbf{H} is the Hamiltonian operator of the system and i and the square root of minus one and Planck's constant (divided by 2π) respectively. The quantity in square brackets is the commutator of its two components, $\mathbf{m}\mathbf{H} - \mathbf{H}\mathbf{m}$.

The natural way to proceed is to assume that this equation is modified in such a way that the right-hand side is some other function of the state operator \mathbf{m} than in the standard form. The objective is to find a form of the function which is compatible

both with what is known of the evolution of thermodynamic systems and, perhaps more important, the dynamics of real microscopic systems. Beretta *et al.* have convinced themselves that the function they are seeking cannot be a linear function of \mathbf{m} . What they propose is the addition to the right-hand side of the quantum equation of motion of a particular function of \mathbf{m} which, by including both the square root and the logarithm of the state operator of the system, is non-linear enough to satisfy anybody's taste.

Almost magically, the system has some of the obviously necessary properties. For example, for a system in a pure quantum state, say that represented by a solution of Schrödinger's equation, the extra terms vanish and the simple form of the equation of motion applies. Similarly, constants of the motion in the new system are also constants of the motion determined by the simpler equation of motion.

What can be said about the entropy? In reality, the state operator \mathbf{m} is the equivalent of what is called the density matrix in quantum statistical mechanics, which why Beretta *et al.* define entropy in terms of the operator analogue, where the definition is the natural logarithm of the operator \mathbf{m} . Specifically, the entropy is the negative of the trace of this operator multiplied by Boltzmann's constant, the authors are able to show it increases (or does not increase) the course of time.

So is this a demonstration that the laws of mechanics and thermodynamics can indeed be combined? Not quite. For one thing, there are various mathematical problems that take some of the steps in the argument conjectural. Worse still, some of the operator functions in the formalism are sometimes undefined. But the authors leave the alert reader changing their minds — the paper now published contains a composite system the treatment in operator language, due to a paper published a year ago.

None of this implies that the arguments about the reconciliation between microscopic reversibility and macroscopic irreversibility will now be stilled. Indeed, while for as long as the present justification of the basis of statistical mechanics holds water, there will be many who say that what Beretta *et al.* have done is strictly unnecessary. But this is a field in which the proof of the pudding is in the eating.

John Maddox

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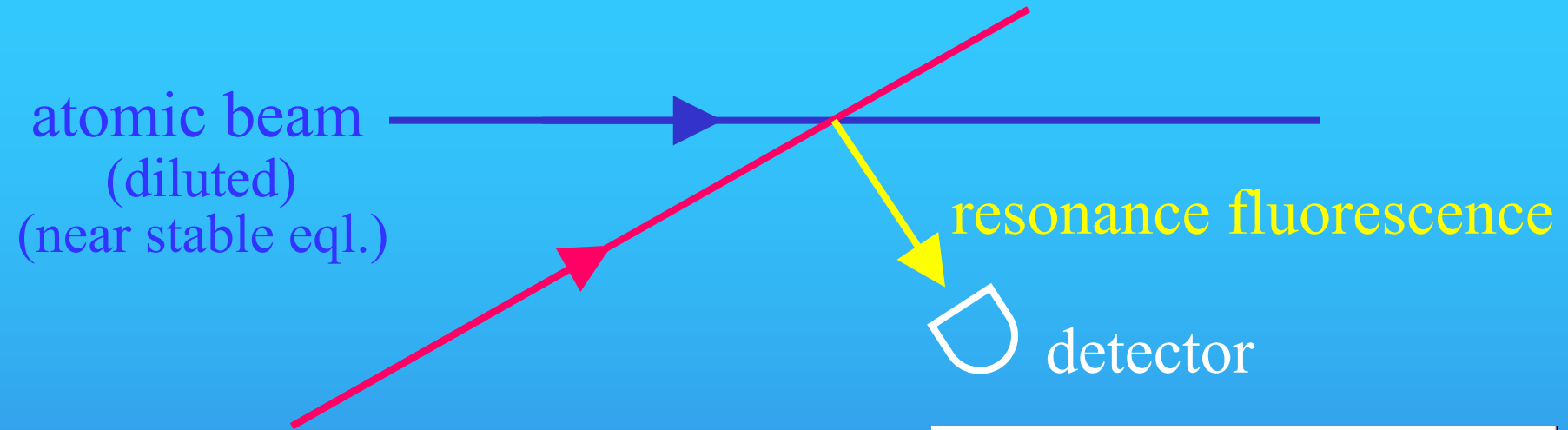
John Maddox



G.P. Beretta, PIAF '09 "New Perspectives on the Quantum State", Perimeter Institute, Sept.27-Oct.2, 2009

References available at: www.quantumthermodynamics.org

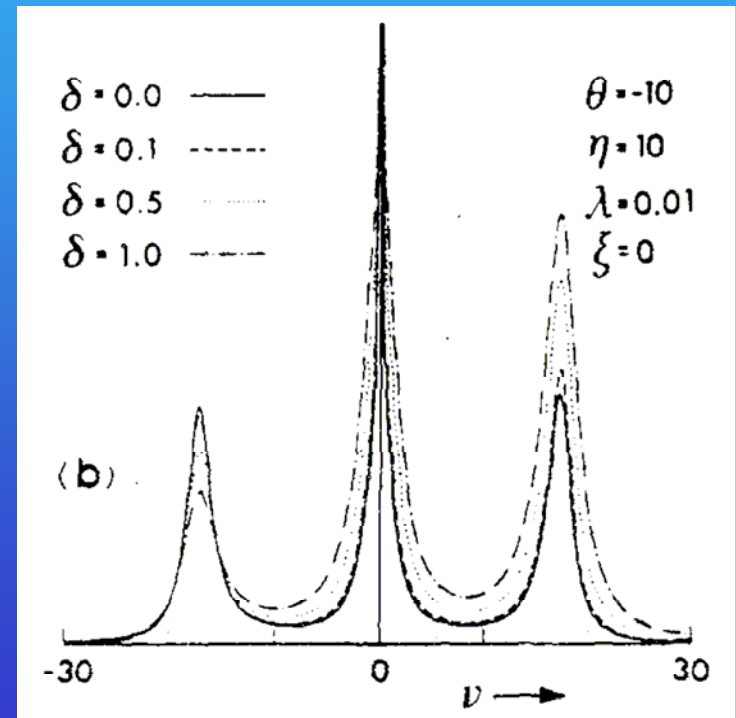
Measurable effects?



Irreversible internal redistribution
implies

asymmetries

in the spectral distribution



Int.J.Theor.Phys., 24, 1233 (1985)

G.P. Beretta, PIAF '09 "New Perspectives on the Quantum State", Perimeter Institute, Sept.27-Oct.2, 2009

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Measurable effects?

laser beam (“probe”)

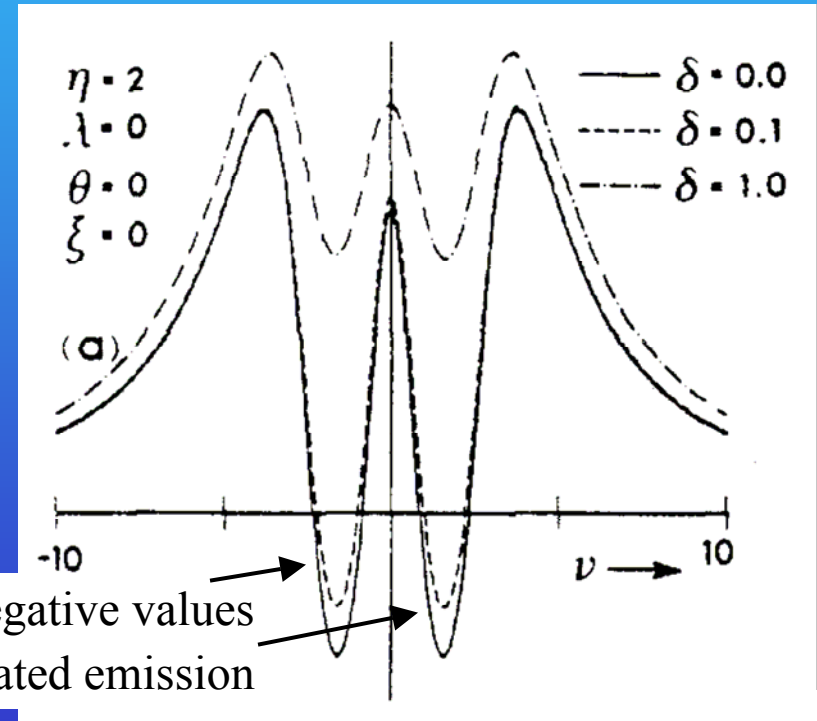
atomic beam
(diluted)
(near stable eql.)

absorption and
stimulated emission

detector

laser beam (“pump”)
on resonance (tuned)

Irreversible internal redistribution
implies
attenuation
of stimulated emission



Int.J.Theor.Phys., 24, 1233 (1985)

G.P. Beretta, PIAF '09 "New Perspectives on the Quantum State", Perimeter Institute, Sept.27-Oct.2, 2009

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Conclusions - “an ontic role of the density operator makes Quantum Thermodynamics fundamental”

- The second law is forced directly into the microscopic laws and emerges as a theorem of the constrained steepest-entropy-ascent (or maximal entropy generation) dynamical law (stability of equilibrium states)
- Entropy emerges from the microscopic level as a measure of the degree of “load sharing” among the particle’s energy levels.
- Irreversibility emerges as a manifestation of spontaneous internal load redistribution among the initially occupied energy levels.
- Yet the dynamical equation is mathematically reversible.
- Nonlinearity requires a non-universal formal structure of the dynamical law. The structure is "model dependent": like the Hamiltonian, it depends on what subsystems are assumed as elementary and separable, i.e., non communicating.
- Standard (pure state) quantum mechanics emerges as the (mildly unstable) boundary solutions (limit cycles) of the more general theory
- The theory is conceptually controversial, but mathematically robust, awaits experimental validation and philosophical scrutiny

