

Title: What if Quantum Thermodynamics were a fundamental extension of Quantum Mechanics?

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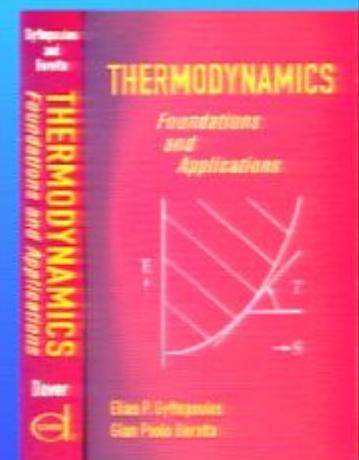
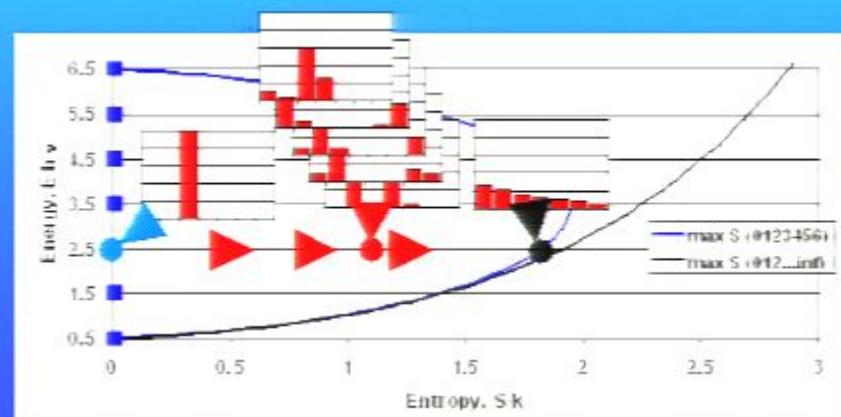
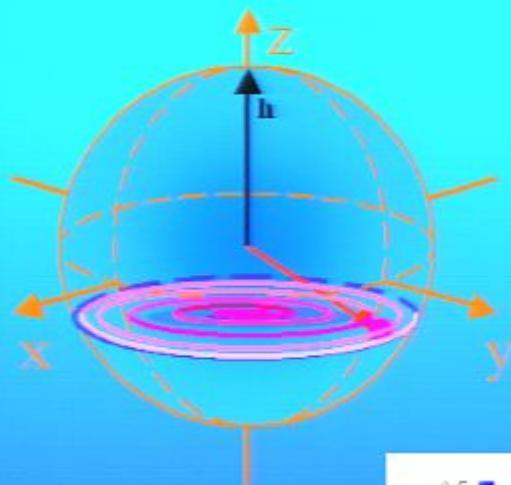
Abstract: What if the second law of thermodynamics, in the hierarchy of physical laws, were at the same level as the fundamental laws of mechanics, such as the great conservation principles? What if entropy were an intrinsic property of matter at the same level as energy is universally understood to be? What if irreversibility were an intrinsic feature of the microscopic dynamical law of all physical objects, including an individual qubit or qudit?

This talk will show how positive answers to these questions need not contradict any of the known results of quantum mechanics. We construct a logically consistent, mathematically sound and definite, physically intriguing, non-relativistic and non-statistical quantum theory, in which the second law of thermodynamics is embedded as a fundamental microscopical law. The theory hinges upon a nonlinear extension of unitary Hamiltonian dynamics which for uncorrelated and noninteracting systems reduces to the usual Schrödinger equation for the zero entropy states, but in general generates a group (not a semi group) of irreversible time evolutions, where the non-Hamiltonian entropy generating term in the evolution equation attracts the state towards the direction of maximal entropy increase. Various examples and features of this highly non-conventional dynamical theory are discussed. References available at <http://www.quantumthermodynamics.org/>

# What if Quantum Thermodynamics were a fundamental extension of Quantum Mechanics?

Gian Paolo Beretta

Università di Brescia, Italy



G.P. Beretta, Seminar "What if Quantum Thermodynamics were a fundamental extension of Quantum Mechanics?"  
Perimeter Institute, Waterloo, Canada, November 8, 2007 - References available at: [www.quantumthermodynamics.org](http://www.quantumthermodynamics.org)

# Outline

- Motivation for a new theory
- Ansatz #1: extension of Quantum Mechanics that builds the 2<sup>nd</sup> law of Thermodynamics directly into microscopic kinematics
- Ansatz #2: steepest-entropy-ascent quantum dynamics that builds irreversibility at the fundamental level, preserving standard QM
- Features of the resulting theory
  - equivalent variational formulation
  - numerical results for a 4-level system
  - stable and unstable equilibrium states and limit cycles
  - mathematical reversibility and the arrow of time
  - time-energy and time-entropy uncertainty relations
  - Onsager relations
  - measurable results



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

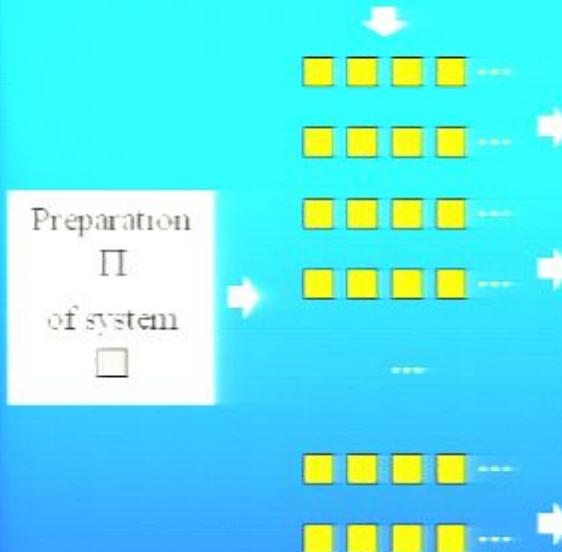
Ensemble  $\mathcal{E}_\Pi$

of identical systems all prepared by  $\Pi$  at time  $t$

Park and Band, FoundPhys.

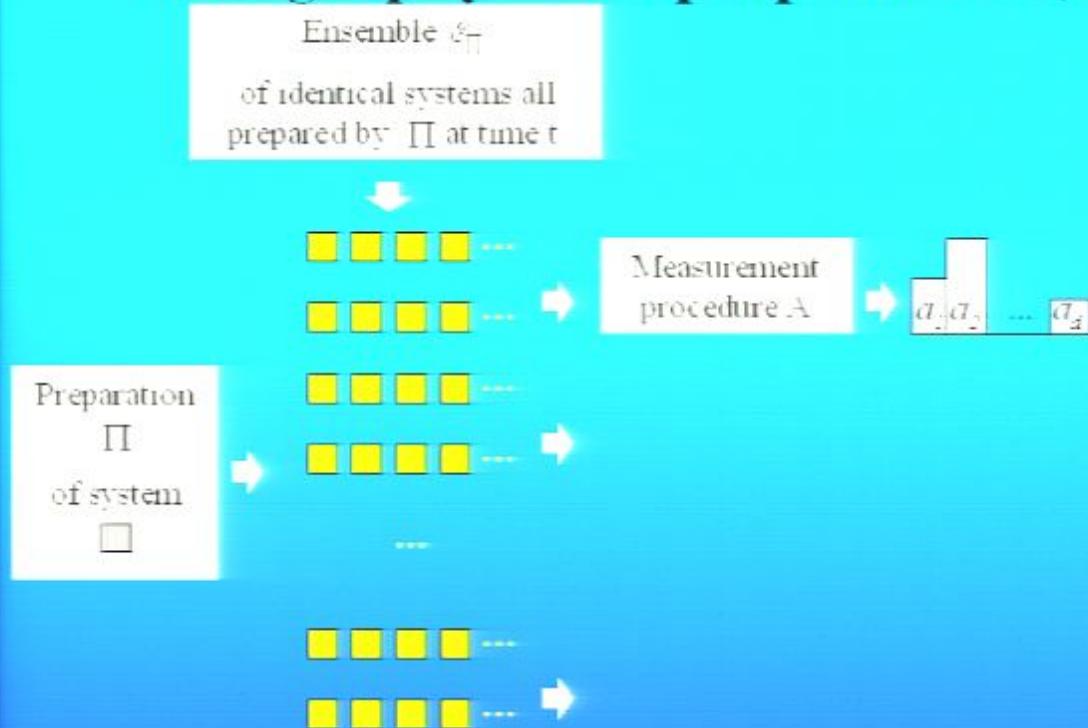
1, 133 (1970); 1, 211 (1971);

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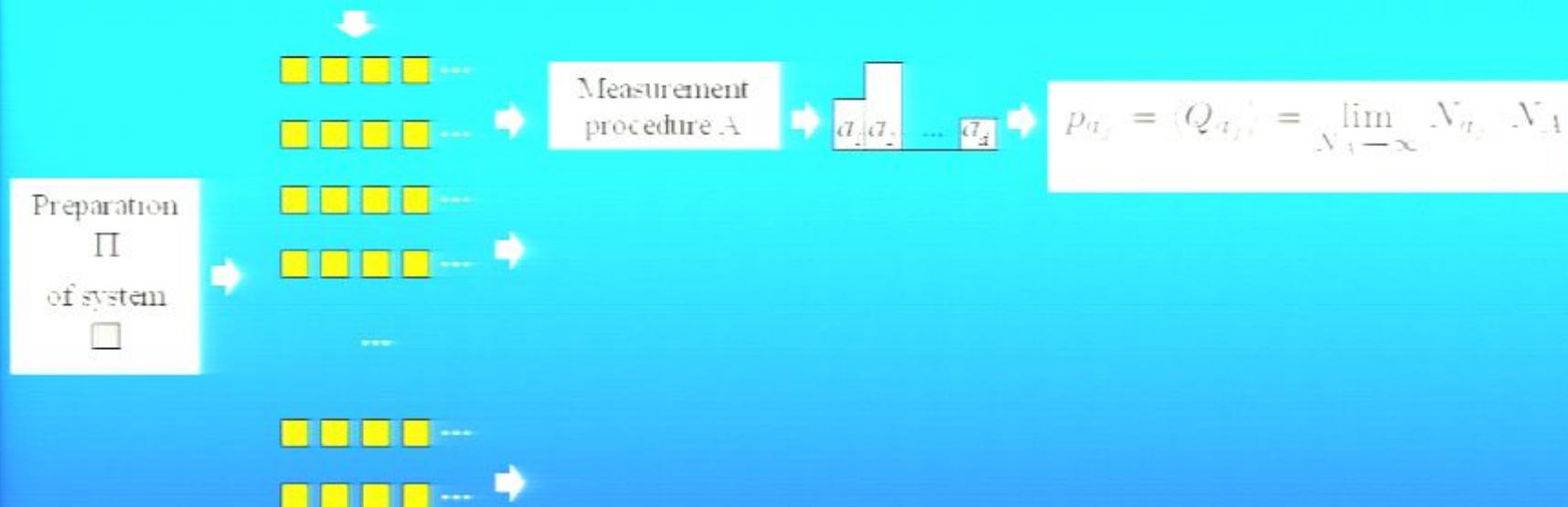
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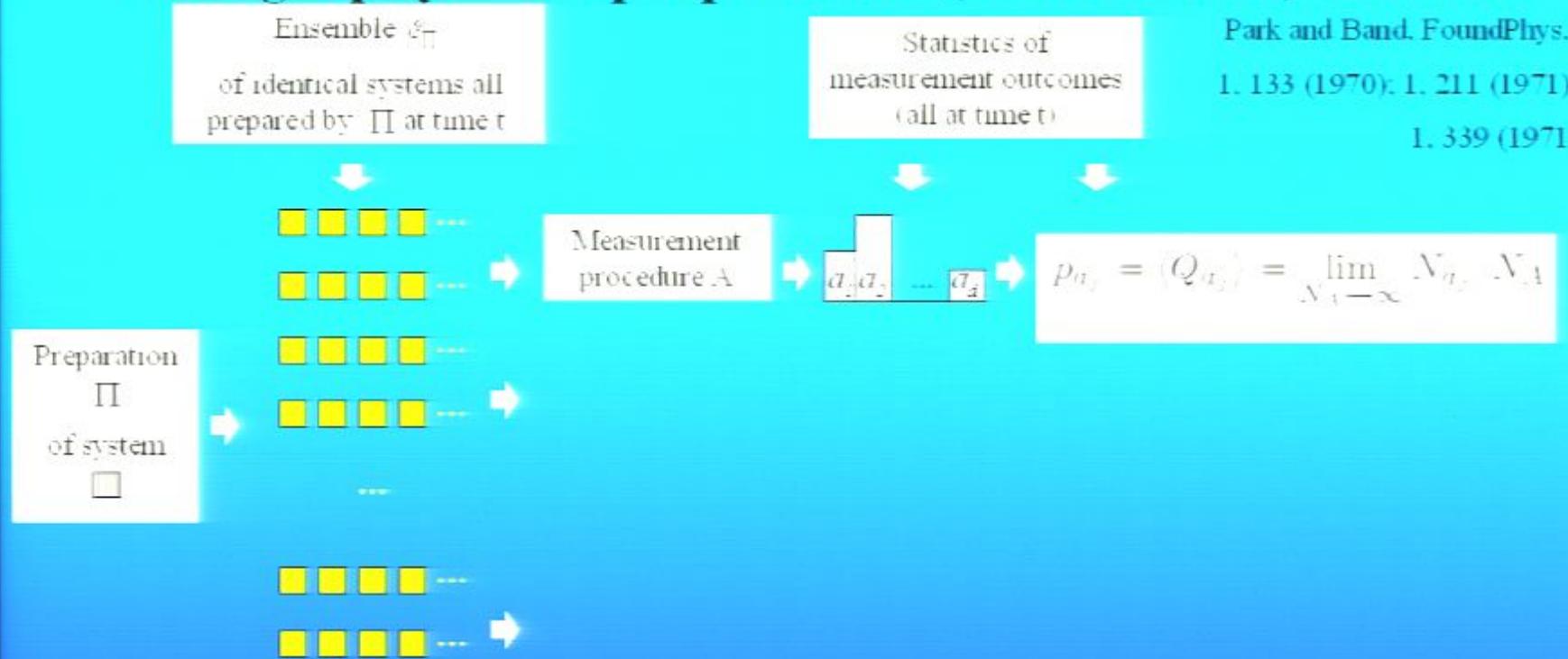
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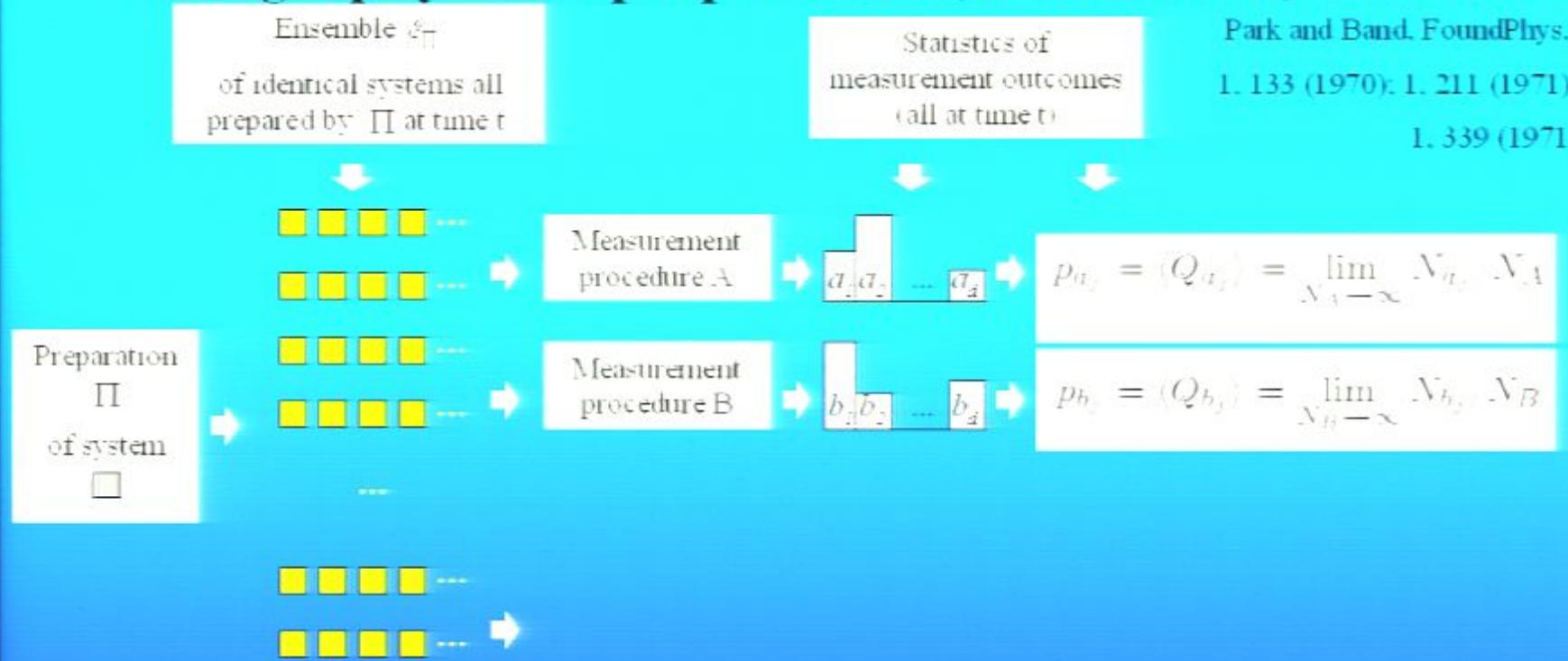
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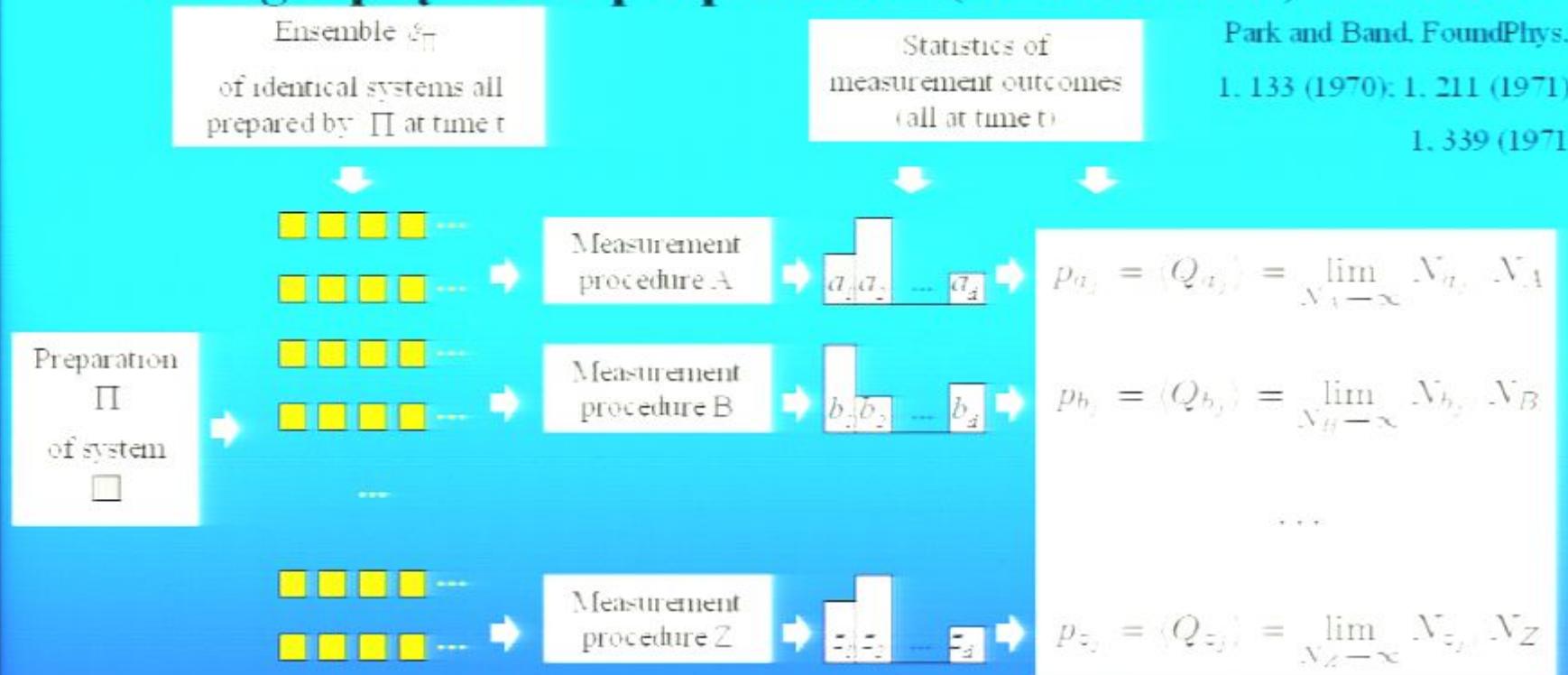
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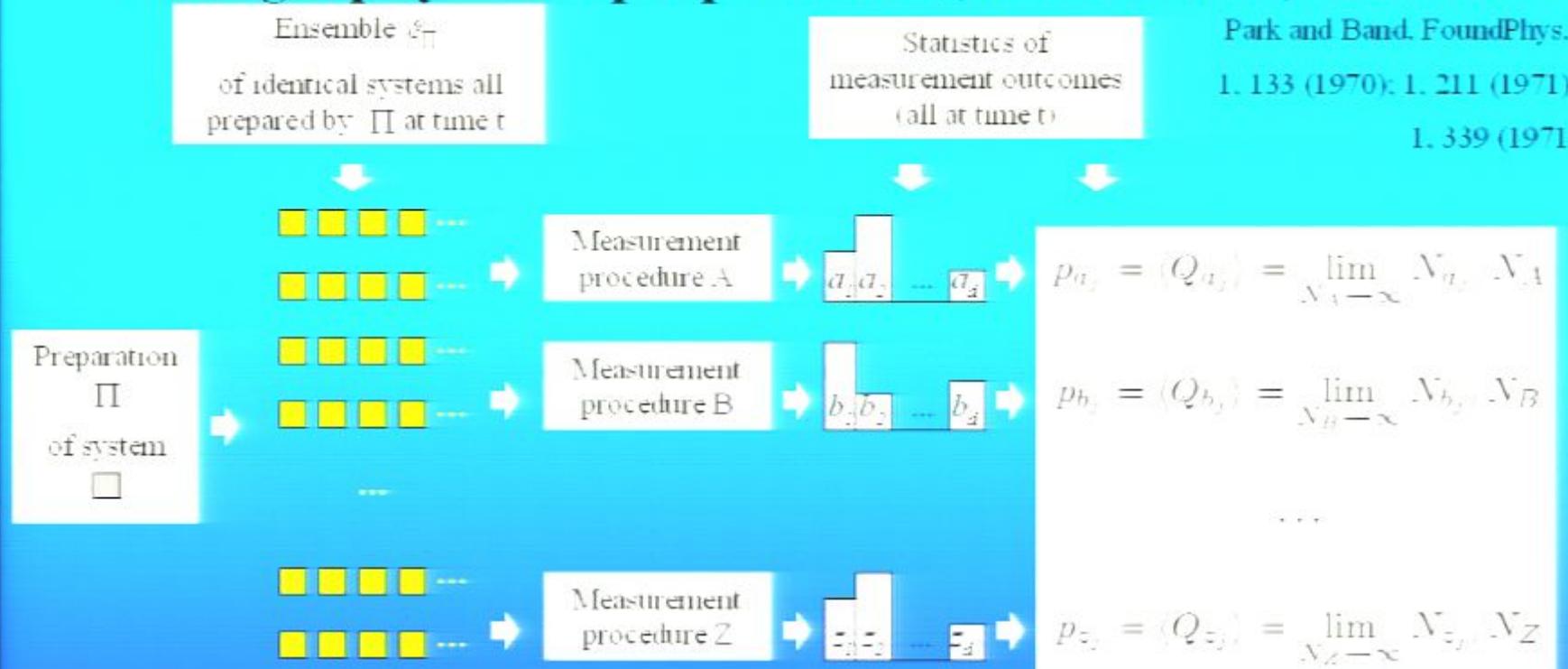
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# “Tomography” of a preparation (or ensemble) at time $t$



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

$$\Pi = \mathcal{E}_\Pi = \{p_{a_1}, \dots, p_{a_n}, p_{b_1}, \dots, p_{b_n}, \dots, p_{z_1}, \dots, p_{z_n}\}$$



# Statistical mixing of preparations (or ensembles)

Preparation  $\Pi$

Preparation

$\Pi_1$

of system



$w_1$



Preparation

$\Pi_2$

of system



$w_2$

For any observable  $A$ , the statistics (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 full statistics is

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



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## Homogeneous vs Heterogeneous preparations (or ensembles)

Given a preparation  $\Pi$ , we may look for *all conceivable decompositions*. We say that  $\Pi$  is *homogeneous* (von Neumann) iff there is no way to obtain the same full statistics from the statistical mixture of two *different* preparations, i.e.,

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



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## Homogeneous preparations (or ensembles) and “states”

For a homogeneous preparation,  $\Pi^0$ , no subdivision into different subensembles is conceivable and, therefore, the entire statistics  $\Pi^0$  can be assigned to (is an intrinsic feature of) each individual member of the ensemble.

Von Neumann, book, engl transl 1932



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But this qualifies to represent the concept of *individual state* only if every heterogeneous preparation (ensemble) admits one and only one decomposition into homogeneous components. Otherwise:

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Schrödinger, PCPS, 32, 446 (1936)

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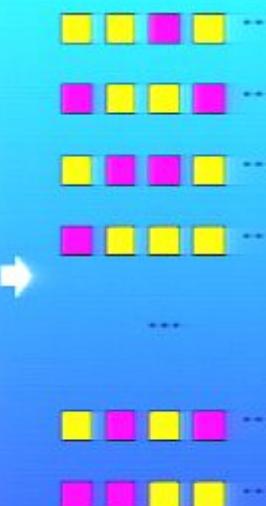
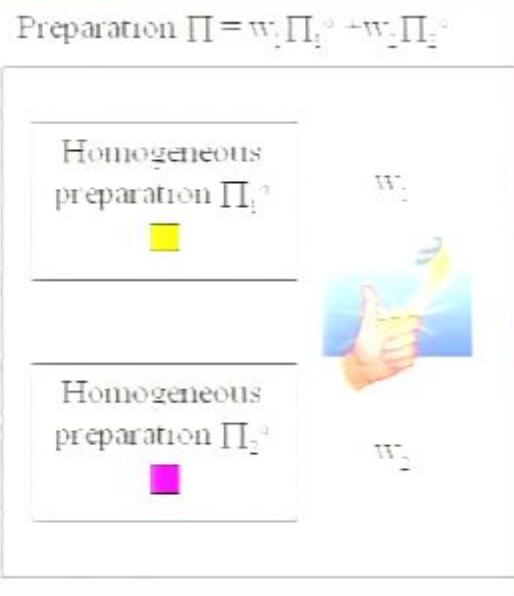


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“State is either or ”



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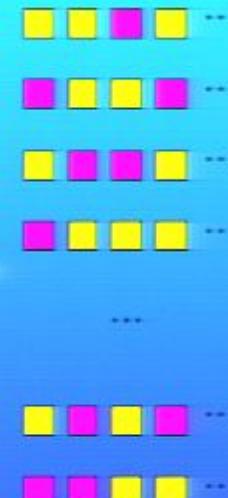
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$w_1$

Homogeneous preparation  $\Pi_2^0$



Preparation  $\Pi = w_3 \Pi_3^0 + w_4 \Pi_4^0$

Homogeneous preparation  $\Pi_3^0$



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Homogeneous preparation  $\Pi_4^0$



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# Traditional construction

## Mechanics:

Homogeneous preparation of a system

Construct	Classical representative	Quantal counterpart
I. System	Phase space	Hilbert space
II. State of system	Phase point ( $q, p$ )	Ray ( $ P\rangle$ )
III. Observable	Function of phase	Hermitian operator with complete orthonormal eigenvector set



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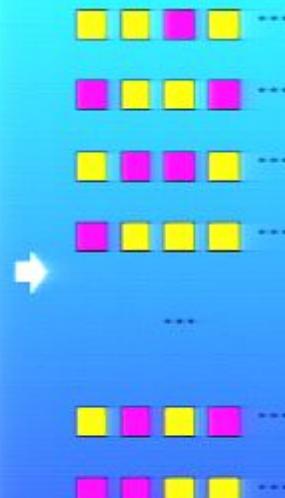
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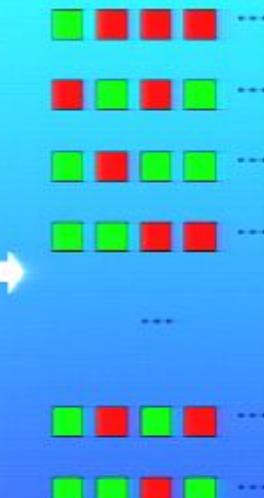
Preparation  $\Pi = w_1 \Pi_1^0 + w_4 \Pi_4^0$

Homogeneous preparation  $\Pi_1^0$



$w_1$

Homogeneous preparation  $\Pi_4^0$



“State is either or ”

contradicts

“State is either or ”



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II. State of system	Phase point $(q, p)$	Ray $  \Psi \rangle$
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## Statistical Mechanics:

Heterogeneous preparation of a system

Construct	Classical	Quantum
IV. Ignorance of true state	Gibbsian coefficient of probability of phase $\rho(q, p)$	Density operator $\hat{\rho} = \sum_i w_i   \phi_i \rangle \langle \phi_i  $



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# Traditional construction

## Mechanics:

Construct	Classical representative	Quantal counterpart
I. System	Phase space	Hilbert space
II. State of system	Phase point ( $q, p$ )	Ray in $\mathcal{H}$
III. Observable	Function of phase	Hermitian operator with complete orthonormal eigenvector set

Homogeneous preparation of a system →

## Statistical Mechanics:

Heterogeneous preparation of a system →

IV. Ignorance of true state

## Classical

Gibbsian coefficient of probability of phase  $\rho(q, p)$

## Quantum

Density operator  
 $\rho = \sum_i w_i |a_n\rangle \langle a_n|$

Unique decomposition?

YES

NO



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# Mixed density operators have multiple decompositions into ‘pure’ ones

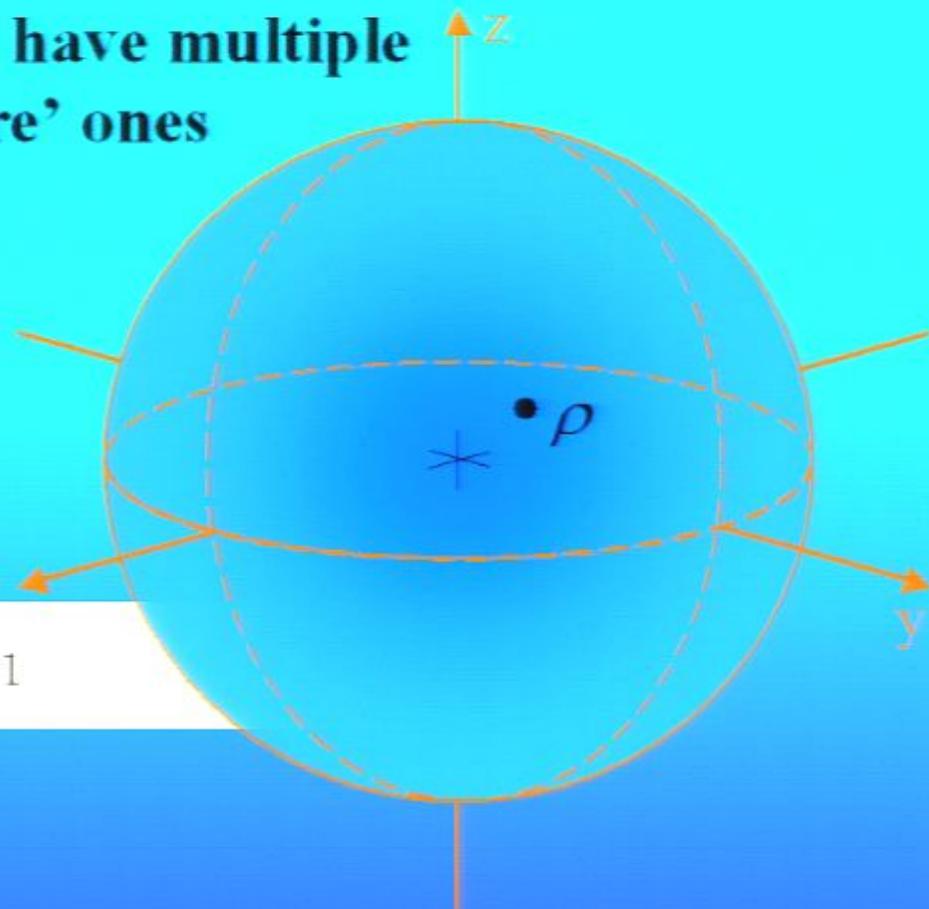
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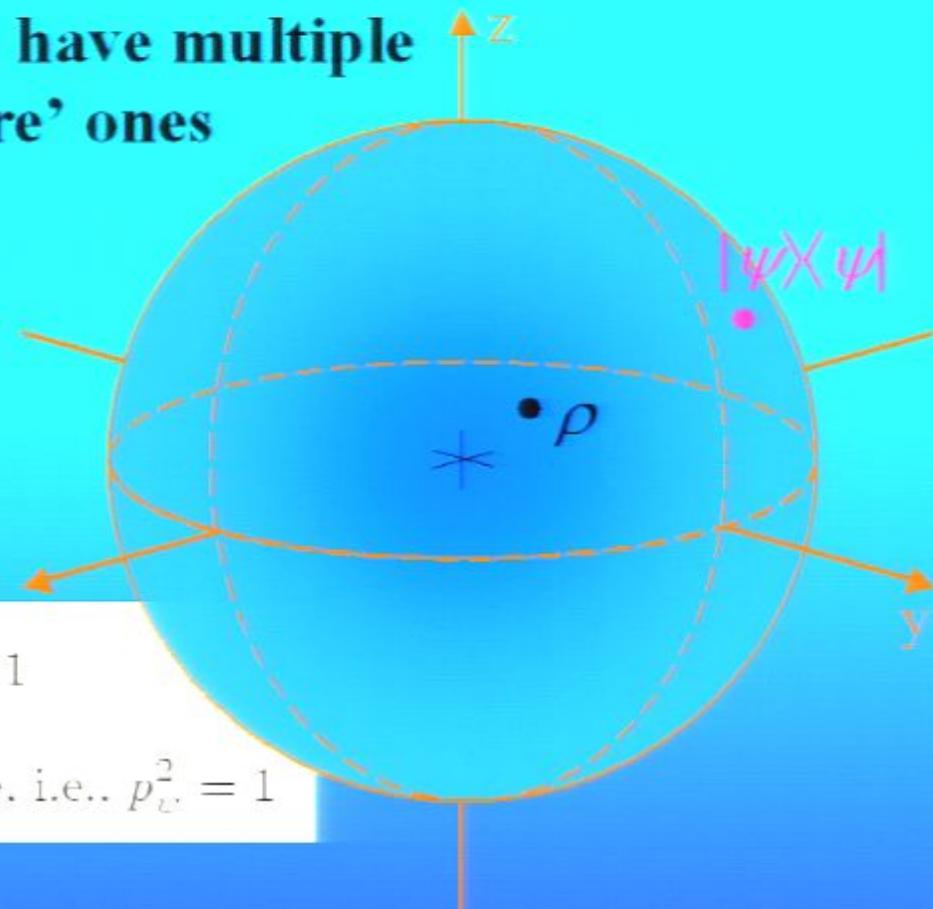
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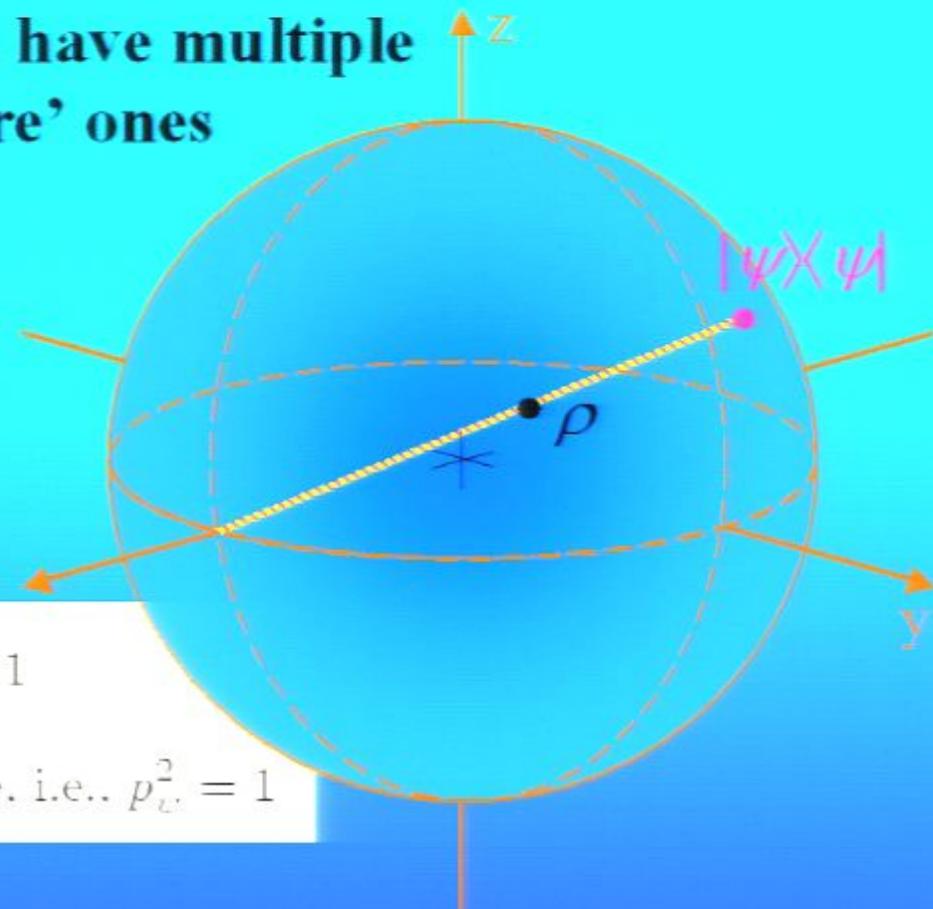
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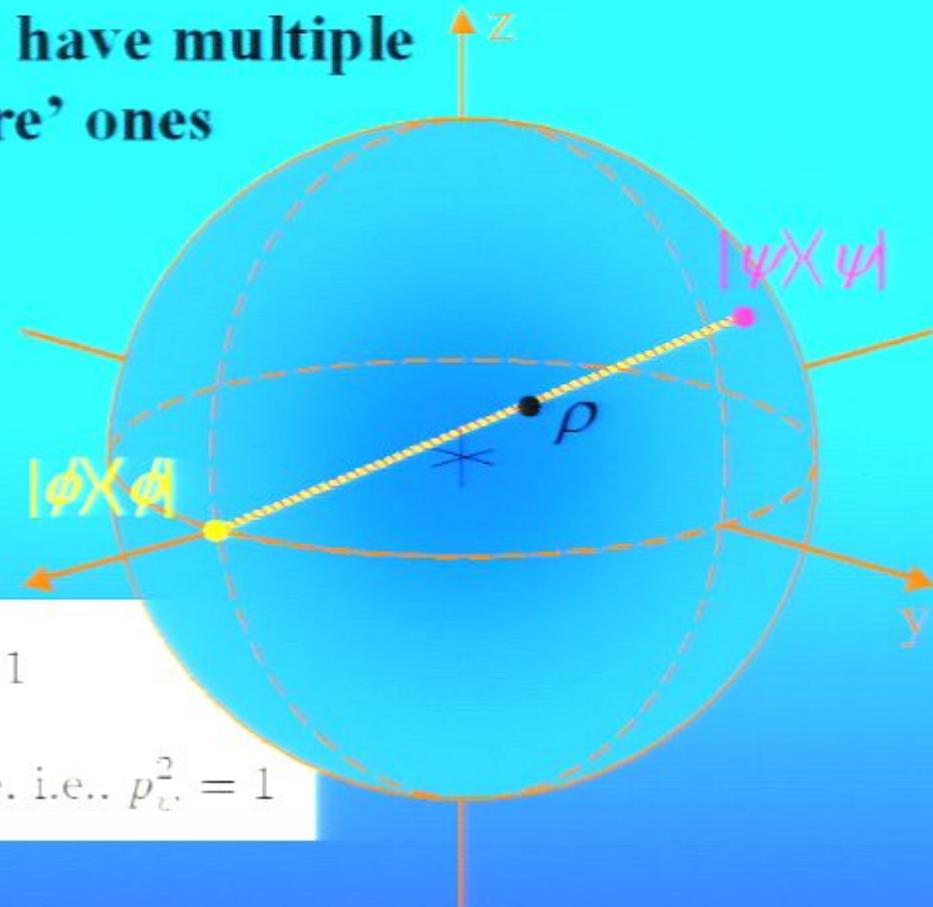
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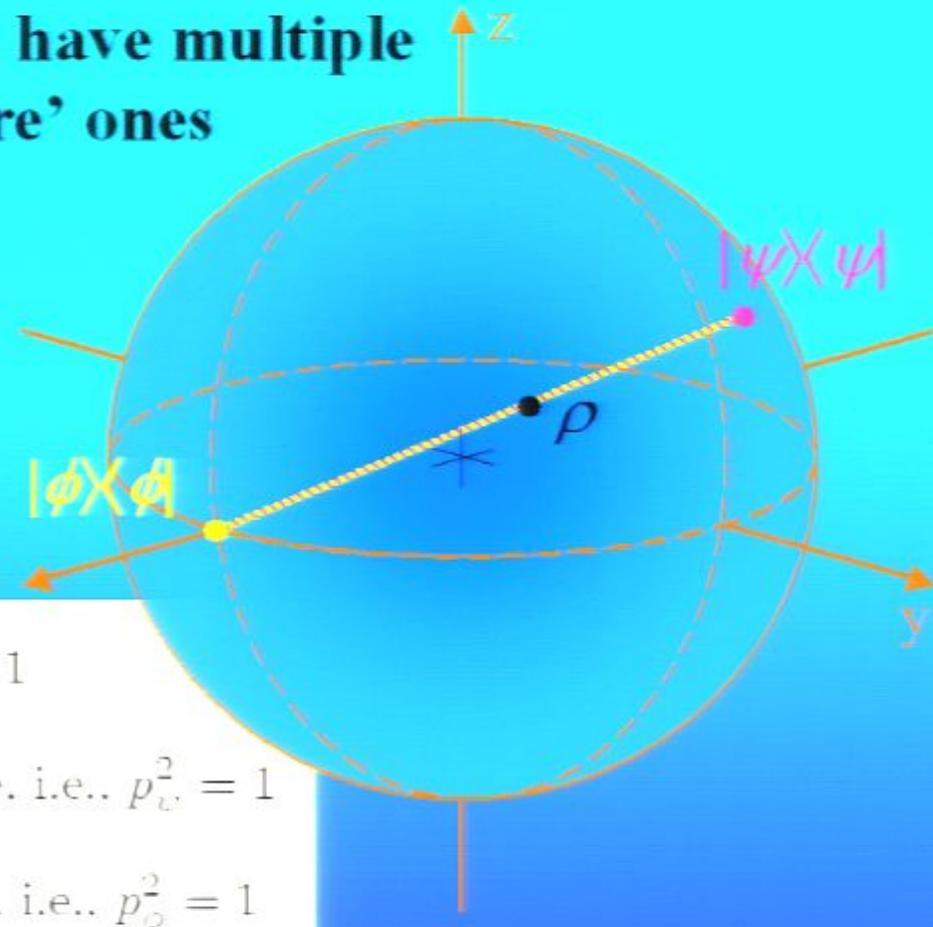
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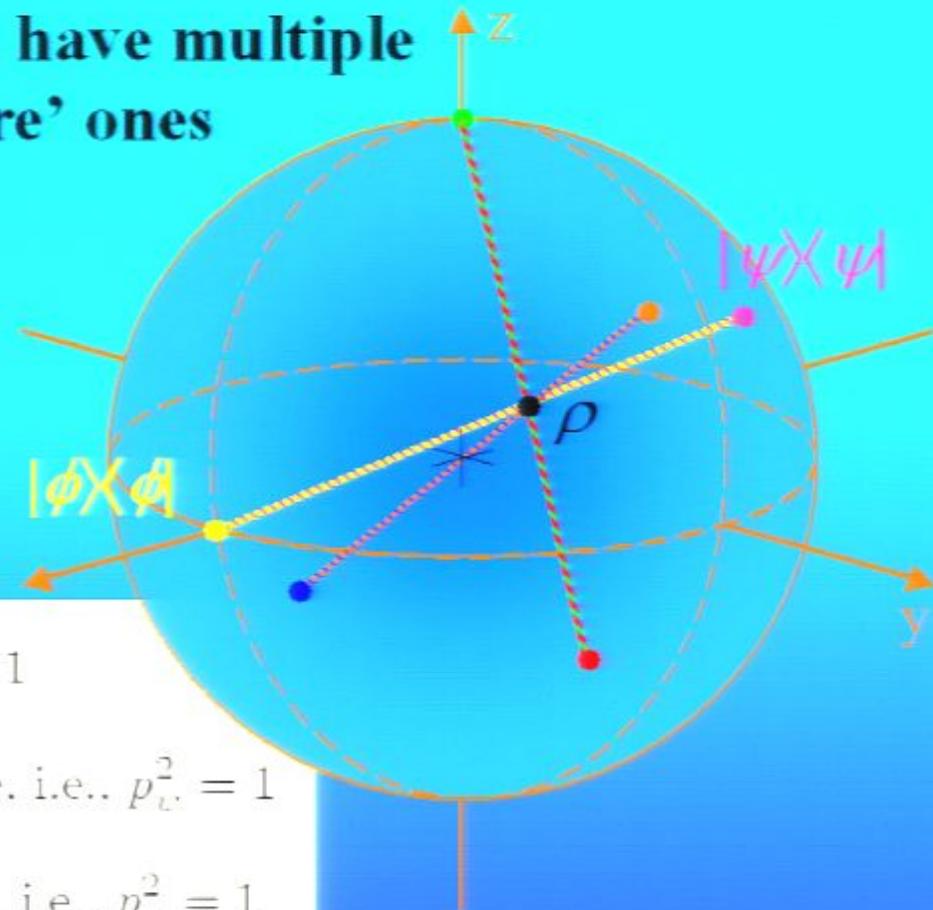
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# Quantum Statistical Mechanics does not conform to the desiderata ... but it is extremely successful in describing thermodynamic equilibrium data

Boltzmann, Fermi-Dirac, Bose-Einstein thermodynamic equilibrium statistics, regularized by:

"Canonical" equilibrium density operators

$$\rho_{ce} = \frac{\exp(-\beta H)}{\text{Tr} \exp(-\beta H)}$$

$\max -\text{Tr} \rho \ln \rho$  subject to  $\text{Tr} \rho H = \langle E \rangle$  and  $\text{Tr} \rho = 1$ .

"Grand canonical" equilibrium density operators

$$\rho_{gec} = \frac{\exp[-\beta(H - \sum_{j=1}^r \mu_j N_j)]}{\text{Tr} \exp[-\beta(H - \sum_{j=1}^r \mu_j N_j)]}$$

$\max -\text{Tr} \rho \ln \rho$  for  $\text{Tr} \rho H = \langle E \rangle$ ,  $\text{Tr} \rho N_j = \langle N_j \rangle$ ,  $\text{Tr} \rho = 1$ .



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# Quantum Statistical Mechanics does not conform to the desiderata ... but it is extremely successful in describing thermodynamic equilibrium data

Boltzmann, Fermi-Dirac, Bose-Einstein thermodynamic equilibrium statistics, regularized by:

"Canonical" equilibrium density operators

$$\rho_{ce} = \frac{\exp(-\beta H)}{\text{Tr} \exp(-\beta H)}$$

$\max -\text{Tr} \rho \ln \rho$  subject to  $\text{Tr} \rho H = \langle E \rangle$  and  $\text{Tr} \rho = 1$ .

"Grand canonical" equilibrium density operators

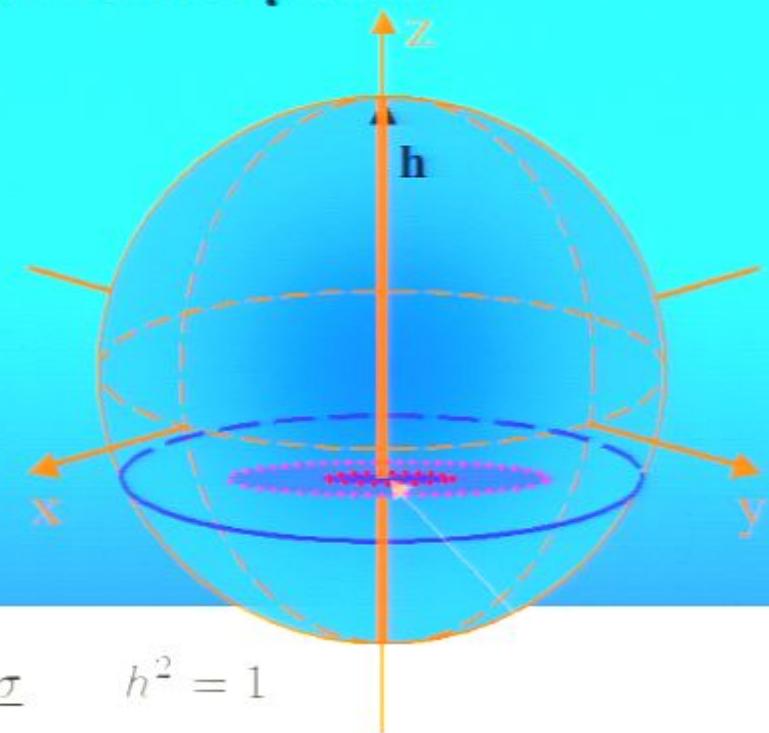
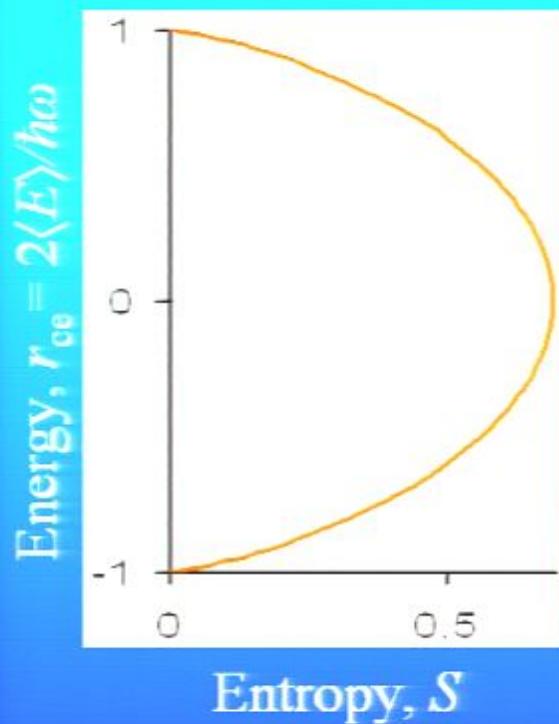
$$\rho_{gce} = \frac{\exp[-\beta(H - \sum_{j=1}^r \mu_j N_j)]}{\text{Tr} \exp[-\beta(H - \sum_{j=1}^r \mu_j N_j)]}$$

$\max -\text{Tr} \rho \ln \rho$  for  $\text{Tr} \rho H = \langle E \rangle$ ,  $\text{Tr} \rho N_j = \langle N_j \rangle$ ,  $\text{Tr} \rho = 1$ .



G.P. Beretta, Seminar "What if Quantum Thermodynamics were a fundamental extension of Quantum Mechanics?"  
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# Quantum Statistical Mechanics, for a single isolated and uncorrelated two-level system



$$H = \frac{1}{2} \hbar \omega \underline{h} \cdot \underline{\sigma} \quad h^2 = 1$$

$$\rho_{ee} = \frac{1}{2}(I + r_{ee} \underline{h} \cdot \underline{\sigma}) \quad r_{ee} = \frac{\langle E \rangle}{\hbar \omega / 2}$$

$$S_{ee} = -k_B \left( \frac{1+r_{ee}}{2} \ln \frac{1+r_{ee}}{2} + \frac{1-r_{ee}}{2} \ln \frac{1-r_{ee}}{2} \right)$$



G.P. Beretta, Seminar "What if Quantum Thermodynamics were a fundamental extension of Quantum Mechanics?"  
Perimeter Institute, Waterloo, Canada, November 8, 2007 - References available at: [www.quantithermodynamics.org](http://www.quantithermodynamics.org)

# Traditional construction

## Mechanics:

Construct	Classical representative	Quantal counterpart
I. System	Phase space	Hilbert space
II. State of system	Phase point ( $q, p$ )	Ray in $\mathcal{H}$
III. Observable	Function of phase	Hermitian operator with complete orthonormal eigenvector set

**Homogeneous preparation of a system** →

## Statistical Mechanics:

**Heterogeneous preparation of a system** →

IV. Ignorance of true state	Gibbsian coefficient of probability of phase $\rho(q, p)$	Density operator $\hat{\rho} = \sum_i w_i  a_i\rangle\langle a_i $
-----------------------------	---	---

**Unique decomposition?**

**YES**

**NO**



Park&Band-FoundPhys-6-157-1976

G.P. Beretta, Seminar "What if Quantum Thermodynamics were a fundamental extension of Quantum Mechanics?"

Perimeter Institute, Waterloo, Canada, November 8, 2007 - References available at: [www.quantumthermodynamics.org](http://www.quantumthermodynamics.org)

# Quantum Thermodynamics as a fundamental extension of Quantum Mechanics

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

## Mechanics:

Homogeneous preparation of a system

## Classical Mechanics

Construct	Classical representative	Quantal counterpart
I. System	Phase space	Hilbert space
II. State of system	Phase point ( $q, p$ )	Density operator
III. Observable	Function of phase	Hermitian operator with complete orthonormal eigenvector set

## Statistical Mechanics:

Heterogeneous preparation of a system

IV. Ignorance of true state

## Classical

Gibbsian coefficient of probability of phase  $\rho(q, p)$

## Quantum

~~Density operator~~  
 $\rho = \sum_n \alpha_n |n\rangle \langle n|$

Unique decomposition?

YES



Park&Band-FoundPhys-6-157-1976

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# Quantum Thermodynamics as a fundamental extension of Quantum Mechanics

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II. State of system	Phase point ( $q, p$ )	Density operator
III. Observable	Function of phase	Hermitian operator with complete orthonormal eigenvector set

## Statistical Mechanics:

Heterogeneous preparation of a system

IV. Ignorance of true state

## Classical

Gibbsian coefficient of probability of phase

## Quantum

Subjective probability distribution defined over the density operators

Unique decomposition?

YES

YES



Park&Band-FoundPhys-6-157-1976

G.P. Beretta, Seminar "What is Quantum Thermodynamics now: a fundamental extension of Quantum Mechanics?"

Perimeter Institute, Waterloo, Canada, November 8, 2007 - References available at: [www.quantumthermodynamics.org](http://www.quantumthermodynamics.org)

# Isolated two-level system, standard Quantum Mechanics

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

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

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

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

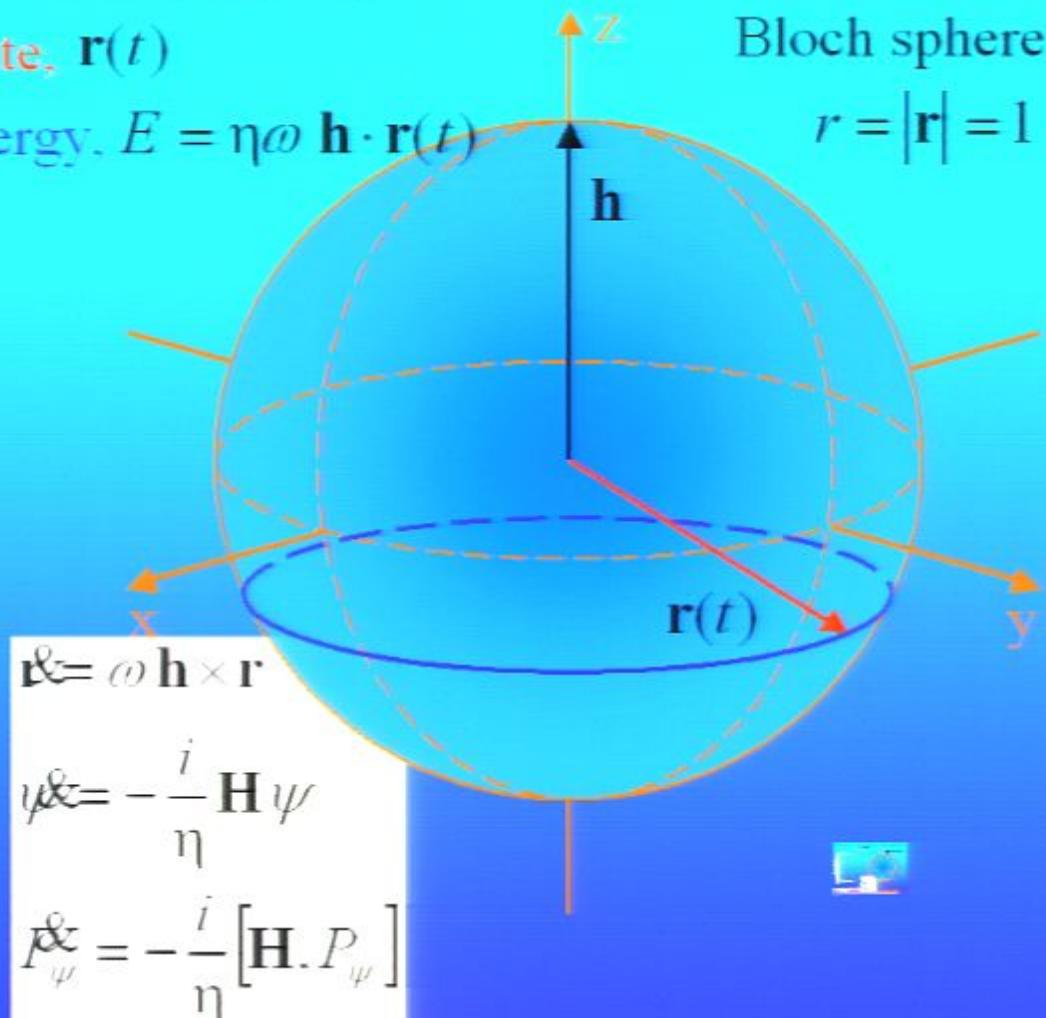
Spin up

Energy,  $2E/\hbar\omega$

0

Spin down

-1



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Perimeter Institute, Waterloo, Canada, November 8, 2007 - References available at: [www.quantumthermodynamics.org](http://www.quantumthermodynamics.org)

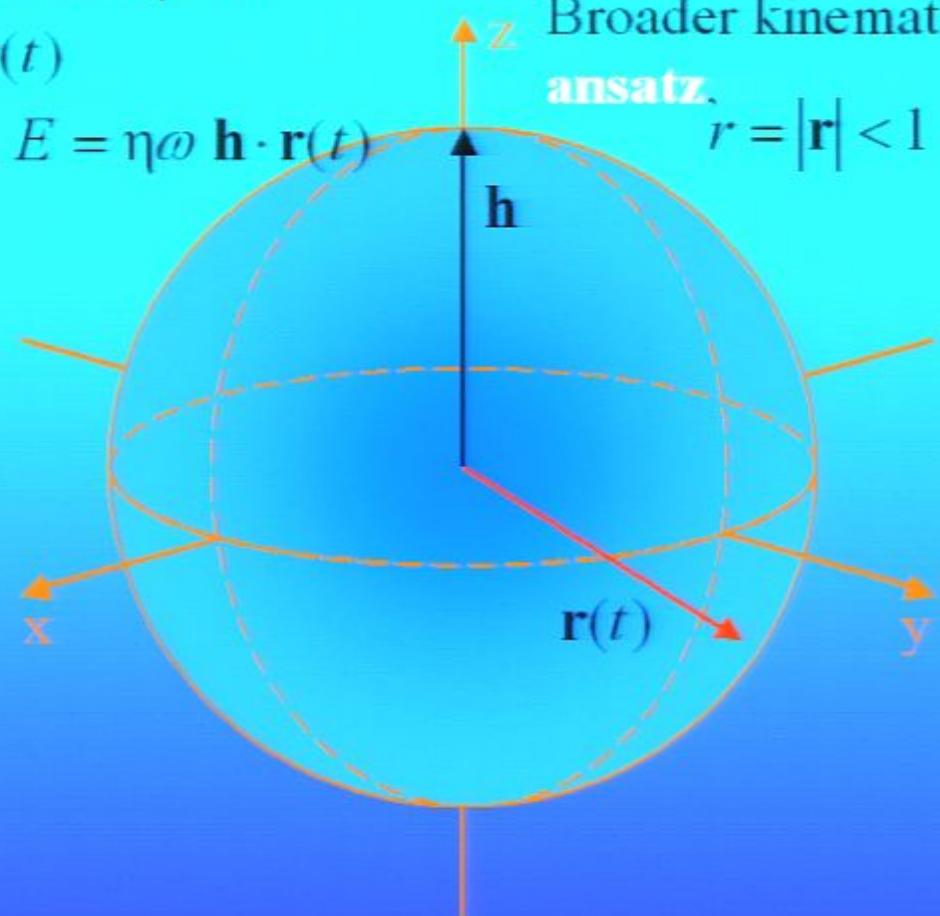
# Isolated two-level system, Quantum Thermodynamics

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

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

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

Broader kinematics  
ansatz,  $r = |\mathbf{r}| < 1$



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

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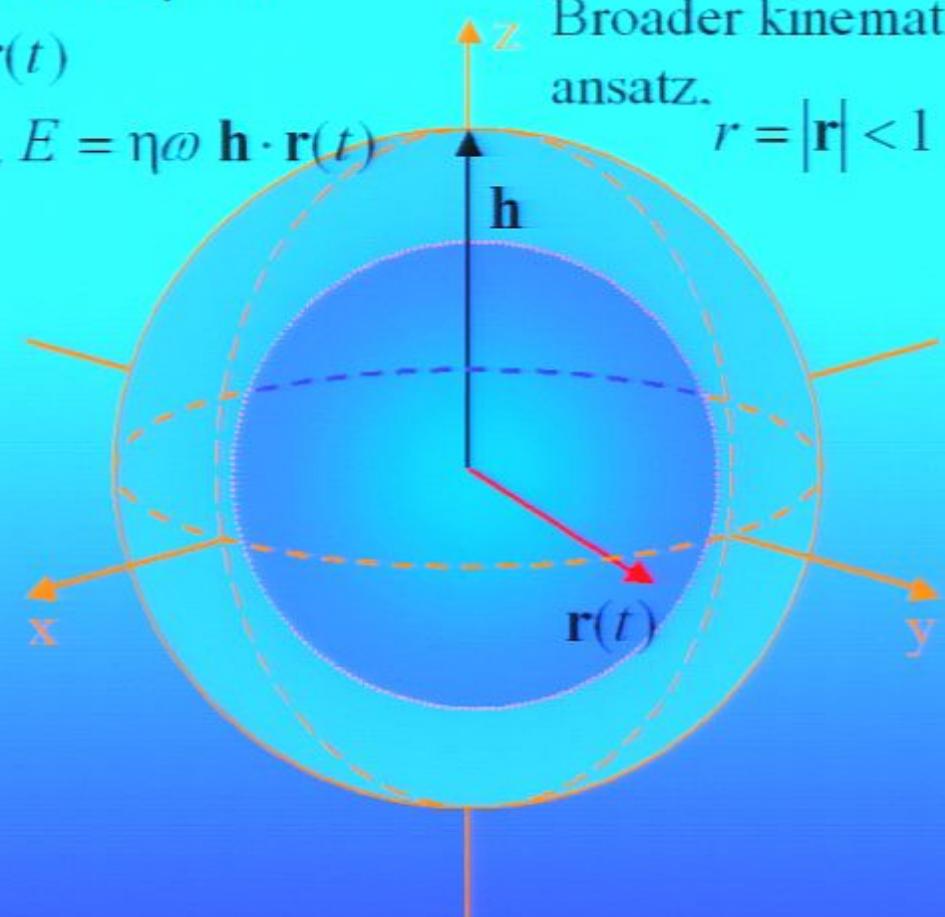
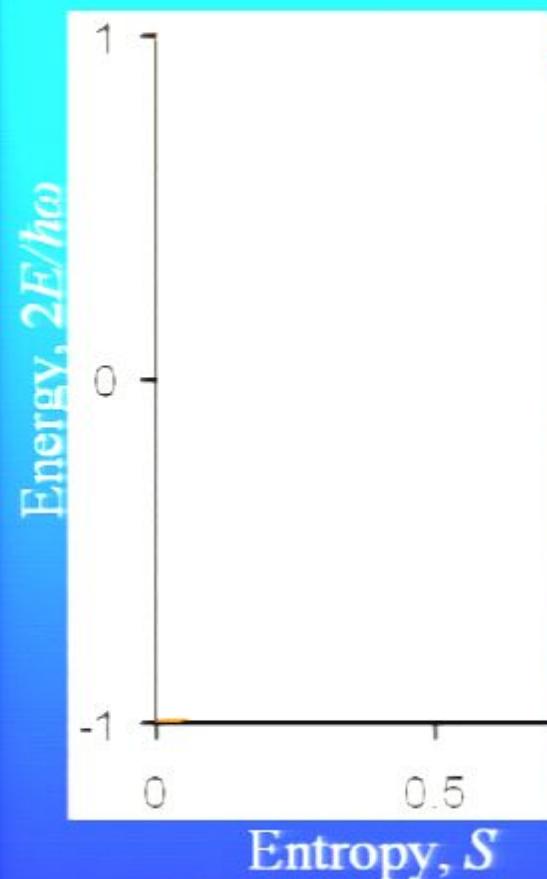
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Hamiltonian,  $\eta\omega \mathbf{h}$

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

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ansatz,  $r = |\mathbf{r}| < 1$



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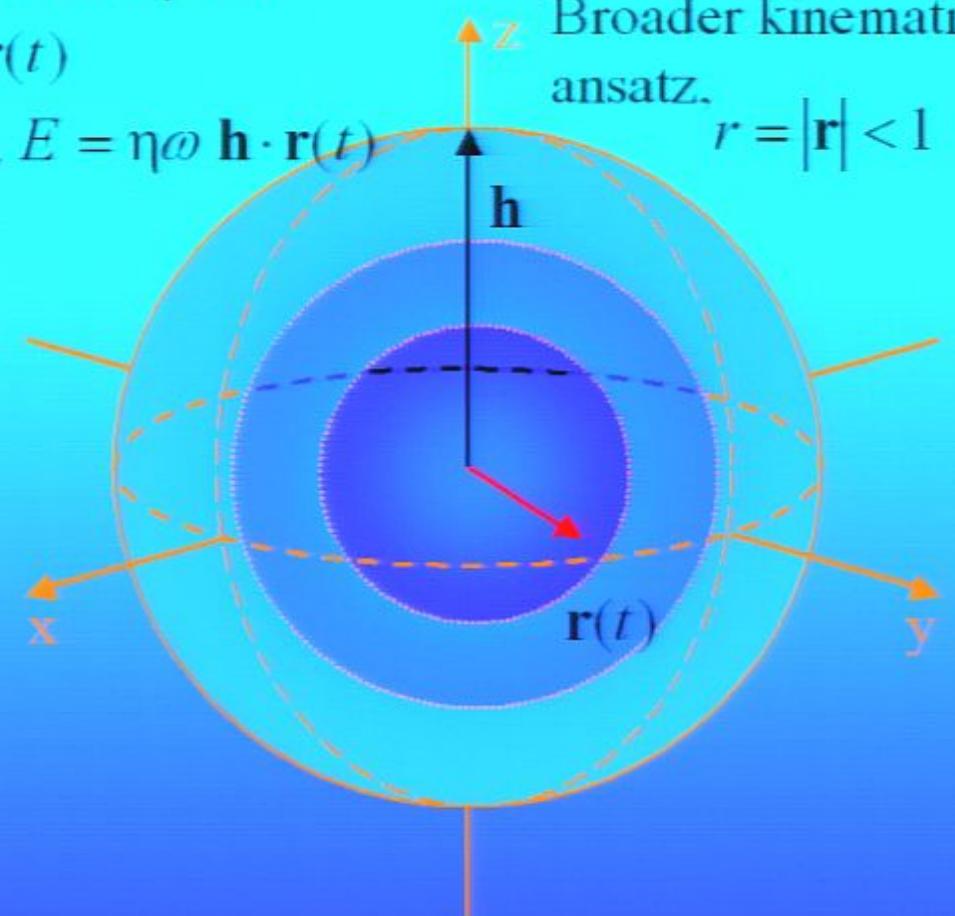
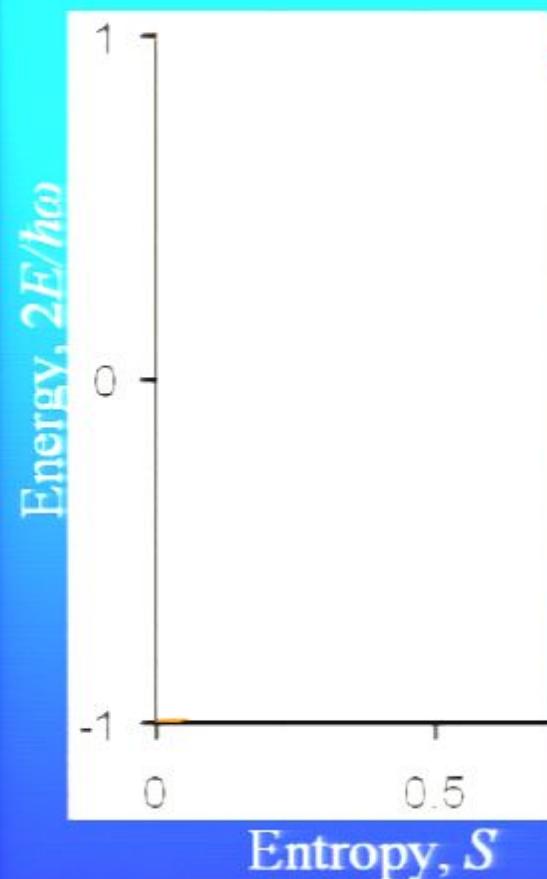
# Isolated two-level system, Quantum Thermodynamics

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

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

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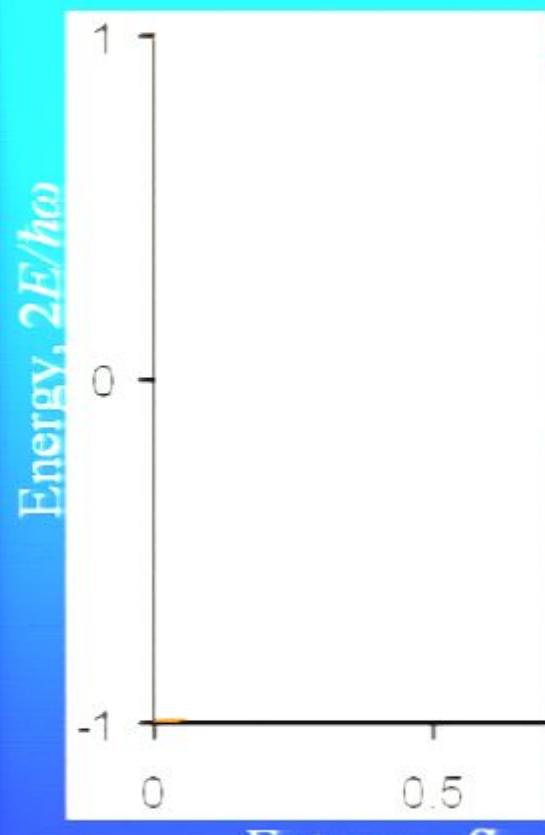
# Isolated two-level system, Quantum Thermodynamics

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

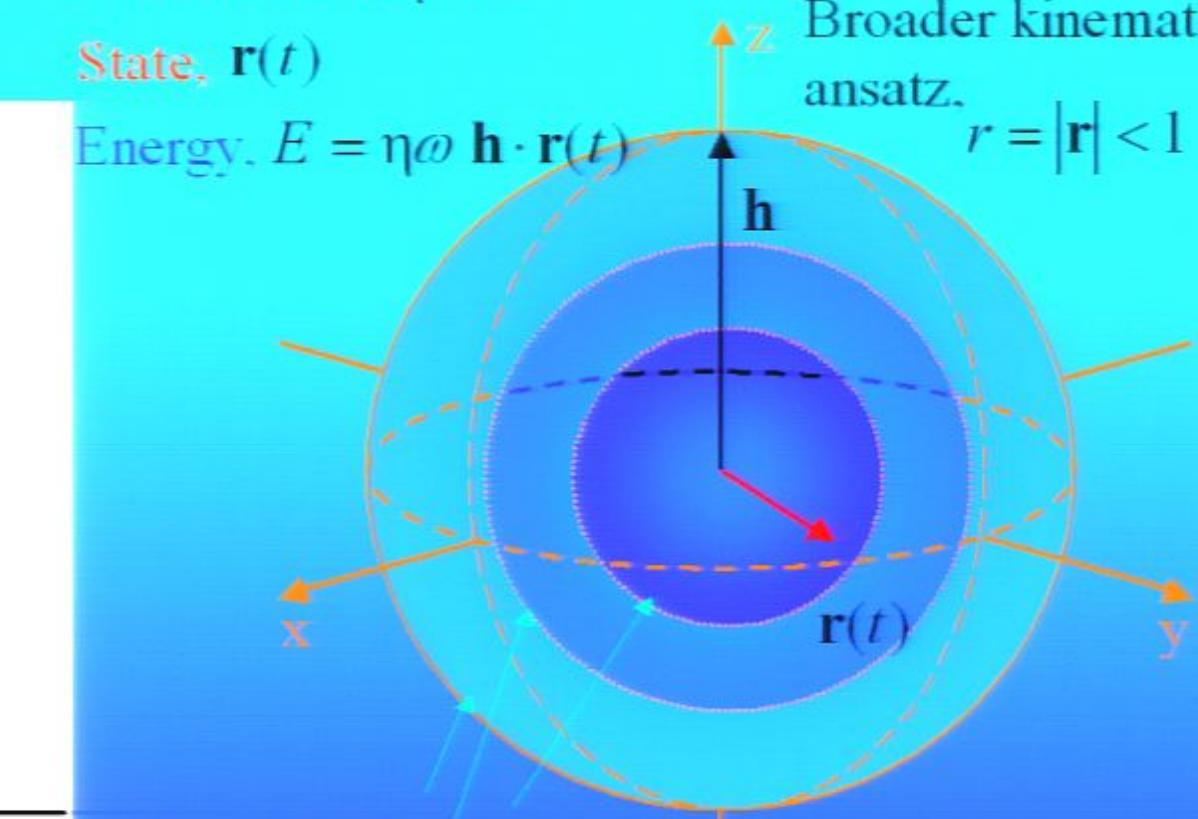
State,  $\mathbf{r}(t)$

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

Broader kinematics  
ansatz,  $r = |\mathbf{r}| < 1$



Isoentropic surfaces



Found.Phys., 6, 15, 127, 439, 561 (1976)

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

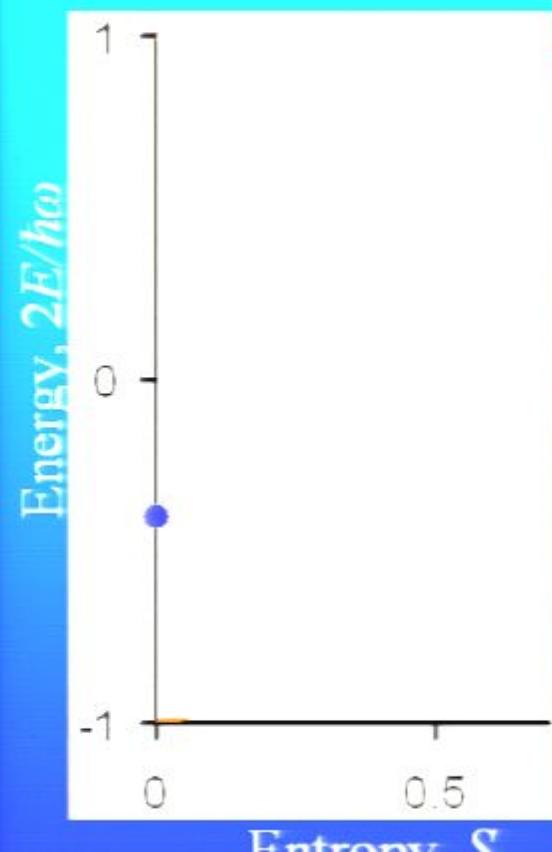
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Hamiltonian,  $\eta\omega \mathbf{h}$

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

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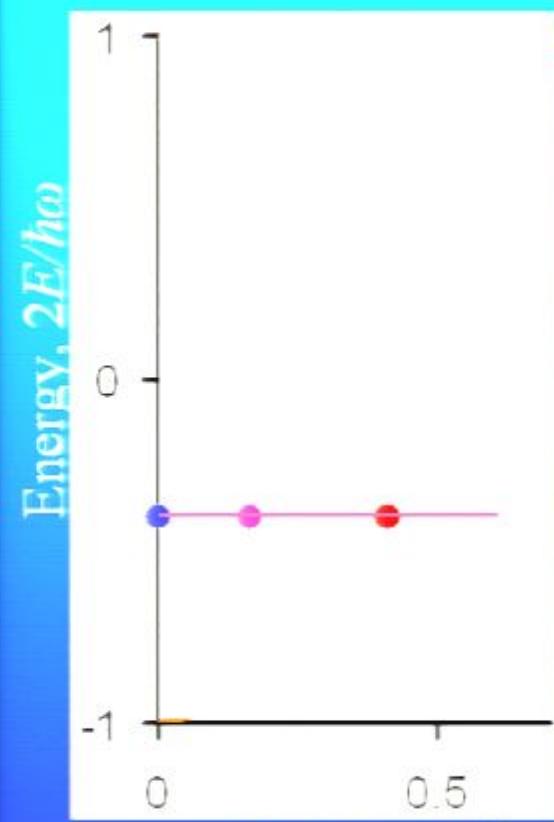
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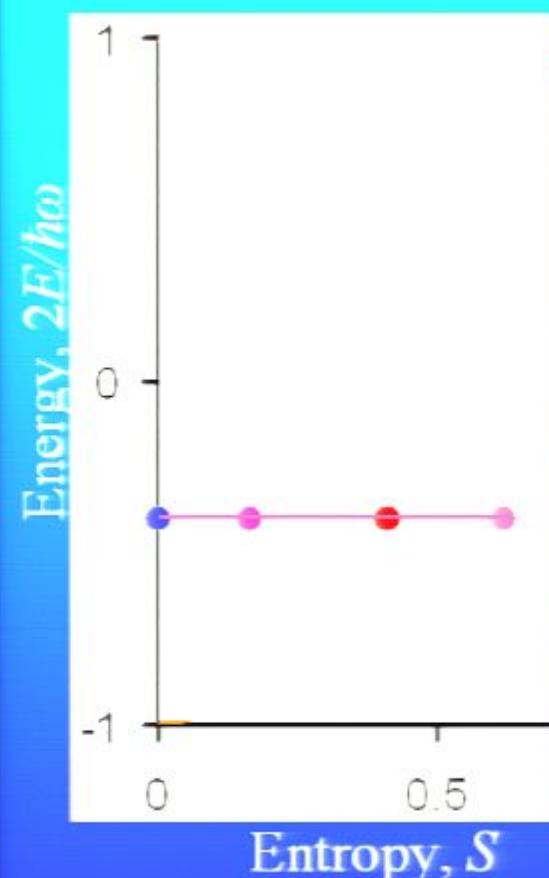
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$$S = -k_B \left( \frac{1+r}{2} \ln \frac{1+r}{2} + \frac{1-r}{2} \ln \frac{1-r}{2} \right)$$

Isoentropic surfaces

Max  $S$  for given  $E$

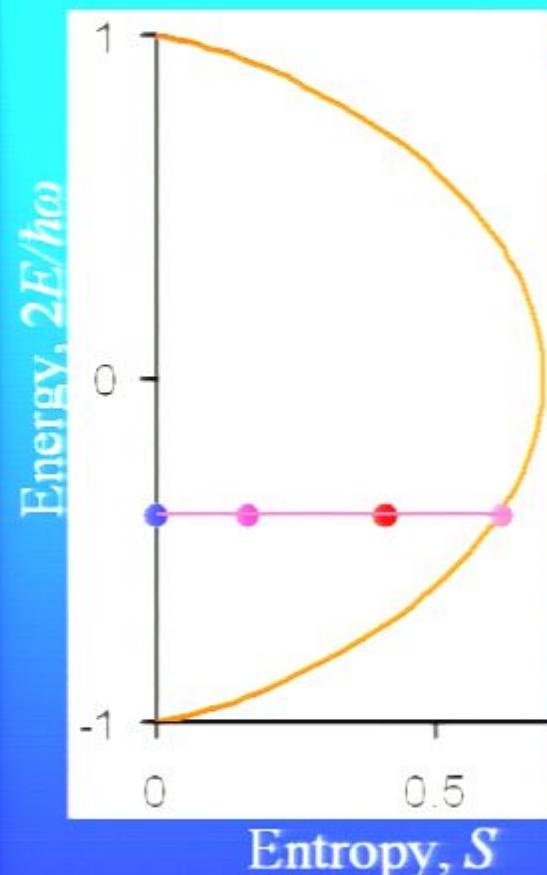
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Hamiltonian,  $\eta\omega \mathbf{h}$

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

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Broader kinematics  
ansatz,  $r = |\mathbf{r}| < 1$



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Max S for given E

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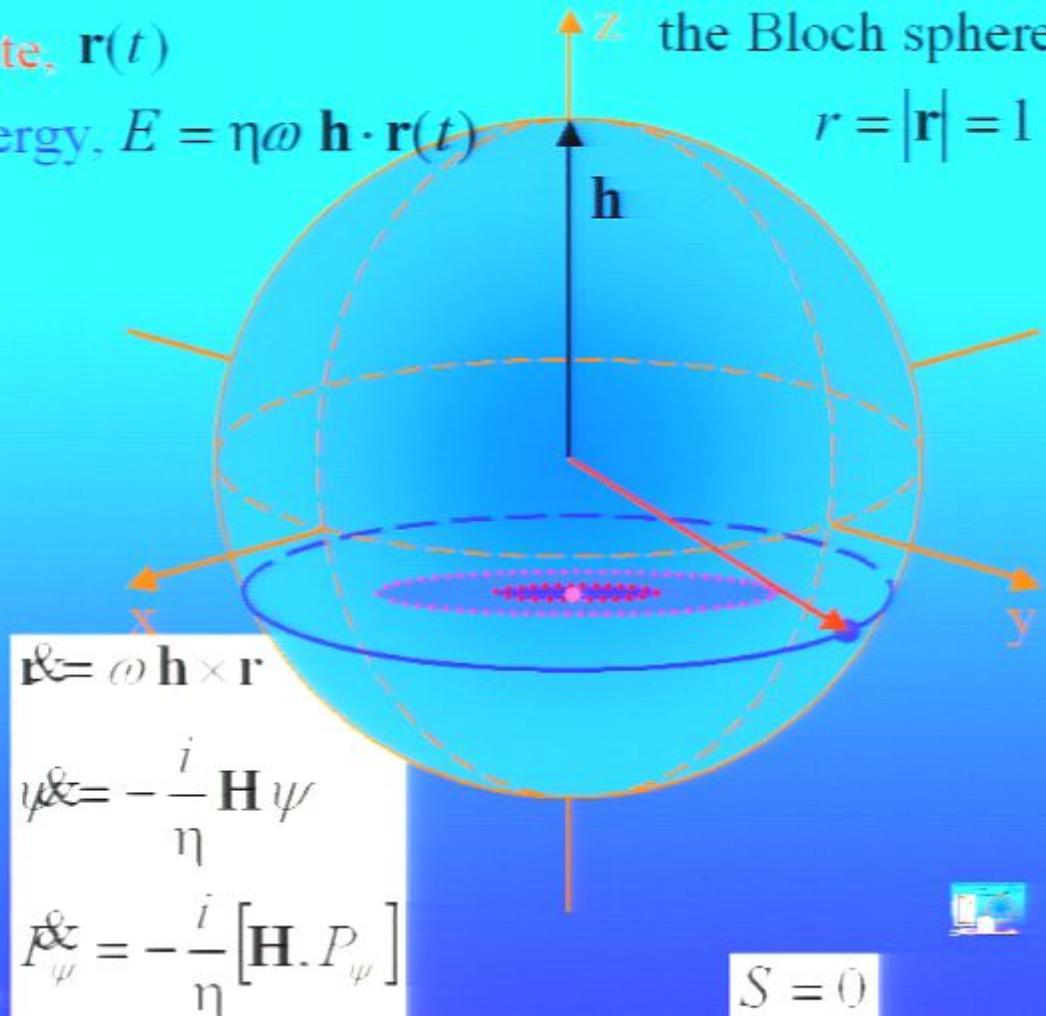
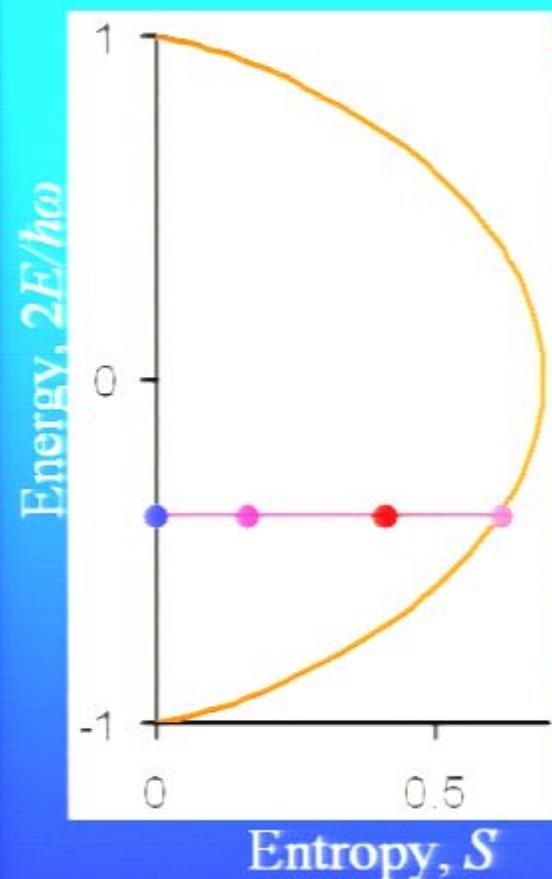
Hamiltonian,  $\eta\omega \mathbf{h}$

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

On the surface of  
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$$r = |\mathbf{r}| = 1$$



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

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## Isolated two-level system, Quantum Thermodynamics

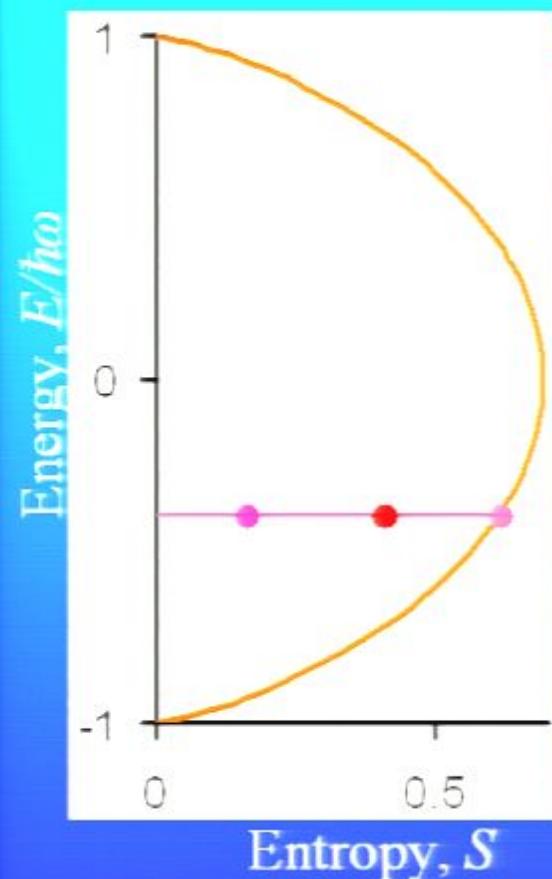
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$$r = |\mathbf{r}| = 1$$



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

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

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

$$S = 0$$



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

G.P. Beretta, Workshop on "Perspectives in Probability Theory and its Connections with Science and Society"  
Levico Terme (Trento), Italy, December 3-7, 2006 - References available at: [www.quantumthermodynamics.org](http://www.quantumthermodynamics.org)

# Isolated two-level system, Quantum Thermodynamics

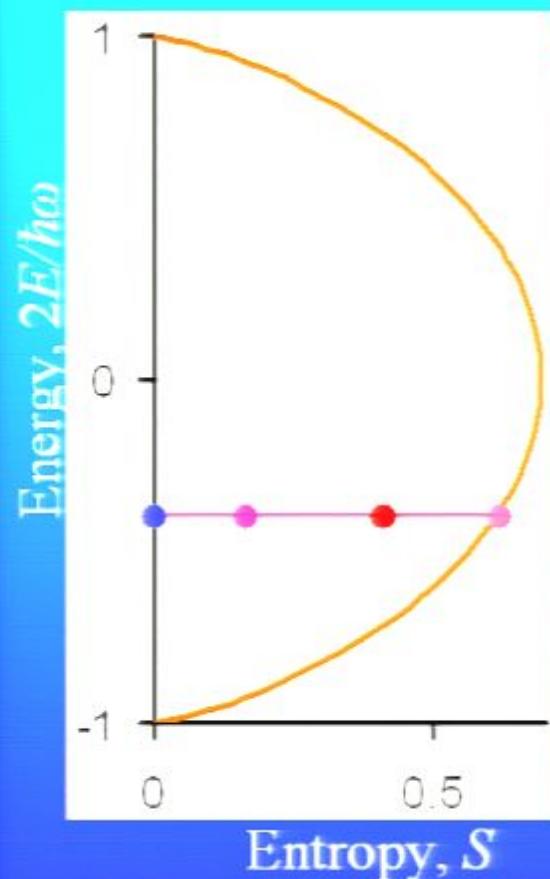
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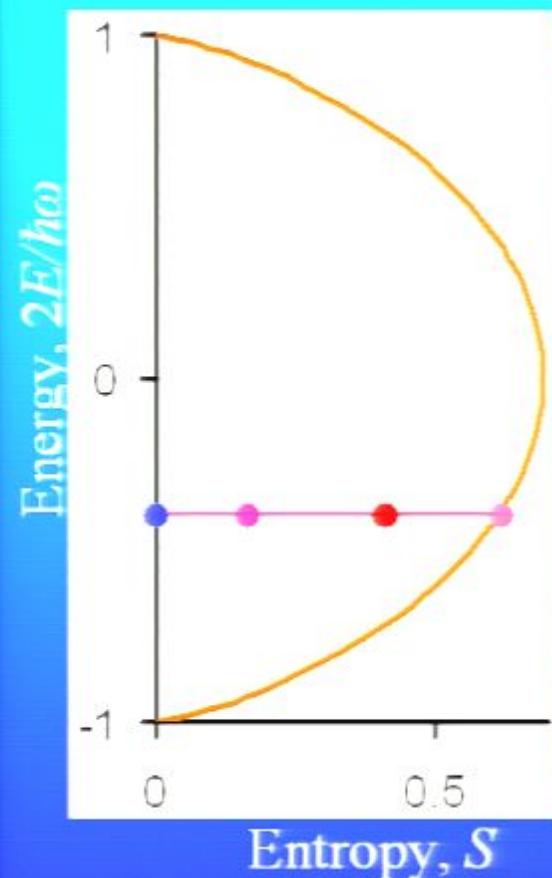
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Energy,  $E = \eta\omega \mathbf{h} \cdot \mathbf{r}(t)$

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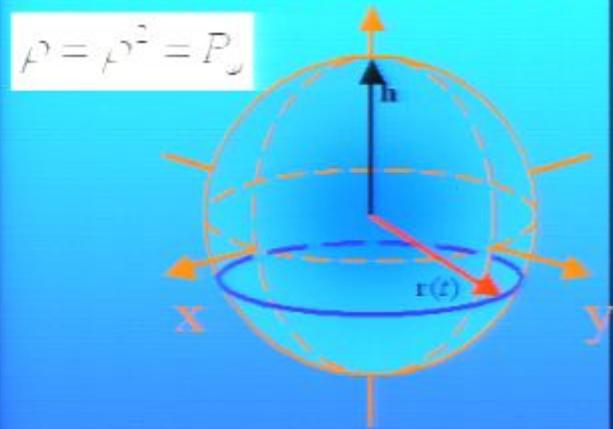
G.P. Beretta, Seminar "What is Quantum Thermodynamics more a fundamental extension of Quantum Mechanics?"  
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If entropy an intrinsic  
property of matter...

Isolated and uncorrelated two-level quantum system (**quBit**)

## Quantum Mechanics

Bloch sphere surface,  $r = 1$



Dynamical law  
(Schrodinger)

$$\dot{\psi} = -\frac{i}{\eta} H \psi$$

$$\dot{P}_y = -\frac{i}{\eta} [H, P_y]$$

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



G.P. Beretta, Seminar "What is Quantum Thermodynamics now: a fundamental extension of Quantum Mechanics?"  
Perimeter Institute, Waterloo, Canada, November 8, 2007 - References available at: [www.quantumthermodynamics.org](http://www.quantumthermodynamics.org)

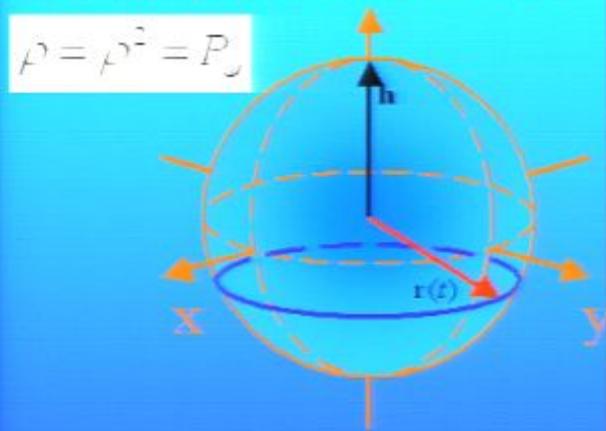
If entropy an intrinsic property of matter...

...is irreversibility an intrinsic feature of microscopic dynamics?

### Isolated and uncorrelated two-level quantum system (quBit)

#### Quantum Mechanics

Bloch sphere surface,  $r = 1$



Dynamical law  
(Schrodinger)

$$\dot{\psi} = -\frac{i}{\eta} H \psi$$

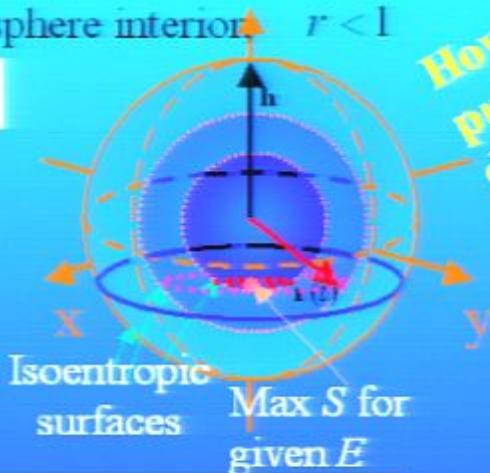
$$\dot{P}_\psi = -\frac{i}{\eta} [H, P_\psi]$$

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

#### Quantum Thermodynamics

Hatsopoulos-Gyftopoulos ansatz:  
also Bloch sphere interior,  $r < 1$

$$\rho = \rho^c$$



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

Dynamical law ?

How can we extend pure state unitary dynamics to include second law?



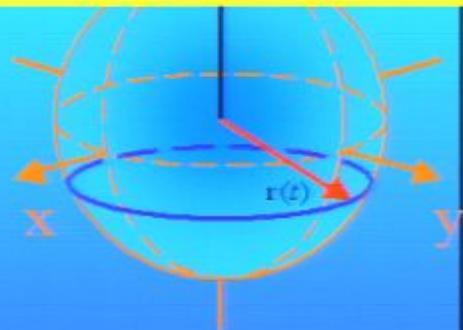
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Fundamental ansatz  
about irreversible  
steepest-entropy-ascent  
quantum dynamics

$$\rho \ln \rho \quad \rho \quad \frac{1}{2} \{H, \rho\}$$

$$\text{Tr} \rho \ln \rho \quad I \quad \text{Tr} \rho H$$

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] - \frac{1}{2} \frac{\text{Tr} \rho H \ln \rho - \text{Tr} \rho H - \text{Tr} \rho H^2}{\text{Tr} \rho H^2 + (\text{Tr} \rho H)^2}$$



Dynamical law  
(Schrödinger)

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

$$\dot{P}_\nu = -\frac{i}{\eta} [H, P_\nu]$$

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

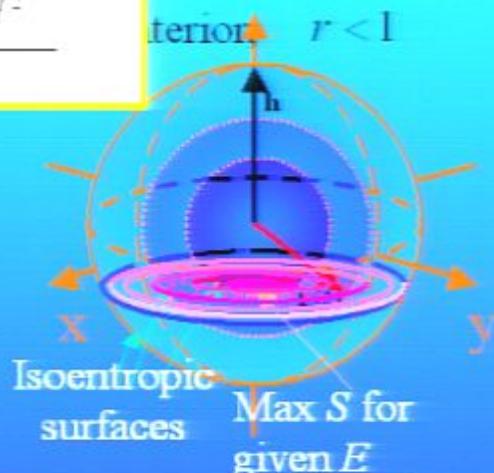
Irreversibility emerges as an intrinsic feature of microscopic dynamics.

tem (quBit)

## rmodynamics

Coulous ansatz:

Interior  $r < 1$



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

Dynamical law

$$\dot{\mathbf{r}} = \omega \mathbf{h} \cdot \mathbf{r} - \frac{f(r)}{\tau} \mathbf{h} \cdot \mathbf{r} \cdot \mathbf{h}$$



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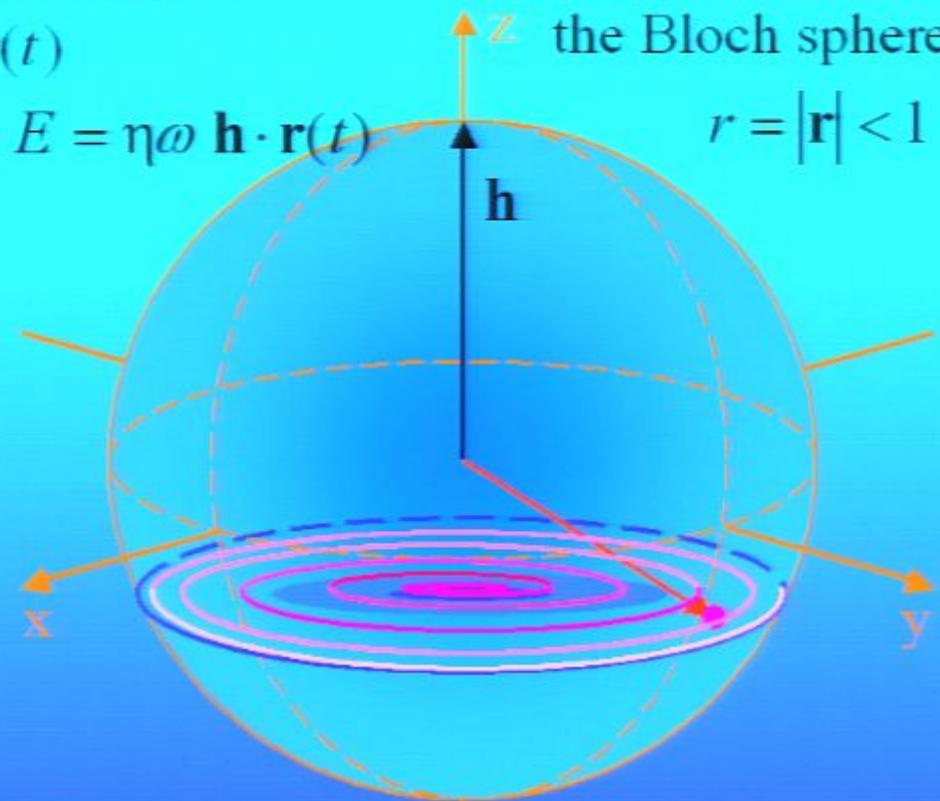
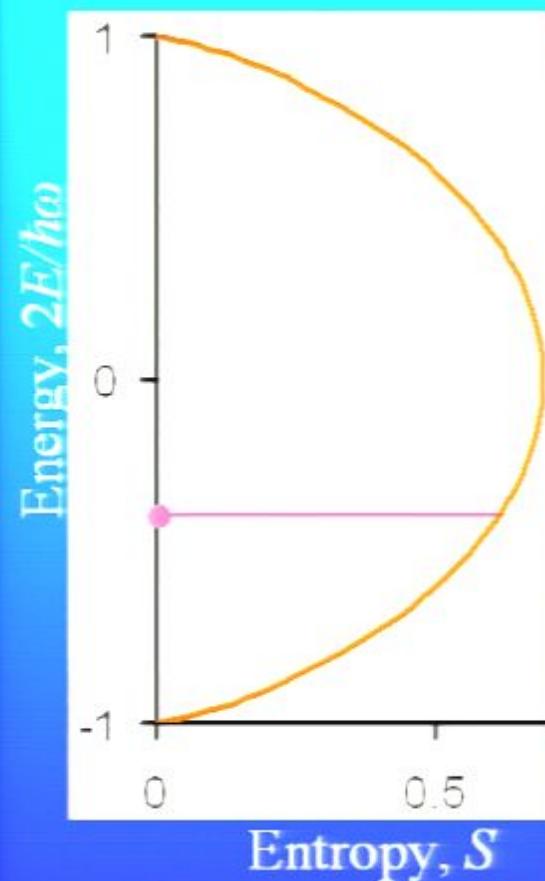
## Isolated two-level system, Quantum Thermodynamics

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

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

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

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



$$\dot{\mathbf{r}} = \omega \mathbf{h} \times \mathbf{r} - \frac{f(r)}{\tau} \mathbf{h} \times \mathbf{r} \times \mathbf{h}$$

$$S \neq 0$$



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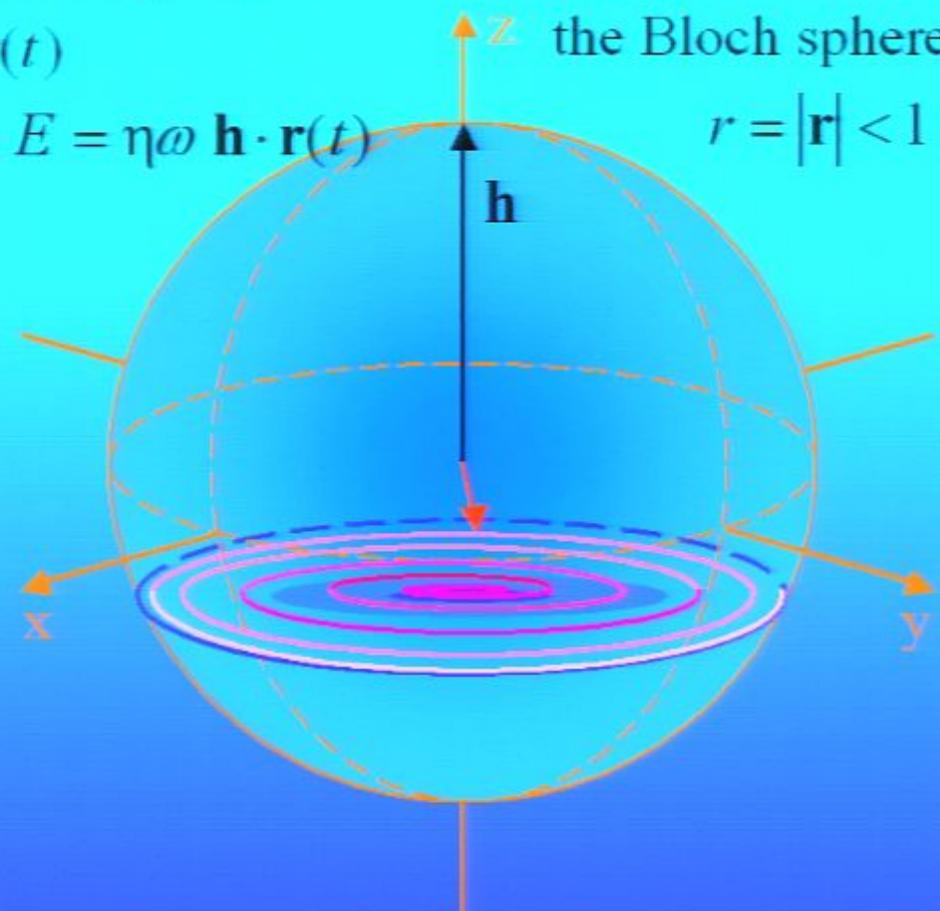
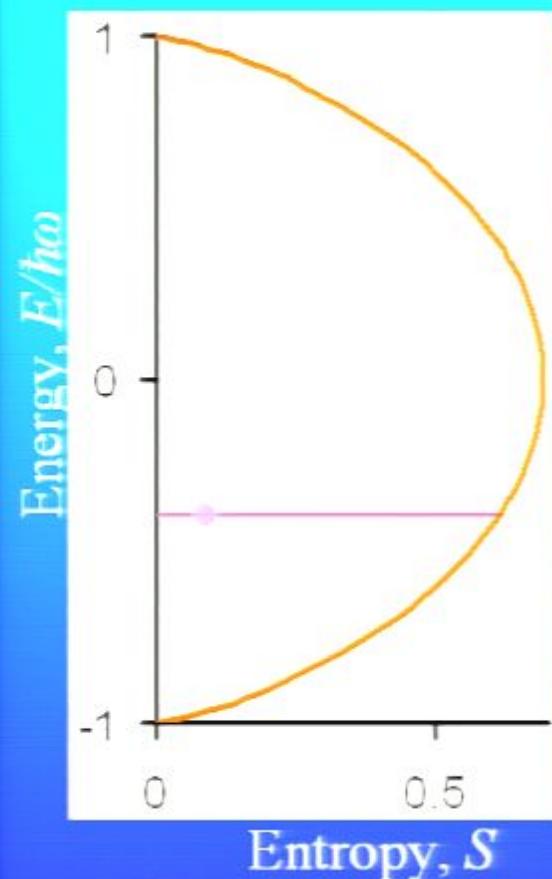
Hamiltonian,  $\eta\omega \mathbf{h}$

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

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

Inside  
the Bloch sphere.

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



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

G.P. Beretta, Workshop on "Perspectives in Probability Theory and its Connections with Science and Society"  
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$$S \neq 0$$

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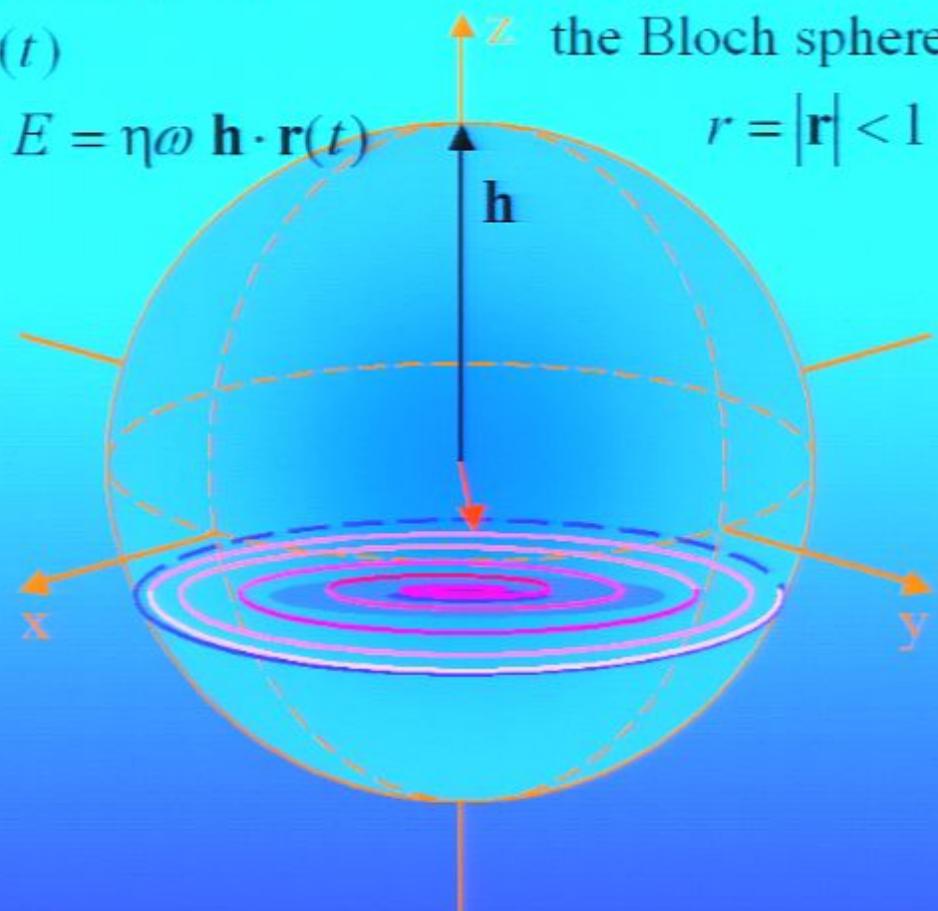
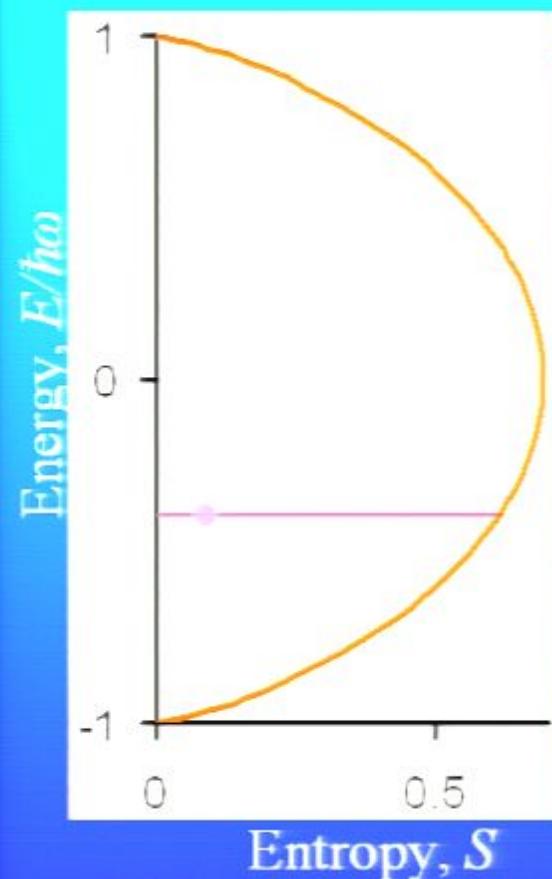
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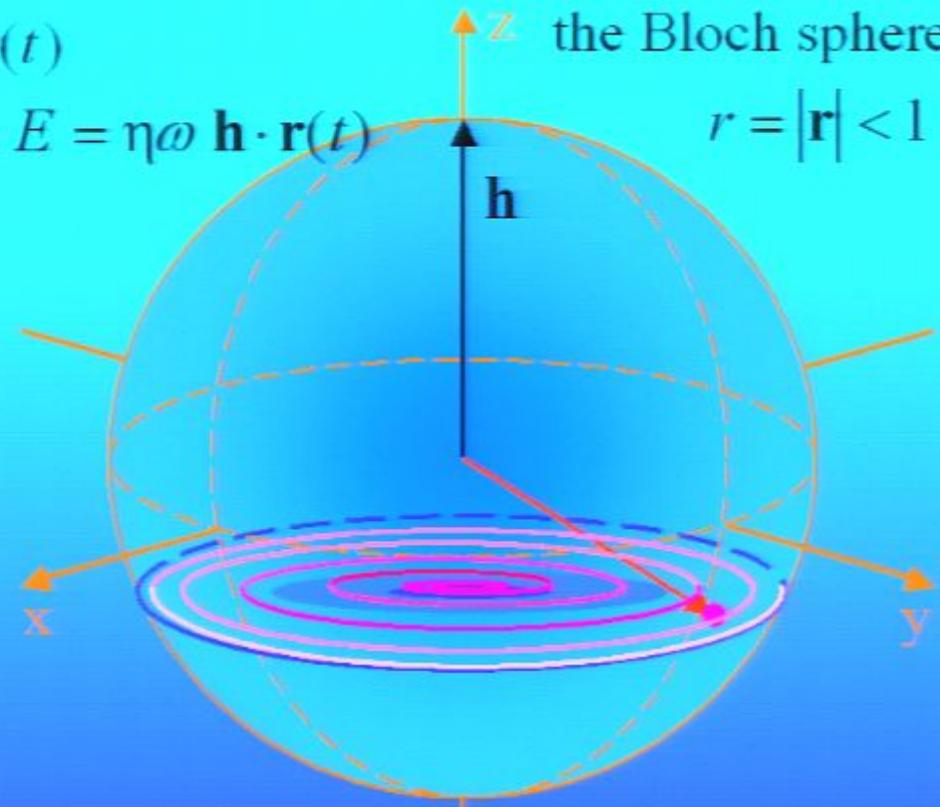
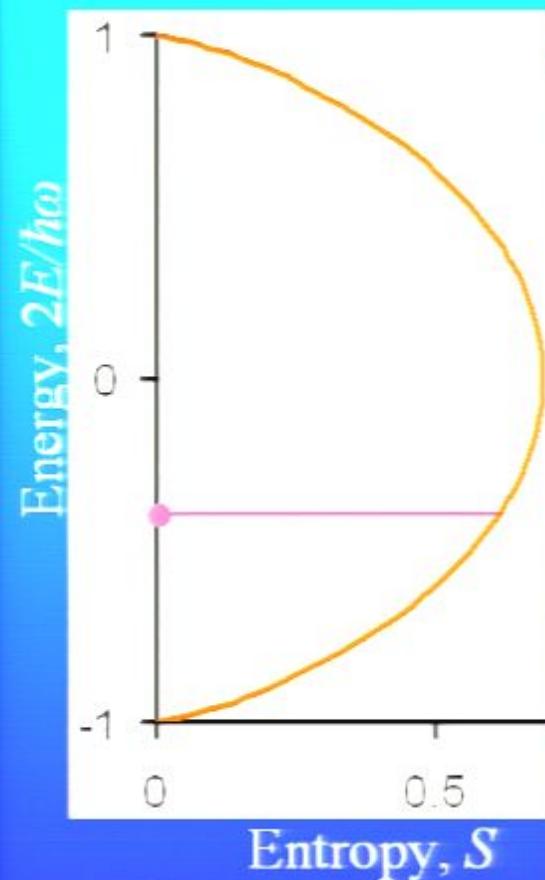
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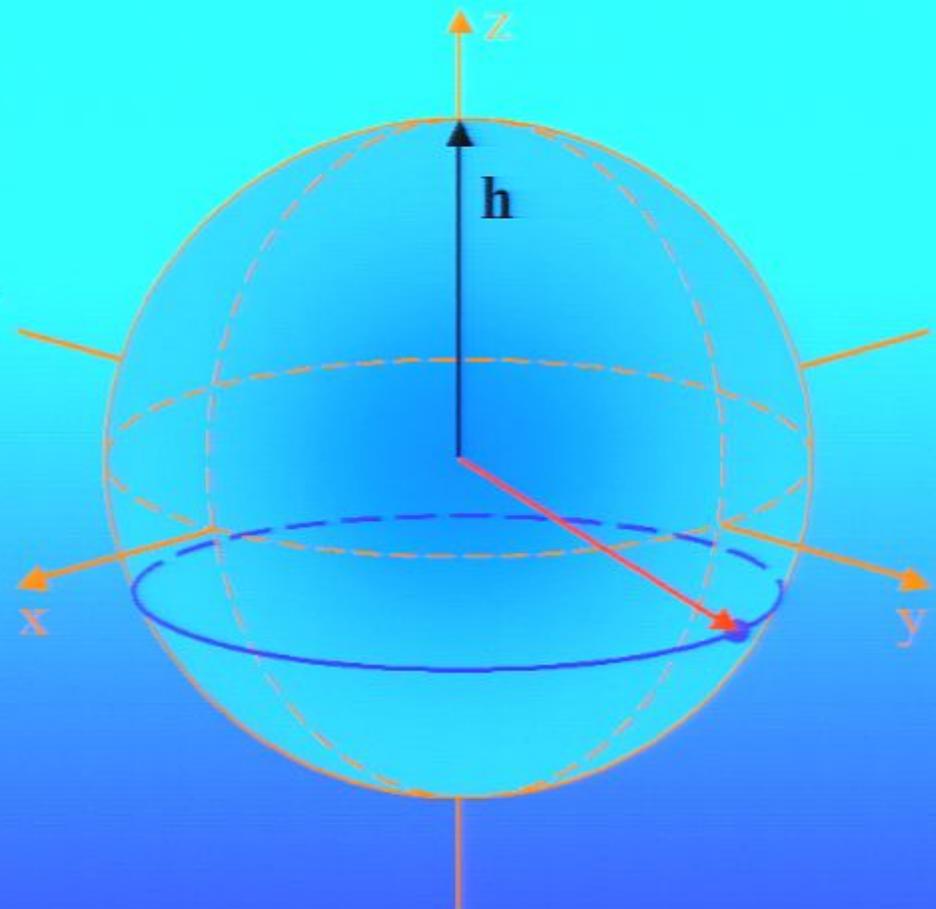
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# Schrödinger's prescient forecast

Proc. Cambridge Phil. Soc., 32, 446 (1936)

“... in a domain which the present theory (Quantum Mechanics) does not cover, there is room for new assumptions without necessarily contradicting the theory in that region where it is backed by experiment.”



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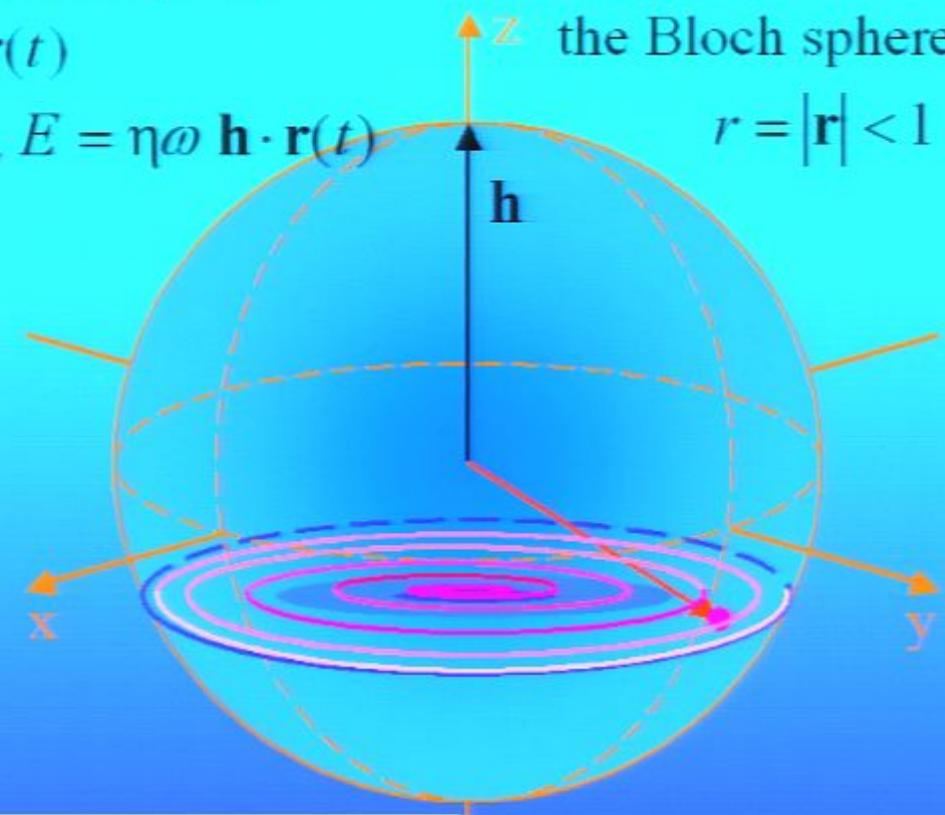
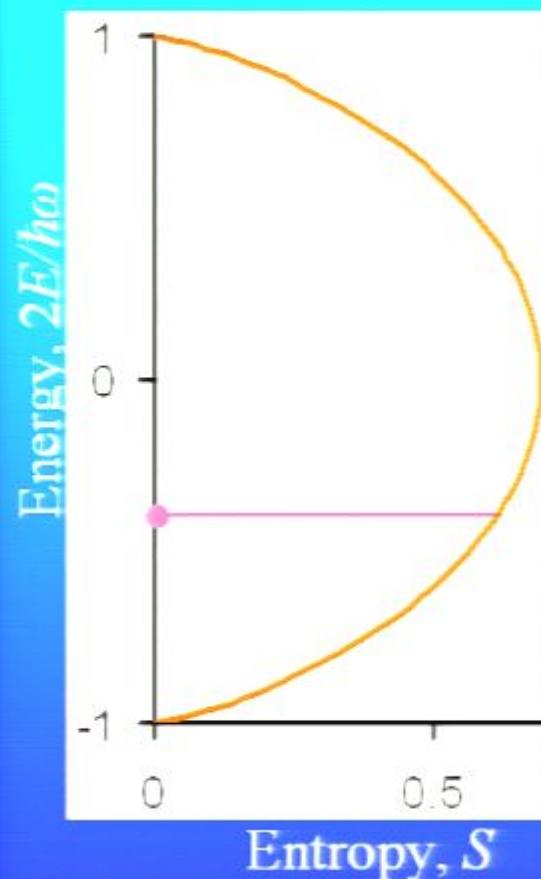
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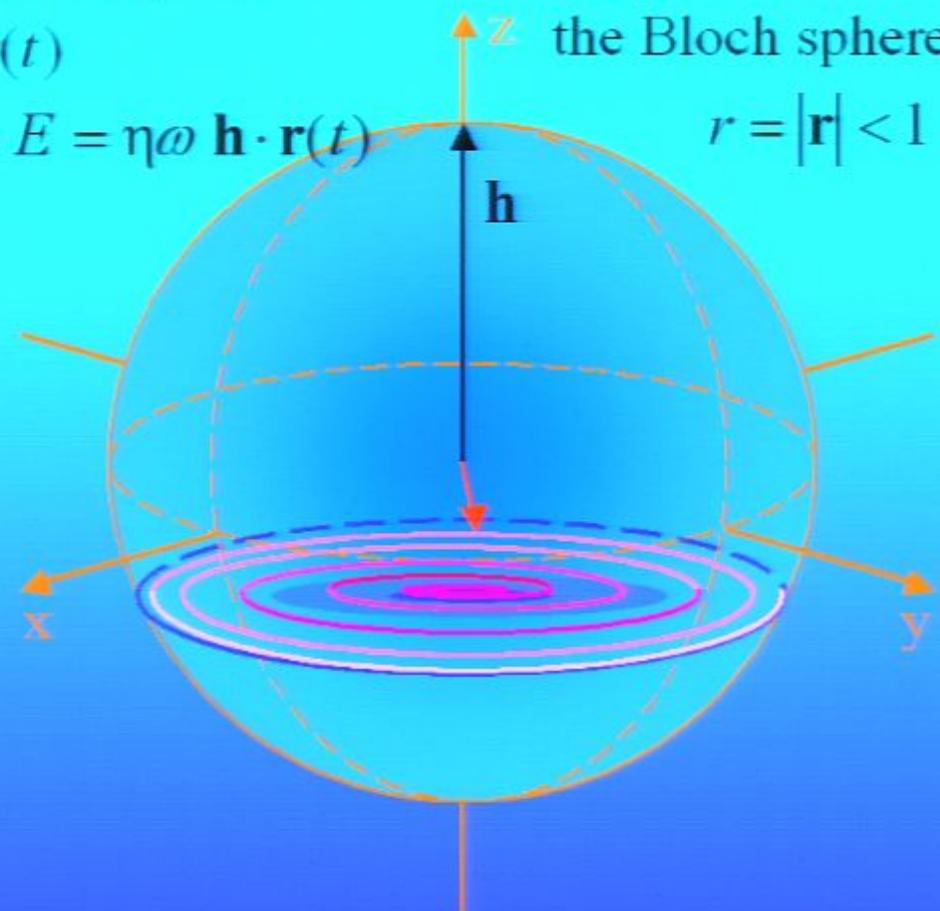
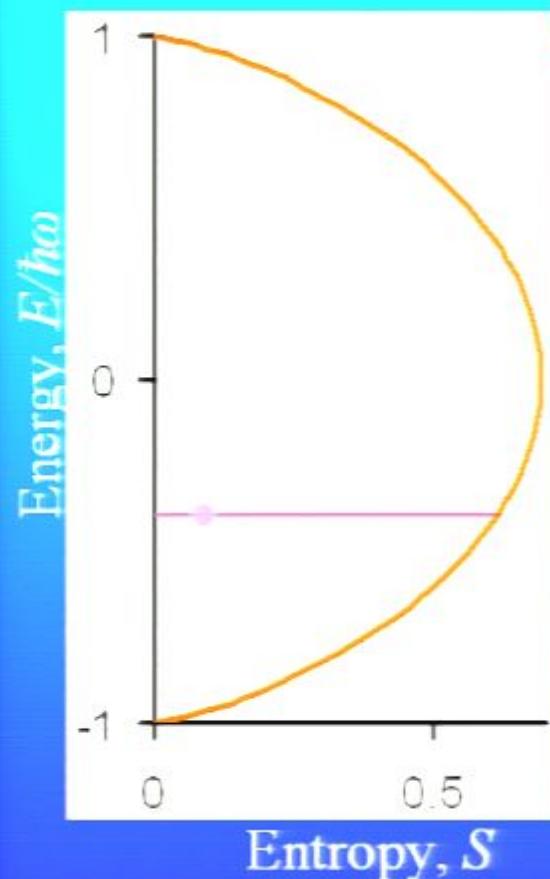
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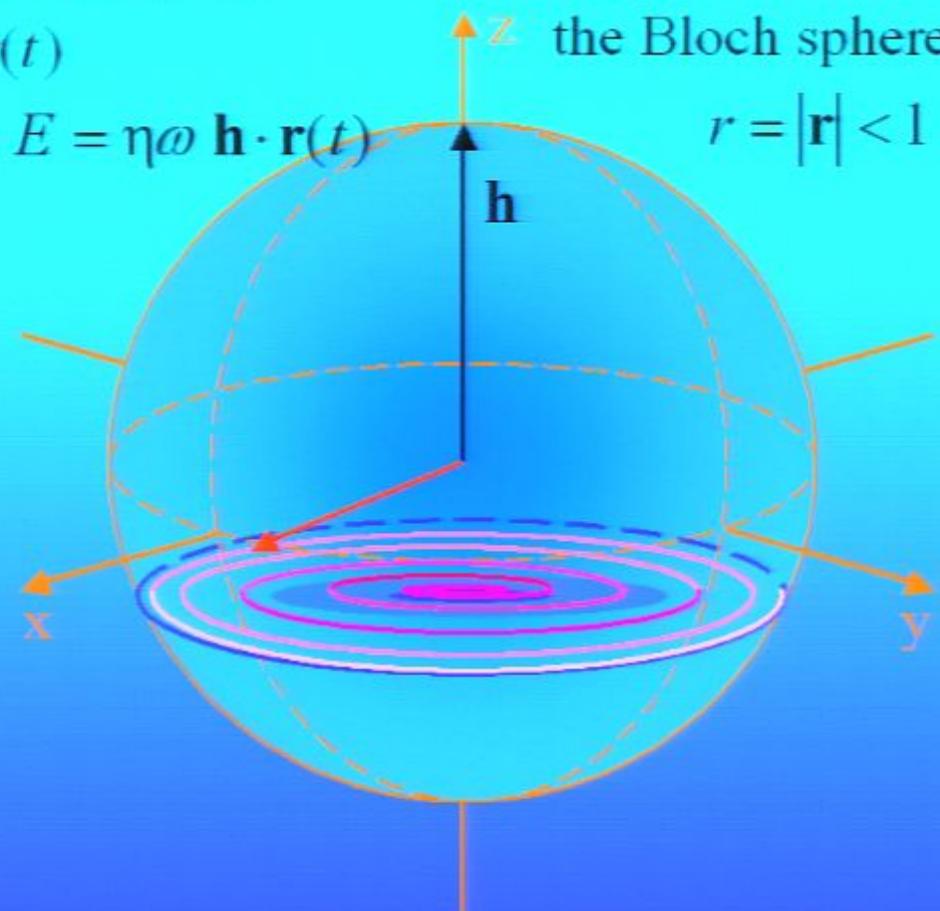
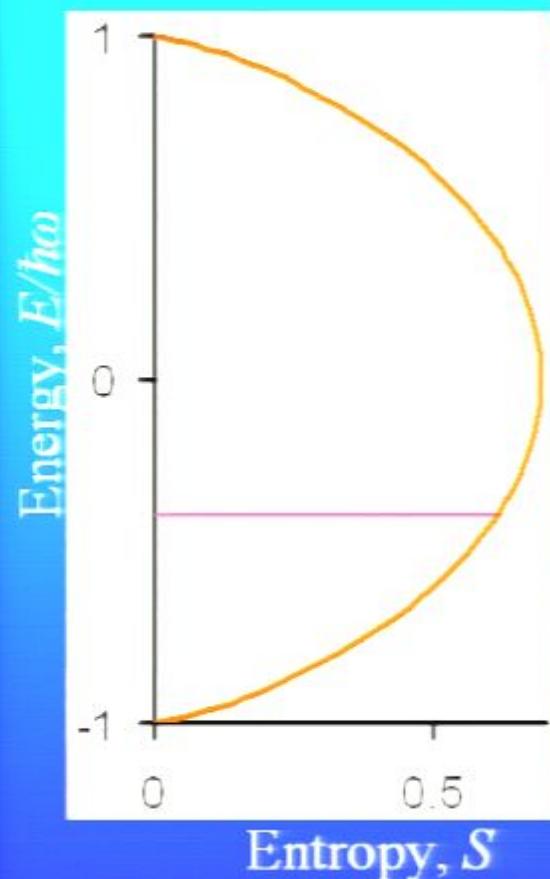
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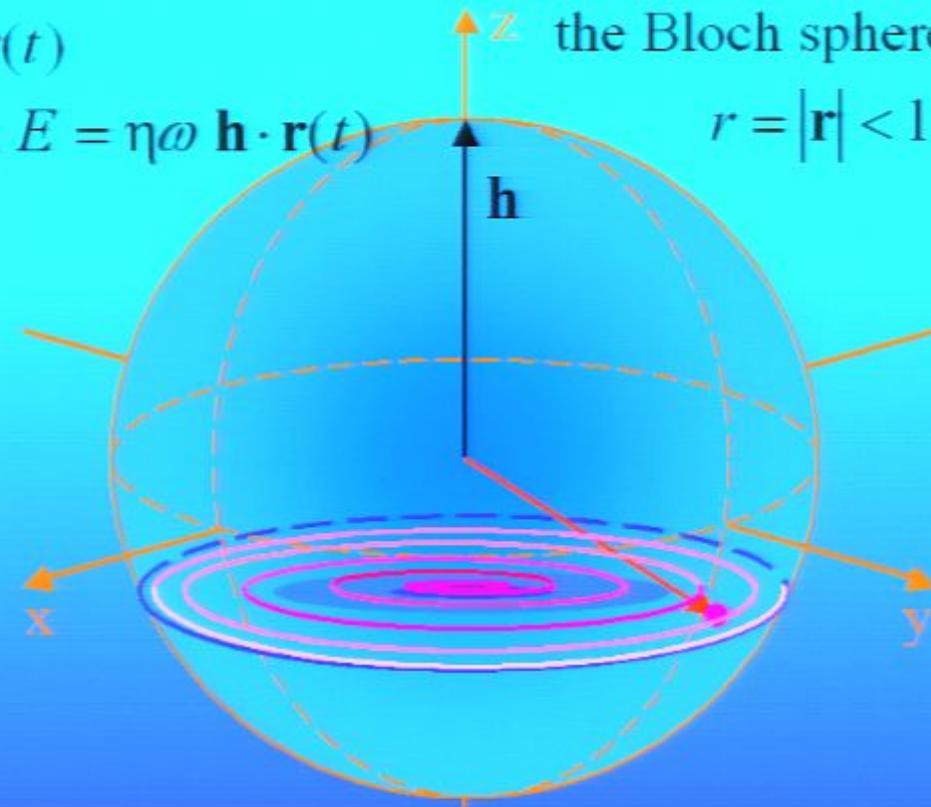
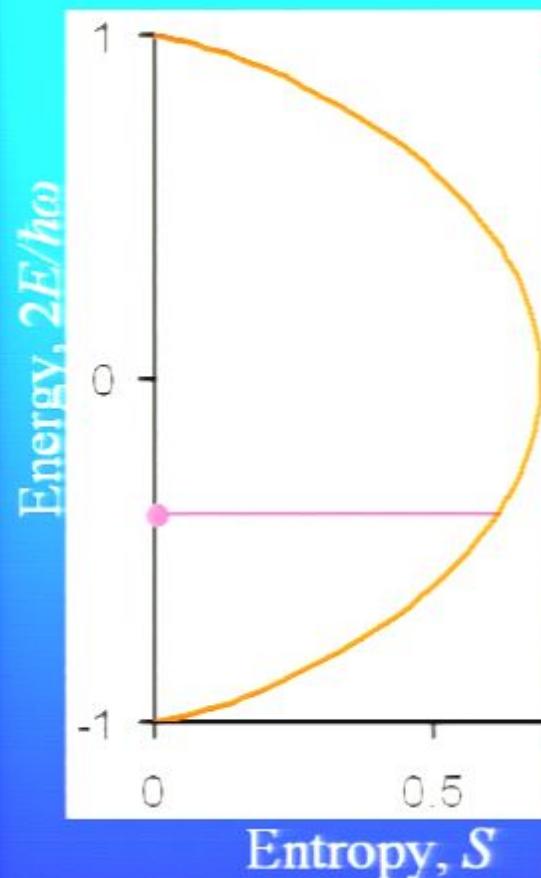
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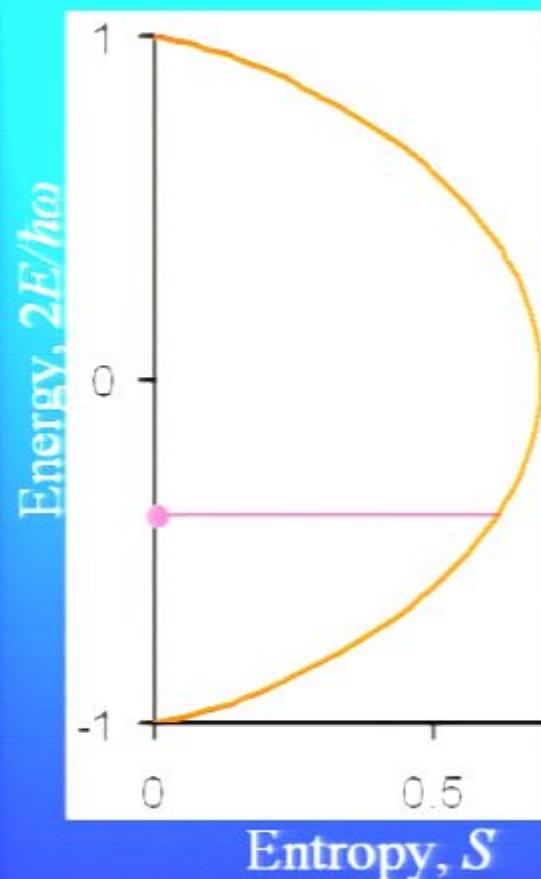
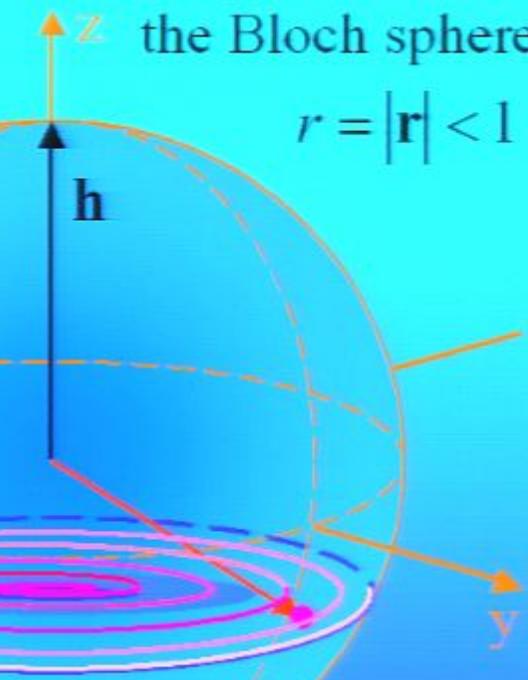
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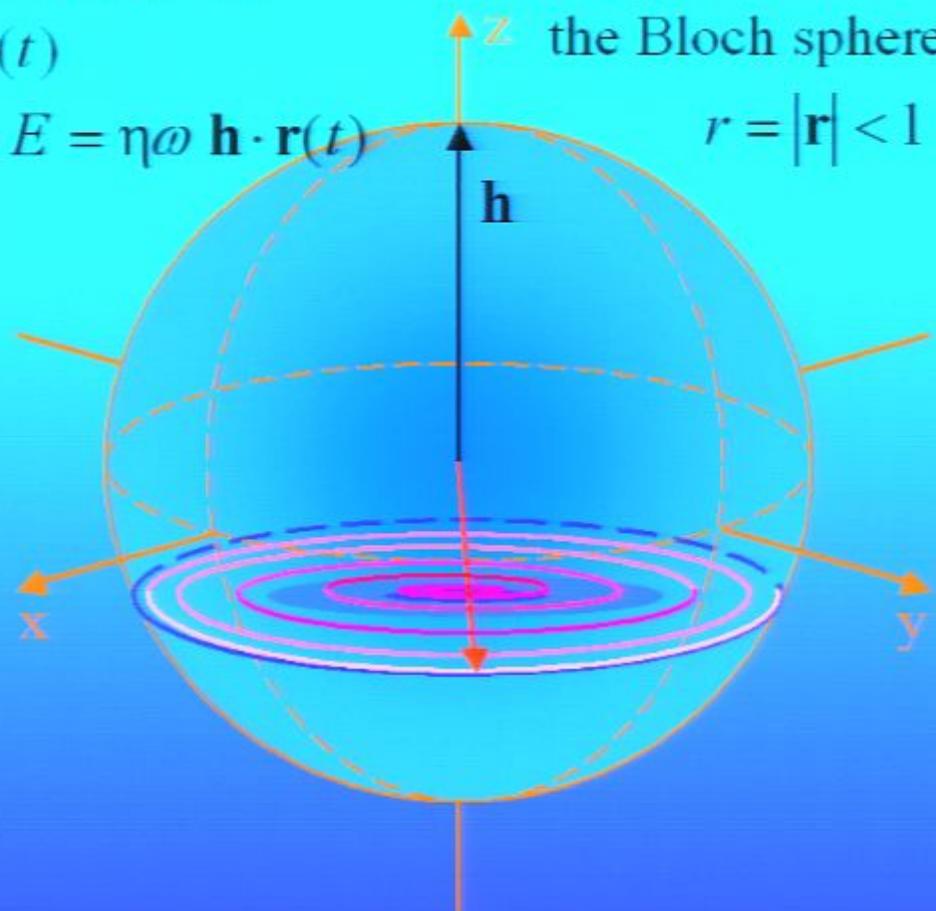
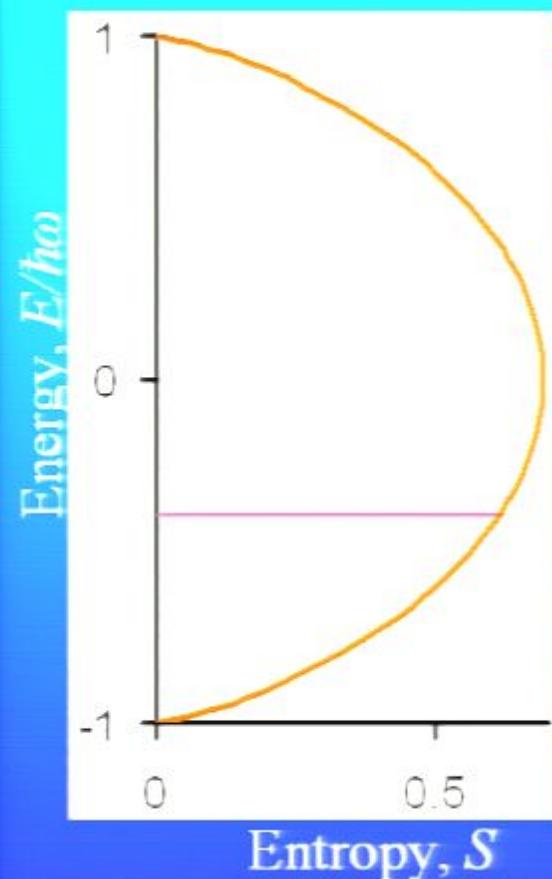
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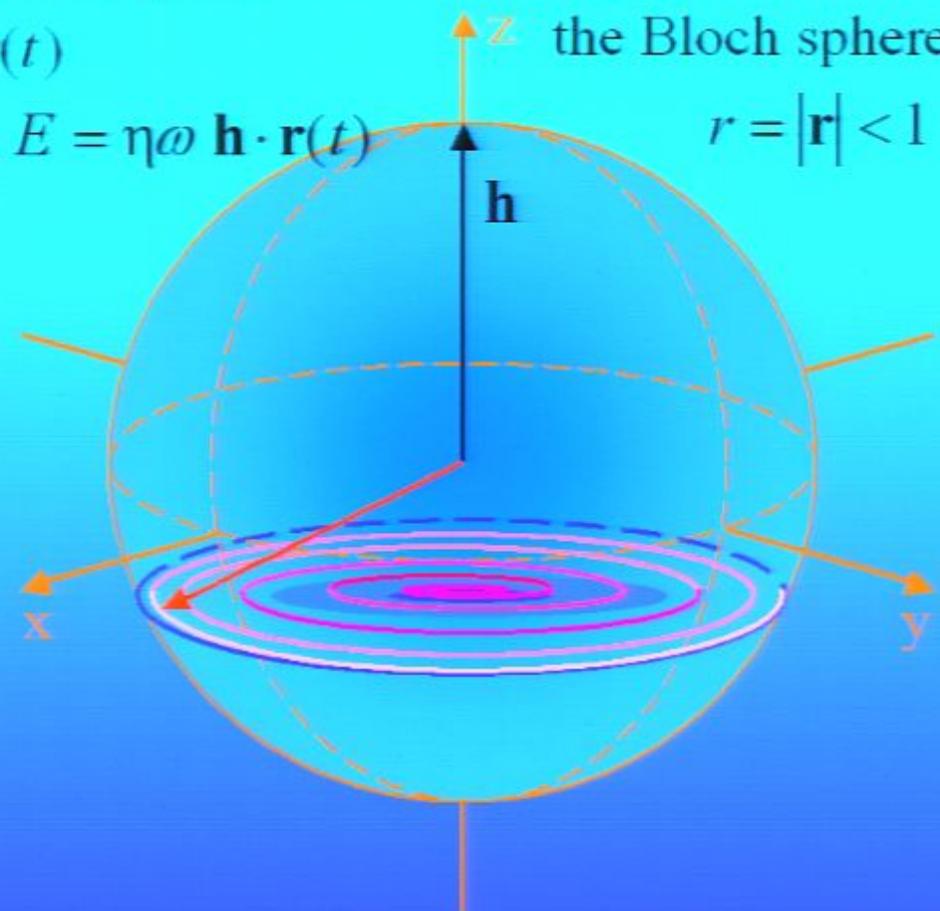
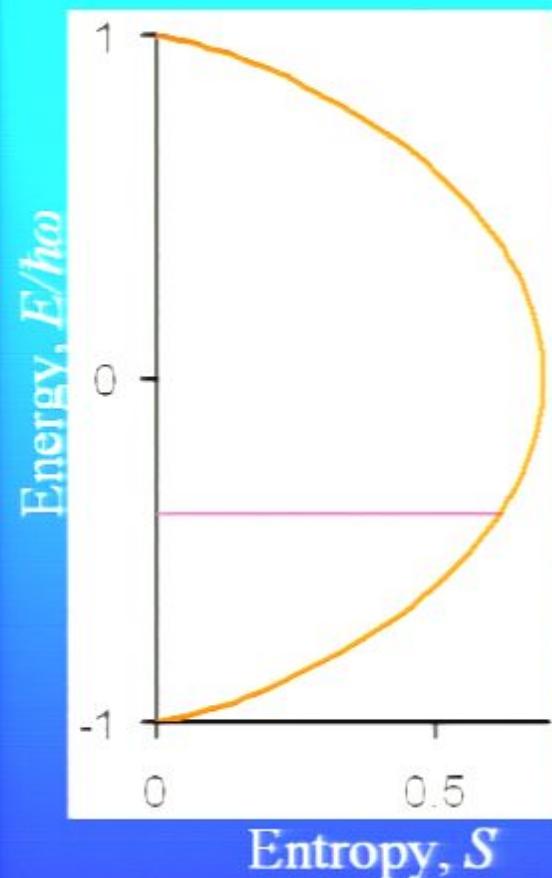
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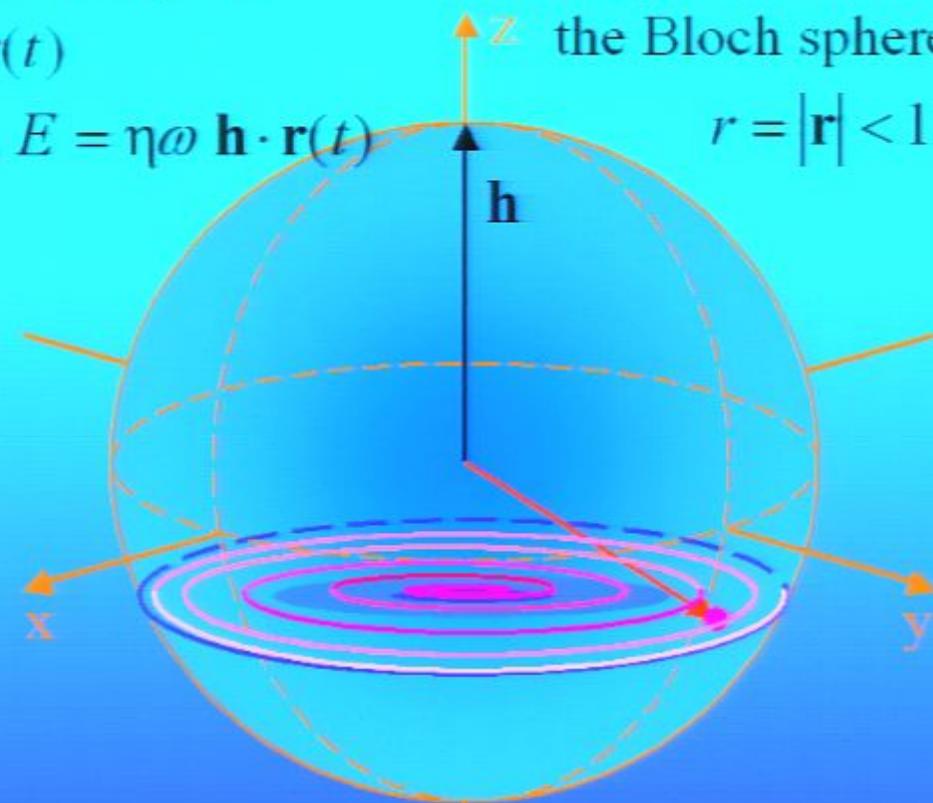
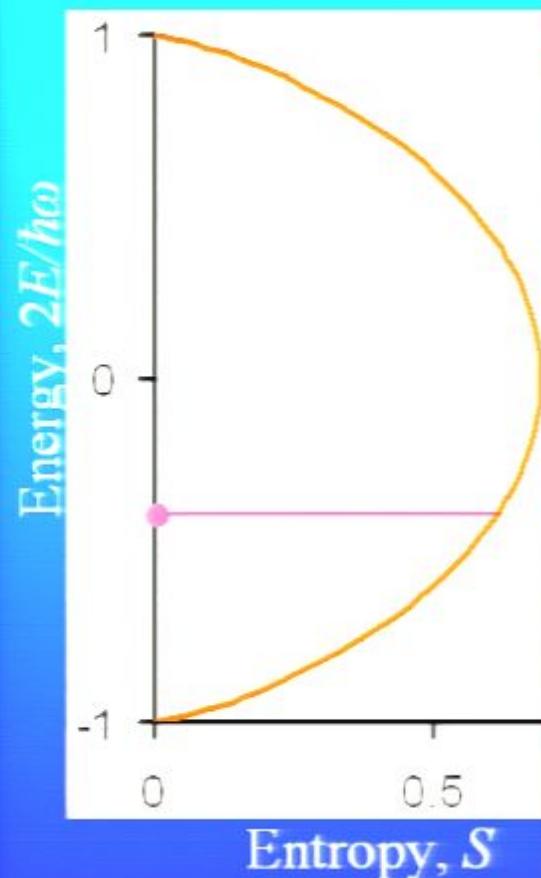
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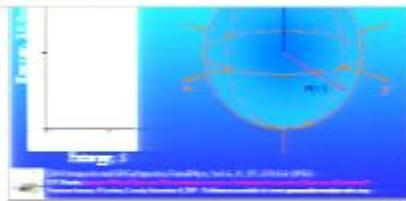
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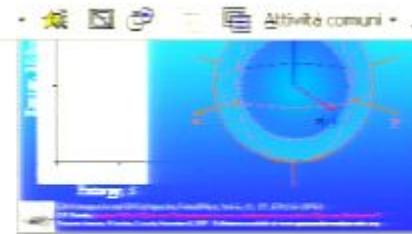




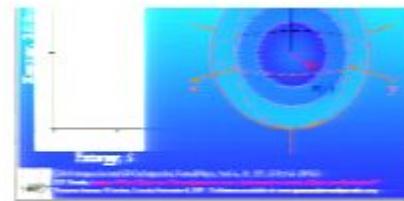
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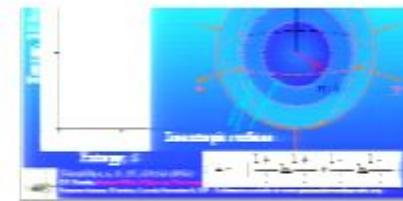
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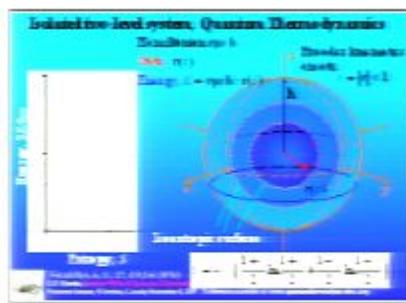
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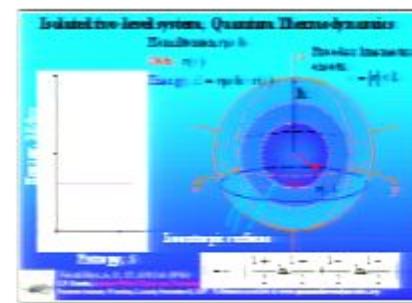
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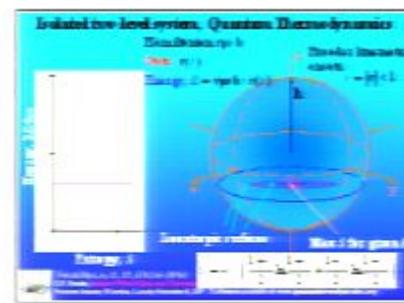
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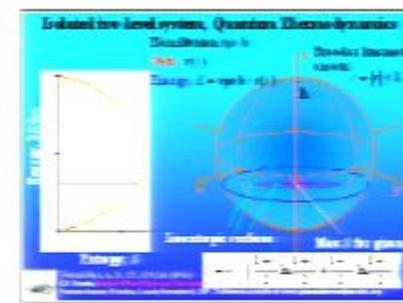
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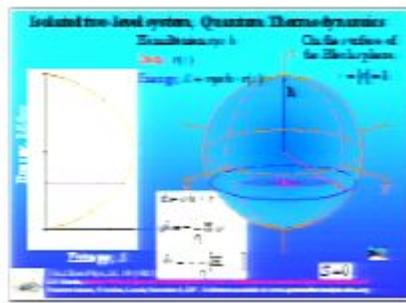
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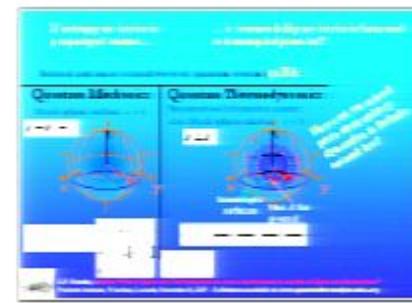
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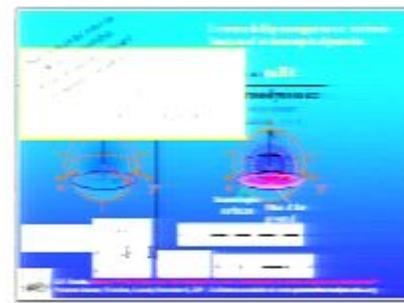
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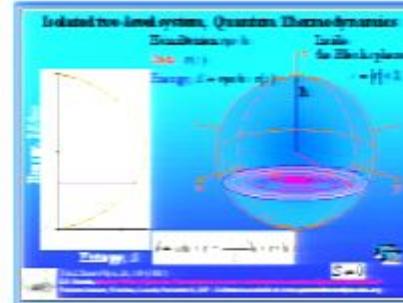
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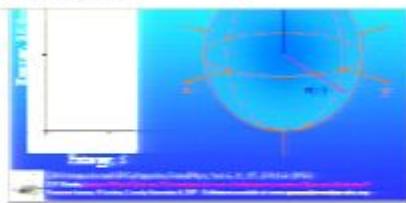
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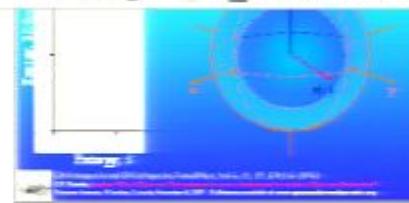
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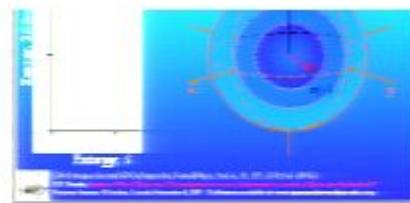
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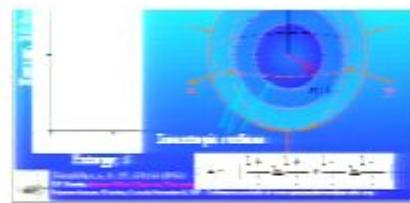
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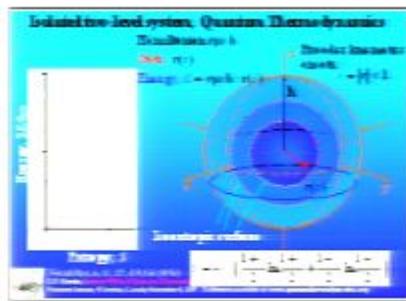
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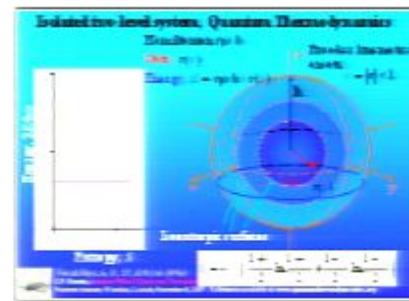
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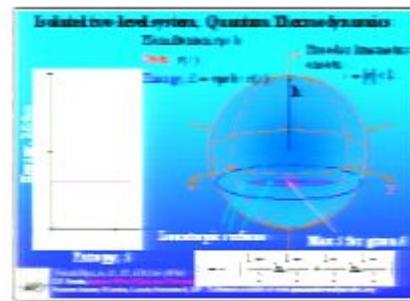
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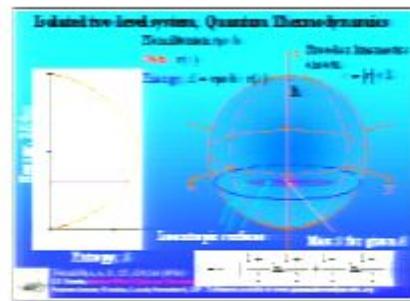
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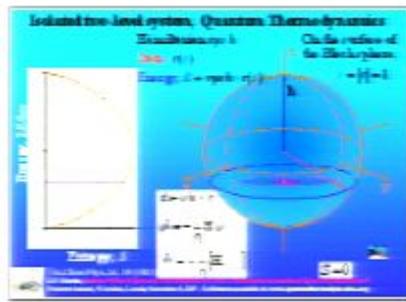
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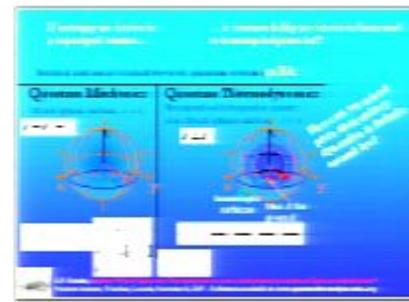
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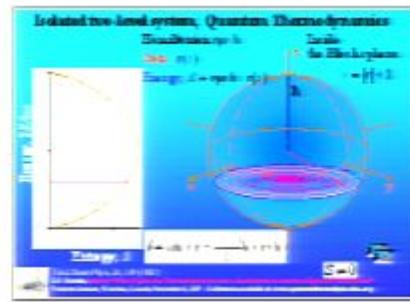
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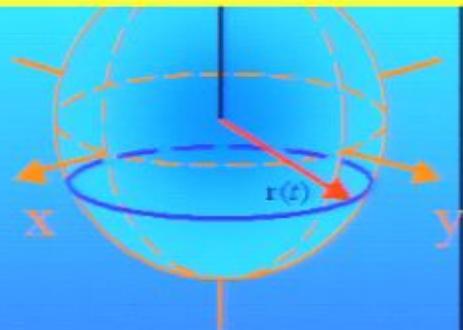
23



24

Fundamental ansatz  
about irreversible  
steepest-entropy-ascent  
quantum dynamics

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] - \frac{1}{2} \frac{\text{Tr}\rho H \ln \rho - \text{Tr}\rho H - \text{Tr}\rho H^2}{\text{Tr}\rho H^2 + (\text{Tr}\rho H)^2}$$



Dynamical law  
(Schrödinger)

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

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

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



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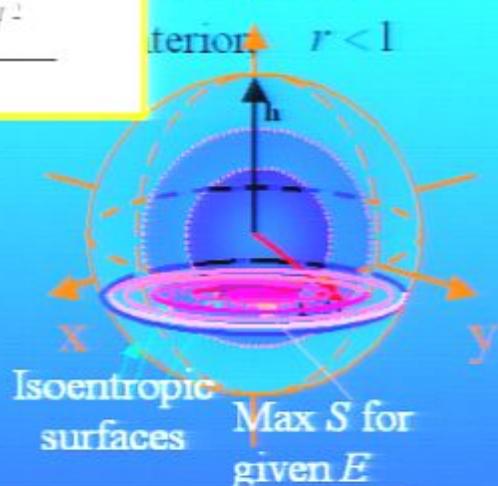
Irreversibility emerges as an intrinsic feature of microscopic dynamics.

tem (quBit)

rmodynamics

Coulomb ansatz:

Interior  $r < 1$



Dynamical law

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

$$\dot{\mathbf{r}} = \omega \mathbf{h} \cdot \mathbf{r} - \frac{f(r)}{\tau} \mathbf{h} \cdot \mathbf{r} \cdot \mathbf{h}$$

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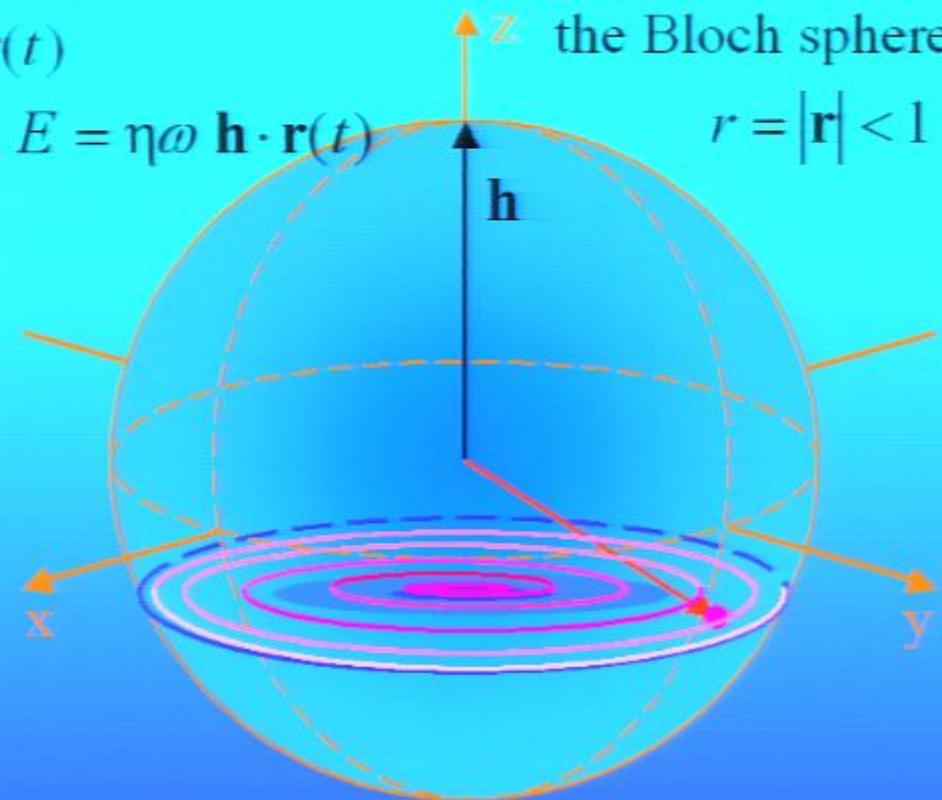
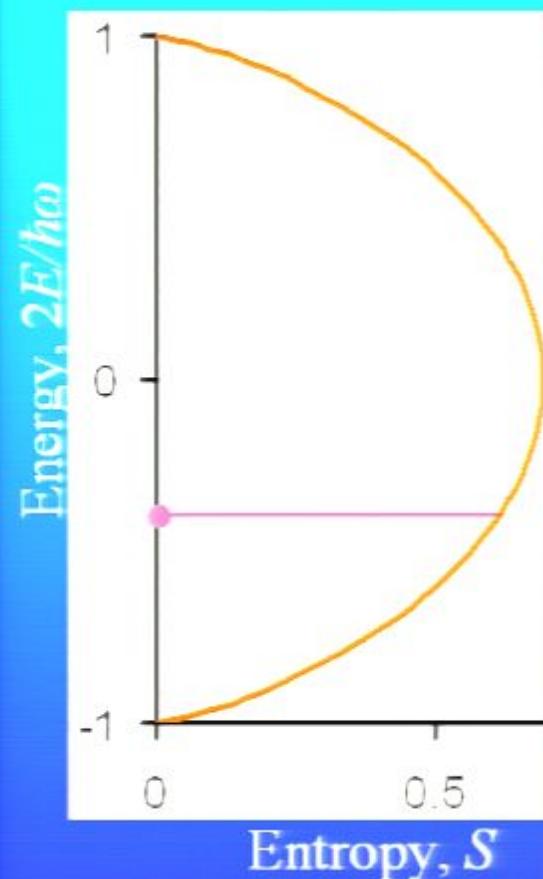
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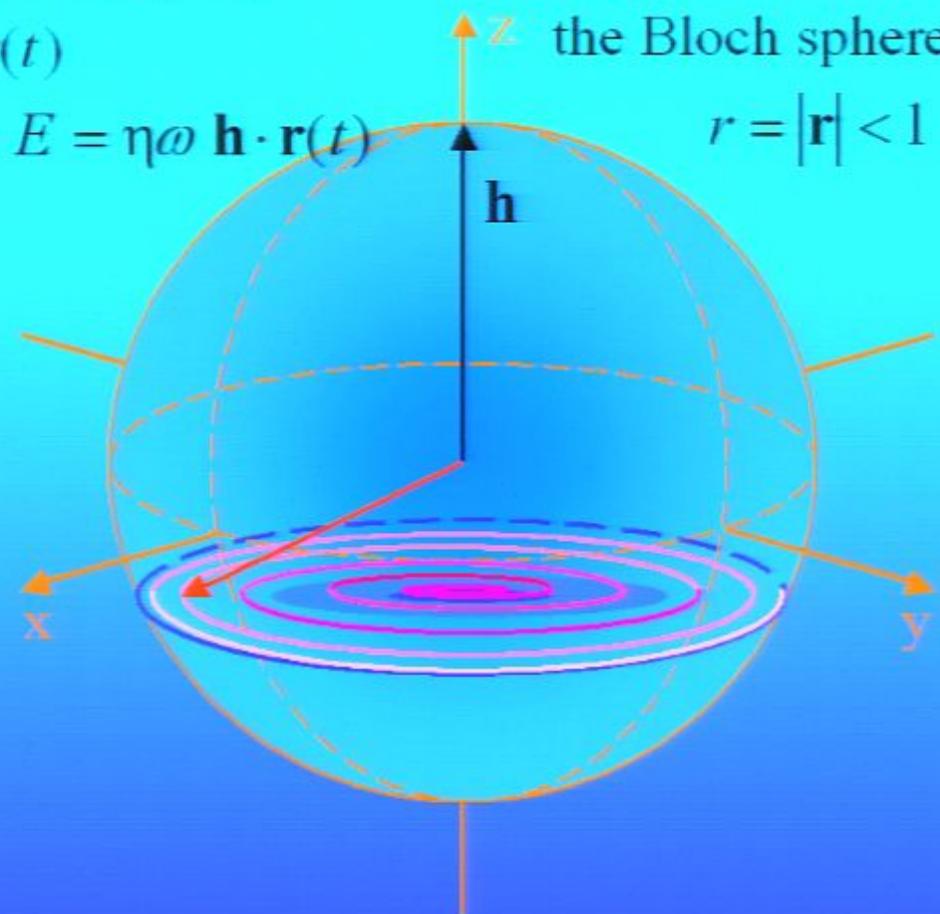
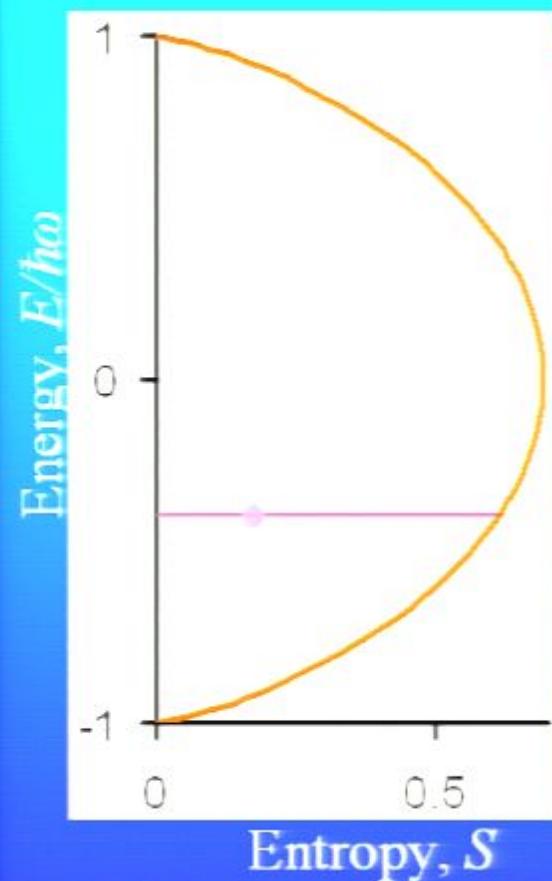
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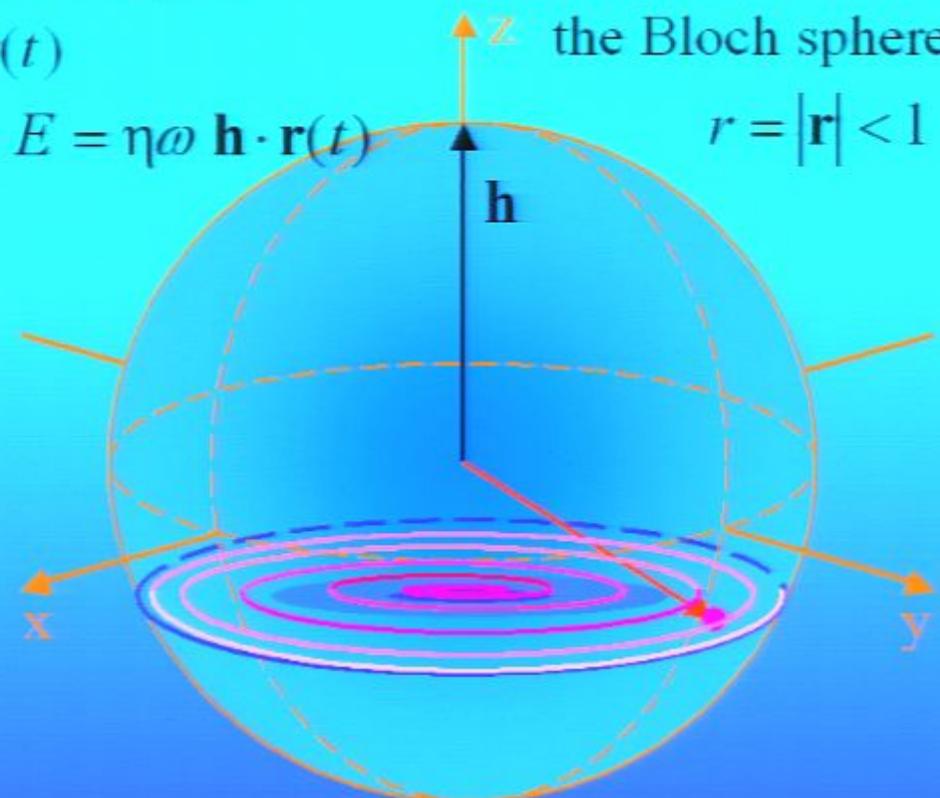
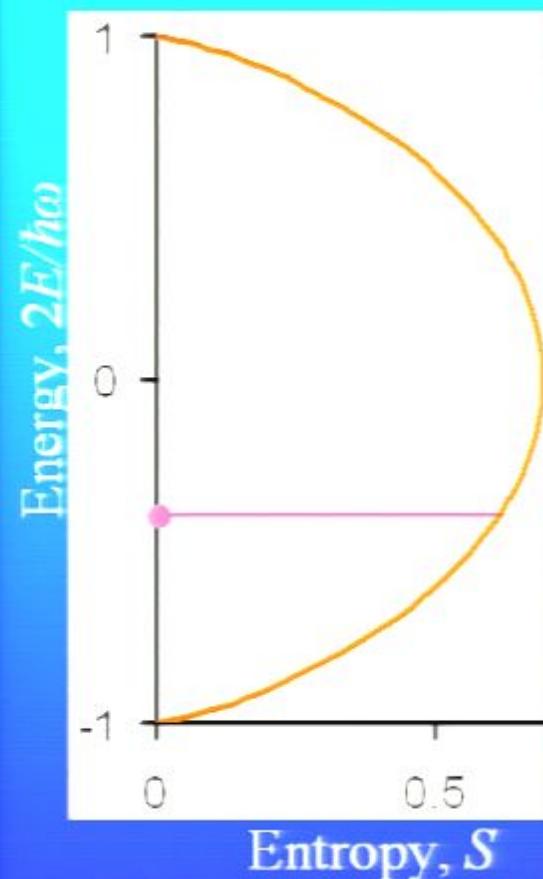
State,  $\mathbf{r}(t)$

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

Inside

the Bloch sphere,

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



$$\mathbf{H} = \omega \mathbf{h} \times \mathbf{r} - \frac{f(r)}{\tau} \mathbf{h} \times \mathbf{r} \times \mathbf{h}$$

$$S \neq 0$$



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

G.P. Beretta, Seminar "What if Quantum Thermodynamics were a fundamental extension of Quantum Mechanics?"  
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## Isolated two-level system, Quantum Thermodynamics

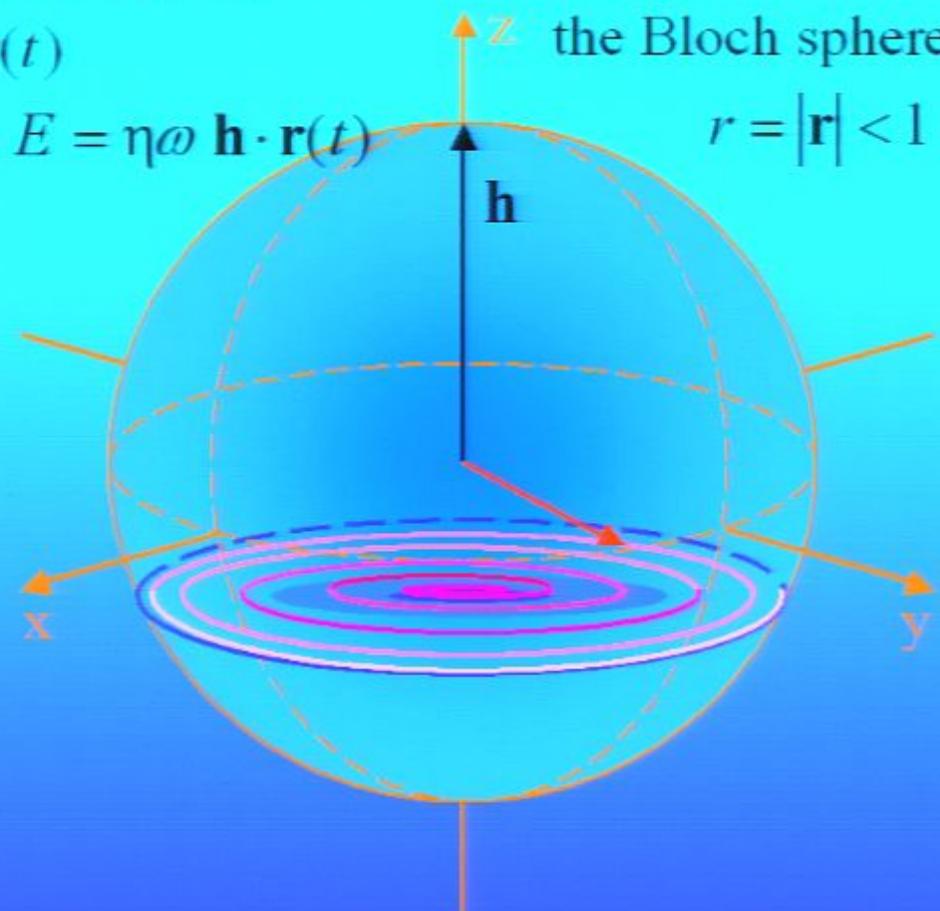
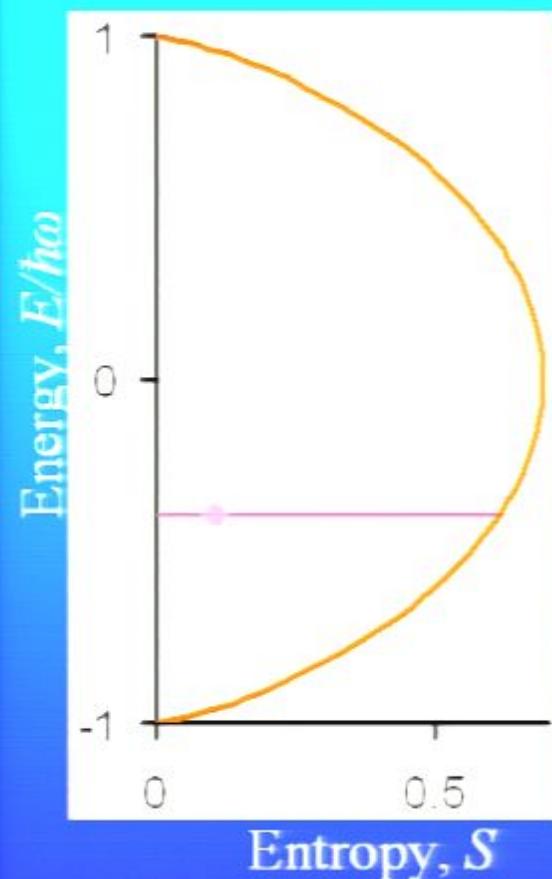
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G.P. Beretta, Workshop on "Perspectives in Probability Theory and its Connections with Science and Society"  
Levico Terme (Trento), Italy, December 3-7, 2006 - References available at: [www.quantumthermodynamics.org](http://www.quantumthermodynamics.org)

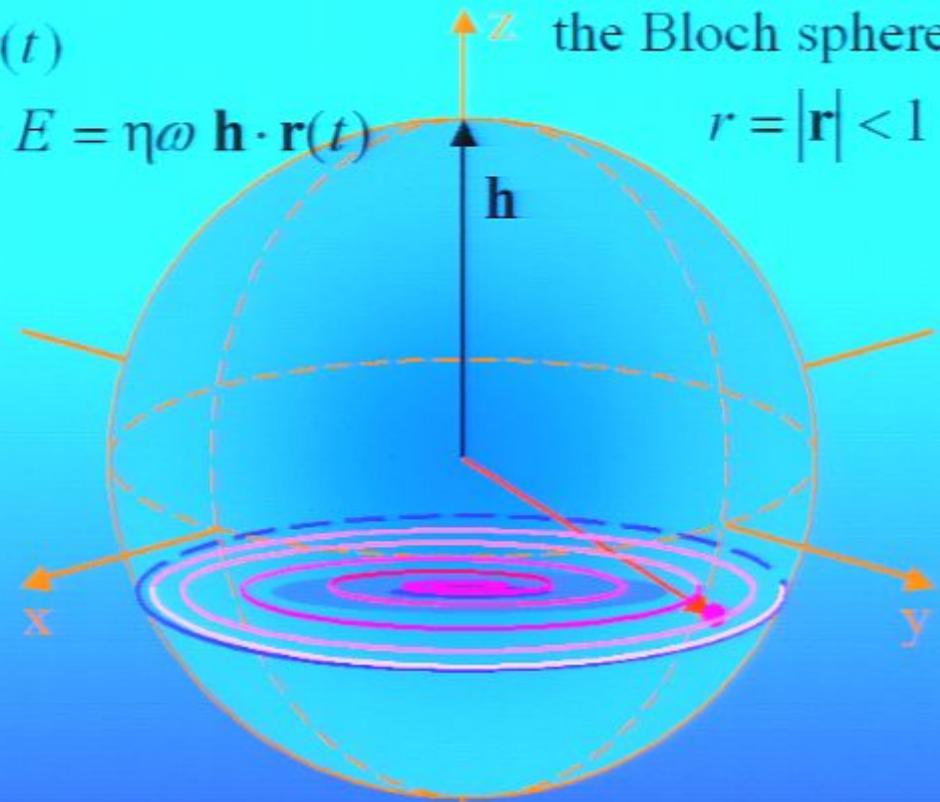
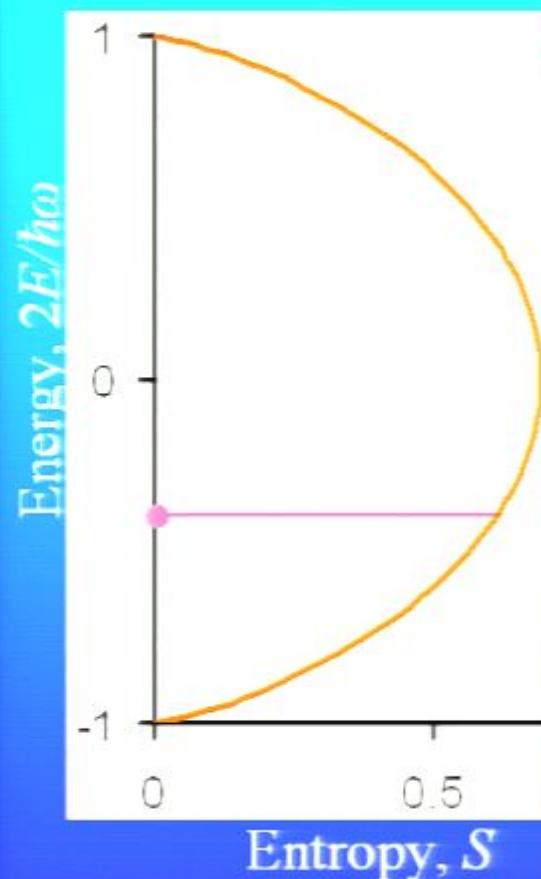
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Int.J.Theor.Phys., 24, 119 (1985)

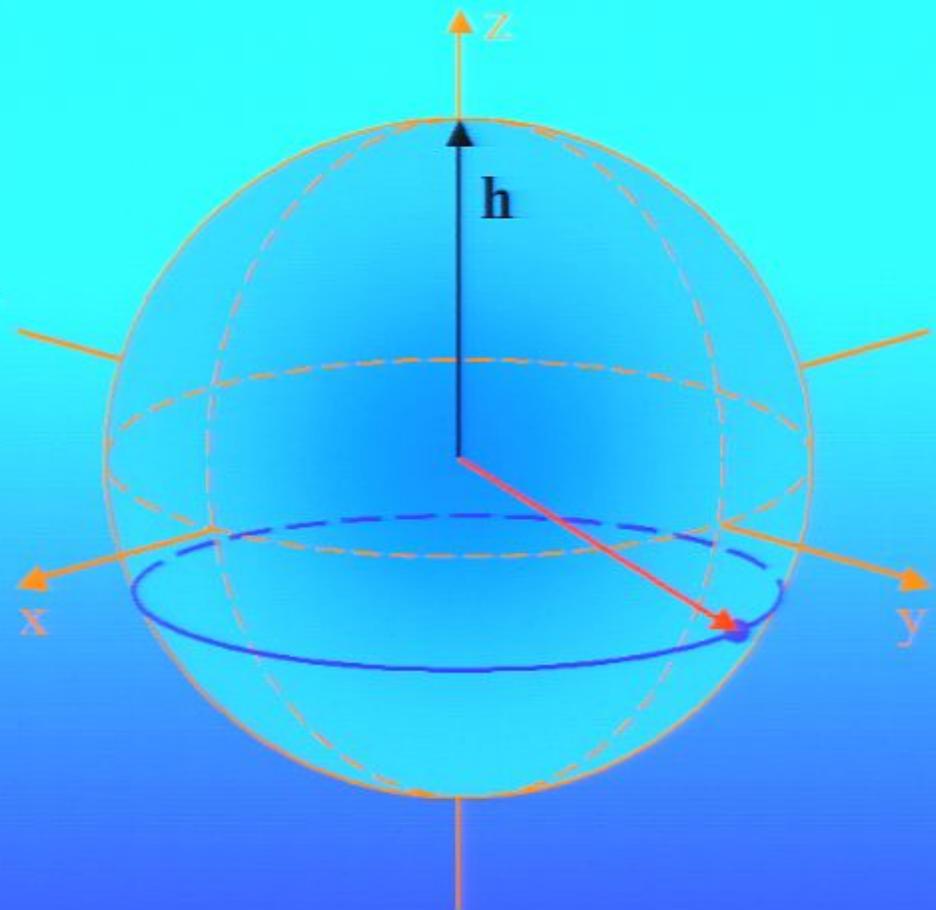
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# Schrödinger's prescient forecast

Proc. Cambridge Phil. Soc., 32, 446 (1936)

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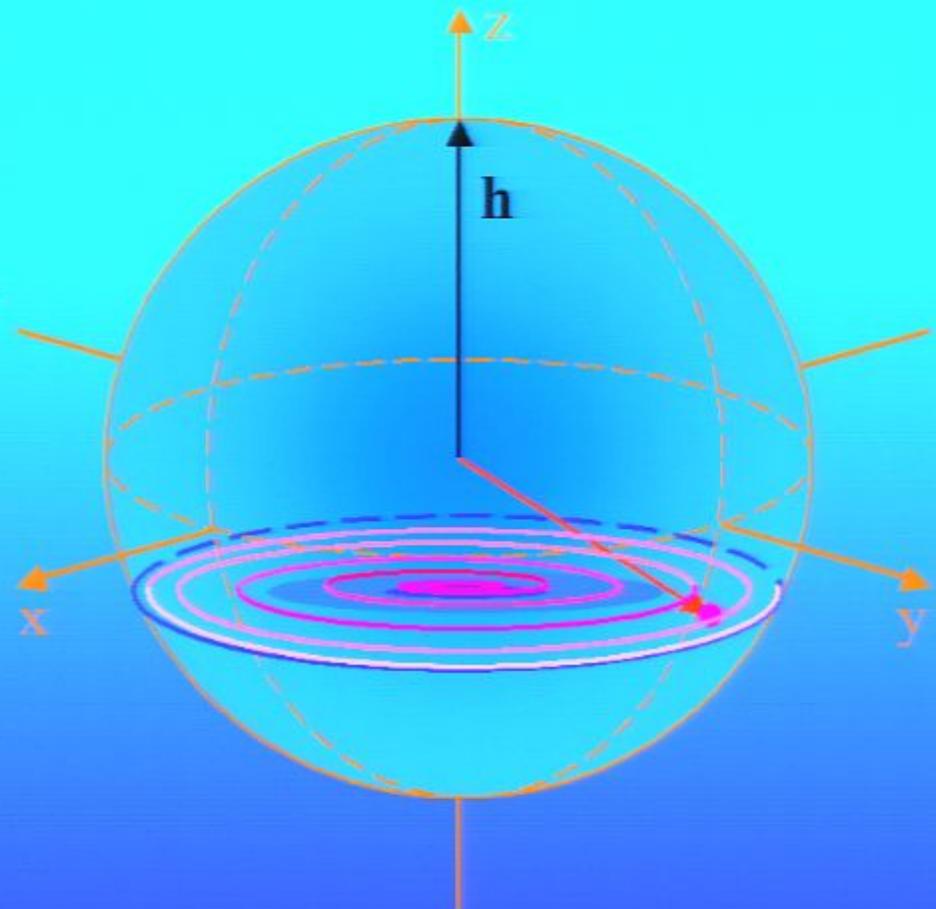


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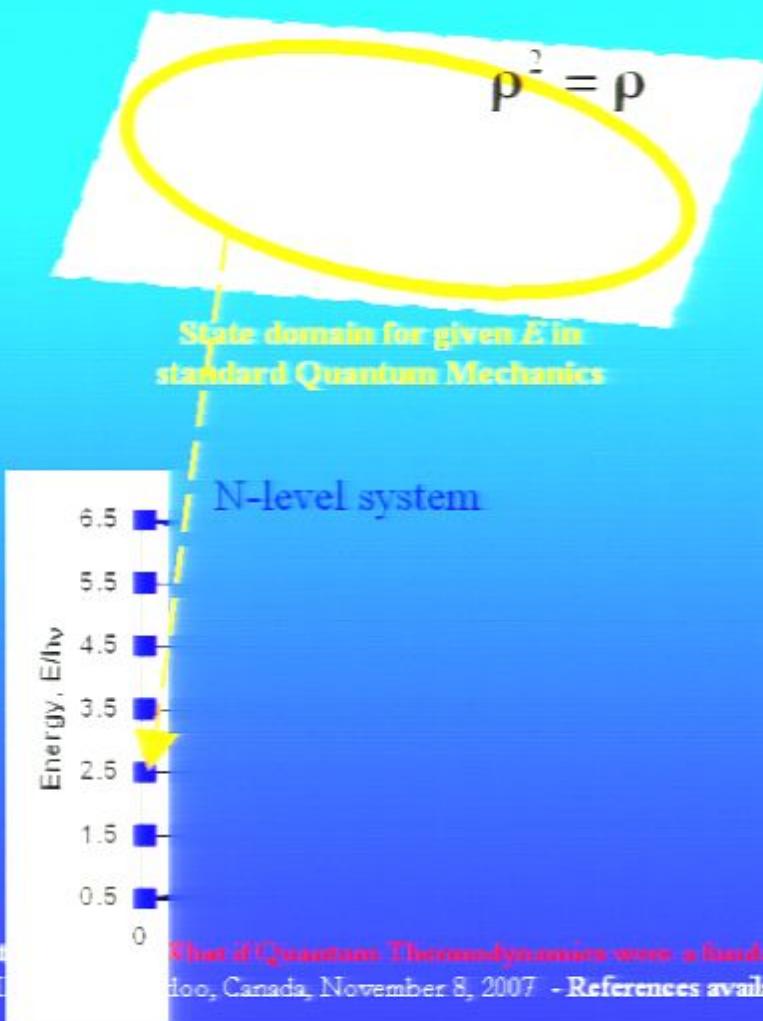
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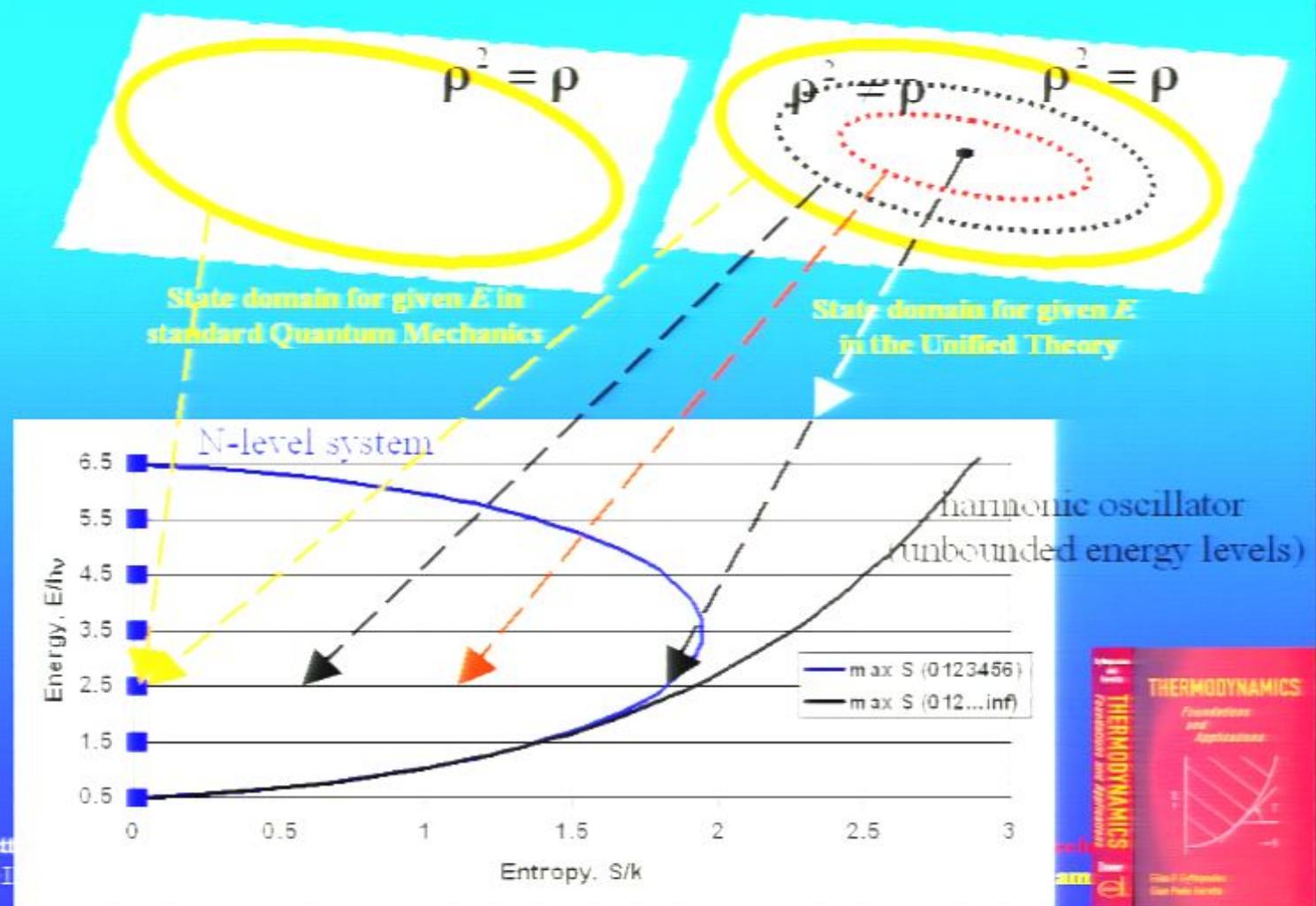
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# Isolated N-level system, Quantum Mechanics



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Perimeter I

# Isolated N-level system, Quantum Thermodynamics

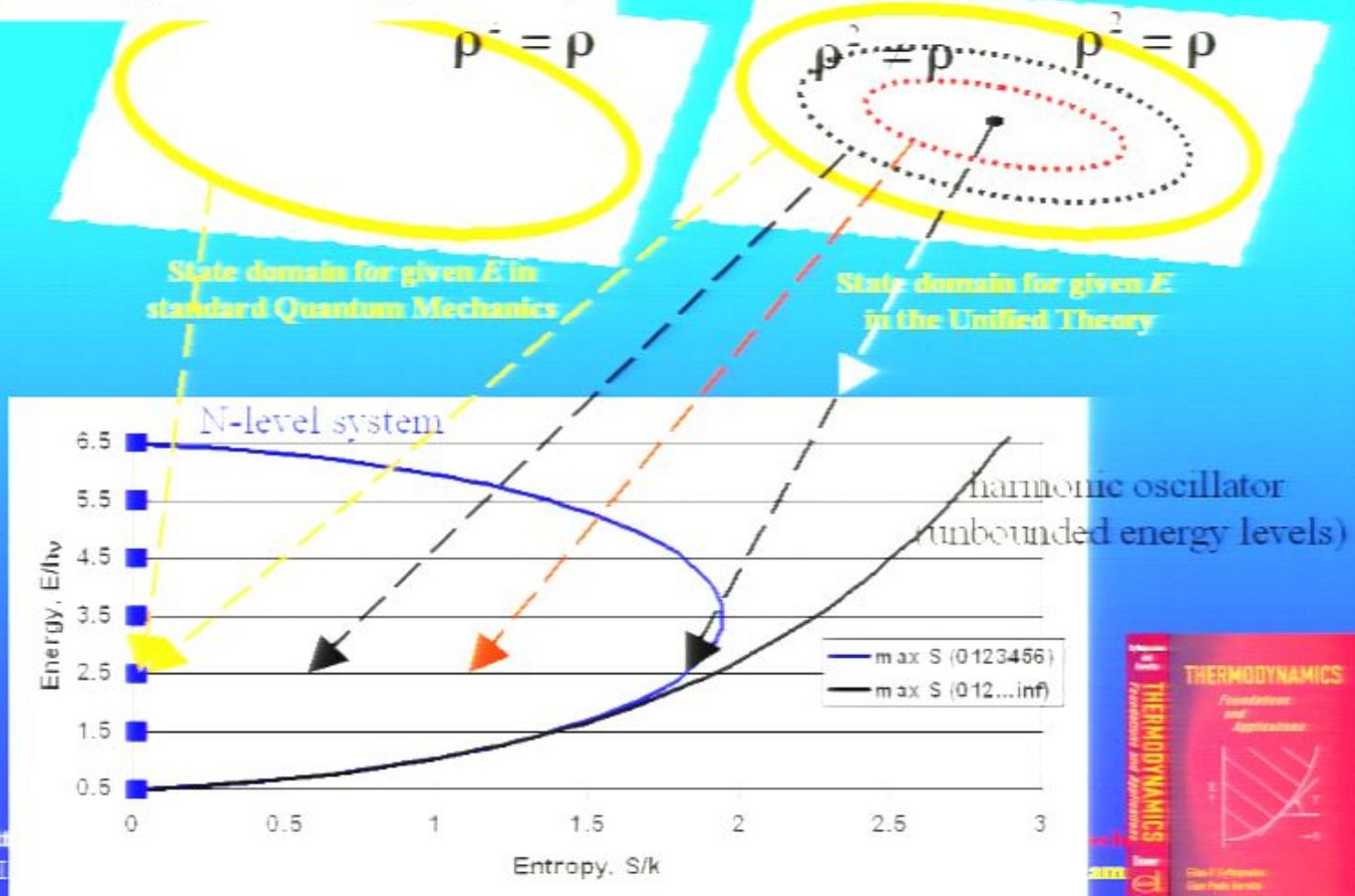


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# Isolated N-level system, Quantum Thermodynamics

energy levels  $e_j$ ,  $j = 1, 2, \dots, N$

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



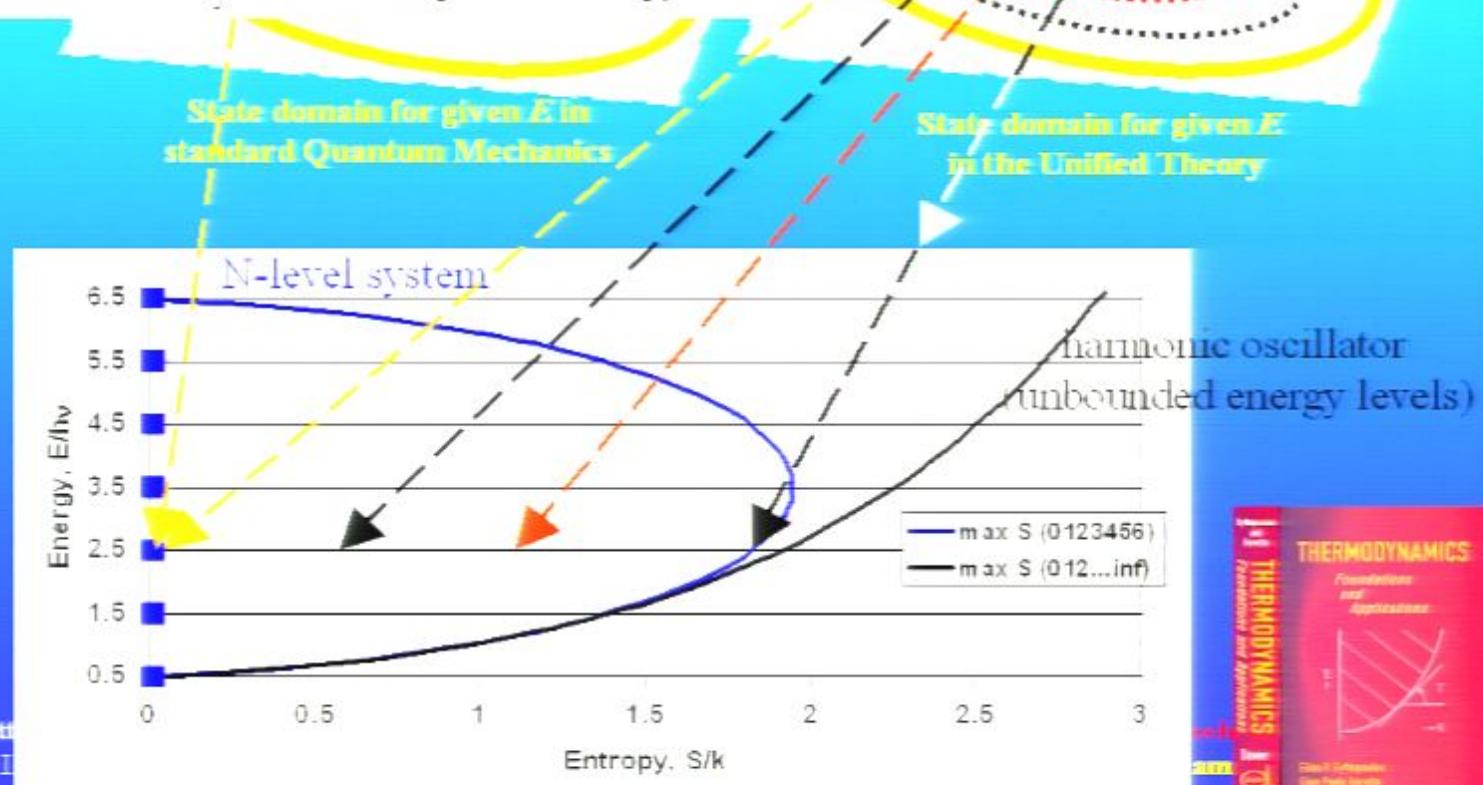
G.P. Beretti  
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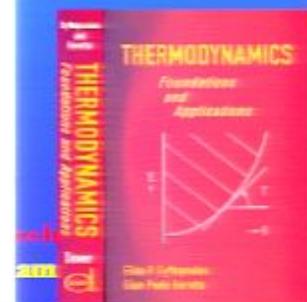
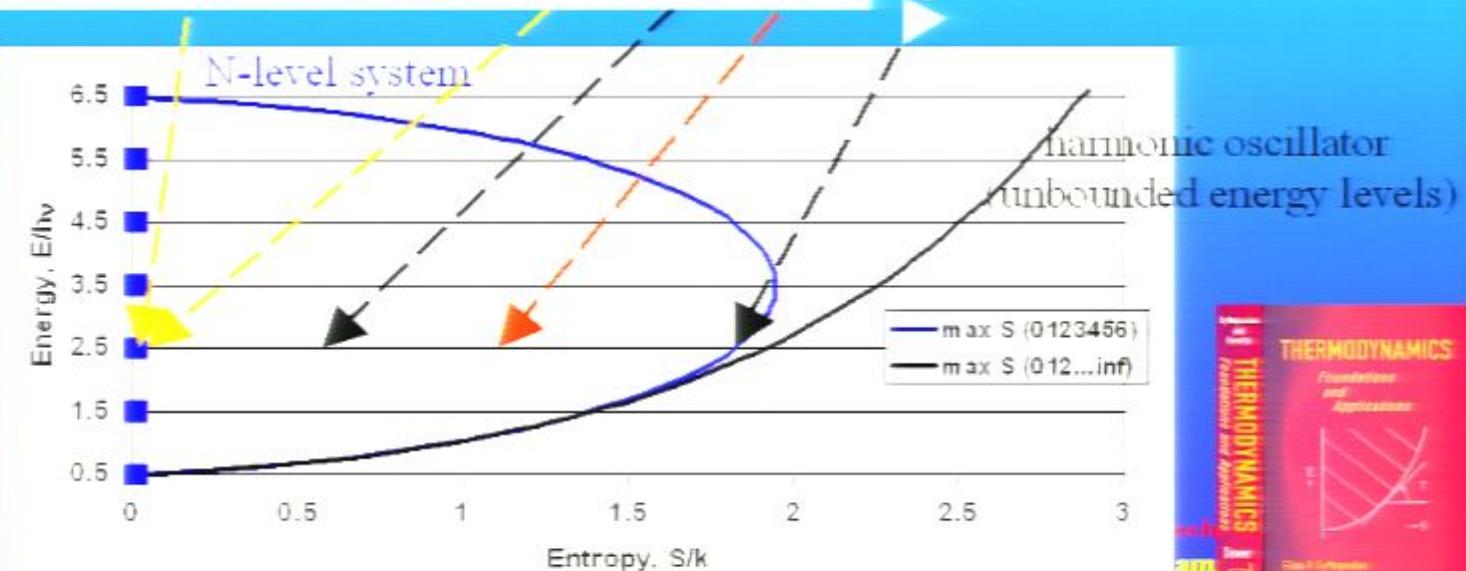
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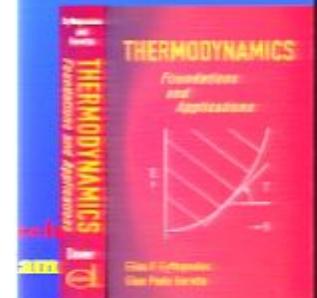
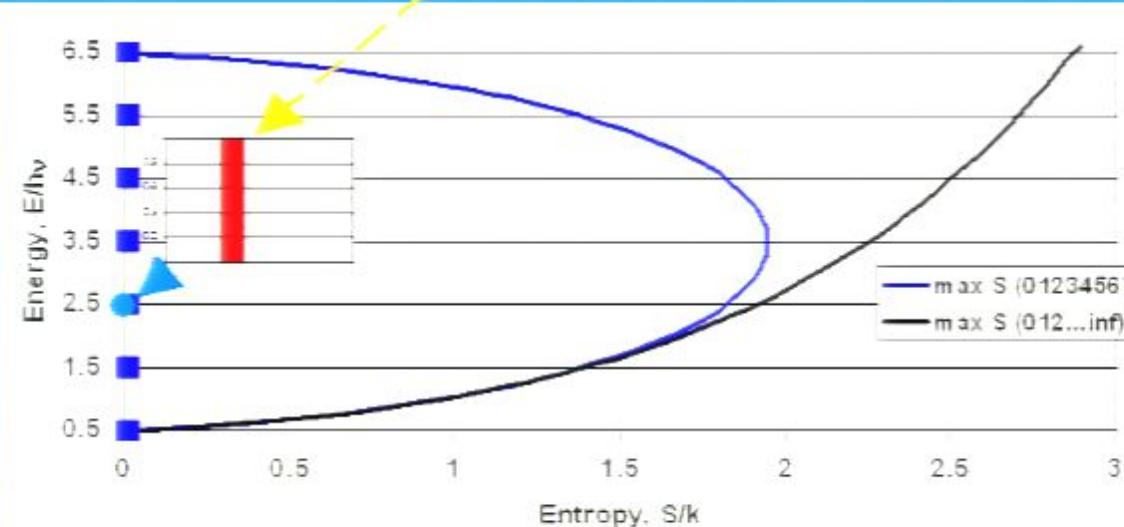
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$$\rho^2 = \rho \quad \rho^2 = \rho$$

State domain for given  $E$  in the Unified Theory



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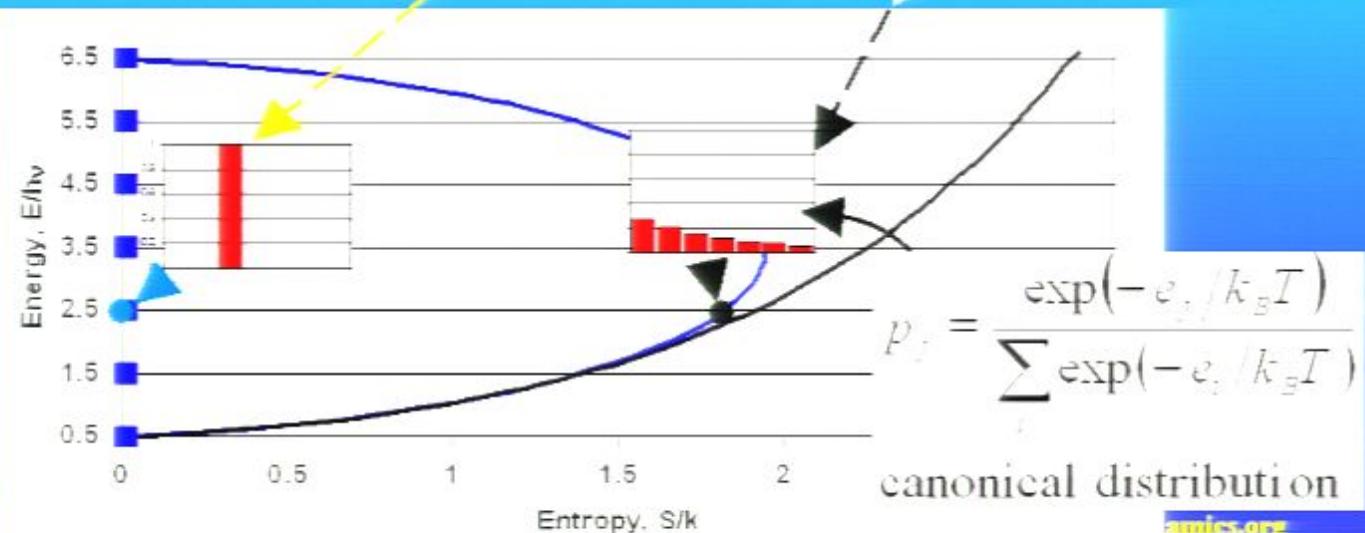
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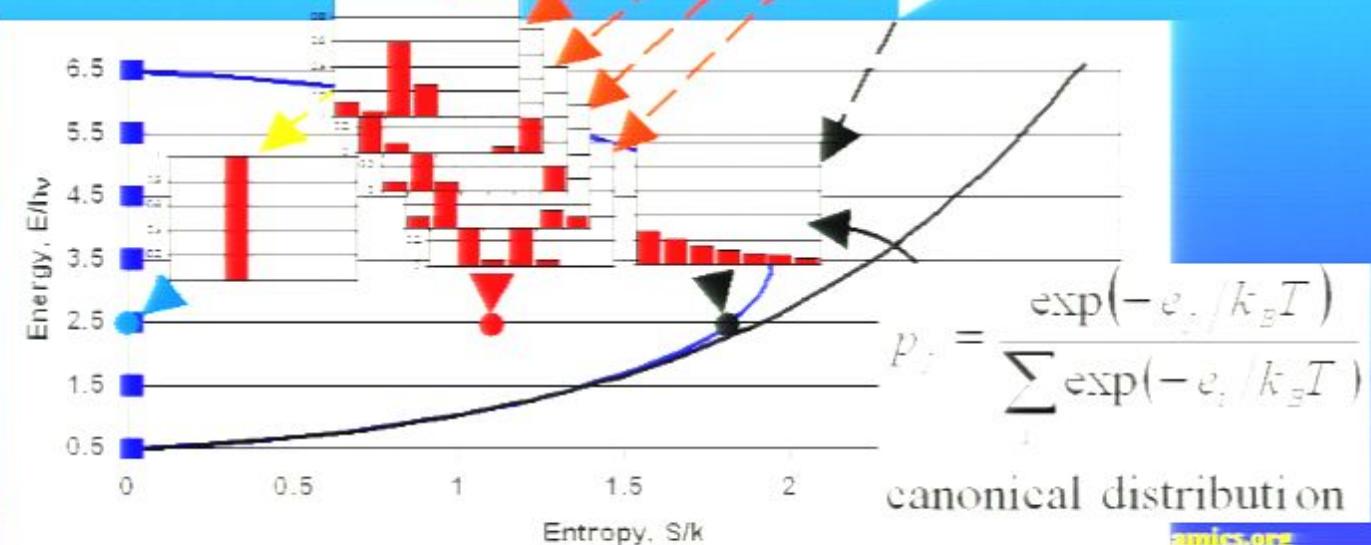
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# Desiderata for a general dynamical law (isolated system)

Mod. Phys. Lett. A, 20, 977 (2005)

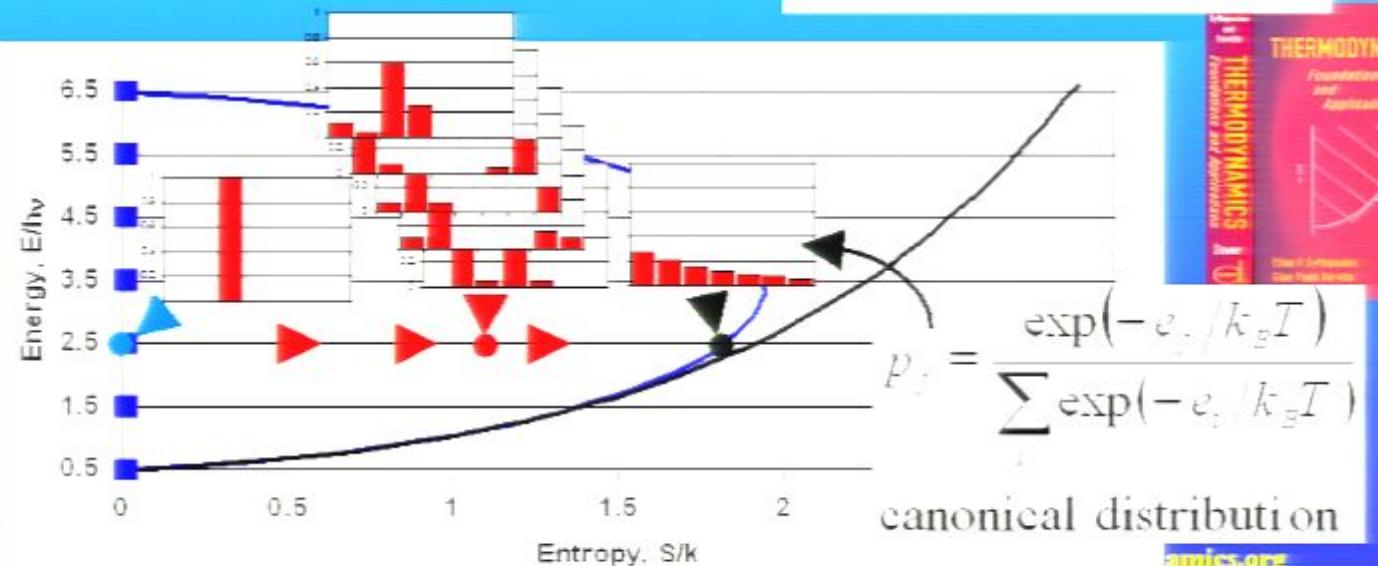
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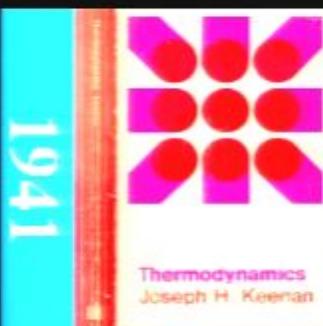
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For each value of  $E = \sum_j p_j e_j$  there must be one and only one stable equilibrium state  
(1965 Hatsopoulos - Keenan statement of the **second law**)



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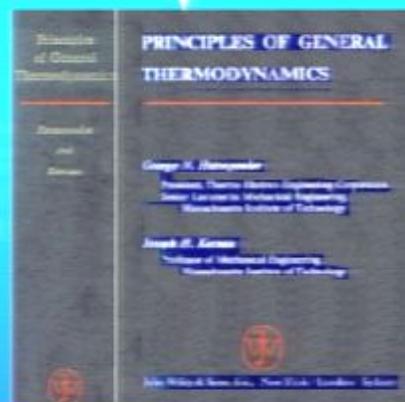


1941

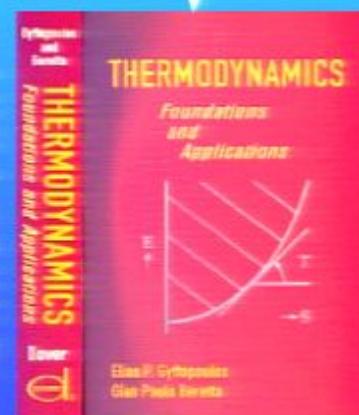
## The Hatsopoulos-Keenan statement of the Second Law and the role of stability at thermodynamic equilibrium

Books by members of the “Keenan school of thermodynamics”

1965

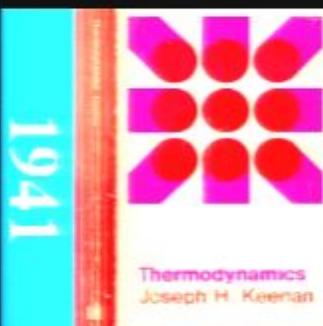


1991 (2005)



G.P. Beretta, Seminar “What is Quantum Thermodynamics more: a fundamental extension of Quantum Mechanics?”  
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Rigorous axiomatic foundations of thermodynamics  
Entropy defined for non-equilibrium states  
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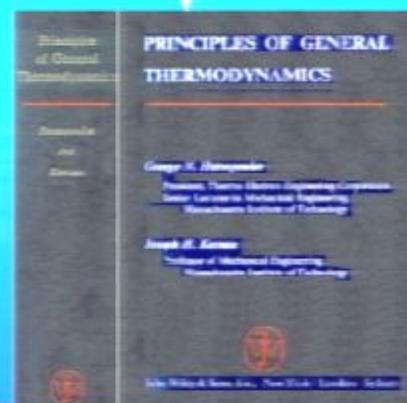


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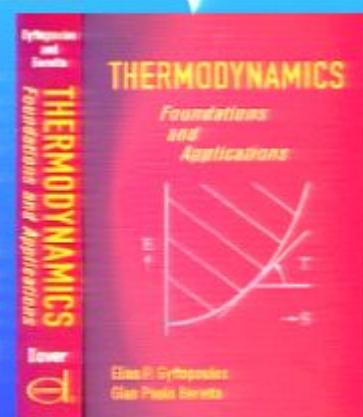
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## Steepest-entropy-ascent dynamical ansatz (isolated system)

$$\rho \ln \rho = \rho - \frac{1}{2}\{H, \rho\}$$

$$\text{Tr} \rho \ln \rho = 1 - \text{Tr} \rho H$$

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] - \frac{1}{2} \frac{\text{Tr} \rho H \ln \rho - \text{Tr} \rho H - \text{Tr} \rho H^2}{\text{Tr} \rho H^2 + (\text{Tr} \rho H)^2}$$

When  $[H, \rho] = 0$

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

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



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

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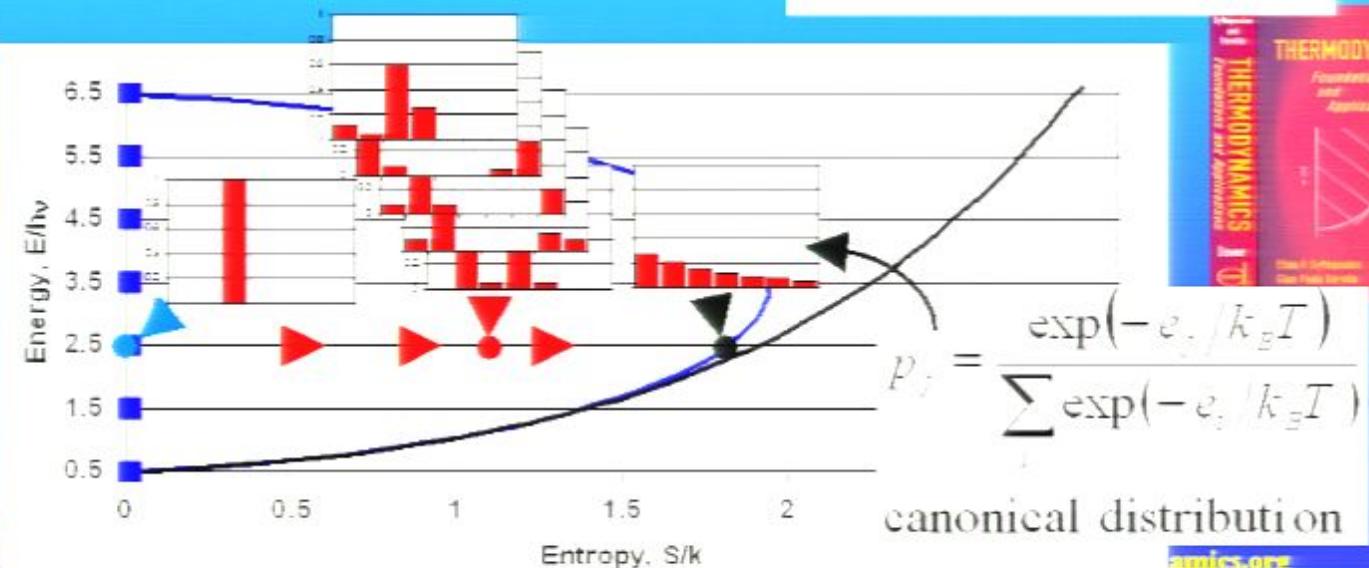
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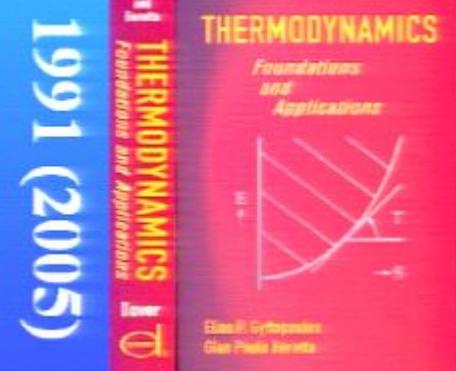
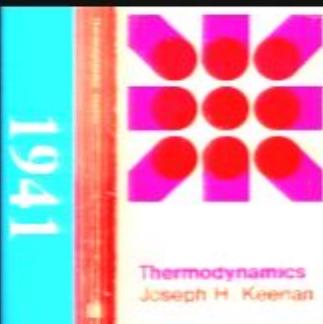
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G.P. Beretti  
Perimeter I



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# Steepest-entropy-ascent dynamical ansatz (isolated system)

$$\begin{aligned} \rho \ln \rho &= -\rho + \frac{i}{\hbar} \{H, \rho\} \\ \text{Tr} \rho \ln \rho &= 1 - \text{Tr} \rho H \\ \frac{d\rho}{dt} = -\frac{i}{\hbar} [H, \rho] - \frac{1}{\tau} \frac{\text{Tr} \rho H \ln \rho - \text{Tr} \rho H - \text{Tr} \rho H^2}{\text{Tr} \rho H^2 - (\text{Tr} \rho H)^2} \end{aligned}$$

When  $[H, \rho] = 0$

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



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# Steepest-entropy-ascent dynamical ansatz (isolated system)

quant-ph-0511091

We assume a dynamical equation of the form

$$\frac{d\rho}{dt} = \omega H^* - \tau H^* \rho \omega^*$$

where  $\omega \in \mathbb{C}$  is an arbitrary complex scaling function,  $H^*$  is Hermitian and  $\tau$  is a real constant.

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

where  $\Delta M(\rho) = P_{\rho>0}M(\rho)P_{\rho>0}$  is Hermitian and  $M(\rho)$  is  $H$ -independent if  $\omega=0$ .

$$\Delta M(\rho) = P_{\rho>0}M(\rho)P_{\rho>0} = P_{\rho>0}M^*(\rho)P_{\rho>0}$$

$$M(\rho) = -k_B P_{\rho>0} \ln \rho - \frac{H}{\theta(\rho)} + \frac{\mu(\rho) + N}{\pi \rho \tau}$$

where  $P_{\rho>0}$  is the projector onto the range of  $\rho$ .  $\propto$

This leads to the set of equations of motion with  $H$  given by the above expression. In particular, we find  $\dot{\rho} = 0$ ,  $\dot{N} = 0$ ,  $\dot{\mu} = 0$  and  $\dot{H} = 0$ . This implies that  $\rho$  is a projector and  $M(\rho)$  is Hermitian. This is the condition of the isolated system. The entropy  $S = -\text{Tr}[\rho \ln \rho]$  is also conserved.



G.P. Beretta  
Perimeter Institute

# Steepest-entropy-ascent dynamical ansatz (isolated system)

$$\rho \ln \rho = \rho - \frac{1}{2}\{H, \rho\}$$

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$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] - \frac{1}{2} \frac{\text{Tr} \rho H \ln \rho - \text{Tr} \rho H - \text{Tr} \rho H^2}{\text{Tr} \rho H^2 + (\text{Tr} \rho H)^2}$$

When  $[H, \rho] = 0$

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

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

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

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

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# Steepest-entropy-ascent dynamical ansatz (isolated system)

quant-ph-0511091

We assume a dynamical equation of the form

$$\frac{d\rho}{dt} = \sqrt{\rho^2 - \tau^2} \partial_\tau \rho + \tau \partial_\tau^2 \rho$$

where  $\tau = \sqrt{\rho^2 - \rho}$  and  $\rho$  is the density matrix of the isolated system. We want to find the most general form of  $\tau$ .

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

where  $H = \frac{1}{2}\rho^{-1/2}P_{\rho>0}H^2P_{\rho>0}\rho^{1/2}$  is the total Hamiltonian and  $\Delta M(\rho) = \rho^{-1/2}M(\rho)\rho^{1/2}$  is the entropy function.

$$\Delta M(\rho) = P_{\rho>0}M(\rho)P_{\rho>0}$$

$$M(\rho) = -k_B P_{\rho>0} \ln \rho - \frac{H}{\theta(\rho)} + \frac{\mu(\rho) + \mathcal{N}}{\theta(\rho)}$$

where  $P_{\rho>0}$  is the projector onto the range of  $\rho$ ,  $\mathcal{N}$  is a constant, and  $\theta(\rho)$  is the denominator of the entropy function. The entropy function depends on  $\rho$  and  $\theta(\rho)$ , and the parameters  $\mu(\rho)$  and  $\mathcal{N}$  are determined by the condition  $\Delta M(\rho) = 0$ . This leads to the following equations:

$$\begin{aligned} \partial_\rho \theta(\rho) &= \frac{1}{\rho} \\ \partial_\rho \mu(\rho) &= \frac{1}{\theta(\rho)} \end{aligned}$$


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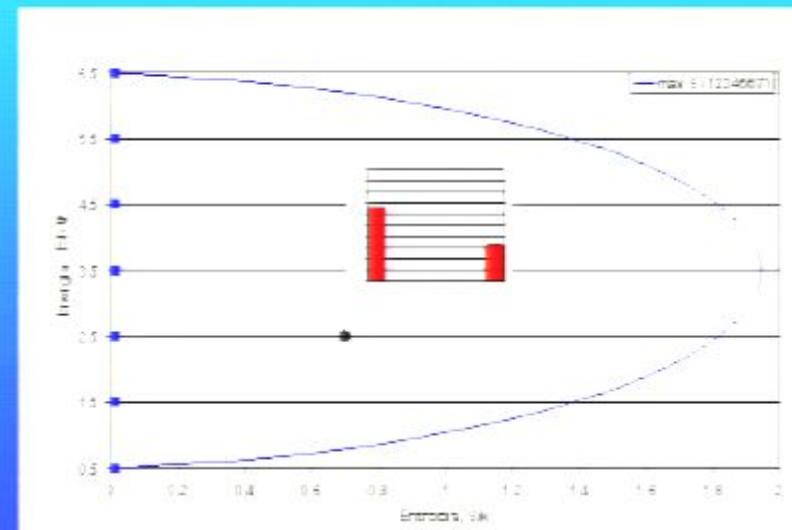
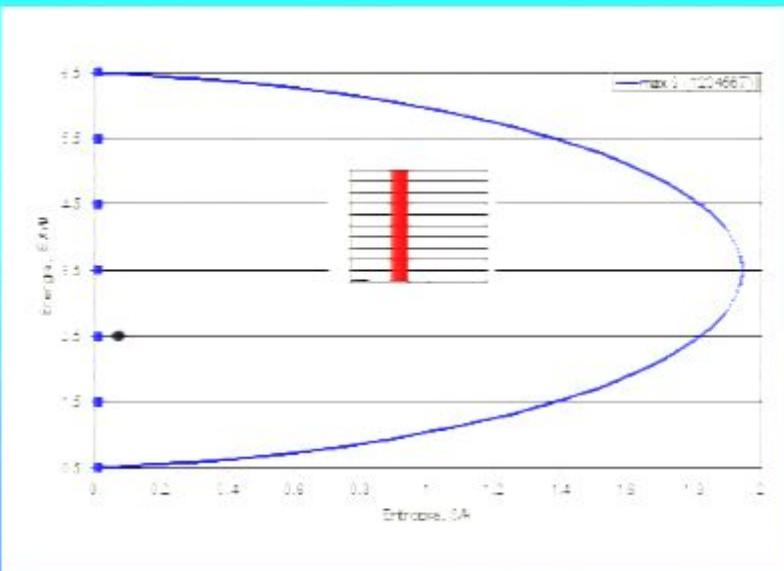
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Ph.D.thesis, MIT (1981), quant-ph/0509116

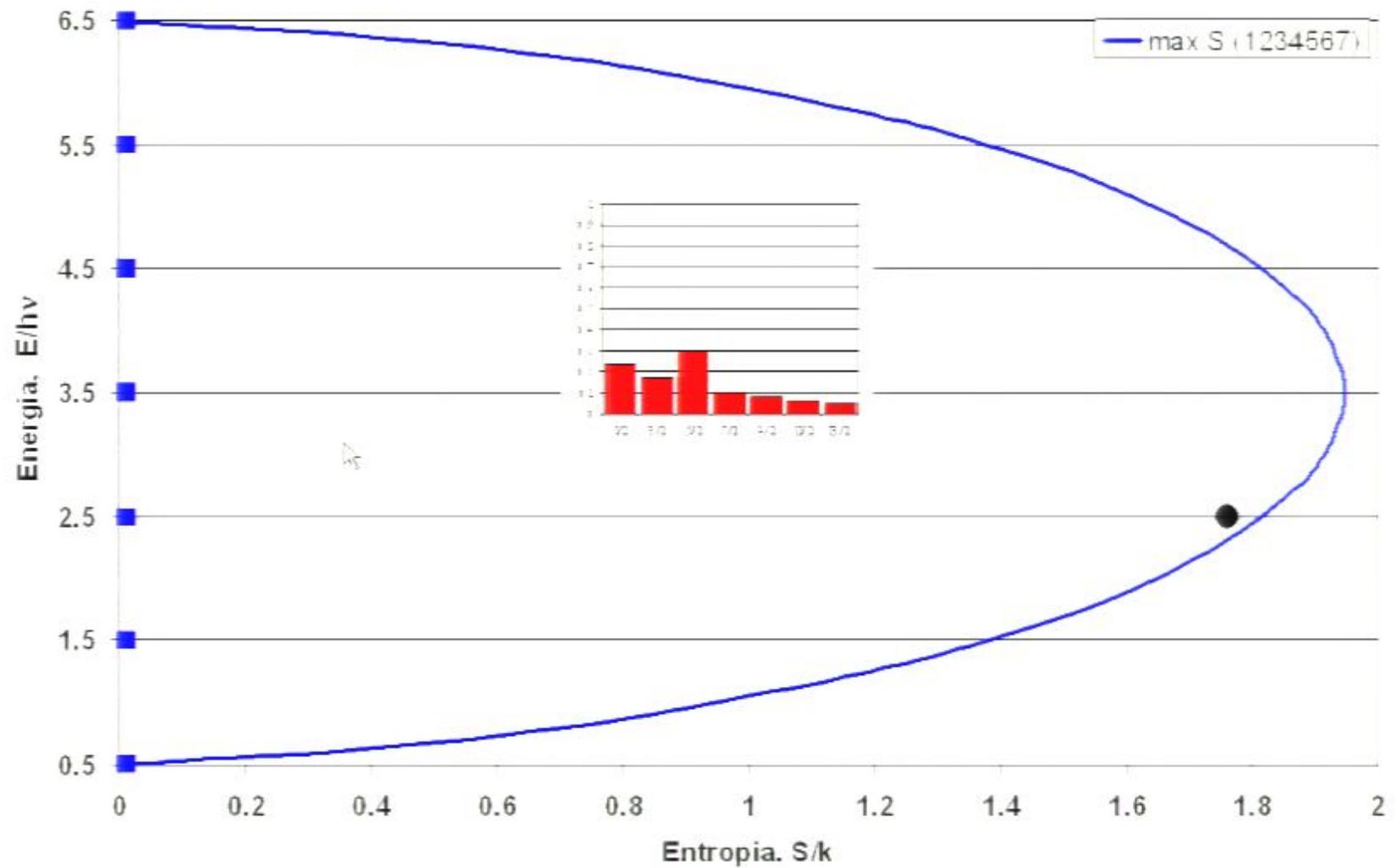
Nuovo Cimento B, 82, 169 (1984); 87, 77 (1985)

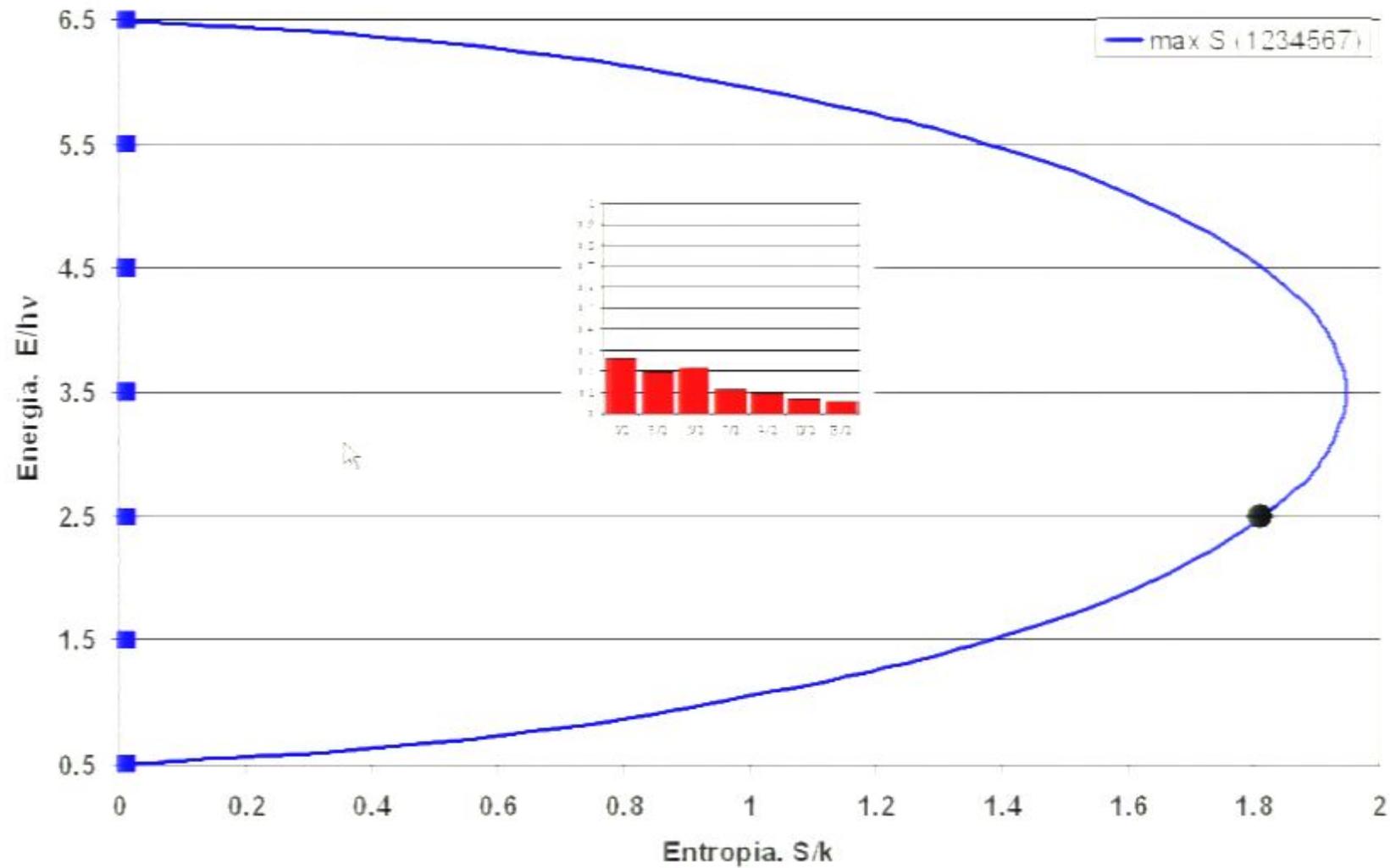
NATO-ASI Lecture Notes, 278, 441 (1986)

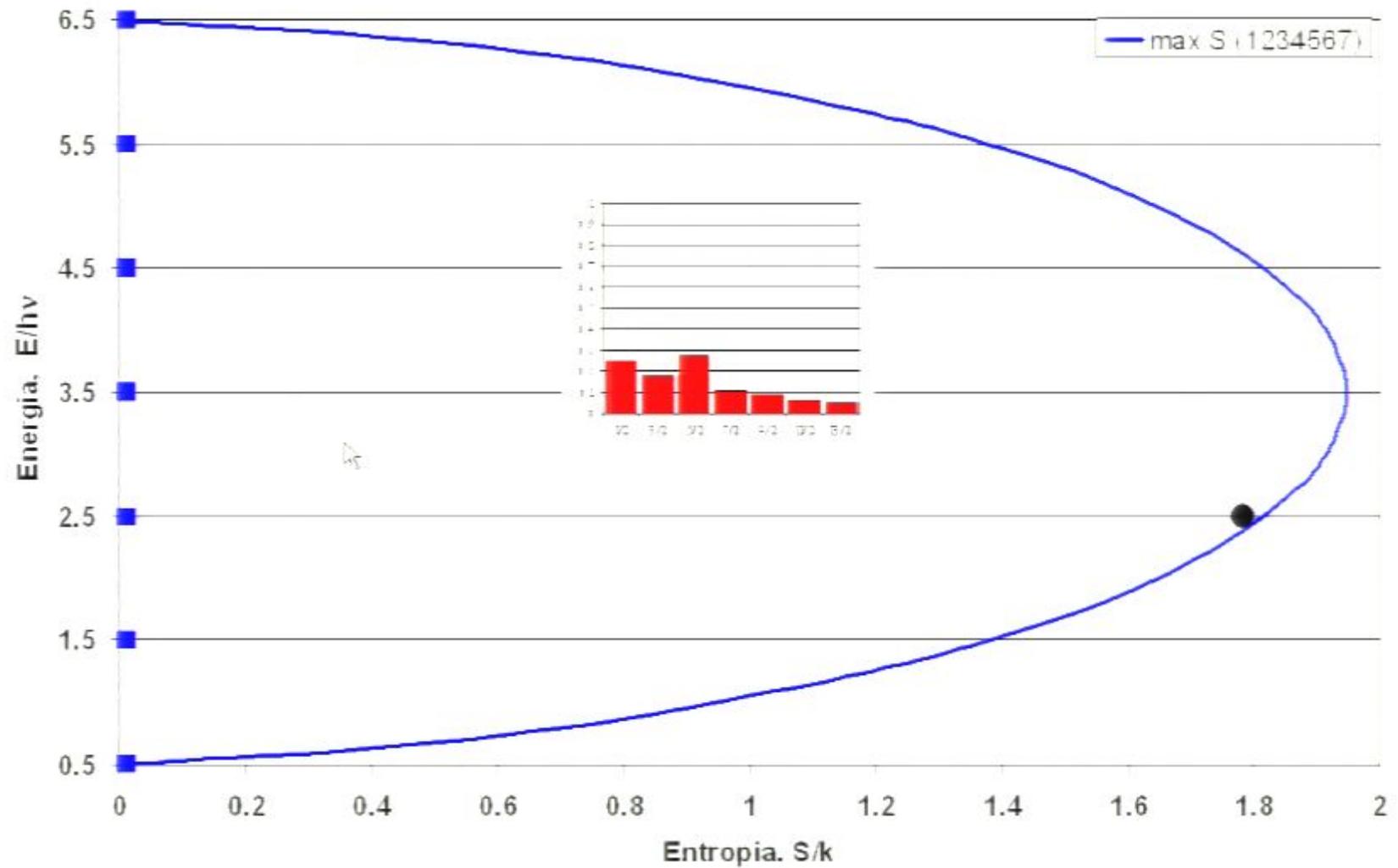
Complete review at quant-ph/0112046

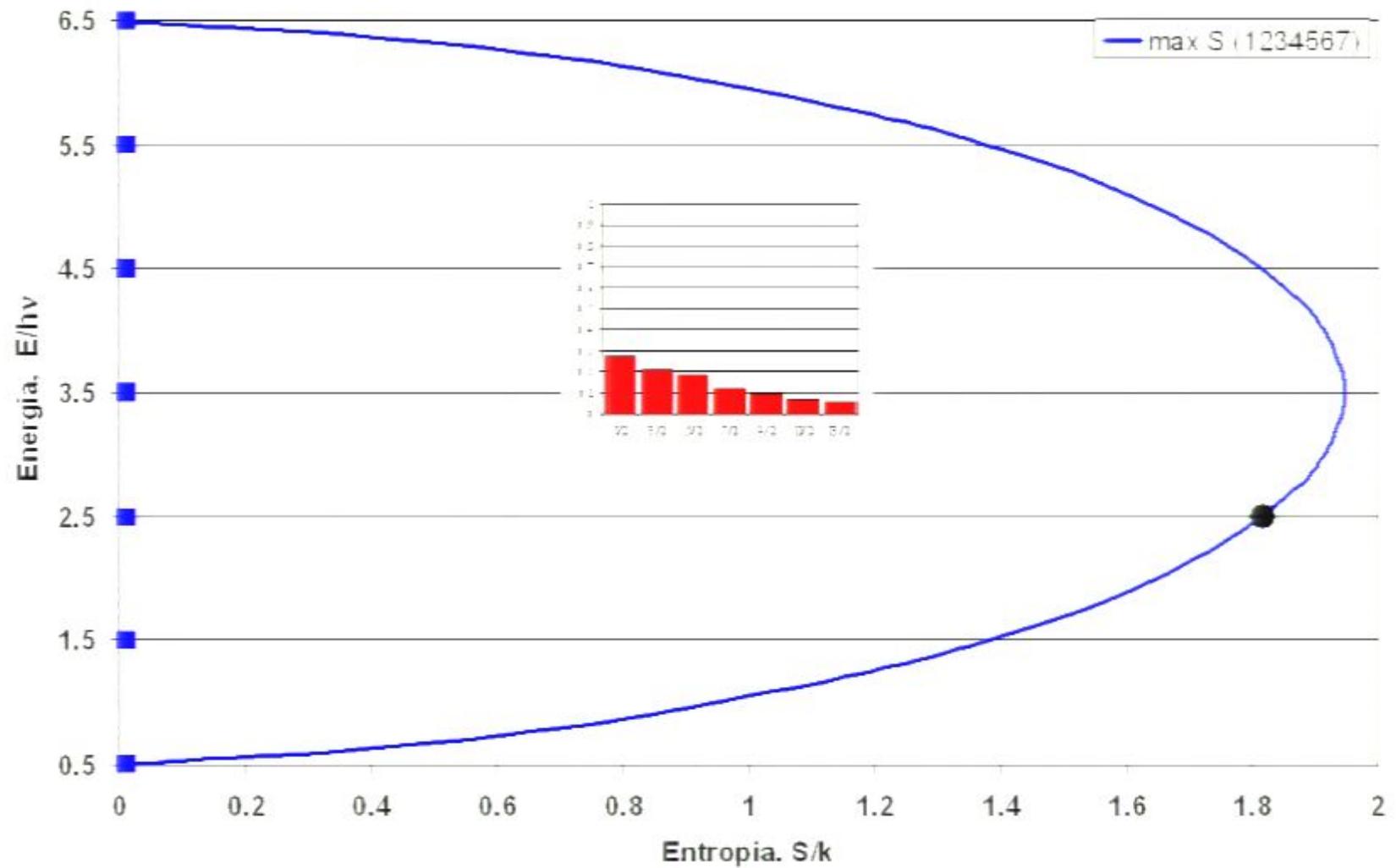


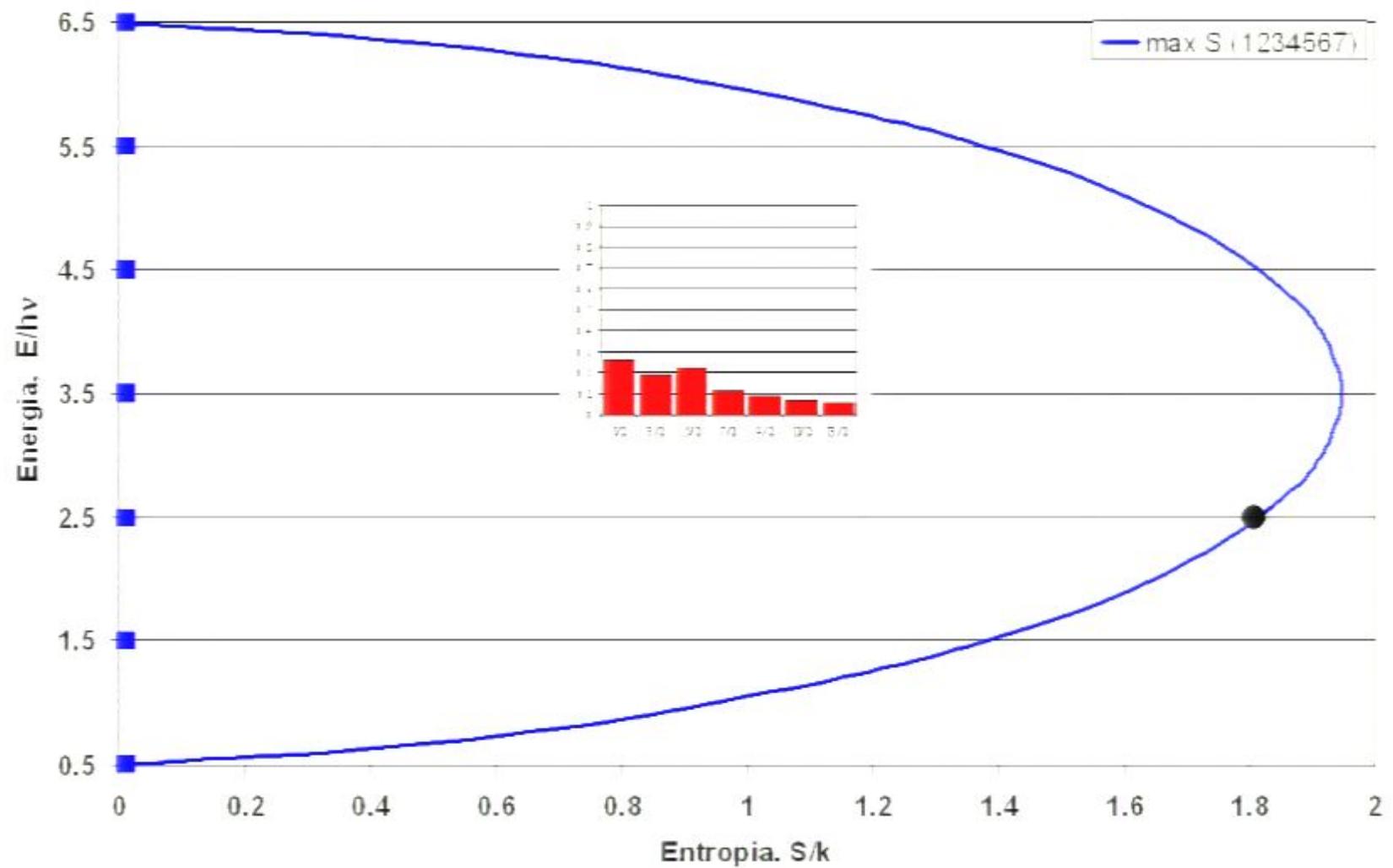
G.P. Beretta, Seminar "What is Quantum Thermodynamics now: a fundamental extension of Quantum Mechanics?"  
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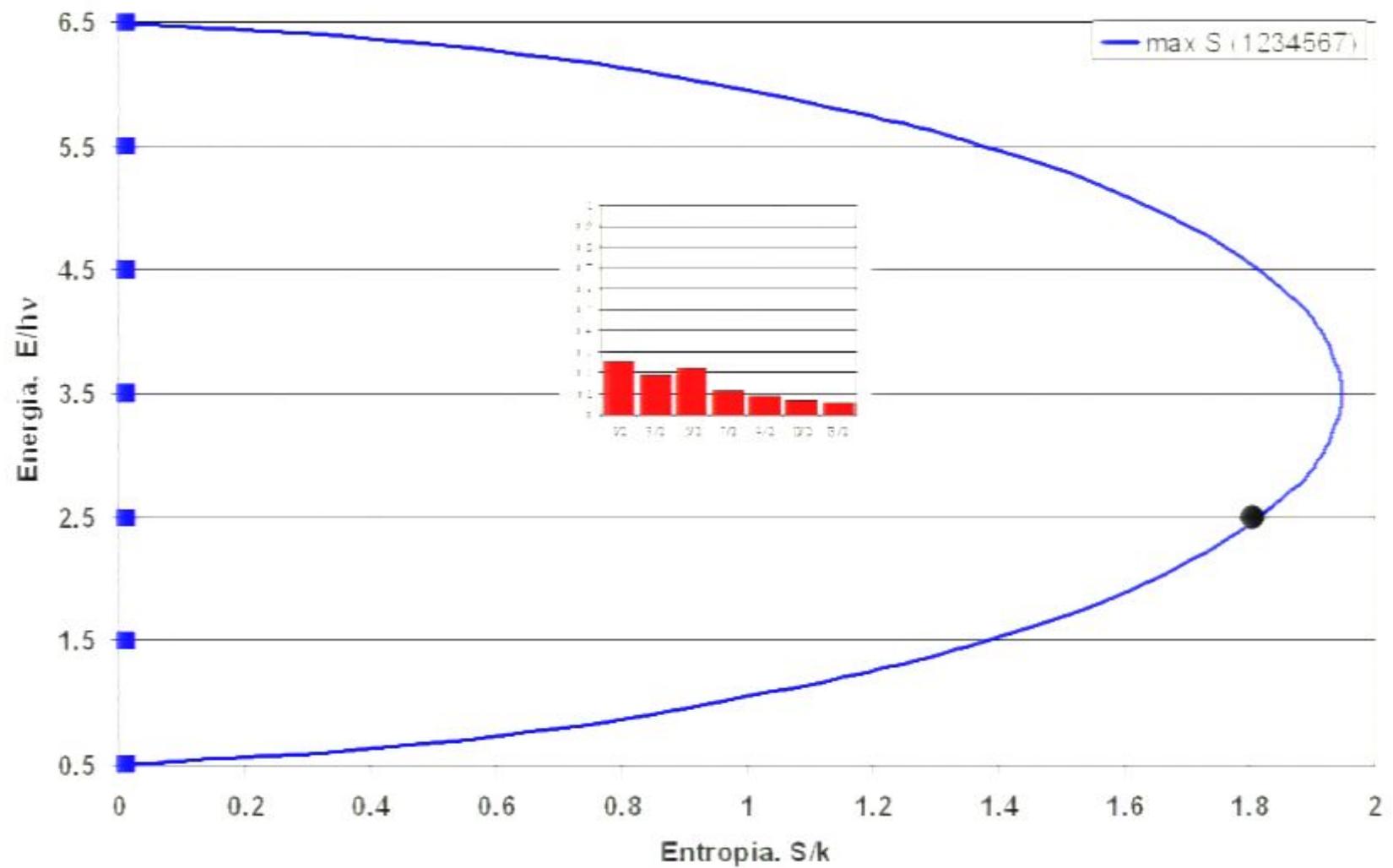












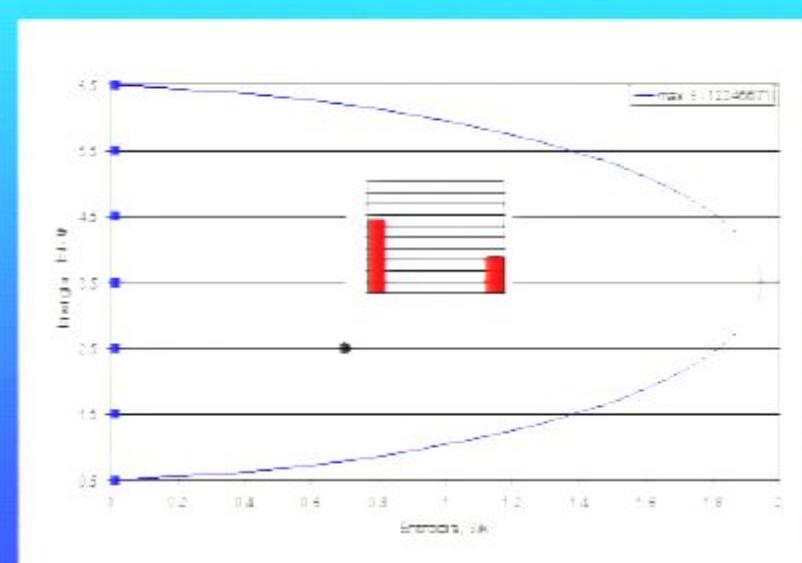
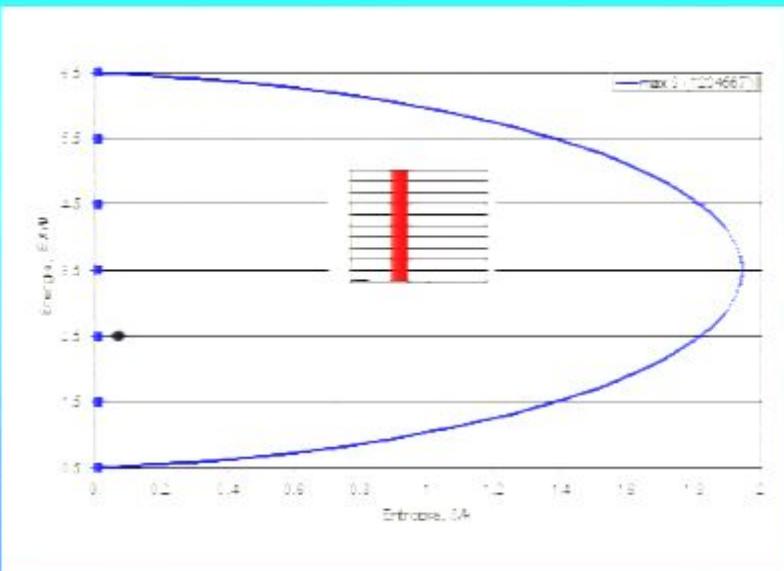
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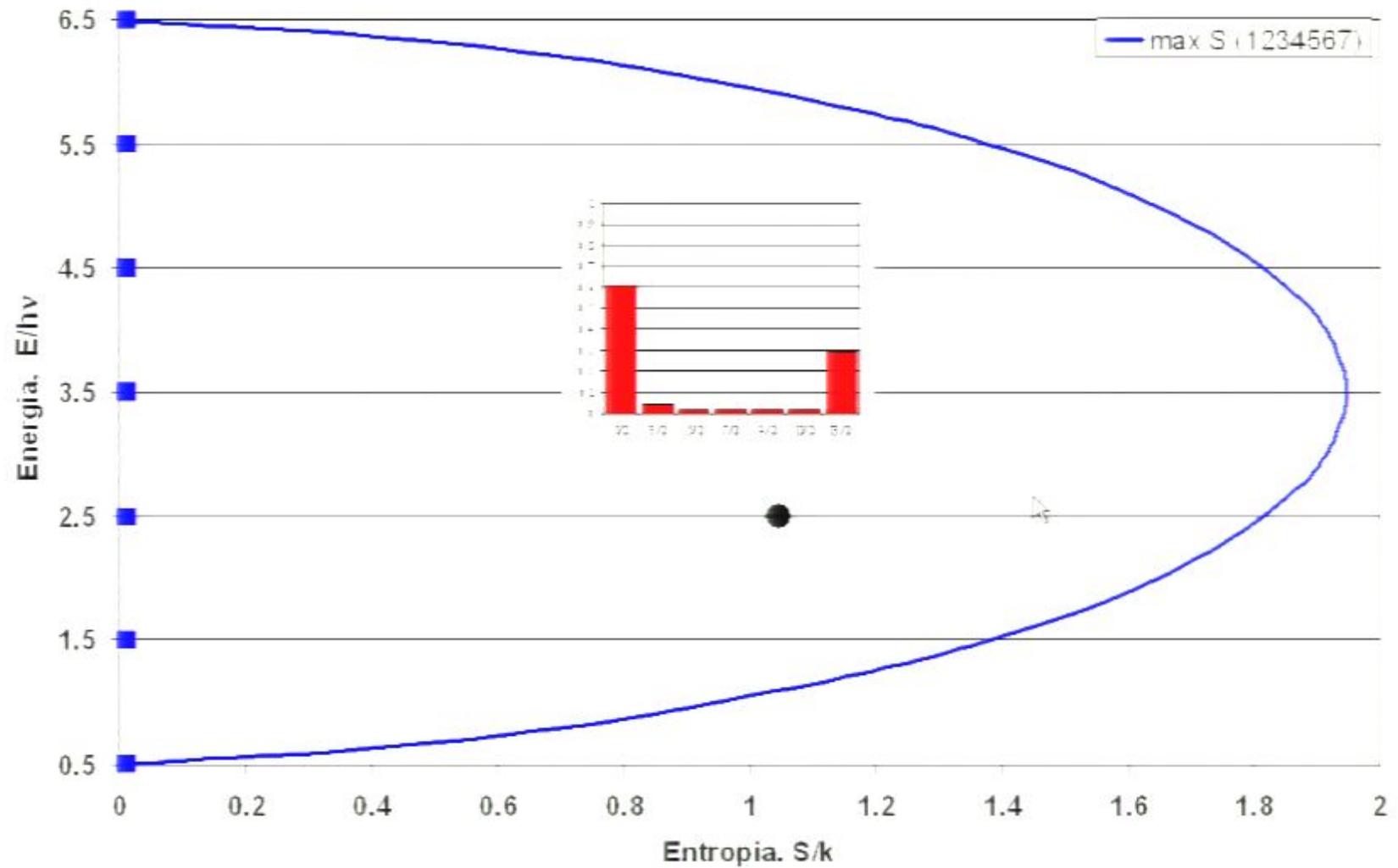
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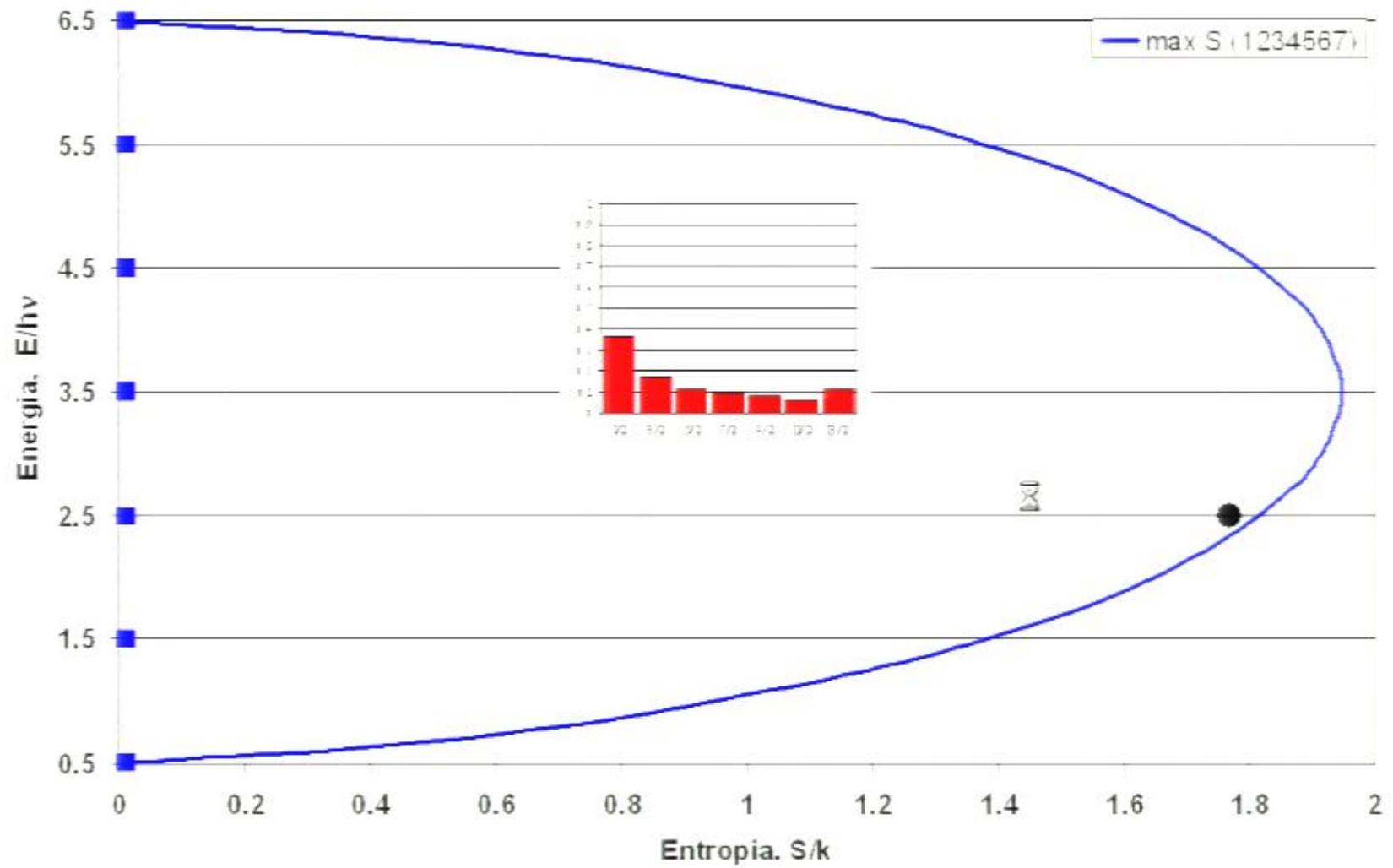
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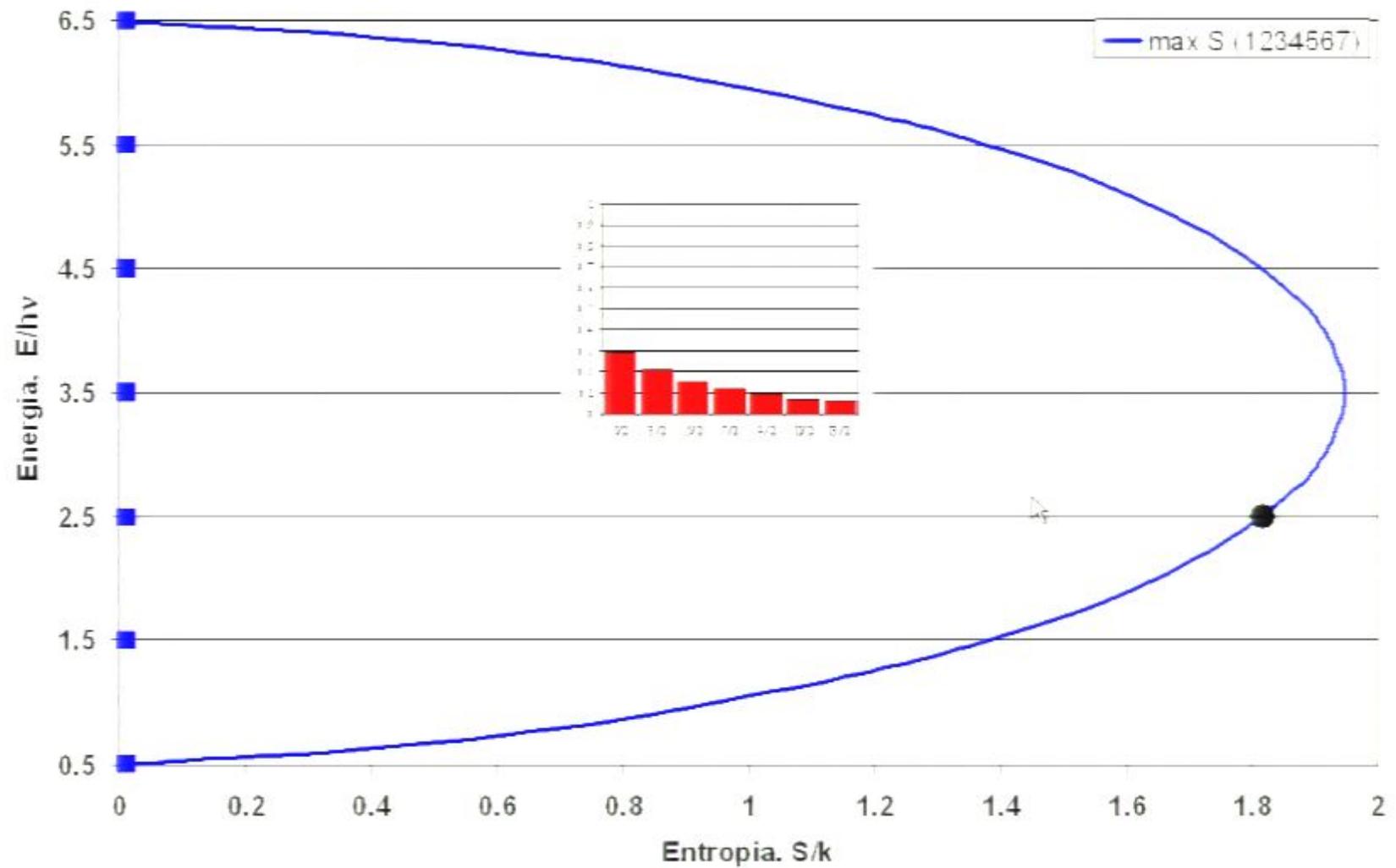
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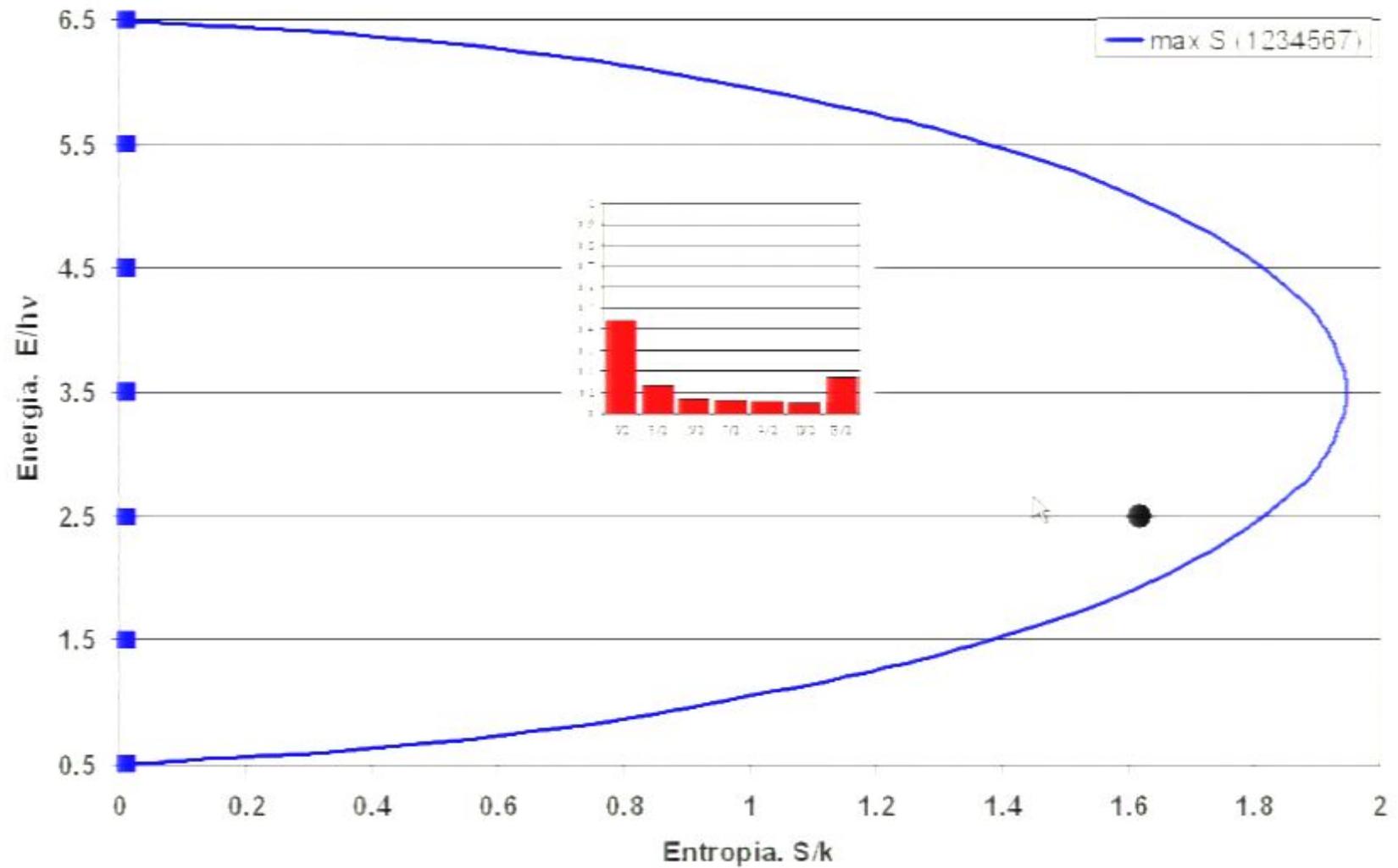


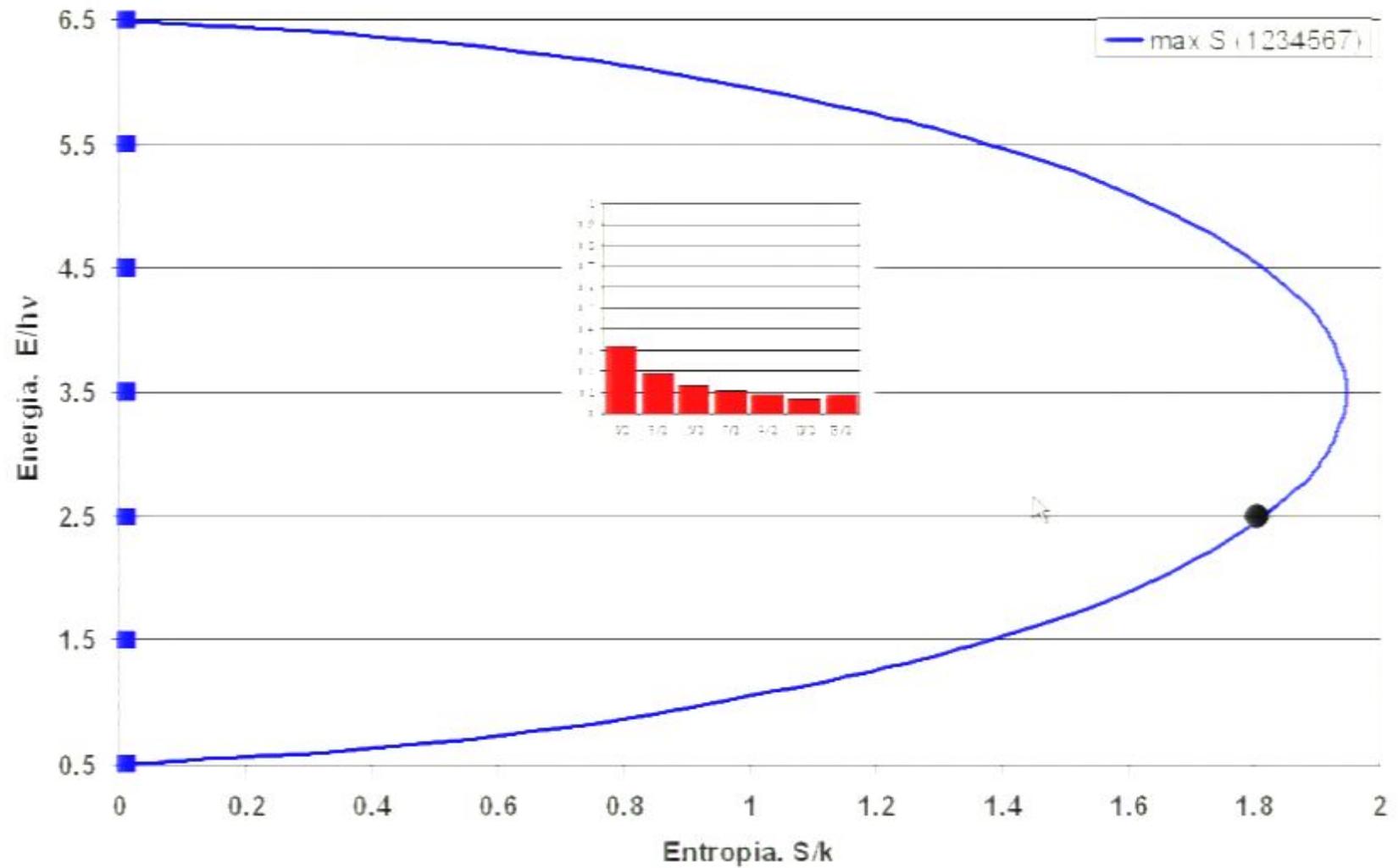
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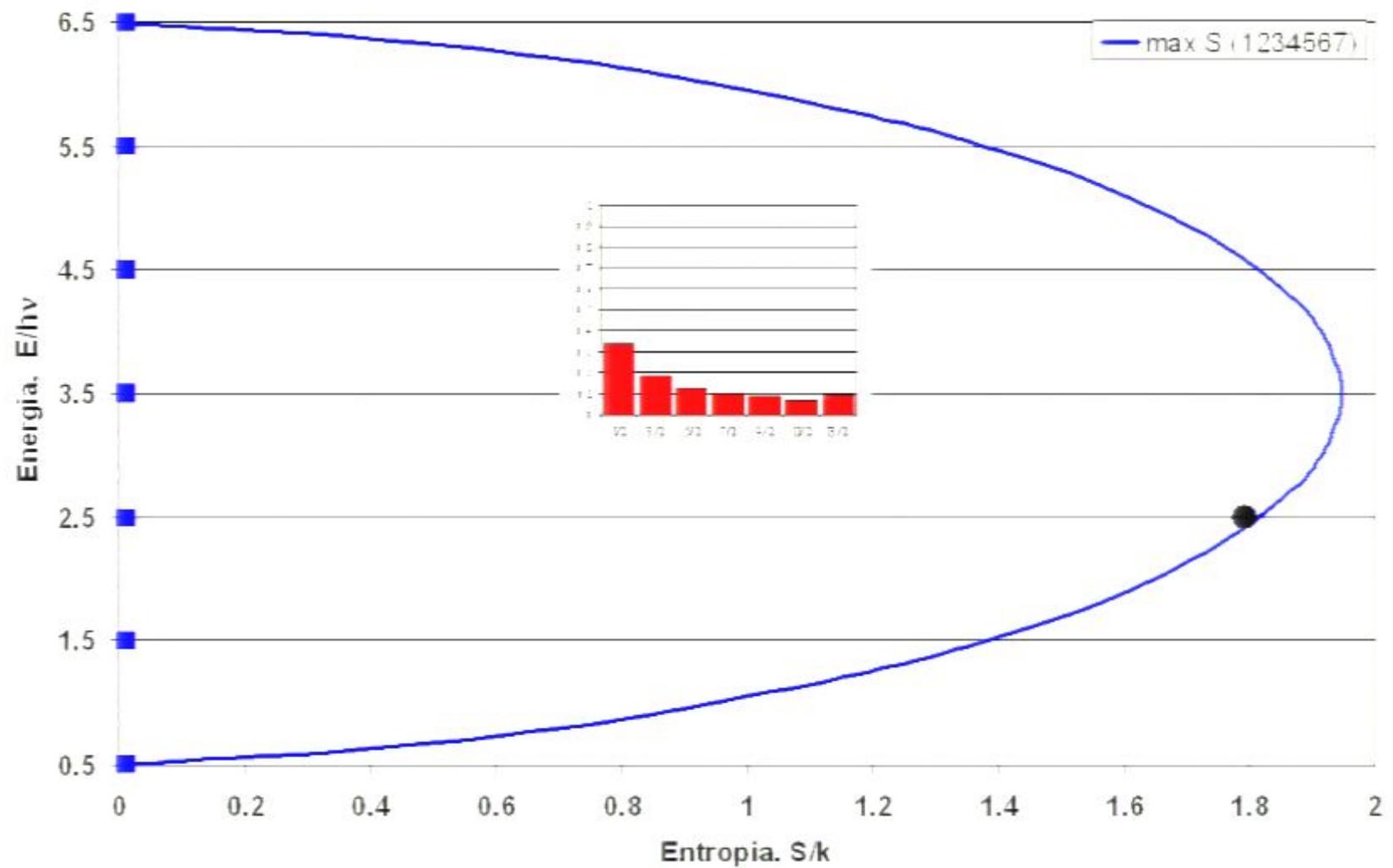


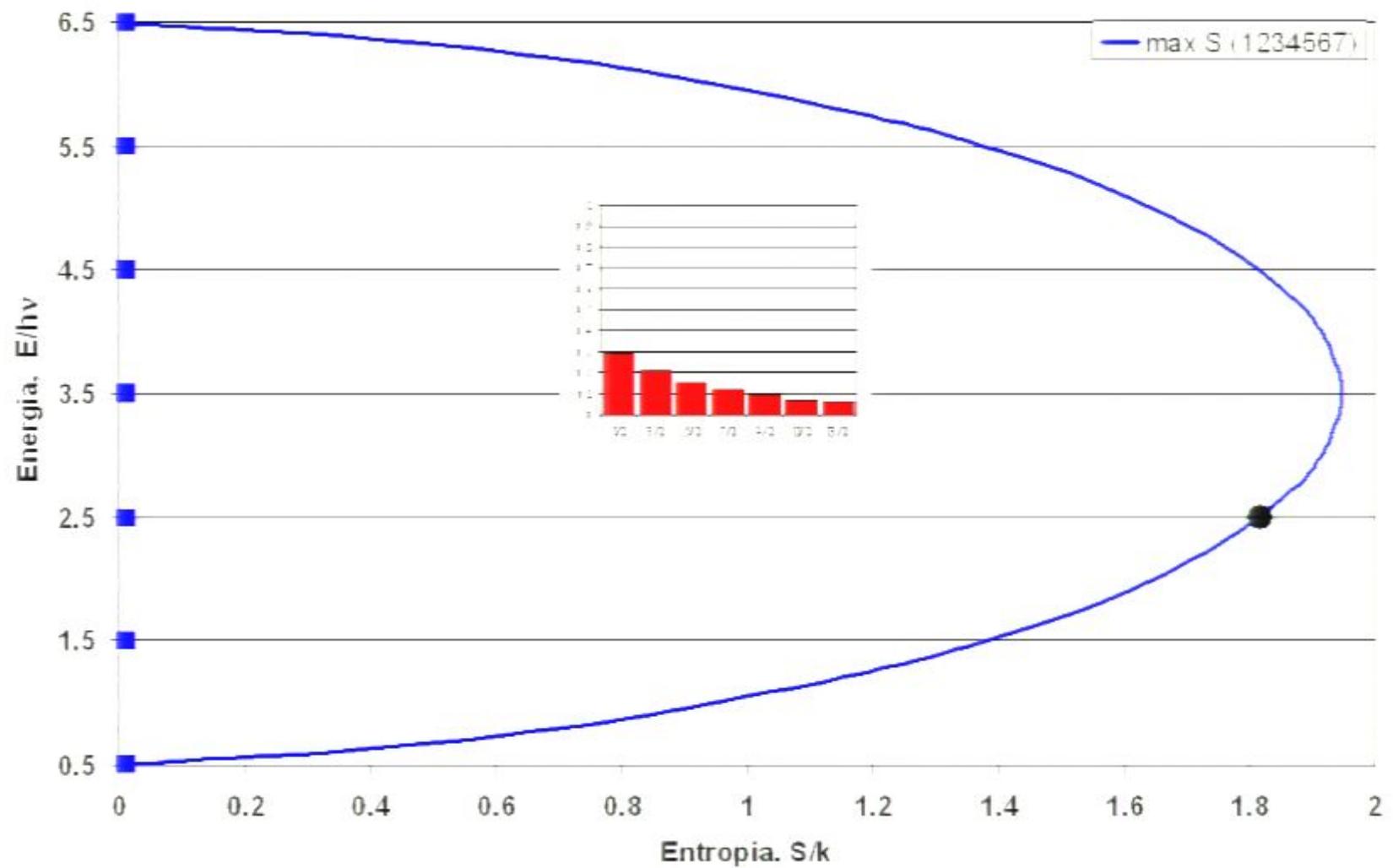












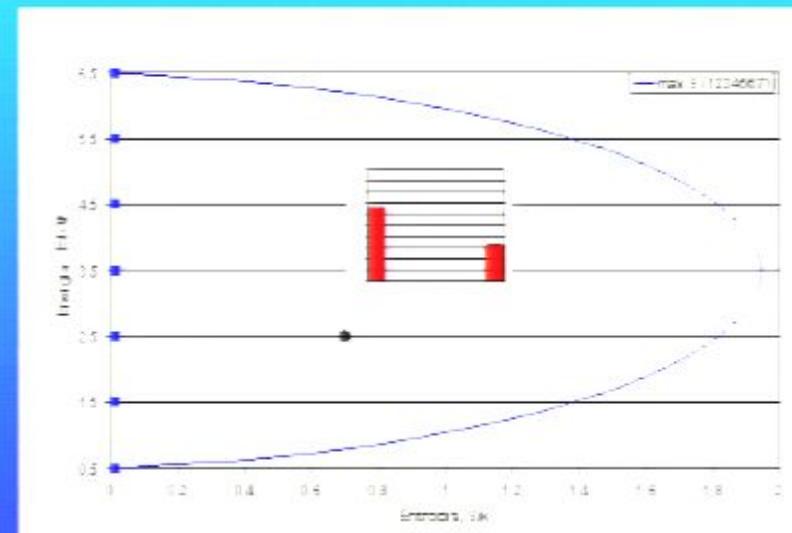
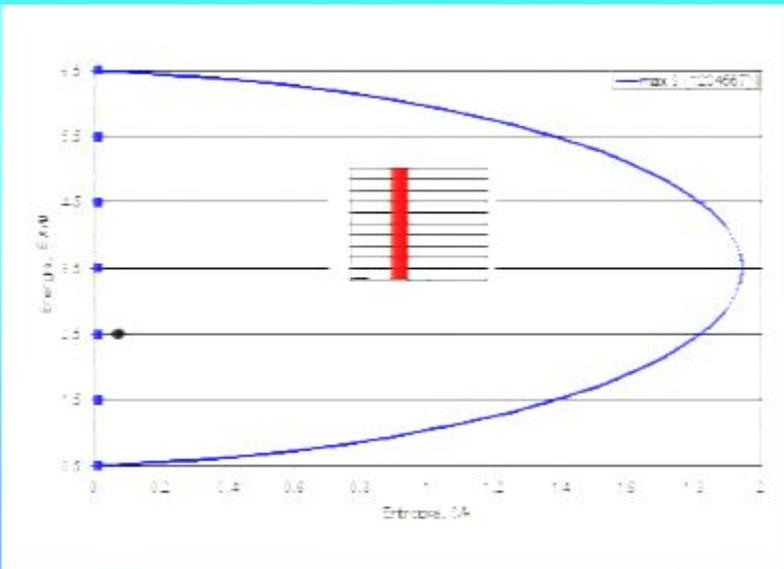
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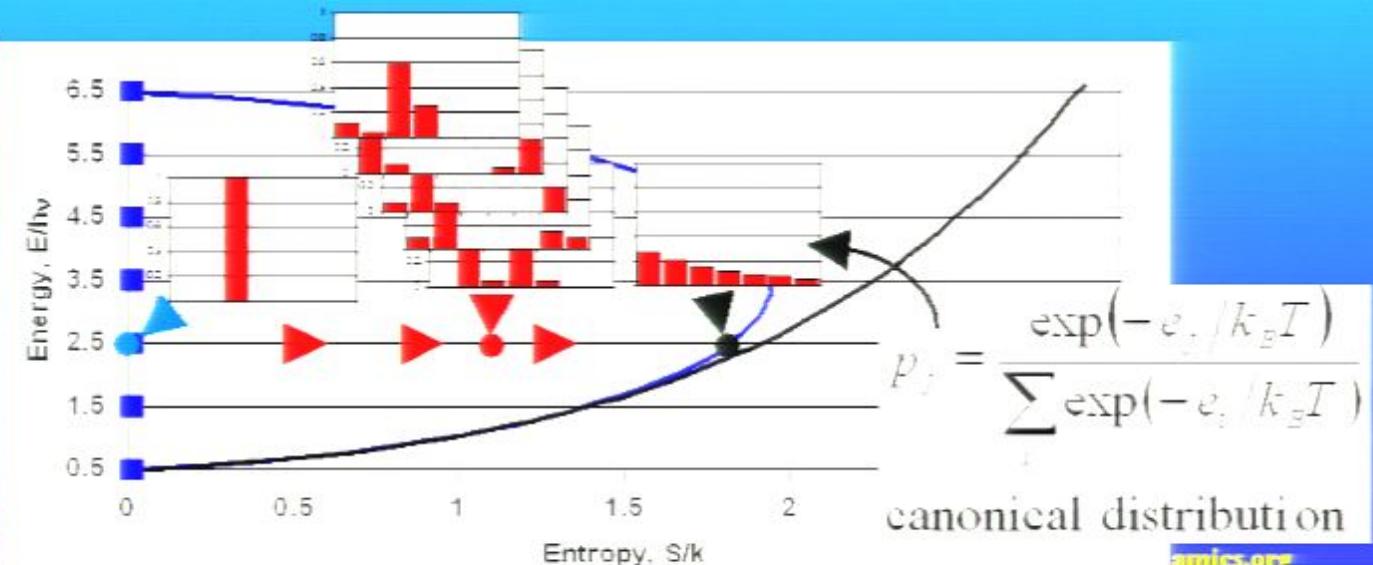
# Desiderata for a general dynamical law (isolated system)

Mod. Phys. Lett. A, 20, 977 (2005)

Energy conservation,  $\frac{d}{dt} \left( \sum_j p_j e_j \right) = 0 \Rightarrow$

Entropy nondecrease,  $\frac{d}{dt} \left( -k_B \sum_j p_j \ln p_j \right) \geq 0 \Rightarrow$

Probability conservation,  $p_j \geq 0, \frac{d}{dt} \left( \sum_j p_j \right) = 0 \Rightarrow$



G.P. Beretti  
Perimeter I

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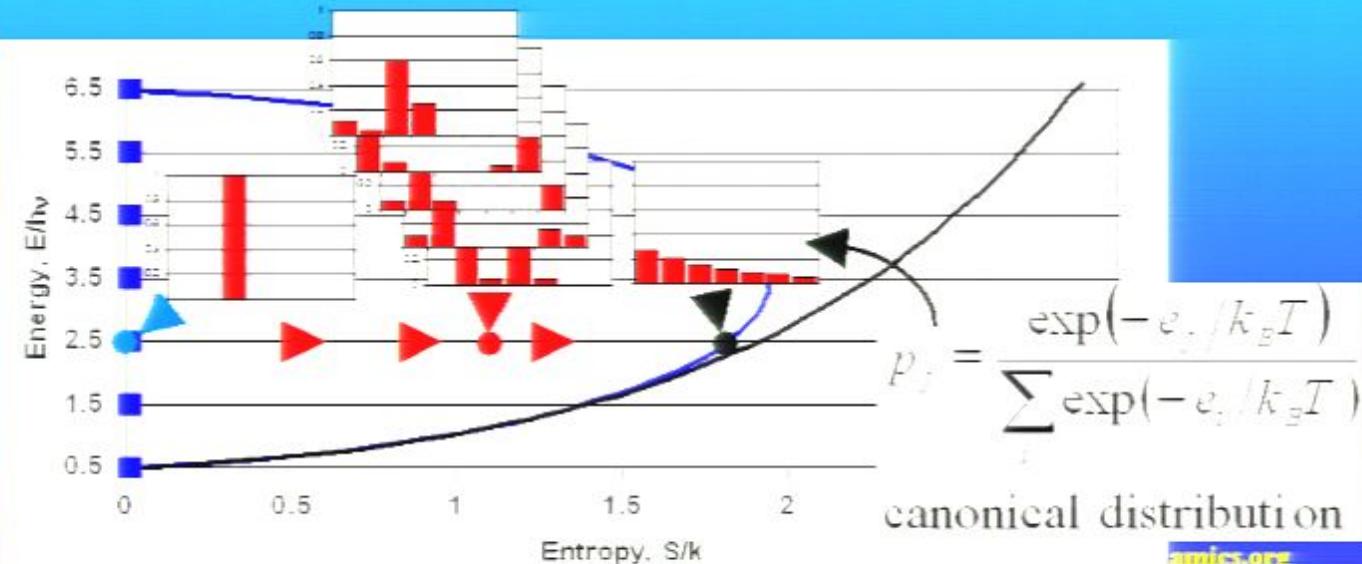
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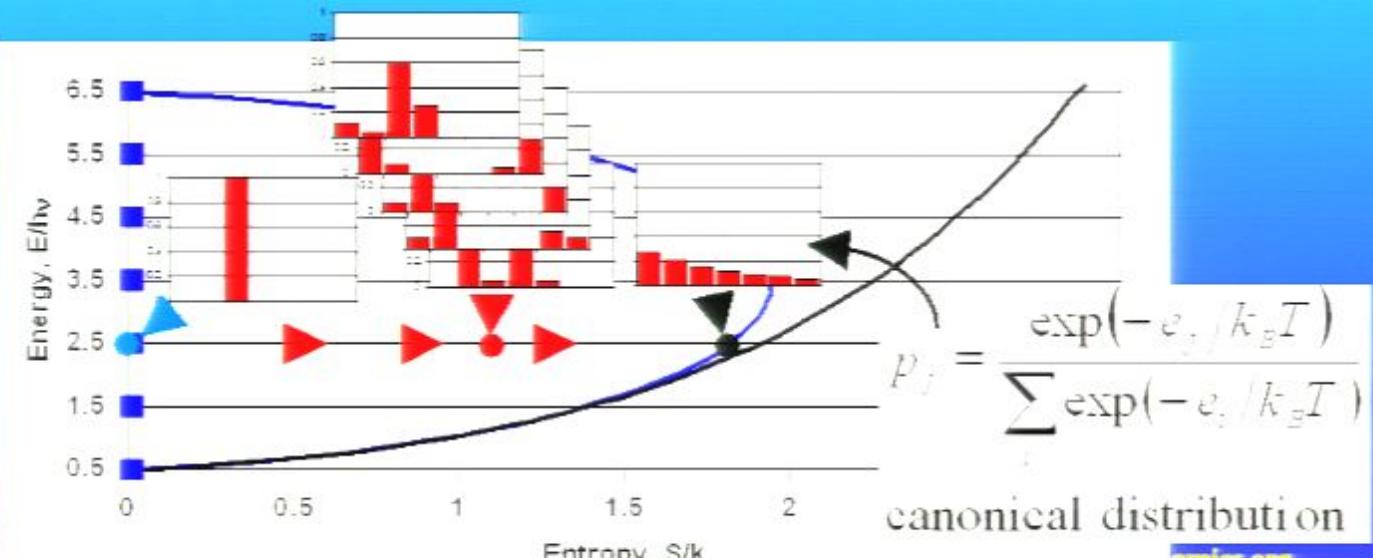
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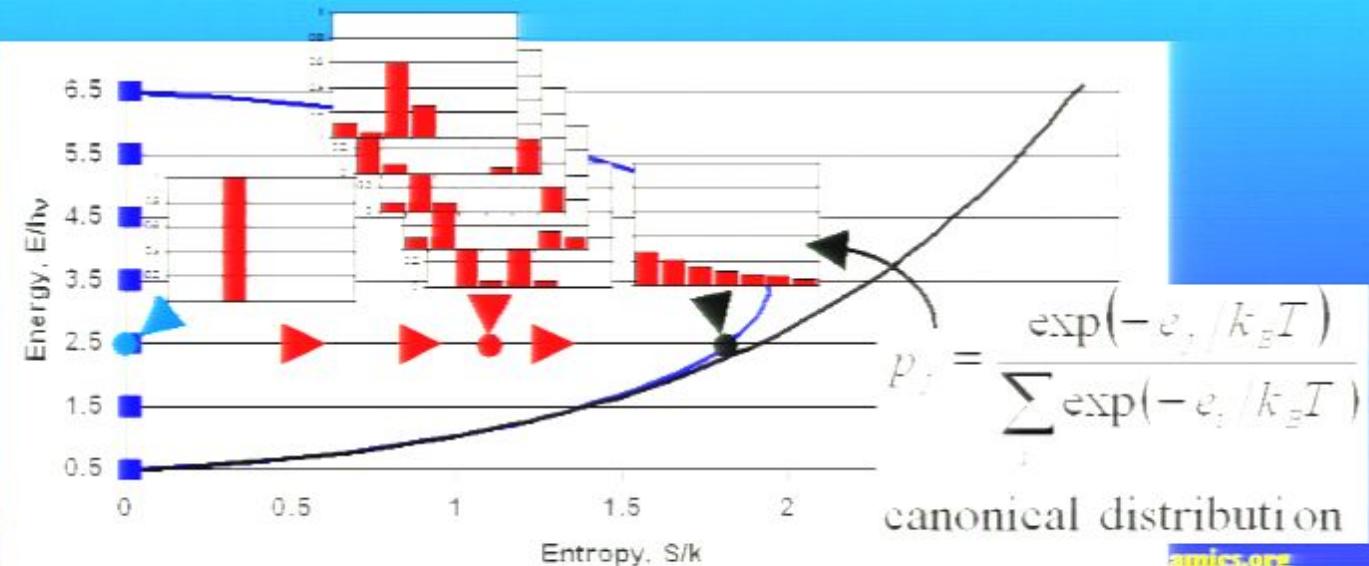
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$$\frac{d}{dt} \left( -k_B \sum_j r_j^2 \ln r_j^2 \right) \geq 0$$

Probability conservation:  $p_j \geq 0, \quad \sum_{j=1}^{N_{\text{max}}} p_j = 1$

$$p_j = r_j^2 \geq 0, \quad \frac{d}{dt} \left( \sum_j r_j^2 \right) = 0$$



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Perimeter I

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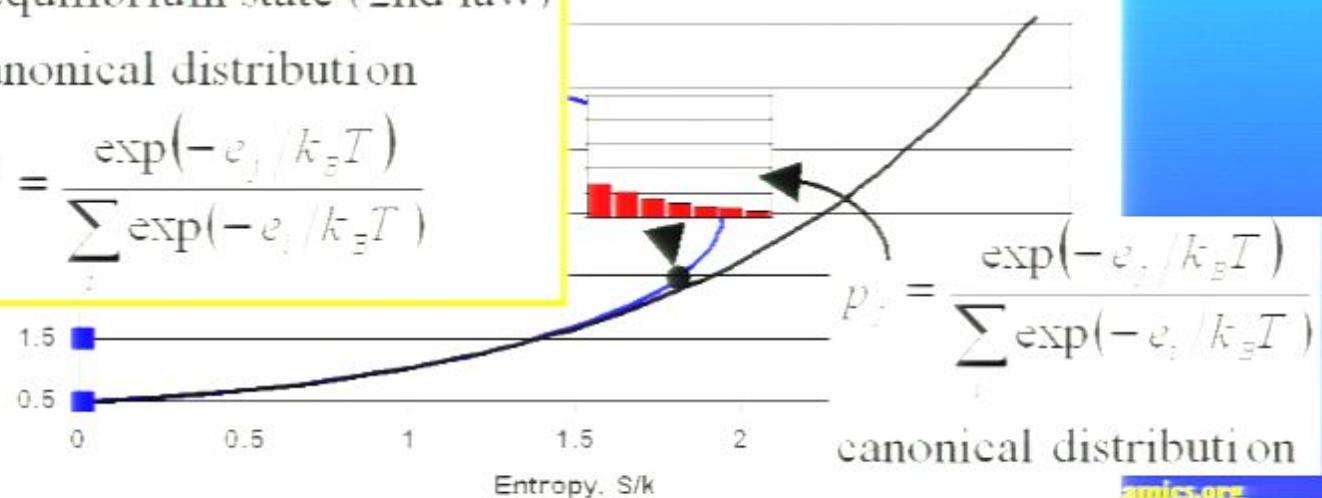
Probability: For each value of  $E = \sum_j p_j e_j$ , there must be one and only one stable equilibrium state (2nd law) with canonical distribution

$$p_j = r_j^2 = \frac{\exp(-e_j/k_B T)}{\sum_i \exp(-e_i/k_B T)}$$

$$p_j = r_j^2 \geq 0, \quad \frac{d}{dt} \left( \sum_j r_j^2 \right) = 0$$



G.P. Beretta  
Perimeter I



# Equivalent variational formulation

Gheorghiu-Svirschevski, Phys Rev A, 63, 054102 (2001)  
quant-ph/0112046

In terms of  $r_j = \sqrt{p_j}$

$$\frac{d}{dt} \left( \sum_j r_j^2 e_j \right) = 0$$

$$\frac{d}{dt} \left( -k_B \sum_j r_j^2 \ln r_j^2 \right) \geq 0$$

$$p_j = r_j^2 \geq 0, \quad \frac{d}{dt} \left( \sum_j r_j^2 \right) = 0$$

steepest - entropy - ascent dynamical ansatz :

$\frac{dr_j}{dt}$  in the direction of  $\max \frac{dS}{dt}$  subject to  $\frac{dE}{dt} = 0$

and  $\frac{dr_j^2}{dt} = \frac{1}{\tau^2}$  where  $\tau > 0$  depends on  $r_j$



G.P. Beretta, Seminar "What if Quantum Thermodynamics were a fundamental extension of Quantum Mechanics?"  
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Variational formulation :

$\max \frac{d}{dt} \left( -k_B \sum_j r_j^2 \ln r_j^2 \right)$  subject to

$$\frac{d}{dt} \left( \sum_j r_j^2 \right) = 0, \quad \frac{d}{dt} \left( \sum_j r_j^2 e_j \right) = 0, \quad \sum_j e_j = 1 \quad \tau^2(r) \quad p_j = r_j^2 \geq 0, \quad \frac{d}{dt} \left( \sum_j r_j^2 \right) = 0$$

In terms of  $r_j = \sqrt{p_j}$

$$\frac{d}{dt} \left( \sum_j r_j^2 e_j \right) = 0$$

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$\max \frac{d}{dt} \left( -k_B \sum_j r_j^2 \ln r_j^2 \right)$  subject to

$$\frac{d}{dt} \left( \sum_j r_j^2 \right) = 0, \quad \frac{d}{dt} \left( \sum_j r_j^2 e_j \right) = 0, \quad \sum_j \lambda_j = 1 - \tau^2(r), \quad p_j = r_j^2 \geq 0, \quad \frac{d}{dt} \left( \sum_j r_j^2 \right) = 0$$

In terms of  $r_j = \sqrt{p_j}$

$$\frac{d}{dt} \left( \sum_j r_j^2 e_j \right) = 0$$

$$\frac{d}{dt} \left( -k_B \sum_j r_j^2 \ln r_j^2 \right) \geq 0$$

$$\frac{\partial}{\partial \lambda_j} \left[ \frac{d}{dt} \left( -k_B \sum_j r_j^2 \ln r_j^2 \right) + \lambda_j \frac{d}{dt} \left( \sum_j r_j^2 e_j \right) + \lambda_j \frac{d}{dt} \left( \sum_j r_j^2 \right) + 2\tau \sum_j \lambda_j e_j \right] = 0$$

$$\frac{\partial}{\partial \lambda_j} \left[ -2k_B \sum_j (r_j^2 - r_j \ln r_j^2) \lambda_j + 2\lambda_j \sum_j r_j e_j + 2\lambda_j \sum_j r_j^2 e_j + 2\tau \sum_j \lambda_j e_j \right] = 0$$

$$-2k_B(r_j^2 - r_j \ln r_j^2) + 2\lambda_j^2 + 2\lambda_j r_j^2 e_j + 2\tau \lambda_j e_j = 0$$

$$\tau \frac{dp_j}{dt} = \tau \frac{dr_j^2}{dt} = 2\tau r_j \dot{e}_j = -k_B p_j \ln p_j - (k_B + \lambda_j) p_j - \lambda_j p_j e_j$$



## Steepest-entropy-ascent dynamical ansatz (isolated system)

$$\begin{aligned} \rho \ln \rho &= \rho - \frac{1}{2}\{H, \rho\} \\ \text{Tr} \rho \ln \rho &= 1 - \text{Tr} \rho H \\ \frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] - \frac{1}{\tau} \frac{\text{Tr} \rho H \ln \rho - \text{Tr} \rho H - \text{Tr} \rho H^2}{\text{Tr} \rho H^2 + (\text{Tr} \rho H)^2} \end{aligned}$$

When  $[H, \rho] = 0$

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



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## Stability of equilibrium states and second law

Indeed, equation (1) preserves the rank and nullity of  $\rho$ , [2], or, as said in Ref. [12], preserves the cardinality of the set of nonzero eigenvalues of  $\rho$ . Because the equation of motion attracts the state operator towards the highest entropy state or limit cycle compatible with the initial mean values of the generators of the motion and the number of zero eigenvalues, a minor perturbation of the state that changes an initially zero eigenvalue to an arbitrarily small non-zero value would cause an irreversible departure of the state towards a different (higher entropy) equilibrium state or limit cycle. Hence, as long as there are zero eigenvalues of  $\rho$ , i.e., unless  $B = I$ , all equilibrium states and limit cycles are unstable. Without this conclusion, we could not claim that the equation of motion entails the second law of thermodynamics (see Appendices A and B, and the original papers, for further discussion of this important point).



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## The two ansatzs of “Quantum Thermodynamics”

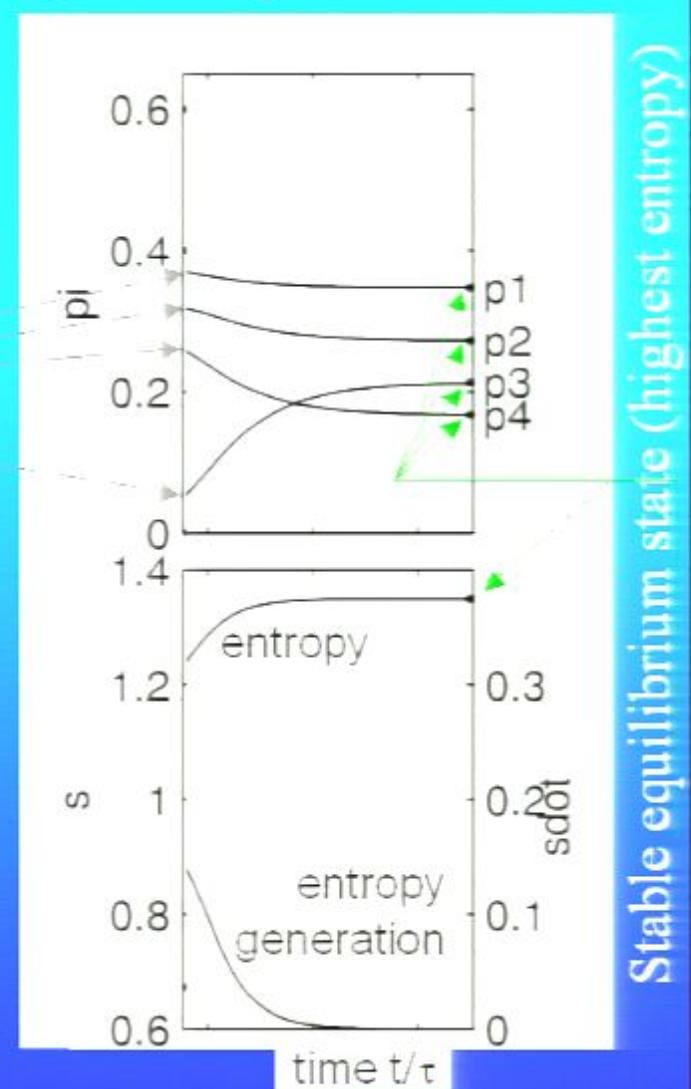
- The second law is forced directly into the microscopic laws and emerges as a theorem of the generalized dynamical law (stability of equilibrium states)
- Entropy emerges from the microscopic level as a measure of the degree of “load sharing” among the energy levels. The higher the sharing the lower the energy available for conversion to work.
- Irreversibility emerges as a manifestation of spontaneous internal load redistribution among the initially occupied energy levels.
- **Experimentally verifiable? Phenomenological or fundamental?**
- If proved not fundamental, the nonlinear dynamical law remains a valuable phenomenological nonlinear master equation, that guarantees all compatibility requirements with thermodynamics.



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# Time dependence of energy-level occupation probabilities

An arbitrary initial distribution (state)



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

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# Time dependence of energy-level occupation probabilities

The trajectory passes  
very close to an  
unstable equilibrium state

An arbitrary initial  
distribution (state)

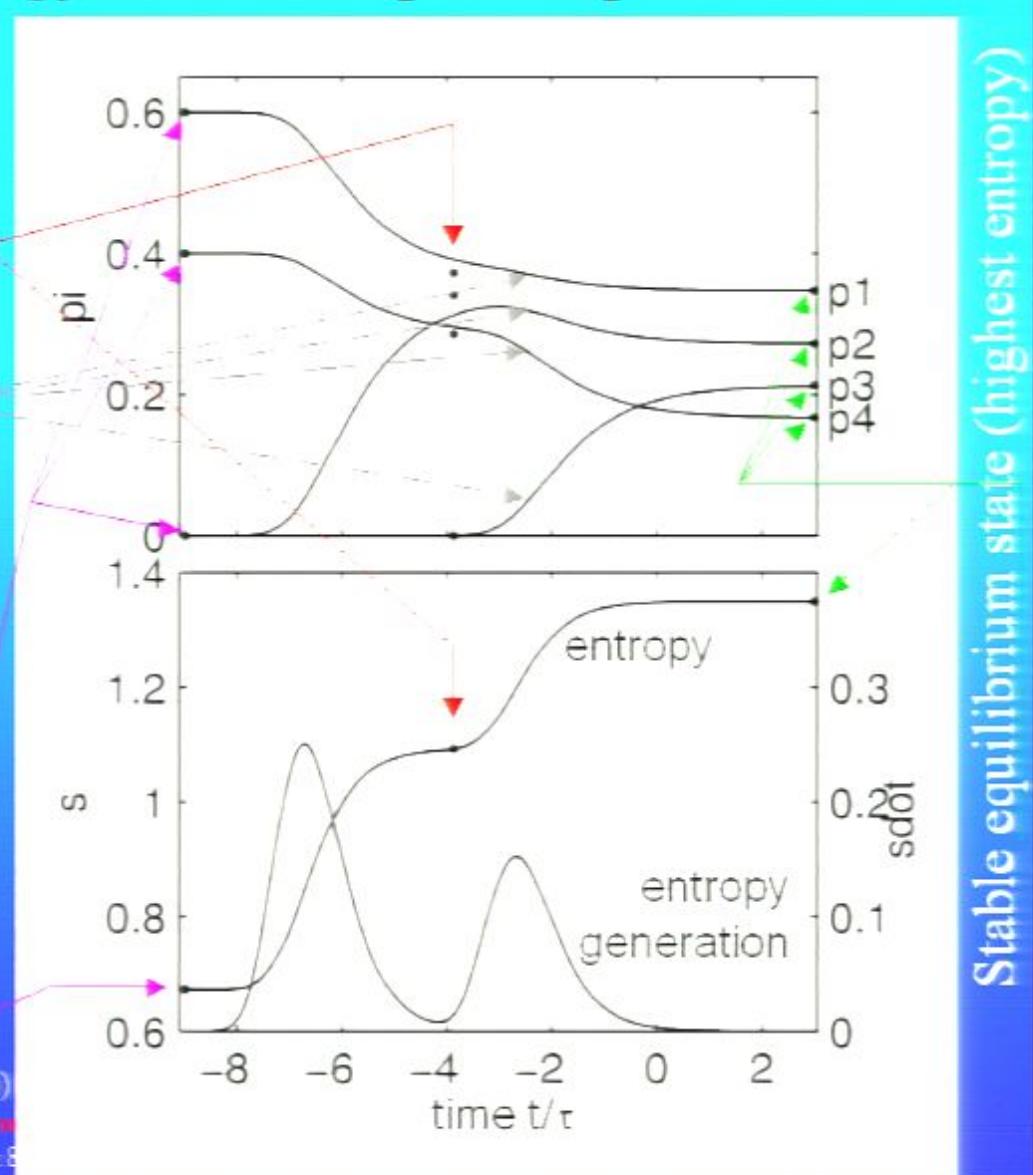
Strong causality:  
**given any initial state the  
trajectory is unique and  
defined for  $-\infty < t < +\infty$**

We can trace back the  
lowest entropy  
'ancestral' state



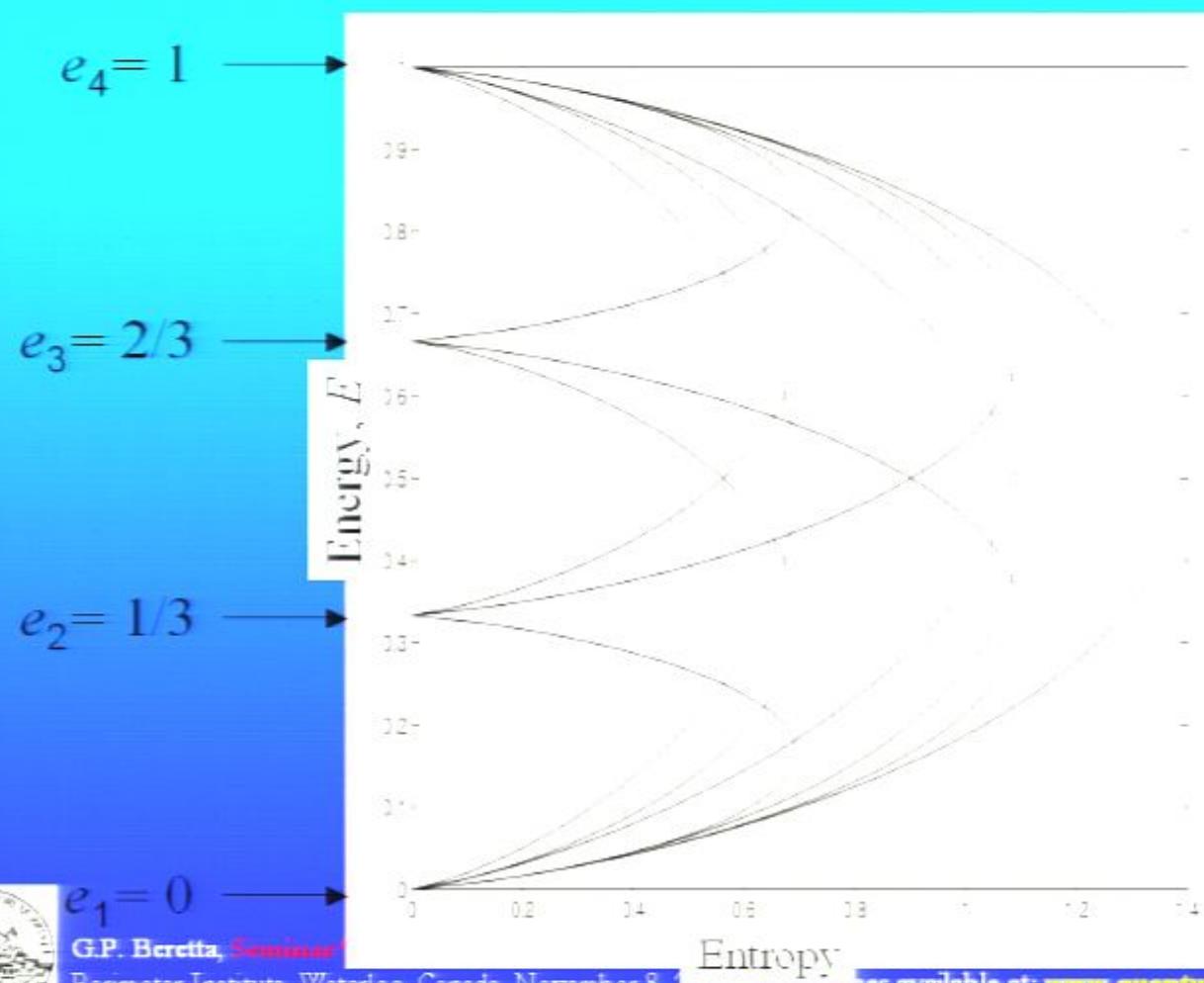
Phys. Rev. E, 73, 026113 (2006)

G.P. Beretta, Seminar "What is Quantum Theory"  
Perimeter Institute, Waterloo, Canada, November 8



# Internal dynamical structure for a 4-level system

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



G.P. Beretta, Seminar

Perimeter Institute, Waterloo, Canada, November 8, 2011

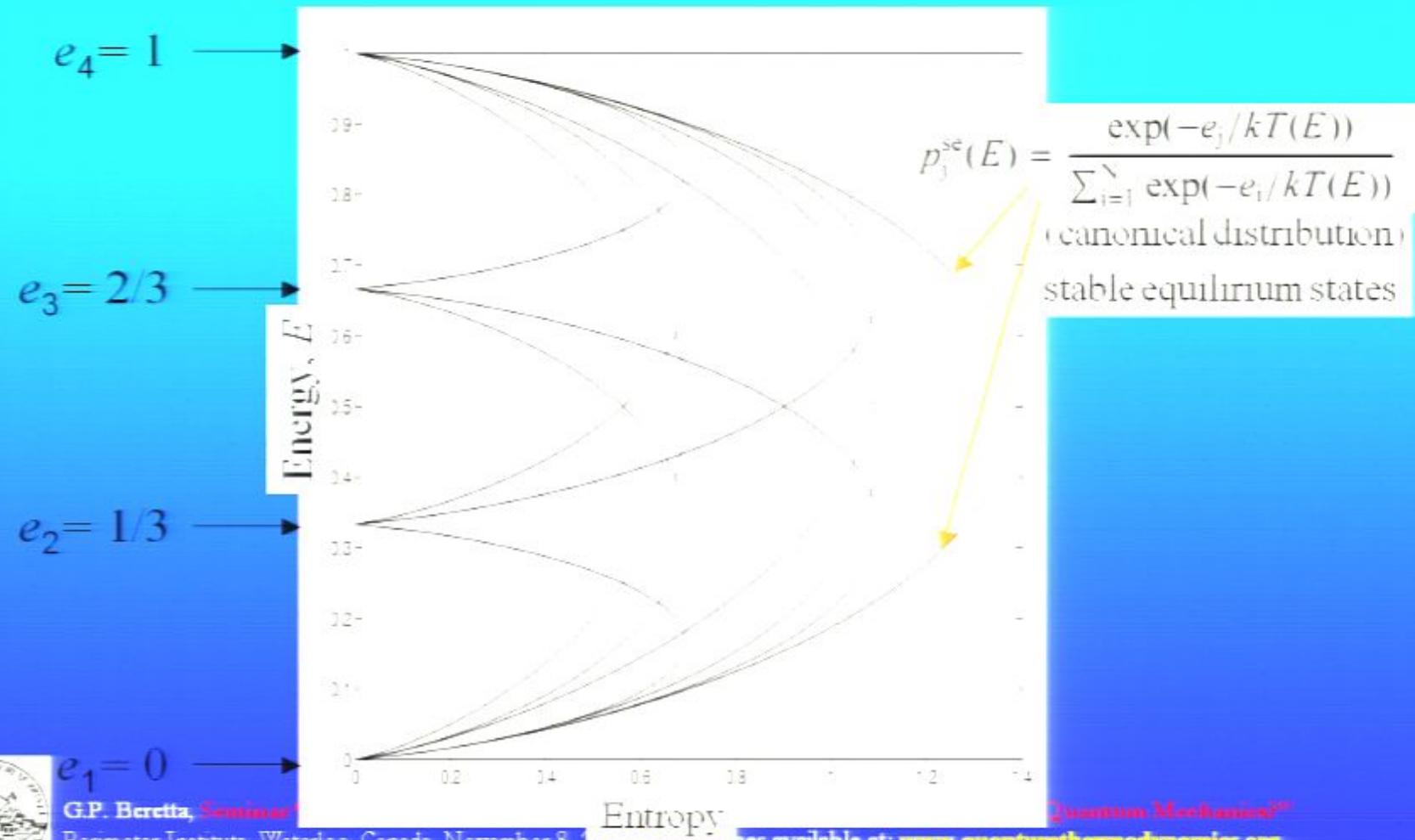
Entropy

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Quantum Mechanics<sup>20</sup>

# Internal dynamical structure for a 4-level system

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



G.P. Beretta, Seminar

Perimeter Institute, Waterloo, Canada, November 8, 2011

Quantum Mechanics<sup>20</sup>

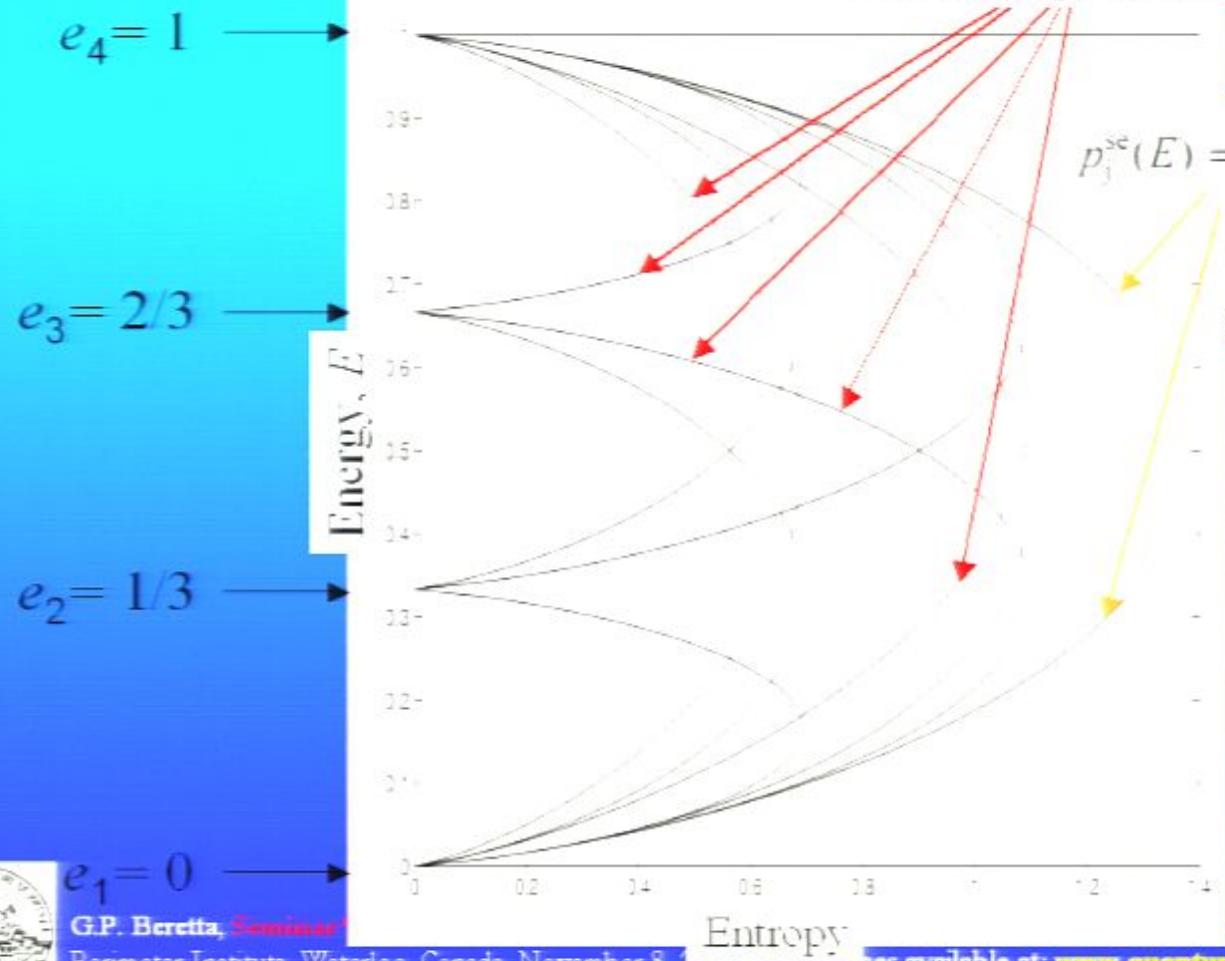
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# Internal dynamical structure for a 4-level system

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



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

(canonical distribution)  
stable equilibrium states



G.P. Beretta, Seminar

Perimeter Institute, Waterloo, Canada, November 8, 2011

Entropy

Quantum Mechanics<sup>20</sup>

Codes available at: [www.quantumthermodynamics.org](http://www.quantumthermodynamics.org)

# Standard Time-Energy Uncertainty Relations

In the Mandelstam-Tamm-Messiah interpretation, for any  $F$  the characteristic time

quant-ph/0511091

$$\tau_F = \Delta_F / |\text{Tr}(\dot{\rho}F)|$$

represents the time required for the mean value  $\langle F \rangle$  to change by an amount equal to the width  $\Delta_F$  of the distribution.  $\tau_F$  is just a feature of the dynamics, a measure of how fast (or slow) the mean value  $\langle F \rangle$  changes with time.



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For Hamiltonian (unitary) time evolution,

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

the “internal” rate of change of  $\langle F \rangle$  is given by

$$\text{Tr}(\dot{\rho}F) = \frac{d}{dt} \langle F \rangle = \langle \dot{F} \rangle = \frac{\langle i[F, H]/2 \rangle}{\hbar/2} = -\frac{\eta_{FH}}{\hbar/2}$$

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# Steepest-entropy-ascent time-energy uncertainty relations

quant-ph-0511091

The internal rate of change of  $\langle F \rangle$  is

$$\text{Tr}(\dot{\rho}F) = \frac{\langle i[F, H]/2 \rangle}{\hbar/2} + \frac{\langle \Delta F \Delta M \rangle}{k_B \tau} = -\frac{\eta_{FH}}{\hbar/2} + \frac{\sigma_{FM}}{k_B \tau} .$$

We obtain the general exact uncertainty relation

$$\tau_F \Delta_H = \frac{\hbar/2}{|c_{FH} + a_+ r_{FM}|}$$

where  $a_+$  is the nonnegative, dimensionless functional

$$a_+ = \frac{\hbar/2}{k_B} \frac{\Delta_M/\tau}{\Delta_H} .$$

In general, if the dynamics is dissipative ( $\tau \neq \infty, a_+ \neq 0$ ) there are density operators for which  $|c_{FH} + a_+ r_{FM}| > 1$  so that  $\tau_F \Delta_H$  takes a value less than  $\hbar/2$  and thus, expectedly, the usual time-energy uncertainty relation is violated. The sharpest general time-energy uncertainty relation always satisfied when both Hamiltonian and dissipative dynamics are active is

$$\left[ \frac{\hbar/2}{\tau_F \Delta_H} \right]^2 \leq 1 + a_+^2 + 2a_+ c_{MH} .$$



G.P. Beretta,  
Perimeter Insti

# Steepest-entropy-ascent time-energy / time-entropy uncertainty relations

quant-ph-0511091

The rate of entropy generation is bounded, i.e..

$$\frac{d\langle S \rangle}{dt} = -k_B \frac{d}{dt} \text{Tr}(\rho \ln \rho) = \frac{\sigma_{MM}}{k_B \tau} \leq \frac{\Delta_S \Delta_M}{k_B \tau} \leq \frac{\sigma_{SS}}{k_B \tau}$$

and we have a time-entropy uncertainty relation

$$\frac{k_B \tau(\rho)}{\tau_S \Delta_S} = r_{SM}^2 \leq r_{SM} \leq 1$$

Moreover, we find the time-energy/time-entropy uncertainty relations

$$\left( \frac{\tau_F \Delta_H}{\hbar/2} \right)^2 + \left( \frac{\tau_F \Delta_S}{k_B \tau(\rho)} \right)^2 \geq 1$$

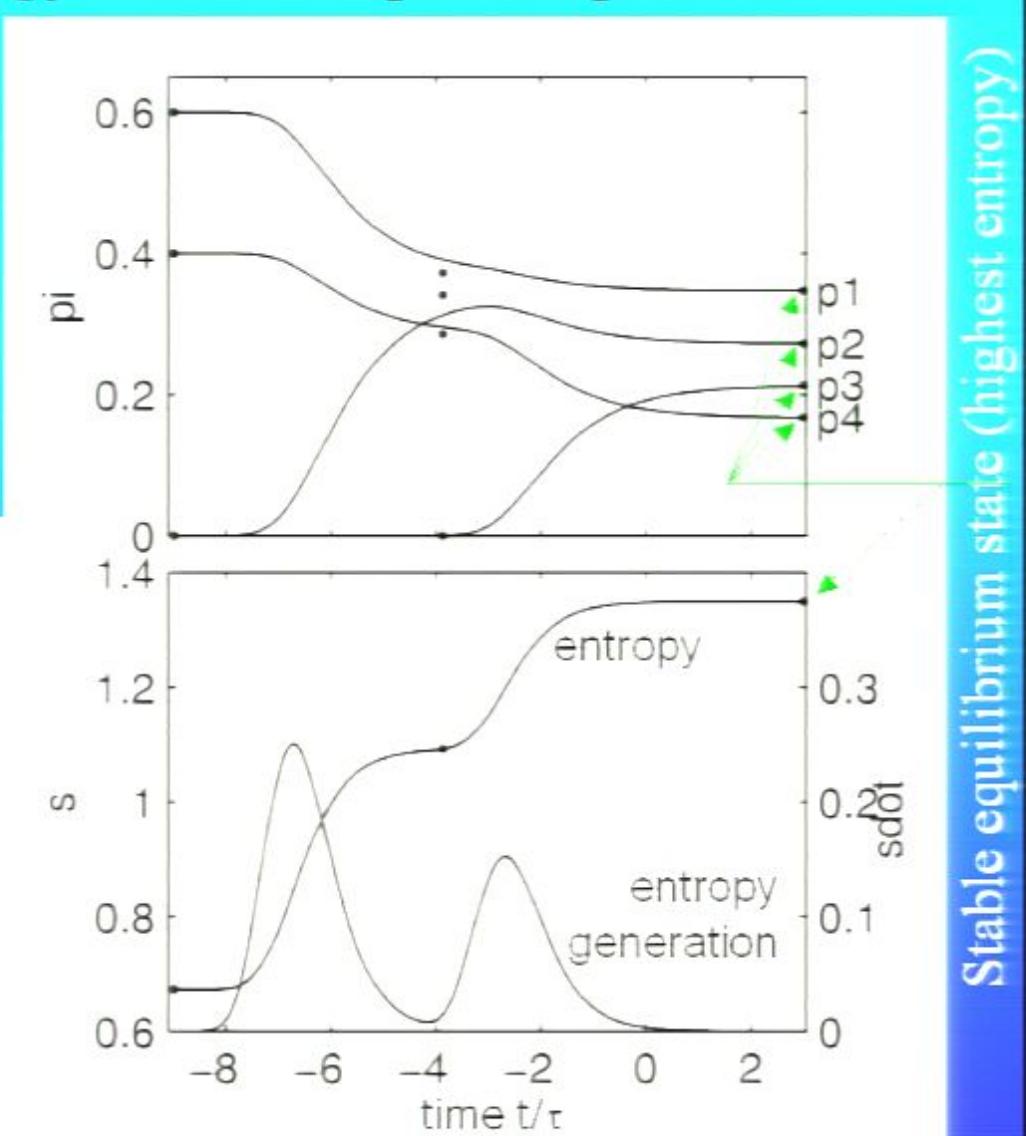
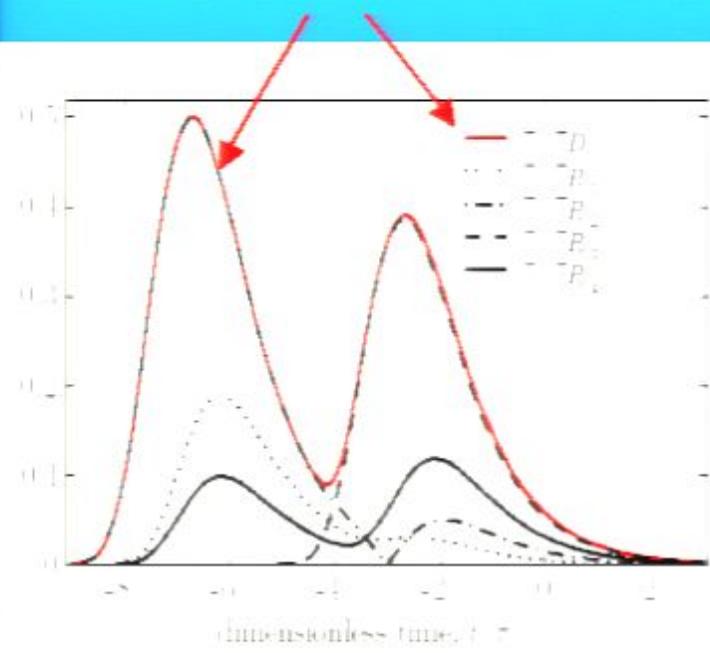


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# Time dependence of energy-level occupation probabilities

quant-ph-0511091

## time-entropy uncertainty bound



Stable equilibrium state (highest entropy)

## Affinities and dissipative rates of change

Any nonequilibrium  $\rho$  can be written as [6]

$$\rho = \frac{B \exp(-\sum_j f_j X_j)}{\text{Tr} B \exp(-\sum_j f_j X_j)} , \quad (3)$$

where the set  $\{f_j, X_j\}$  spans the real space  $\mathcal{L} \subset \mathcal{H}$ . Hence,

$$\sqrt{\rho} \ln \rho = -f_0 \sqrt{\rho} + \sum_j f_j \sqrt{\rho} X_j , \quad (4)$$

$$x_j(\rho) = \text{Tr}(\rho X_j) , \quad (5)$$

$$s(\rho) = k_B f_0 + k_B \sum_j f_j x_j(\rho) , \quad (6)$$

$$\text{where } k_B f_j = \left. \frac{\partial s(\rho)}{\partial x_j(\rho)} \right|_{x_i \neq j(\rho)} \quad (7)$$

may be interpreted as a generalized affinity or force, and

$$\frac{Dx_i(\rho)}{Dt} = 2(E_D | \sqrt{\rho} X_i) . \quad (8)$$

is the dissipative rate of change of property  $x_j(\rho)$ .



## Generalized Onsager conductivities and reciprocity

The rate of entropy change may be rewritten as a quadratic form of the generalized affinities,

$$\frac{ds(\rho)}{dt} = k_B \sum_i \sum_j f_i f_j L_{ij}(\rho) . \quad 47$$

Being a Lorentz matrix, " $L_{ij}(\rho)$ " has non-negative definite determinant  $\det(L_{ij}(\rho))_B \geq 0$ , strict positive iff all operators  $L_{ij}(\lambda^i \lambda^j)_B$  are linearly independent, in which case Eq.(47) may be solved to yield

$$f_j = \sum_i L_{ij}^{-1}(\rho) \frac{Dx_i(\rho)}{Dt} \quad 48$$

and the rate of entropy change can be written as a quadratic form of the dissipative rates

$$\frac{ds(\rho)}{dt} = k_B \sum_i \sum_j L_{ij}^{-1}(\rho) \frac{Dx_i(\rho)}{Dt} \frac{Dx_j(\rho)}{Dt} . \quad 49$$



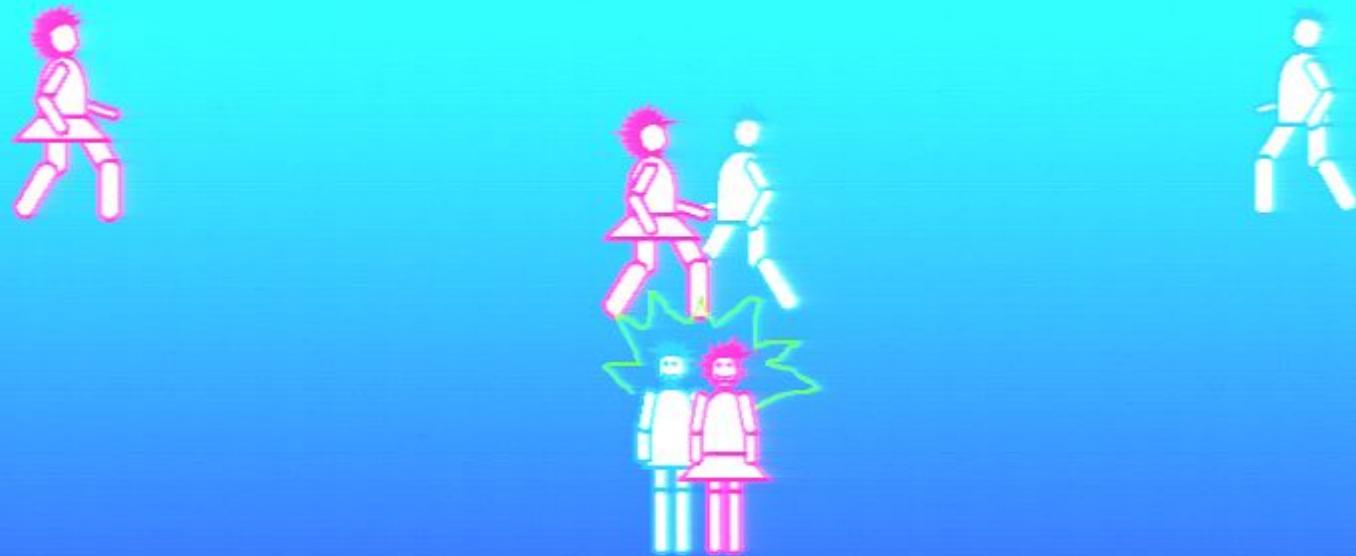
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STEEPEST-ENTROPY-ASCENT DYNAMICS FOR COMPOSITE SYSTEMS.  
NO-SIGNALING CONDITION AND LOCAL EFFECTS OF CORRELATIONS



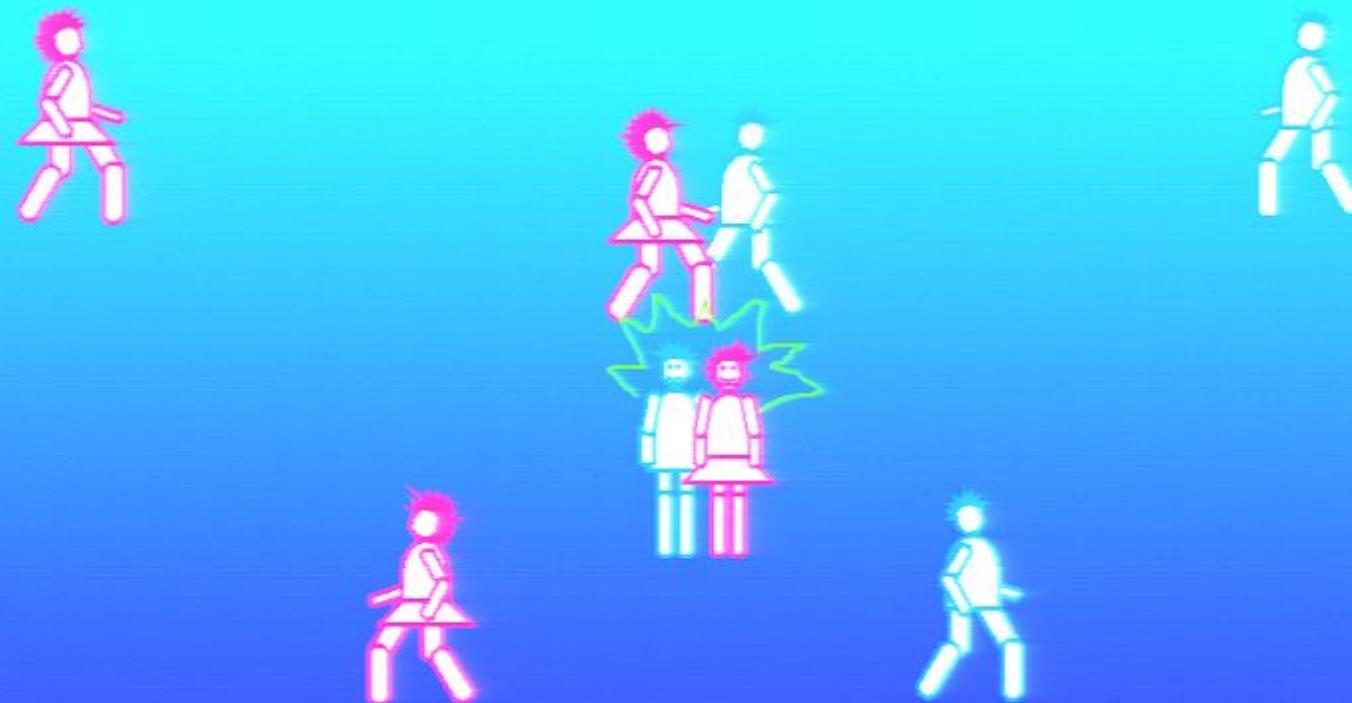
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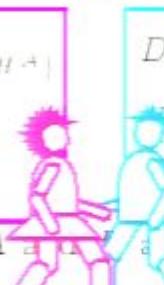
$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho] + \frac{1}{2k_B\tau_A}(\sqrt{\rho_A}D_A + D_A^\dagger\sqrt{\rho_A}) \otimes \rho_B + \frac{1}{2k_B\tau_B}\rho_B \otimes (\sqrt{\rho_B}D_B + D_B^\dagger\sqrt{\rho_B})$$



$$D_A = [\sqrt{\rho_A}(S)^A, -\mathcal{L}_{(\sqrt{\rho_A}\sqrt{\rho_B})}H^A]$$

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

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



$$D_B = [\sqrt{\rho_B}(S)^B, -\mathcal{L}_{(\sqrt{\rho_A}\sqrt{\rho_B})}H^B]$$

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

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



All zero entropy states ( $\rho^2 = \rho$ ), even if  $A$  and  $B$  are entangled, obey the Schrödinger equation  $\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho]$ .



**G.P. Beretta, See [here]<sup>20</sup> that if Quantum Thermodynamics were a fundamental extension of Quantum Mechanics, it<sup>21</sup>**  
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$V_{AB} = 0$  does not imply  $\frac{d\rho_A}{dt} \cancel{\neq} f(\rho_A)$  if  $\rho \neq \rho_A \otimes \rho_B$



$$\frac{d\rho_A}{dt} = f_A(\rho)$$

where  $f_A(\rho)$  is independent of any operator on  $\mathcal{H}_B$



G.P.H

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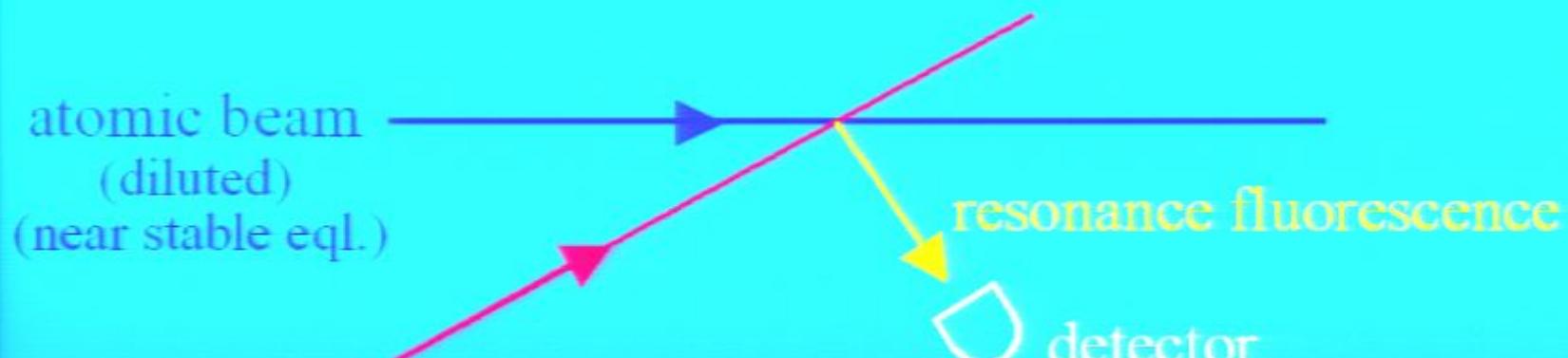
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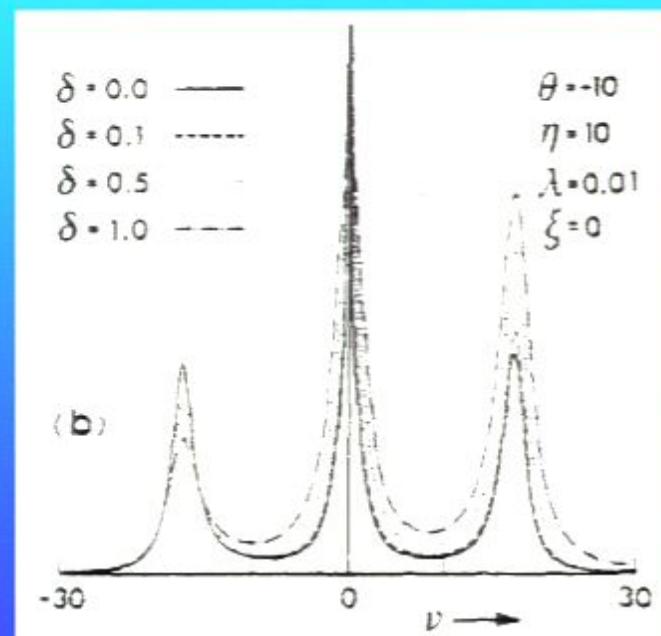
## Measurable effects?



atomic beam  
(diluted)  
(near stable eq.)

laser beam ("pump")  
off resonance (detuned)

Irreversible internal redistribution  
implies  
asymmetries  
in the spectral distribution



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

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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.*



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



G.P. Beretta, Seminar "What is Quantum Thermodynamics now: a fundamental extension of Quantum Mechanics?"  
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## Separability: structure of the equation of motion for...

$$\frac{d\rho}{dt} = \sqrt{\rho} E + E^\dagger \sqrt{\rho} , \quad E_D = \frac{1}{2k_B\tau(\rho)} [\sqrt{\rho} S]_{-\mathcal{L}\{\sqrt{\rho} R_i\}} .$$

$$E = E_H + E_D , \quad \{\sqrt{\rho} R_i\} = \text{linear span of } \sqrt{\rho} I, \sqrt{\rho} H, \sqrt{\rho} N_k$$

$$E_H = i\sqrt{\rho} H/\hbar , \quad (F|G) = \text{Tr}(F^\dagger G + G^\dagger F)/2 .$$

$$S = -k_B P_{\text{Ran } \rho} \ln \rho .$$

**...an indivisible system**

$$\frac{d\rho}{dt} = \sqrt{\rho} E + E^\dagger \sqrt{\rho} , \quad \mathcal{H} = \mathcal{H}^1 \otimes \mathcal{H}^2 \otimes \cdots \otimes \mathcal{H}^M = \mathcal{H}^J \otimes \mathcal{H}^J .$$

$$E = E_H + E_D , \quad \sqrt{\rho} E_D = \sum_{J=1}^M \sqrt{\rho_J} E_{DJ} \otimes \rho_{\overline{J}} .$$

$$E_H = i\sqrt{\rho} H/\hbar .$$

$$S = -k_B P_{\text{Ran } \rho} \ln \rho , \quad E_{DJ} = \frac{1}{2k_B\tau_J(\rho)} [\sqrt{\rho_J} (S)^J]_{-\mathcal{L}\{\sqrt{\rho_J} (R_{iJ})^J\}} .$$

$$\mathcal{L}\{\sqrt{\rho_J} (R_{iJ})^J\} = \text{lin. span of } \sqrt{\rho_J} I_J, \sqrt{\rho_J} (H_J)^J, \sqrt{\rho_J} (N_{kJ})^J$$

$$(F_J|G_J)_J = \text{Tr}_J(F_J^\dagger G_J + G_J^\dagger F_J)/2 .$$

$$(R_{iJ})^J = \text{Tr}_{\overline{J}}[(I_J \otimes \rho_{\overline{J}}) R_{iJ}] .$$

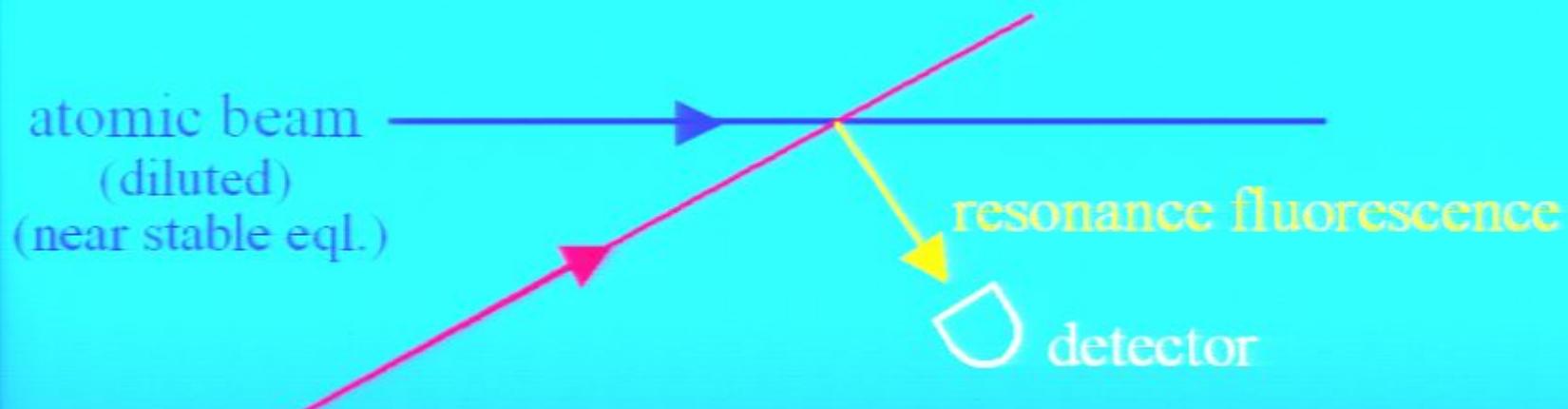
$$(S)^J = \text{Tr}_{\overline{J}}[(I_J \otimes \rho_{\overline{J}}) S] .$$



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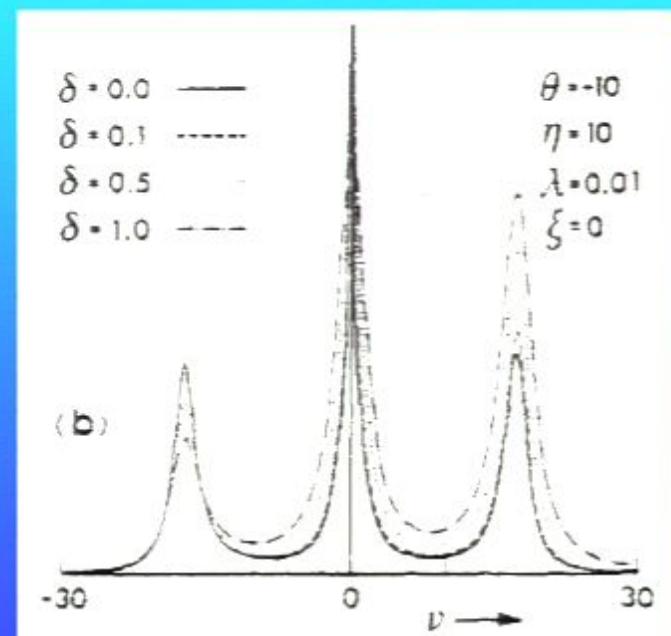
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