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

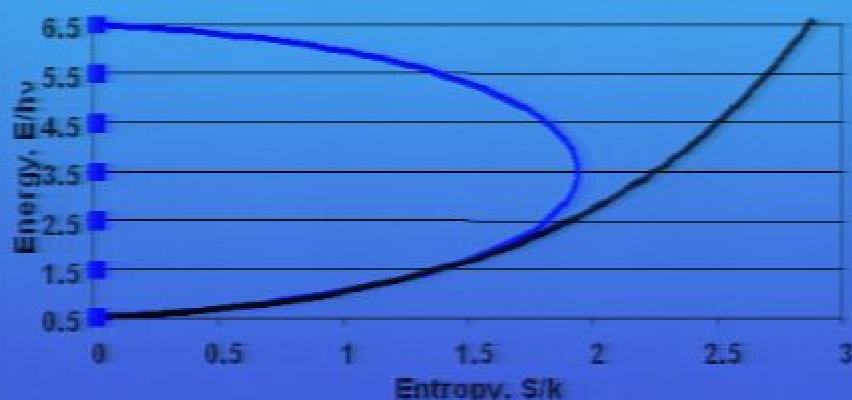
Date: Oct 01, 2009 09:30 AM

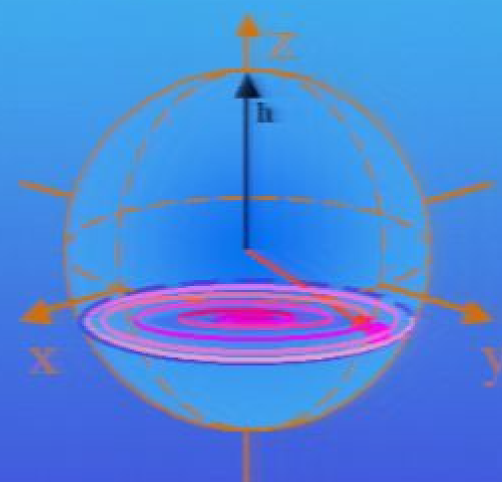
URL: http://pirsa.org/09100088

Abstract: Perhaps the earliest explicit ansatz of a truly ontic status for the density operator has been proposed in [G.N. Hatsopoulos and E.P. Gyftopoulos, Found. Phys., Vol.6, 15, 127, 439, 561 (1976)]. Their self-consistent, unified quantum theory of Mechanics and Thermodynamics hinges on: (1) modifyng the ‘state postulate’ so that the full set of ontic individual states of a (strictly isolated and uncorrelated) quantum system is one-to-one with the full set of density operators (pure and mixed); and (2) complementing the remaining usual postulates of quantum theory with an ‘additional postulate’ which effectively seeks to incorporate the Second Law into the fundamental level of description. In contrast with the epistemic framework, where the linearity of the dynamical law is a requirement, the assumed ontic status of the density operator emancipates its dynamical law from the restrictive requirement of linearity. Indeed, when the ‘additional postulate’ is replaced by the dynamical ansatz of a (locally) steepest entropy ascent, nonlinear evolution equation for the density operator proposed in [G.P. Beretta, Sc.D. thesis, M.I.T., 1981, e-print quant-ph/0509116; and follow-up papers], the (Hatsopoulos-Keenan statement of the) Second Law emerges as a general theorem of the dynamics (about the Lyapunov stability of the equilibrium states). As a result, the ontic status is acquired not only by the density operator, but also by the entropy (which emerges as a microscopic property of matter, at the same level as energy), and by irreversibility (which emerges as a microscopic dynamical effect). This “adventurous scheme ... may end arguments about the arrow of time -- but only if it works” [J. Maddox, Nature, Vol.316, 11 (1985)]. Indeed, the scheme resolves both the Loschmidt paradox and the Schroedinger-Park paradox about the concept of ‘individual quantum state’. However, nonlinearity imposes a high price: the maximum entropy production (MEP) dynamical law does not have a universal structure like that of the Liouville-von Neumann equation obeyed by the density operator within the epistemic (statistical mechanics) view. Instead, much in the same way as the implications of the Second Law depend on the assumed model of a given physical reality, the MEP dynamical law for a composite system is model dependent: its structure depends on which constituent particles or subsystems are assumed as elementary and separable, i.e., incapable of no-signaling violations. See www.quantumthermodynamics.org for references.

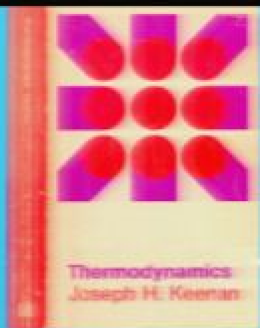
Mechanics and Thermodynamics fundamentally united by density operators with an ontic status obeying a locally maximum entropy production dynamics. But at what price?

Gian Paolo Beretta
Università di Brescia, Italy



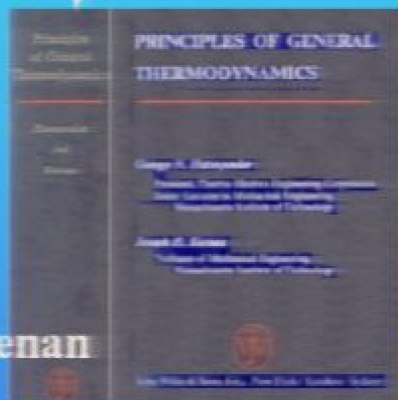


The Keenan school of Thermodynamics
from engineering, to physics, to mathematical-physics, and back!



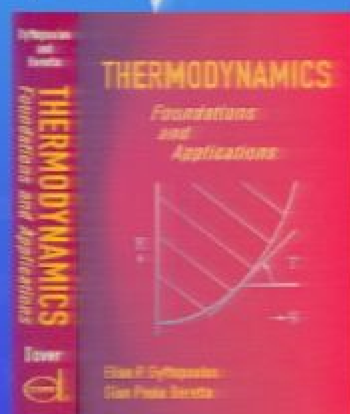
Keenan

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

References available at: **www.quantumthermodynamics.org**

Outline

1) Notion of individual state and the known conceptual problem in QSM

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) Notion of individual state and the known conceptual problem in QSM

2) An ansatz (1976) allows to embed Thermodynamics into Quantum Theory

- Ontic status of density operators and microscopic entropy

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Part I

1) Notion of individual state and the known conceptual problem in QSM

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

Ensemble E_{Π} of identical systems all prepared by Π at time t

Statistics of measurement outcomes (all at time t)

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

Preparation Π of system

Measurement procedure A → $a_1\, a_2 \ldots a_d$ → $p_{a_j} = \langle Q_{a_j} \rangle = \lim_{N_A \to \infty} N_{a_j}/N_A$

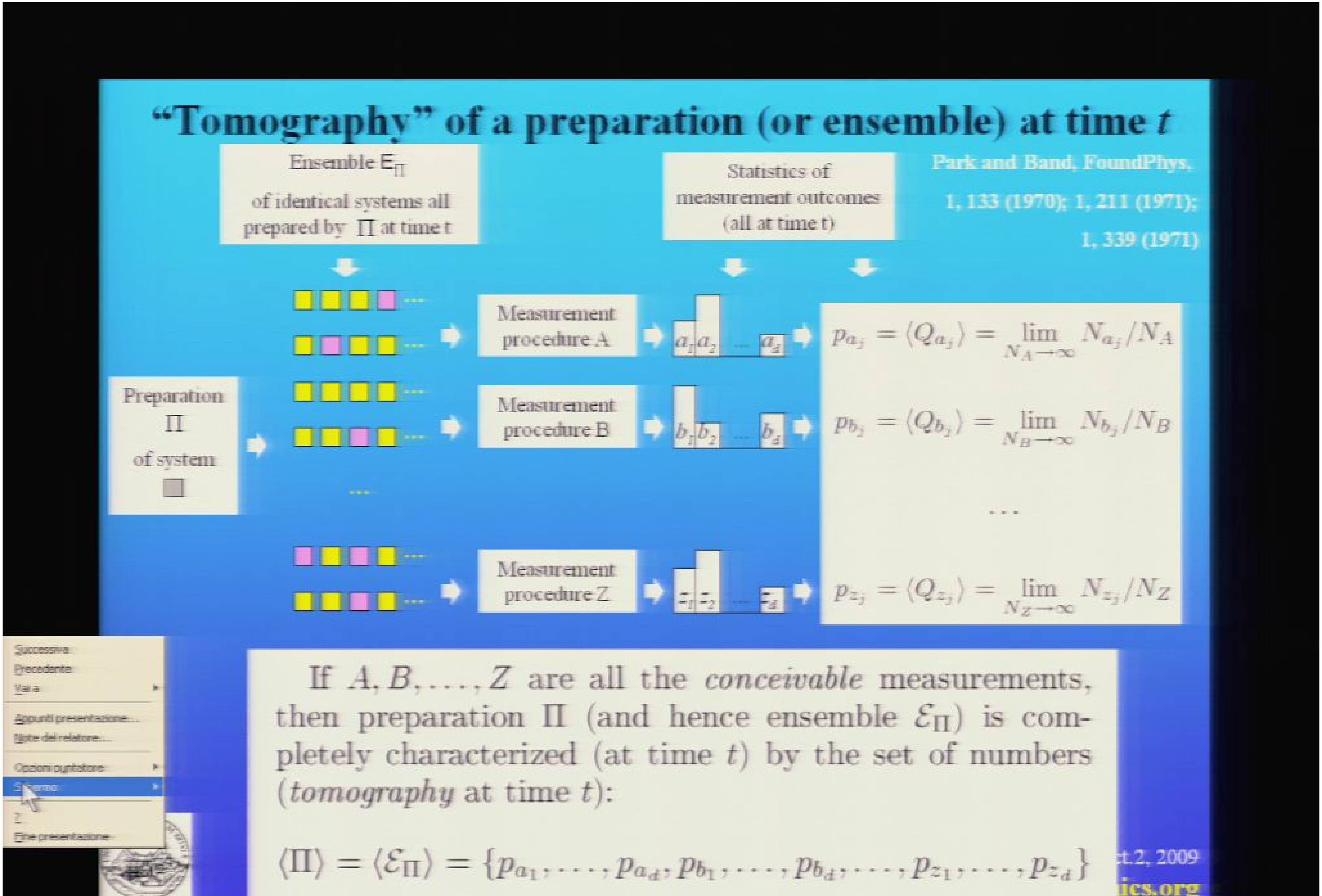
Measurement procedure B → $b_1\, b_2 \ldots b_d$ → $p_{b_j} = \langle Q_{b_j} \rangle = \lim_{N_B \to \infty} N_{b_j}/N_B$

...

Measurement procedure Z → $z_1\, z_2 \ldots z_d$ → $p_{z_j} = \langle Q_{z_j} \rangle = \lim_{N_Z \to \infty} N_{z_j}/N_Z$

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

$$\langle \Pi \rangle = \langle \mathcal{E}_{\Pi} \rangle = \{p_{a_1}, \ldots, p_{a_d}, p_{b_1}, \ldots, p_{b_d}, \ldots, p_{z_1}, \ldots, p_{z_d}\}$$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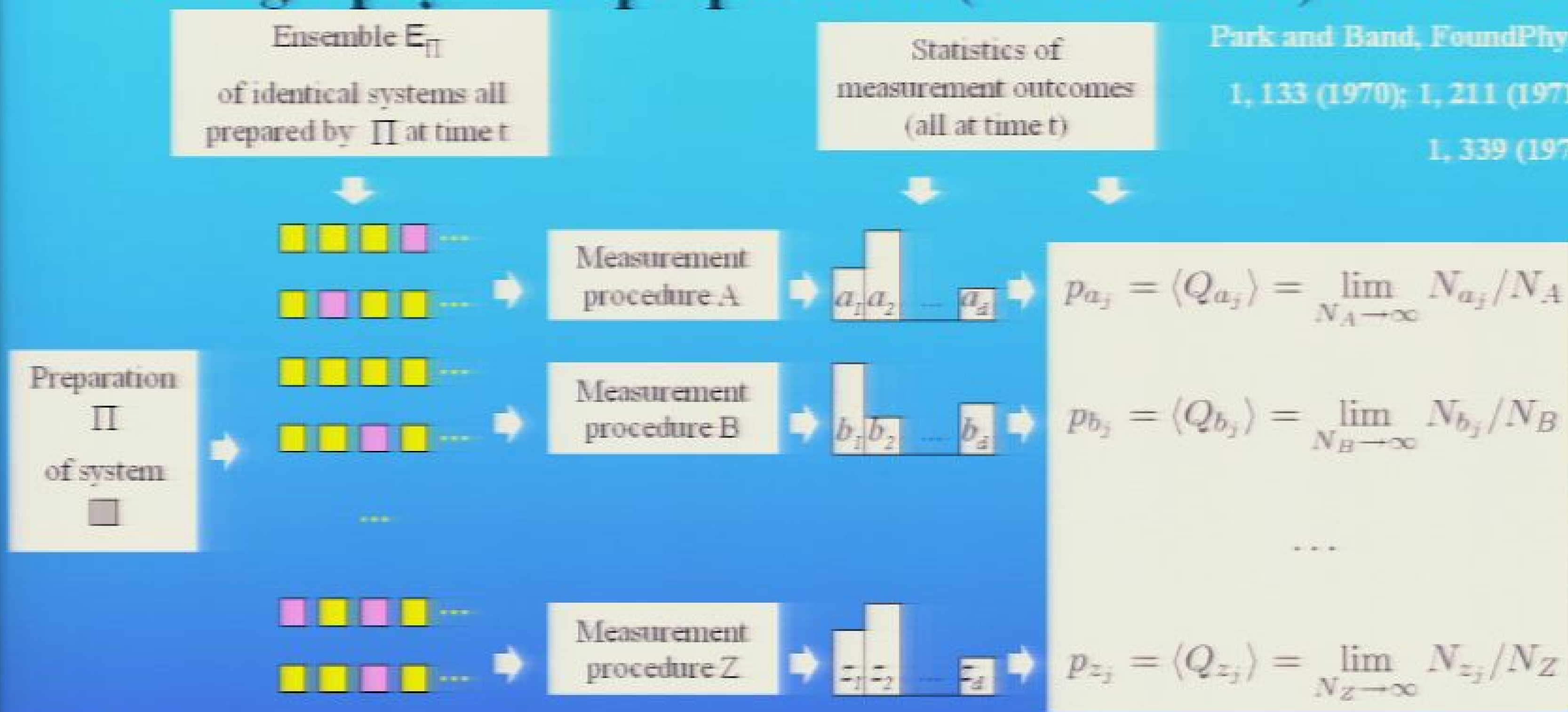
Successiva
Precedente
Vai a
Appunti presentazione...
Note del relatore...
Opzioni puntatore
Schermo
Fine presentazione

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

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



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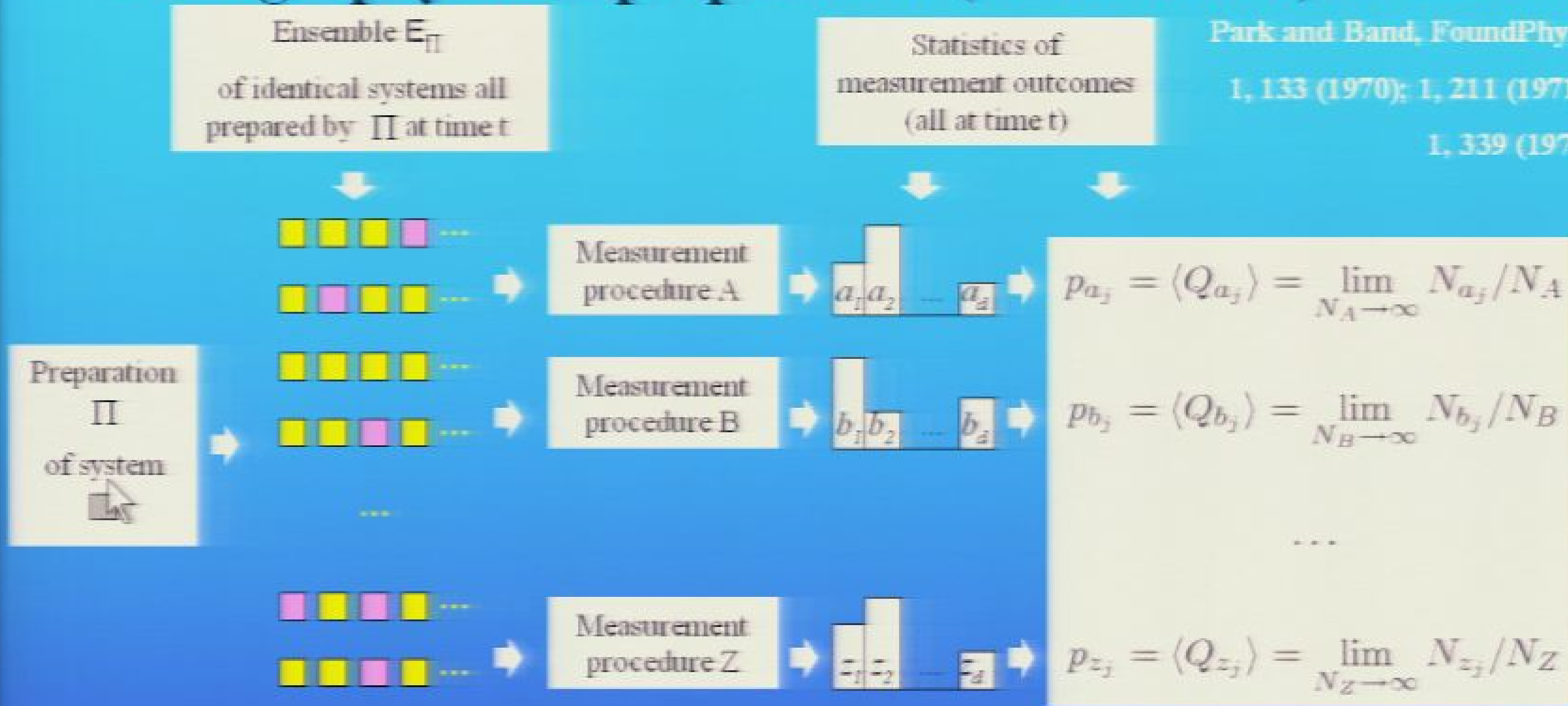

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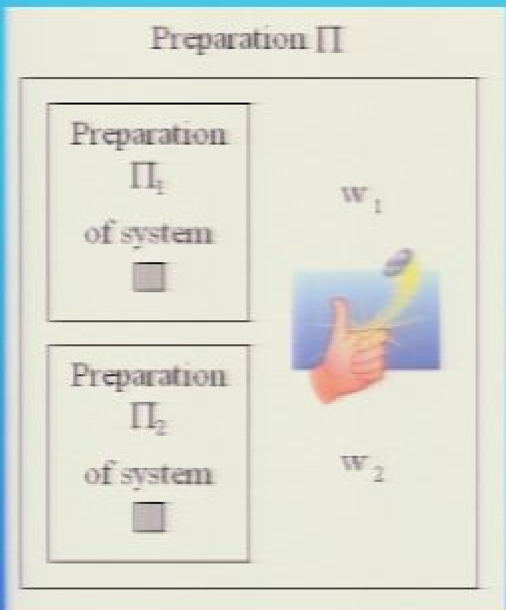
Statistical mixing of preparations (or ensembles) and the notion of homogeneous preparation



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

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

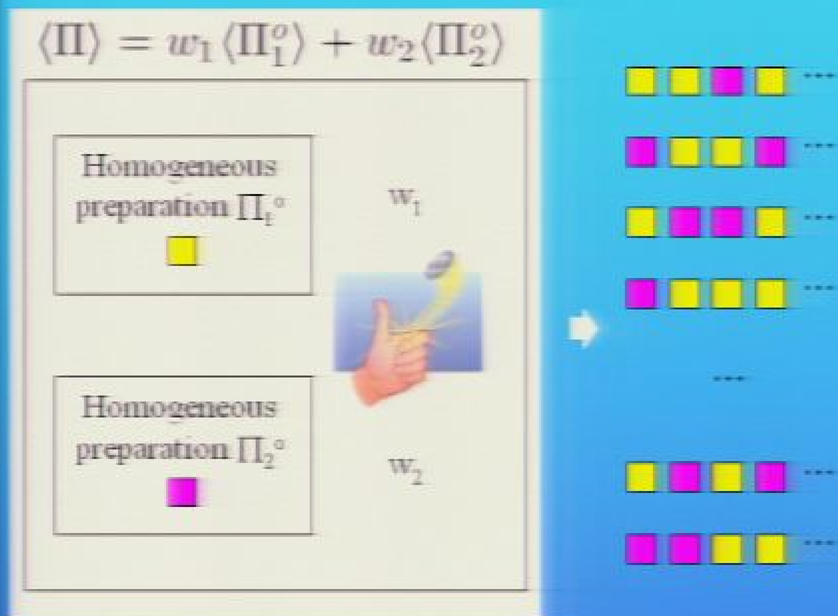
Given a preparation Π, we may look for *all conceivable decompositions*. A preparation is *homogeneous* (von Neumann), denoted Π^o, iff there is no conceivable way to obtain the same tomography from a notrivial statistical mixture of two *different* preparations (different means *with different tomography*),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

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

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.*

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

The notion of quantum state is incompatible with QSM



"State is either ■ or ■"

Schrödinger, PCPS, 32, 446 (1936)

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

quant-ph/0509116

ModPhysLettA, 21, 2799 (2006)

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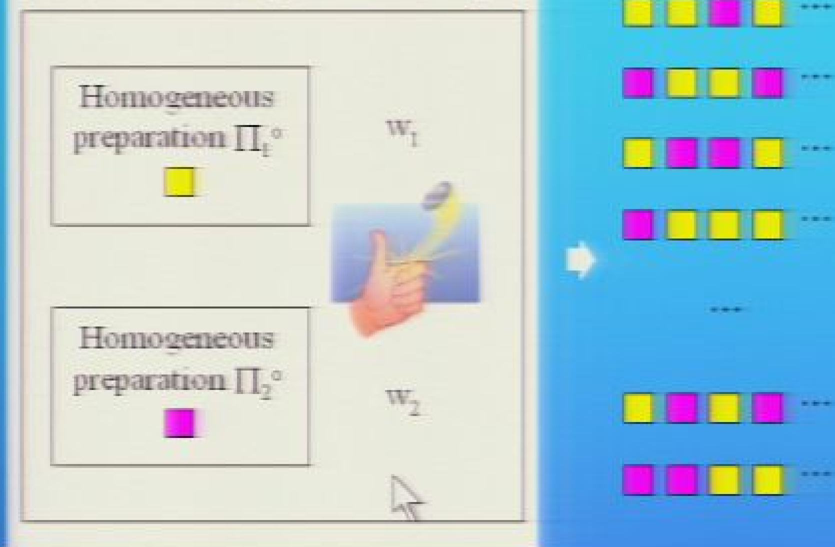
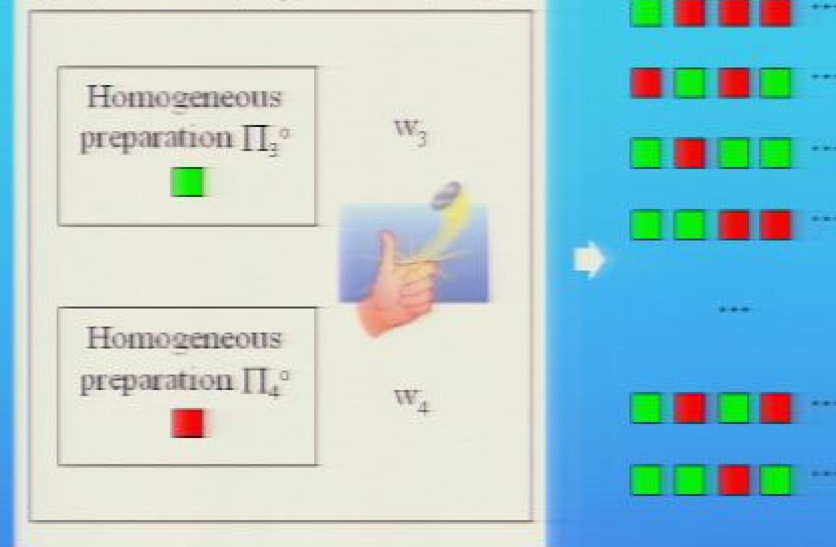
$\langle \Pi \rangle = w_1 \langle \Pi_1^o \rangle + w_2 \langle \Pi_2^o \rangle$



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



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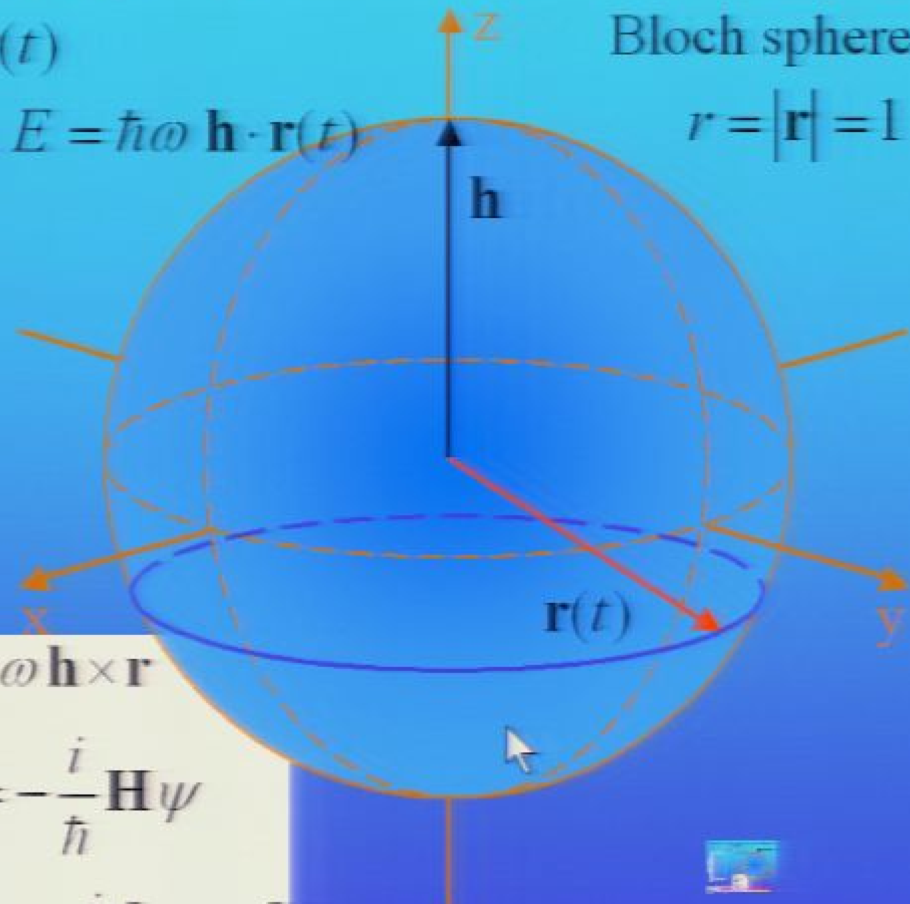
Isolated and uncorrelated 2-level particle

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

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

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

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



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

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

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

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

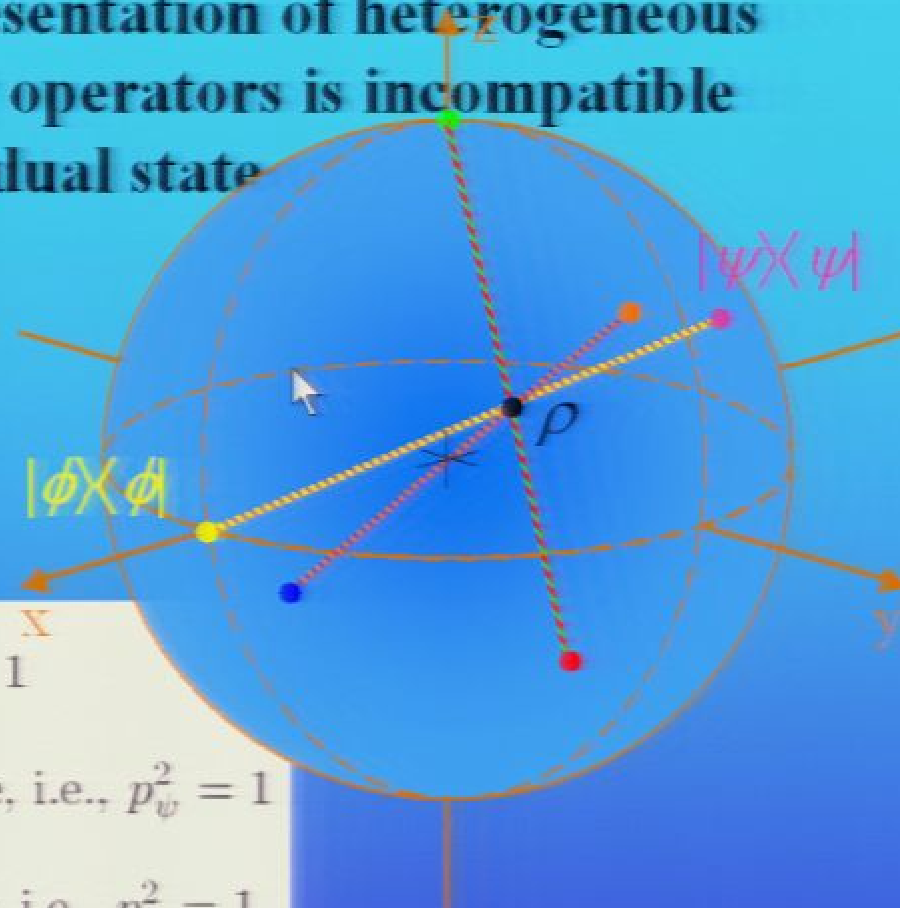
Schrödinger, PCPS, 32, 446 (1936)

ParkBand-FoundPhys-6-157-1976

many others later

quant-ph/0509116

ModPhysLettA-21-2799-2006



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

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

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

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

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

PhD Thesis (1981), quant-ph/0509116

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 $\mu_1 = \mu_2 = \mu^o$;

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

$$f(\mu) = \sum_j w_j(\mu) f(\mu_j^o) \qquad \sum_j w_j = 1,\, w_j \geq 0 \tag{1}$$

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.

Heterogeneous preparations in QSM should instead be represented by probability density distributions over the manifold of possible ontic QM 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):

$$\alpha \Longrightarrow |\psi_\alpha\rangle\langle\psi_\alpha| \qquad |\psi\rangle \Longrightarrow \alpha_{|\psi\rangle}$$

Representation of a **homogeneous preparation**

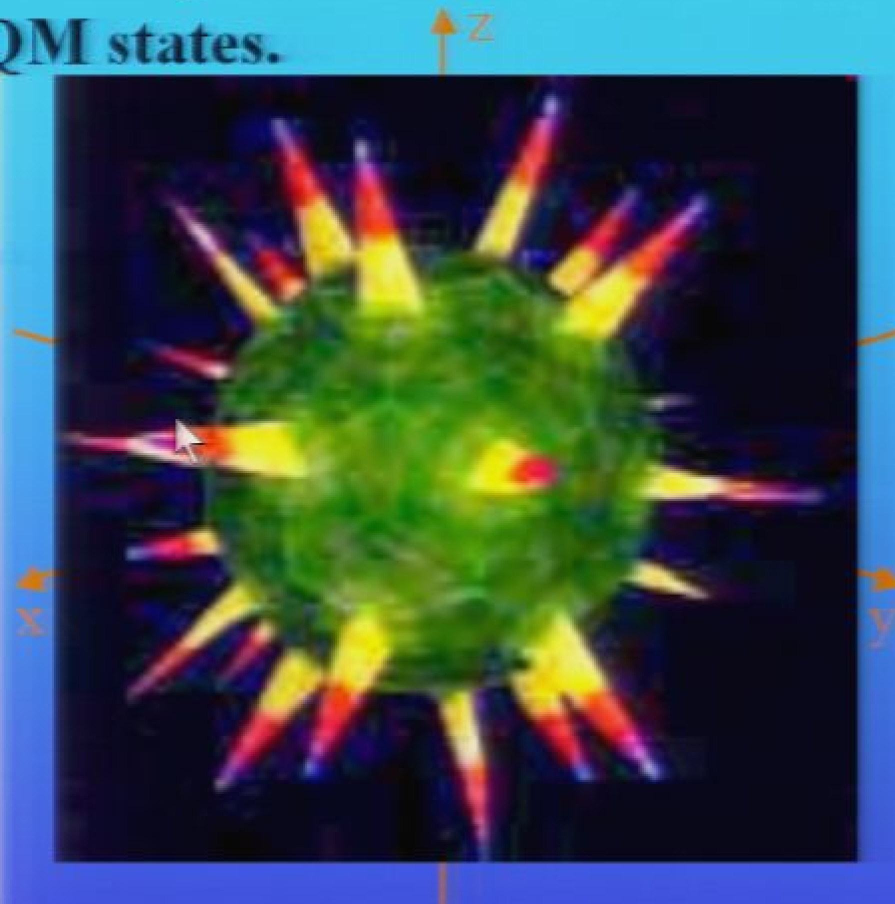
$$w(\mu^o_{|\psi\rangle},\alpha) = \delta(\alpha - \alpha_{|\psi\rangle})$$

Notice: only for **linear observables**,

$$f_L(\mu^o_{|\psi\rangle}) = \mathrm{Tr}(L|\psi\rangle\langle\psi|)$$

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

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



"...on the Quantum State", Perimeter Institute, Sept.27-Oct.2, 2009

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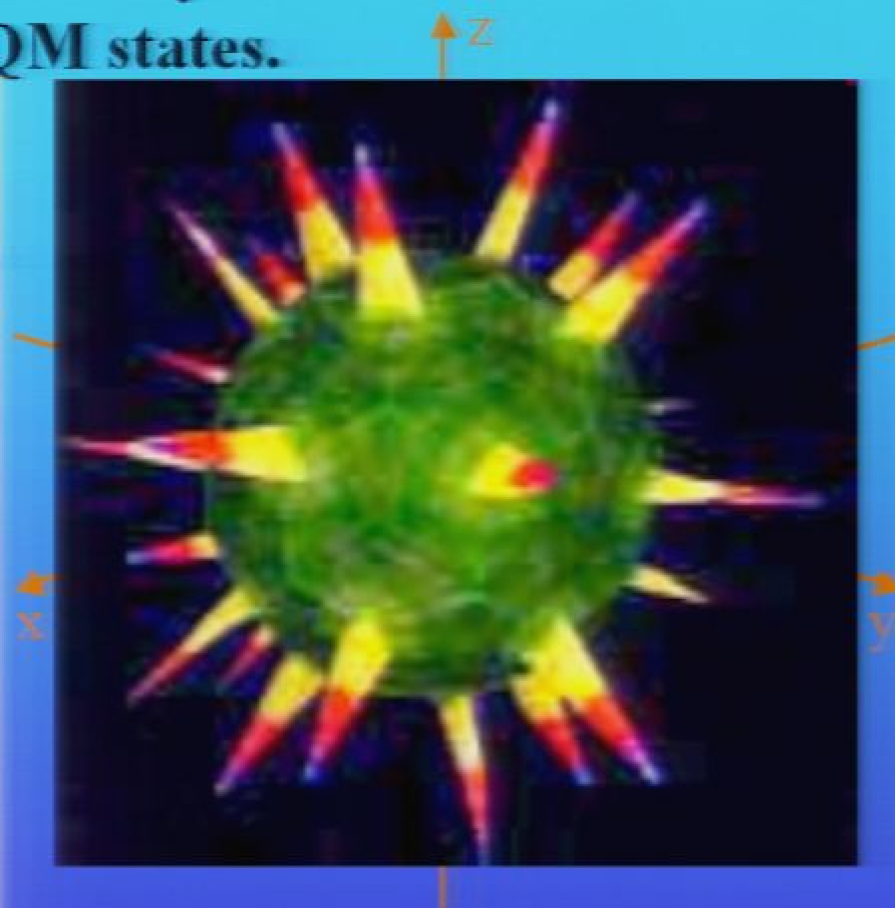


Is this a fundamental indication (theorem) there must exist some measurable observables which need to be represented by **nonlinear** functionals of $|\psi\rangle\langle\psi|$?

Part II

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

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

To unite Mechanics and Thermodynamics it is sufficient to assume the existence of more ontic states than in QM

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

- 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 **<u>not</u>** 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 $-k_B \mathrm{Tr}\, \rho \ln\rho$ as an ontic physical quantity, like energy or mass.
- $-k_B \mathrm{Tr}\, \rho \ln\rho$ is **<u>not</u>** understood as measuring how broad is an epistemic probability distribution.

Isolated and uncorrelated 2-level particle

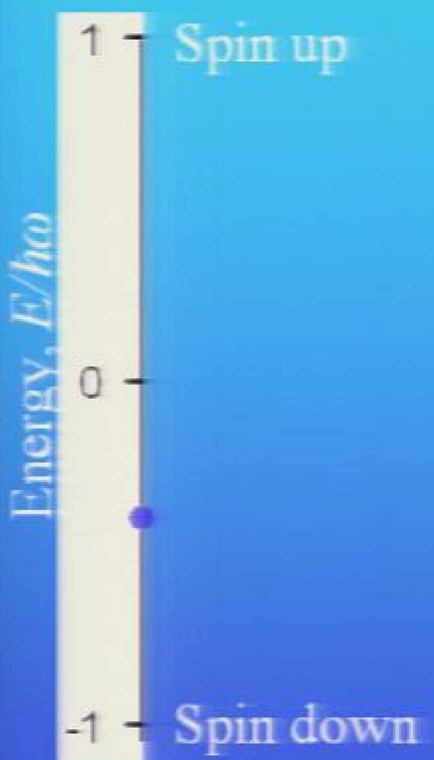
Hamiltonian, $\hbar\omega\,\mathbf{h}$

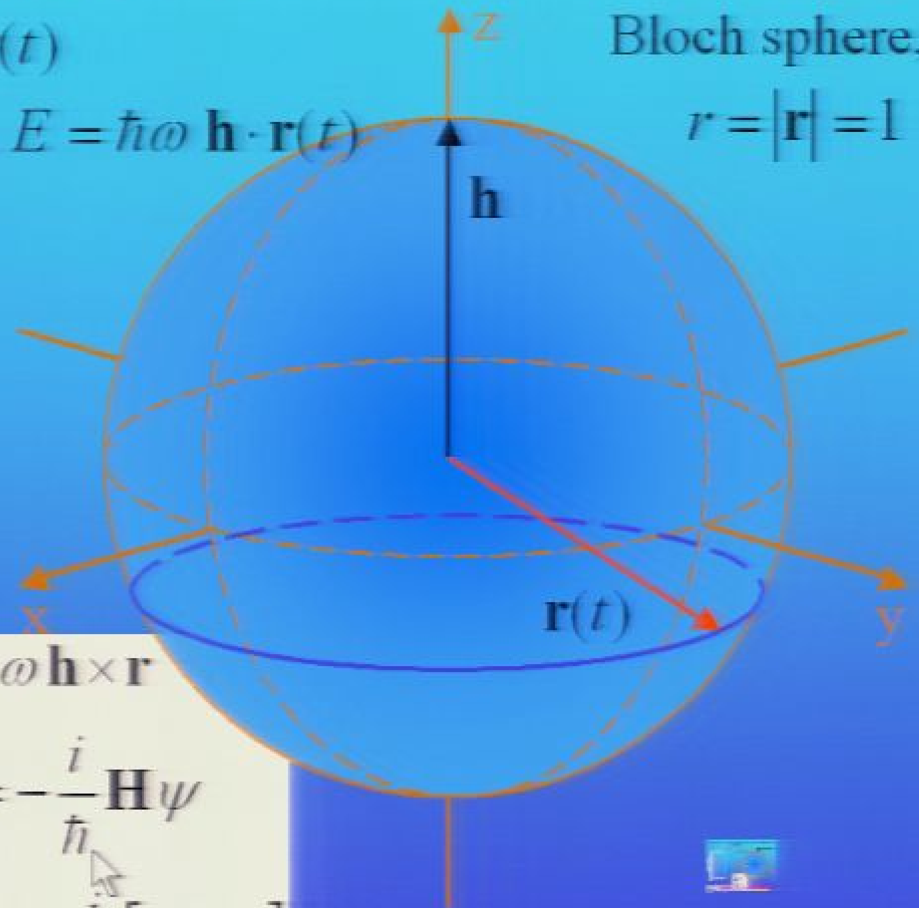
State, $\mathbf{r}(t)$

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

Bloch sphere,

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





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

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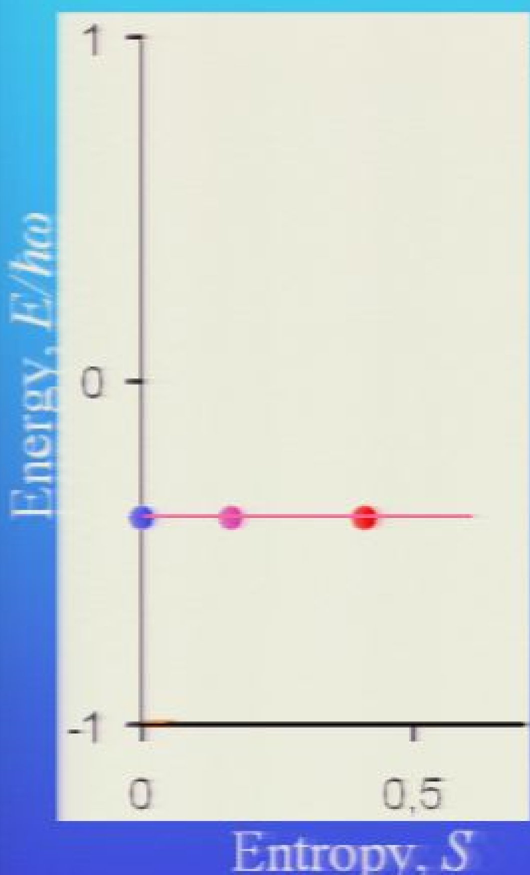
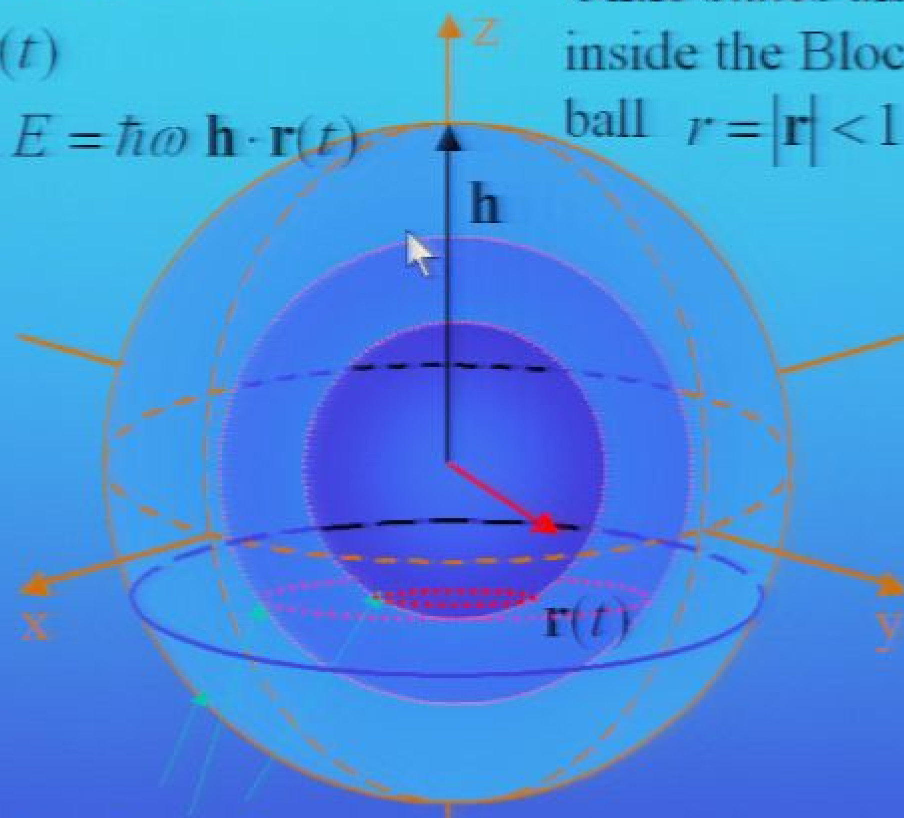
Ontic states also inside the Bloch ball $r = |\mathbf{r}| < 1$





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

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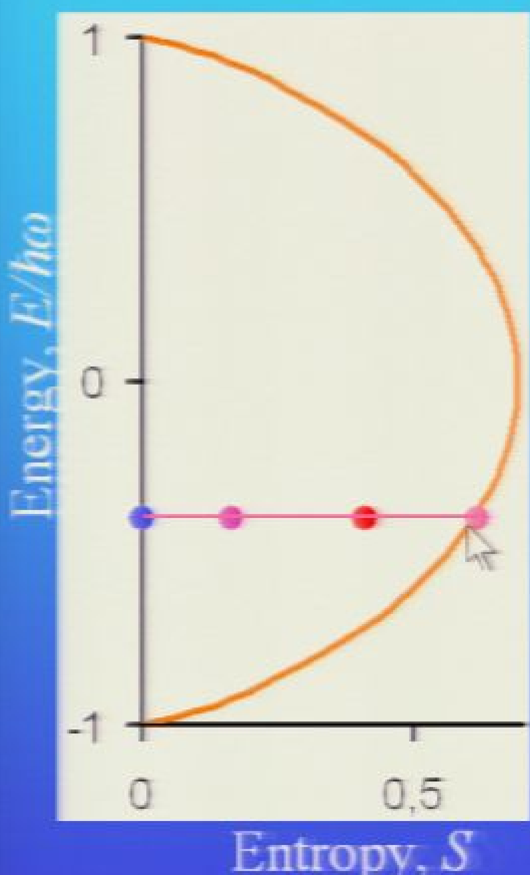

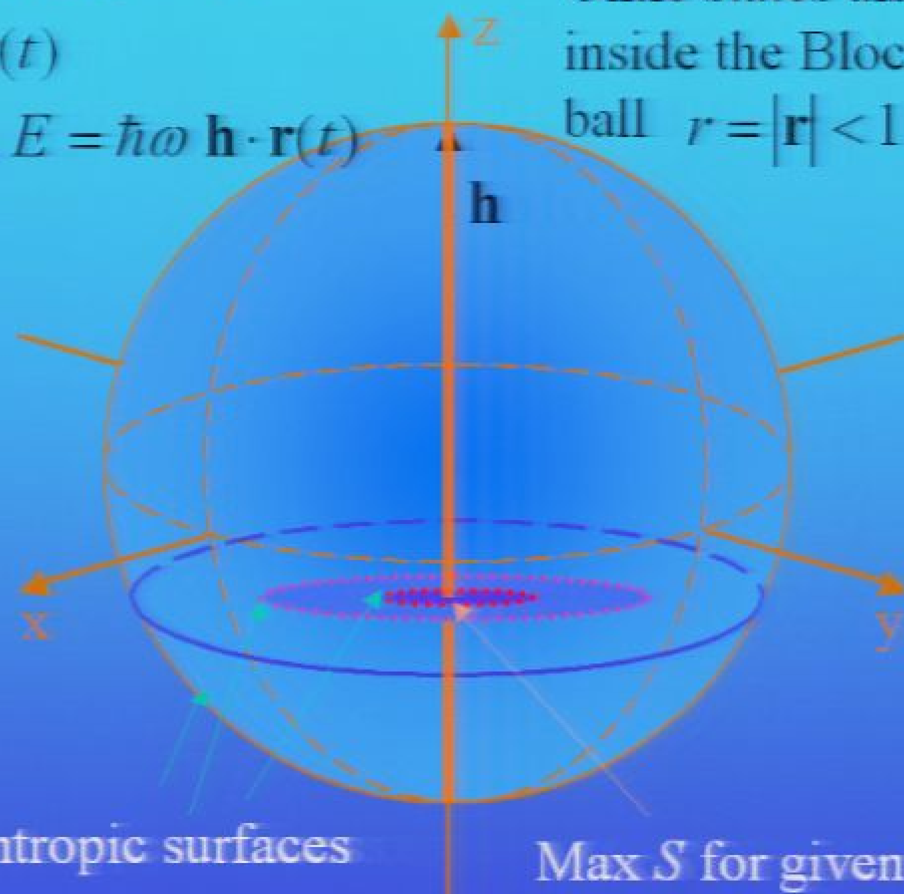

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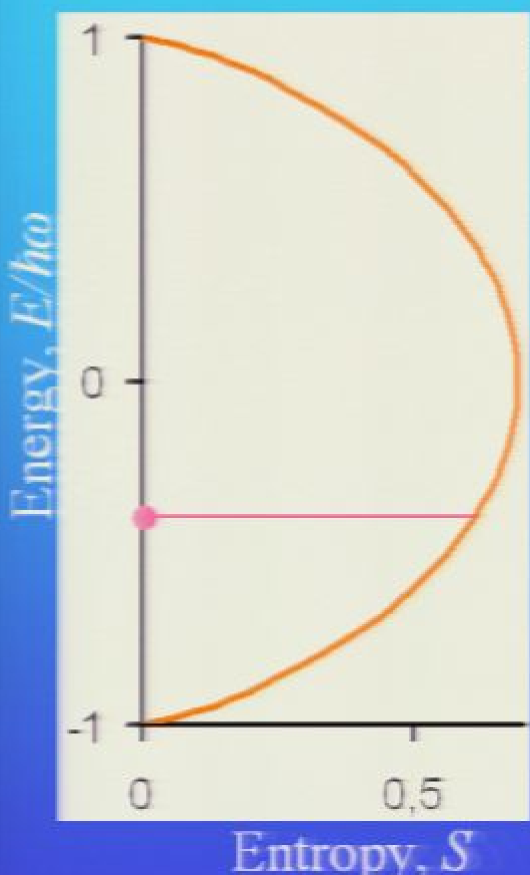
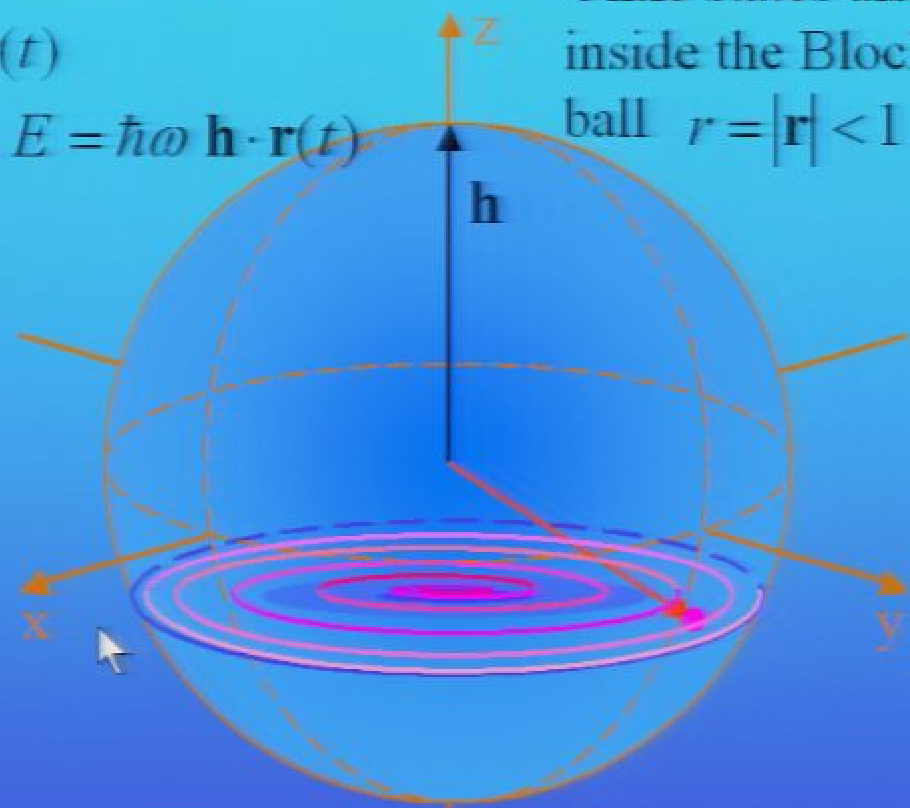




$$\dot{\mathbf{r}} = \omega\,\mathbf{h}\times\mathbf{r} - \frac{f(r)}{\tau}\mathbf{h}\times\mathbf{r}\times\mathbf{h}$$

$S \neq 0$

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

Isolated two-level system, Quantum Thermodynamics

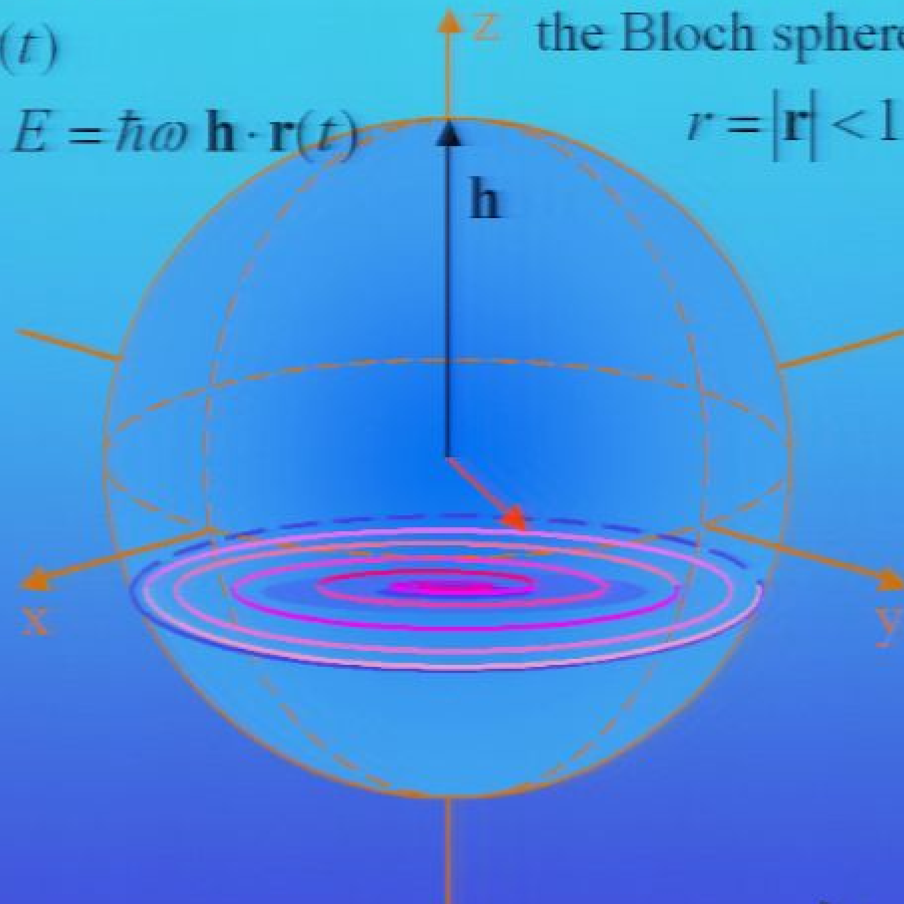
Hamiltonian, $\hbar\omega\,\mathbf{h}$

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

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

Inside the Bloch sphere,

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



$S \neq 0$

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

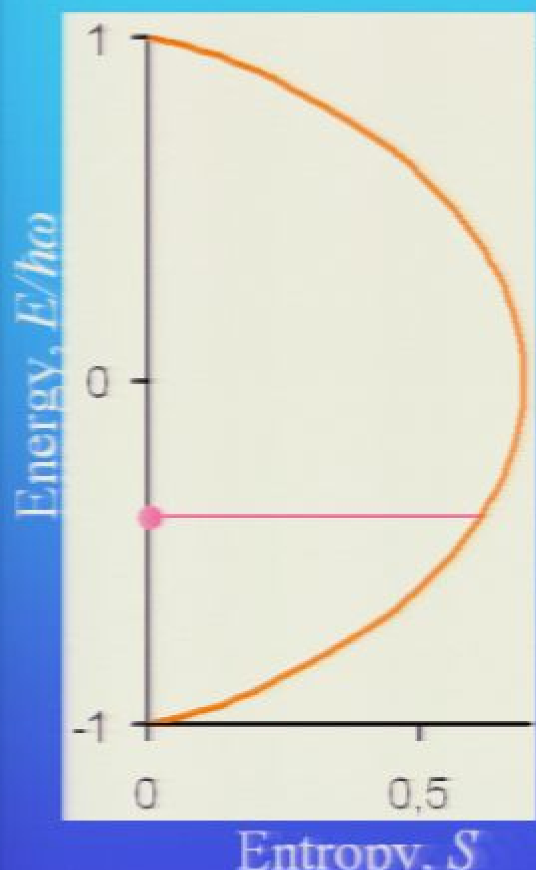
Isolated and uncorrelated 2-level particle

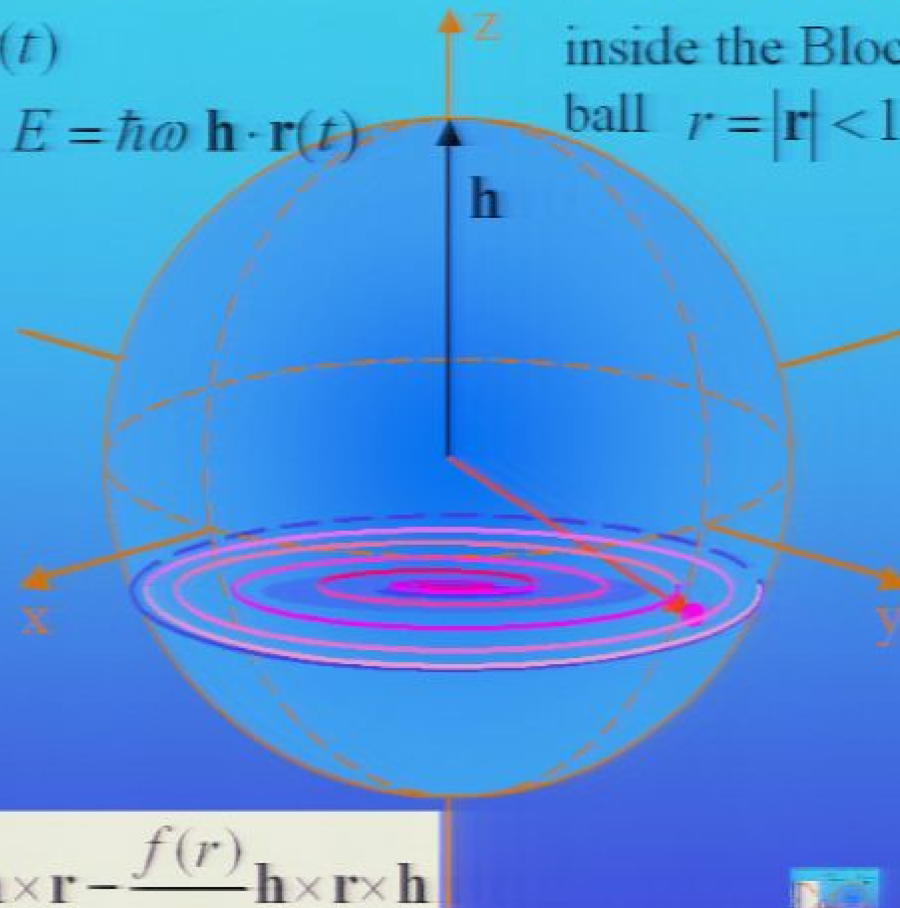
Hamiltonian, $\hbar\omega\,\mathbf{h}$

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

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

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





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

Isolated and uncorrelated 2-level particle

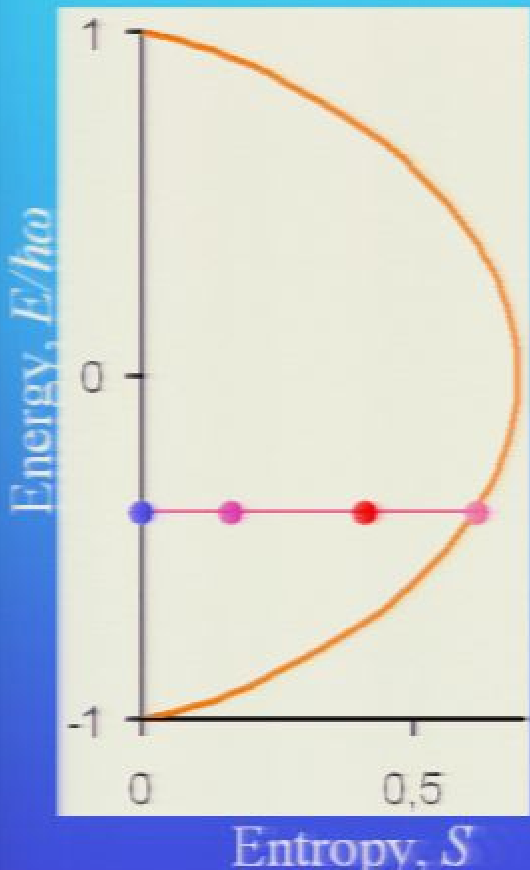
Hamiltonian, $\hbar\omega\,\mathbf{h}$

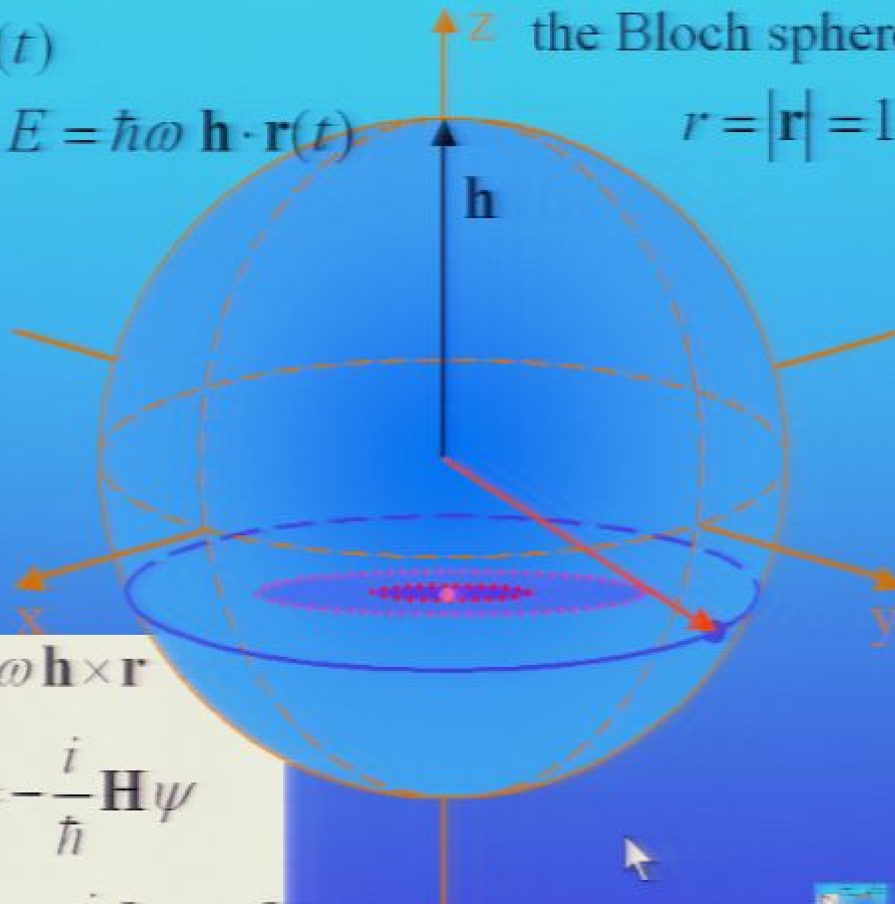
State, $\mathbf{r}(t)$

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

On the surface of the Bloch sphere.

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





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

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

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

$S = 0$

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

References available at: **www.quantumthermodynamics.org**

Ontic interpretation of the eigenvalues of ρ

Isolated and uncorrelated N-level particle

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

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

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

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

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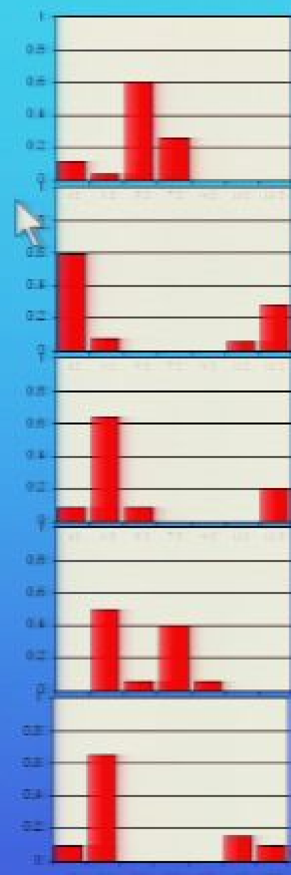


Example, N=7, different distributions with same E and S

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

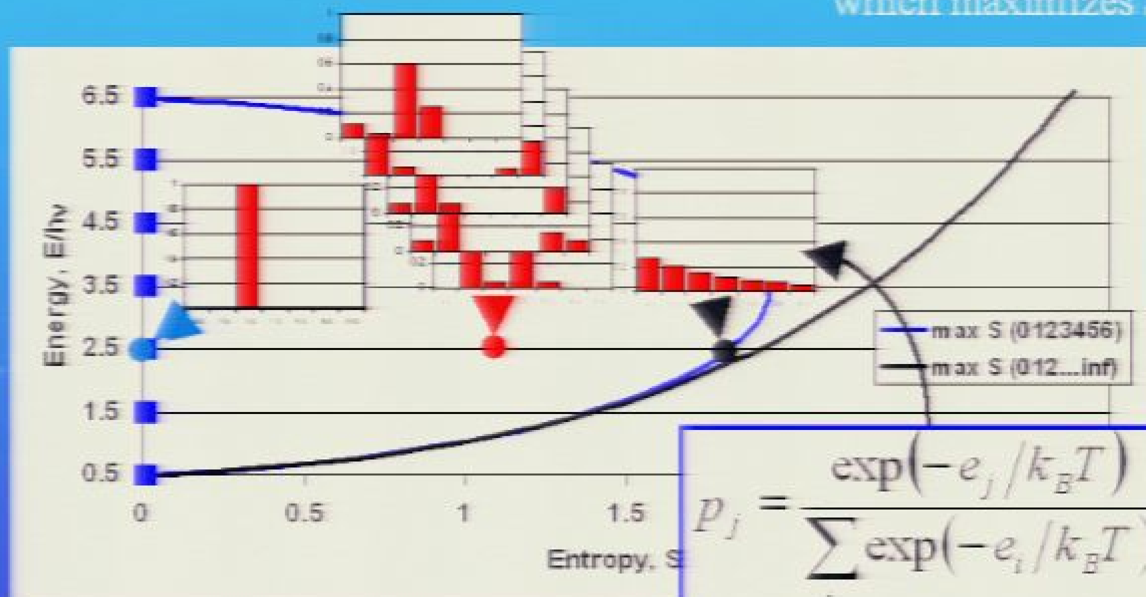
p_j eigenvalues of $\boldsymbol{\rho}$ (for simplicity, assume $\boldsymbol{\rho}\mathbf{H} = \mathbf{H}\boldsymbol{\rho}$)

$E = \sum_j p_j e_j$ energy

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

In 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 $\boldsymbol{\rho}\mathbf{H}=\mathbf{H}\boldsymbol{\rho}$, 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

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

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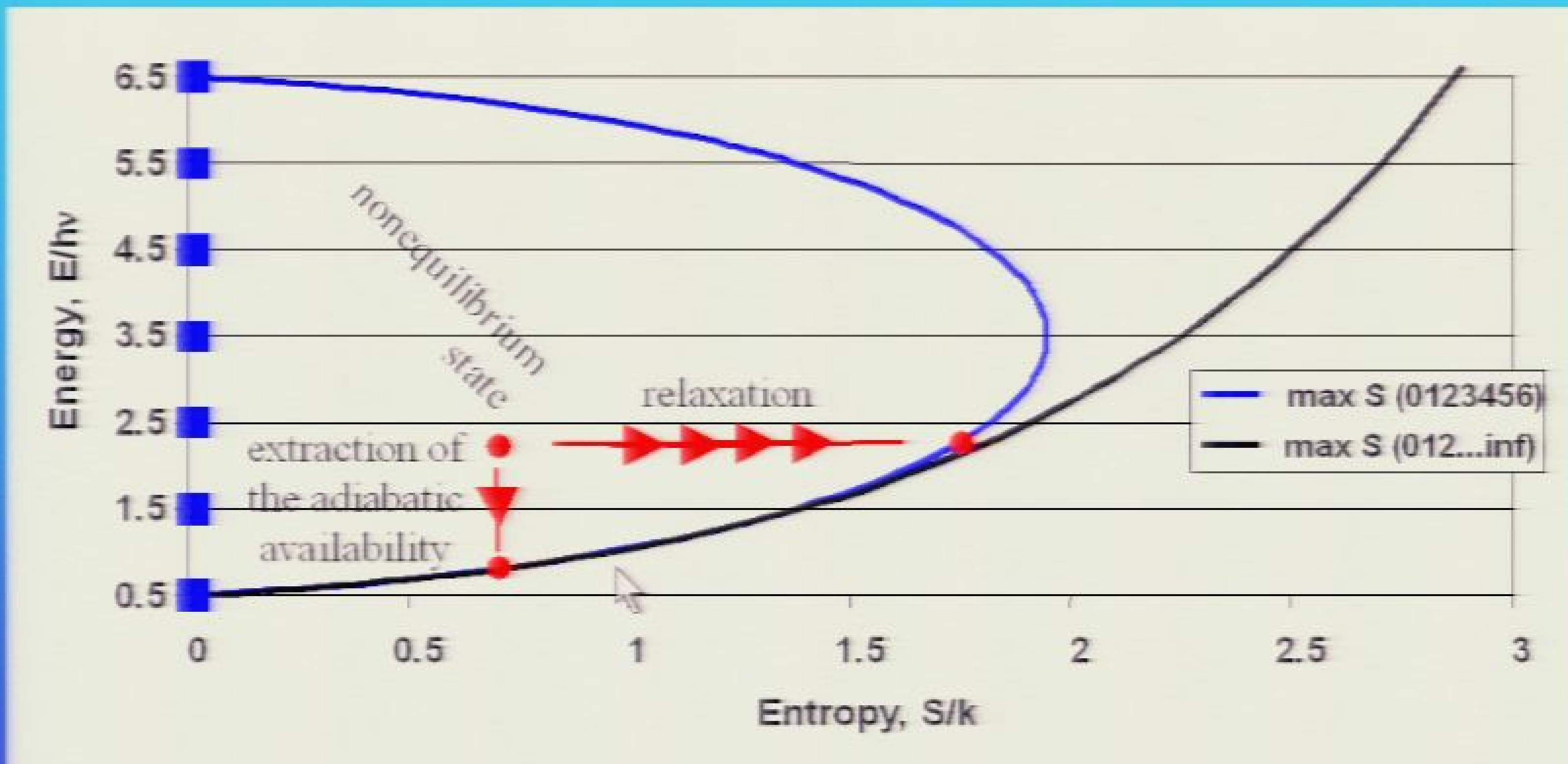
References available at: **www.quantumthermodynamics.org**

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



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

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

p_j eigenvalues of $\boldsymbol{\rho}$ (for simplicity, assume $\boldsymbol{\rho}\mathbf{H} = \mathbf{H}\boldsymbol{\rho}$)

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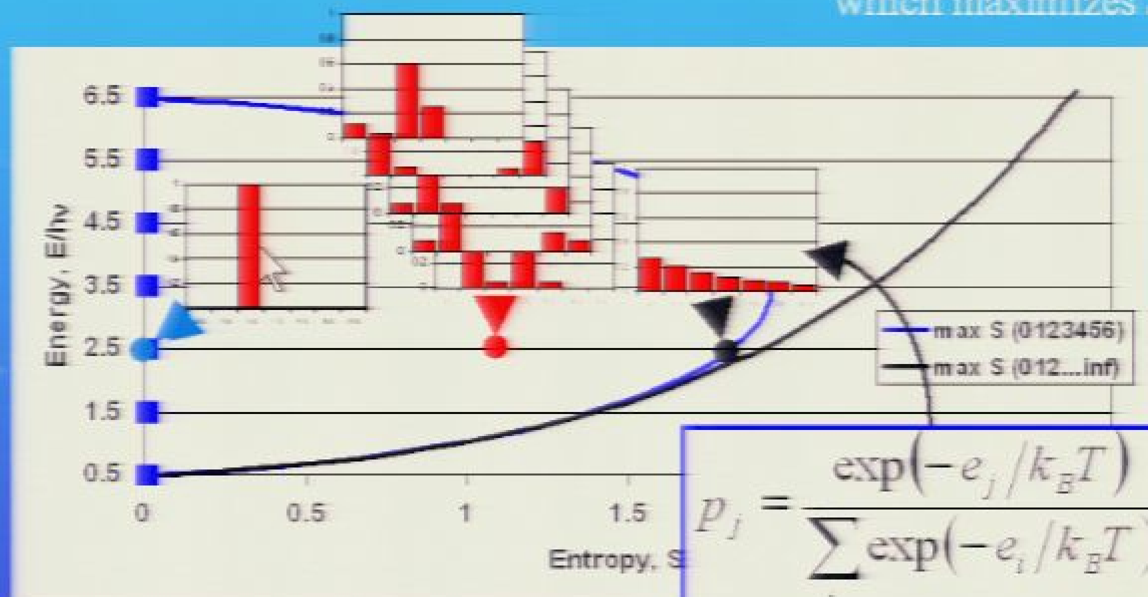

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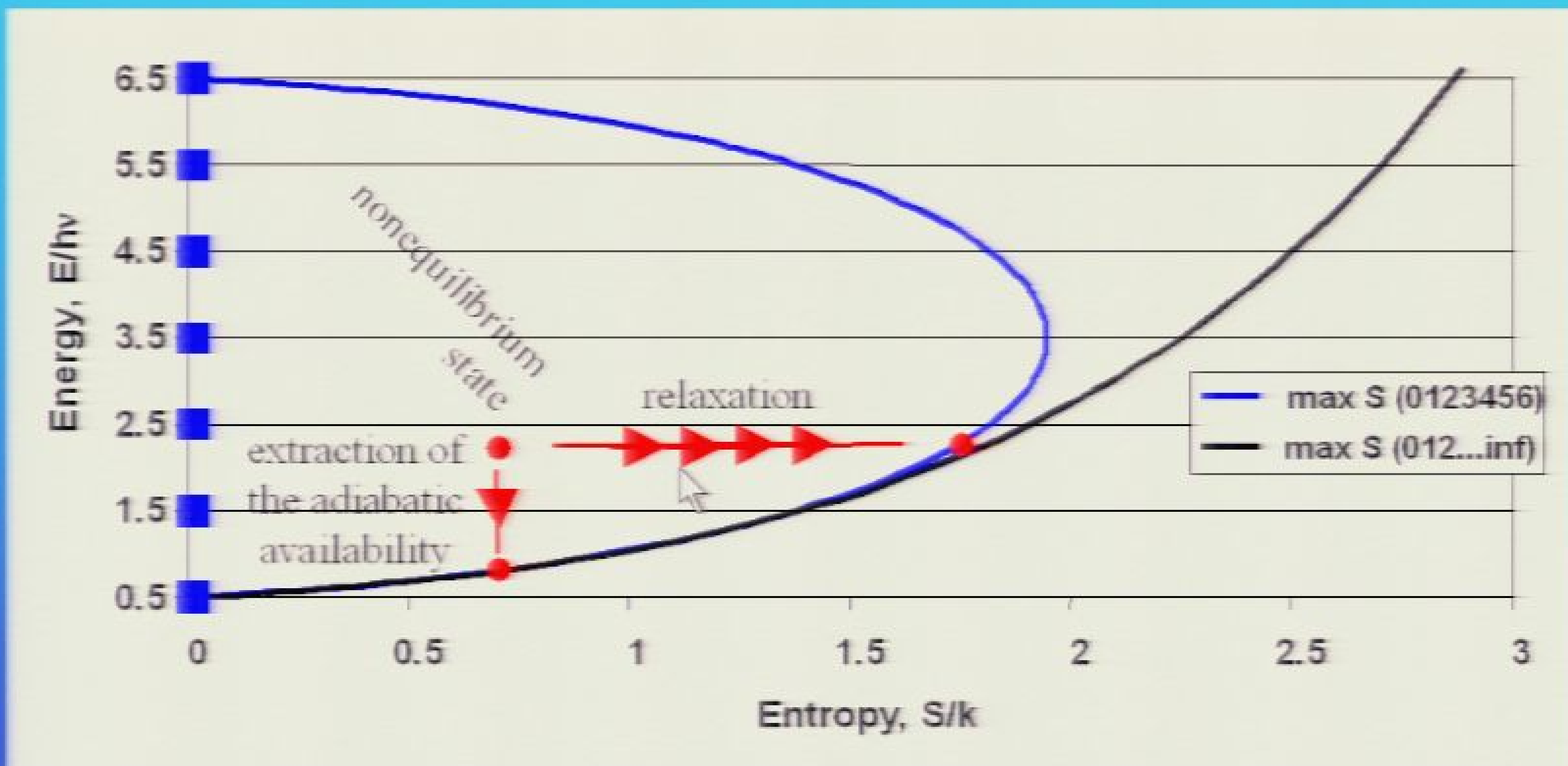

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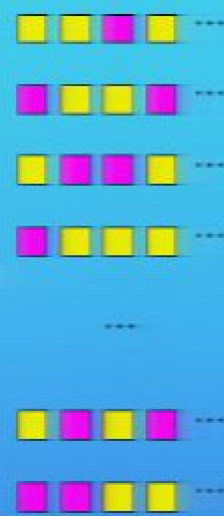
No need for linearity of the dynamical law

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

Homogeneous preparation Π_1° ■ (yellow) — $\rho_1(t)$ — w_1

Homogeneous preparation Π_2° ■ (magenta) — $\rho_2(t)$ — w_2



"State at time t is either ■ or ■"

The density operator

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

does **not** represent the heterogeneous preparation

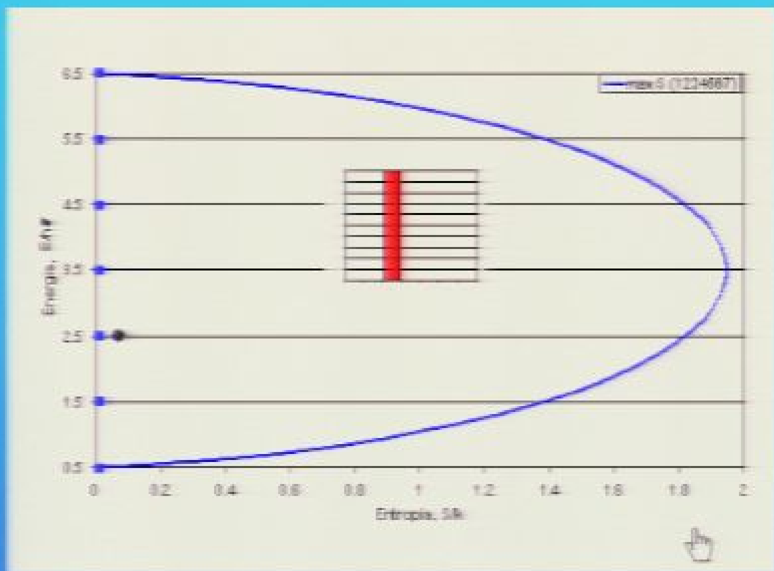
$$\langle \Pi \rangle_t = w_1 \langle \Pi_1^o \rangle_t + w_2 \langle \Pi_2^o \rangle_t$$

The description must be such that

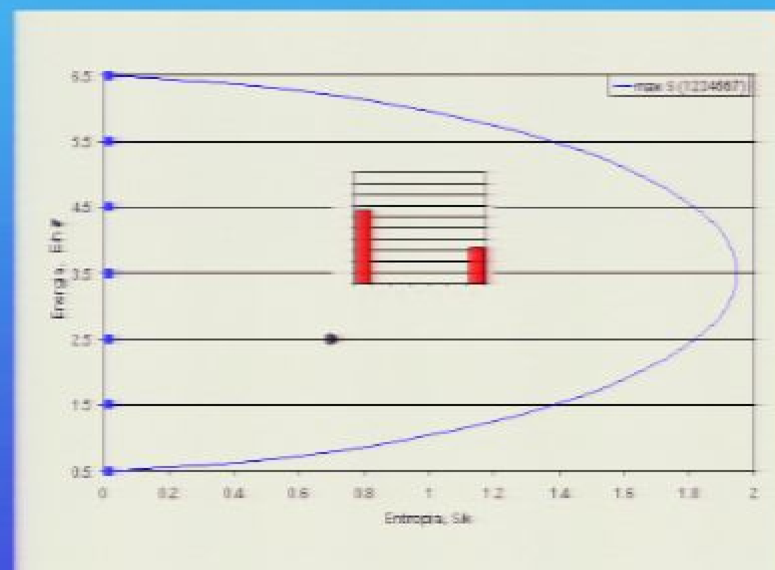
$$\frac{d\langle \Pi \rangle_t}{dt} = w_1 \frac{d\langle \Pi_1^o \rangle_t}{dt} + w_2 \frac{d\langle \Pi_2^o \rangle_t}{dt}$$

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

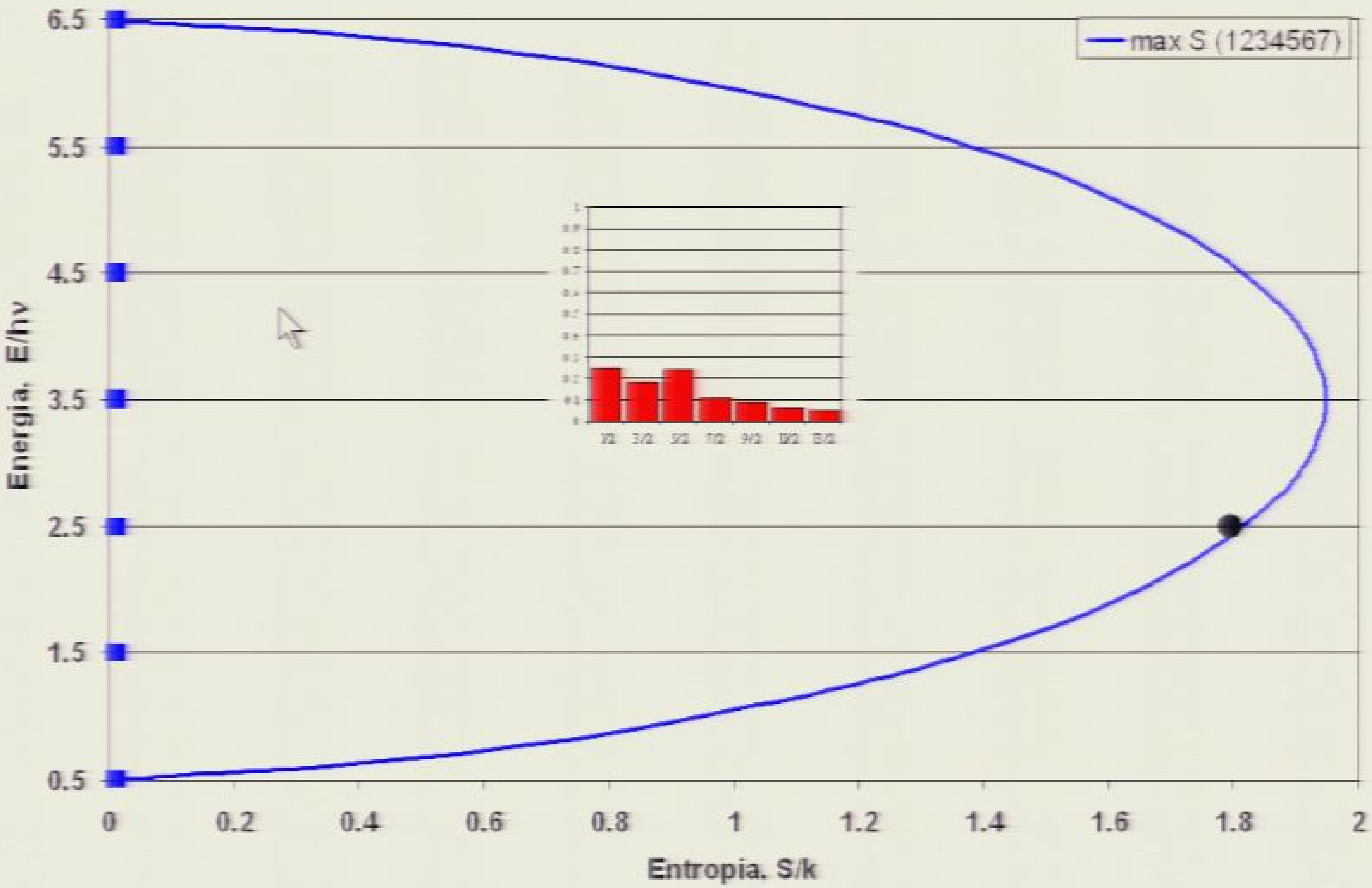
Giving an "ontic" status to irreversibility



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 ?



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 acecssible to the particle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Energia, E/hv
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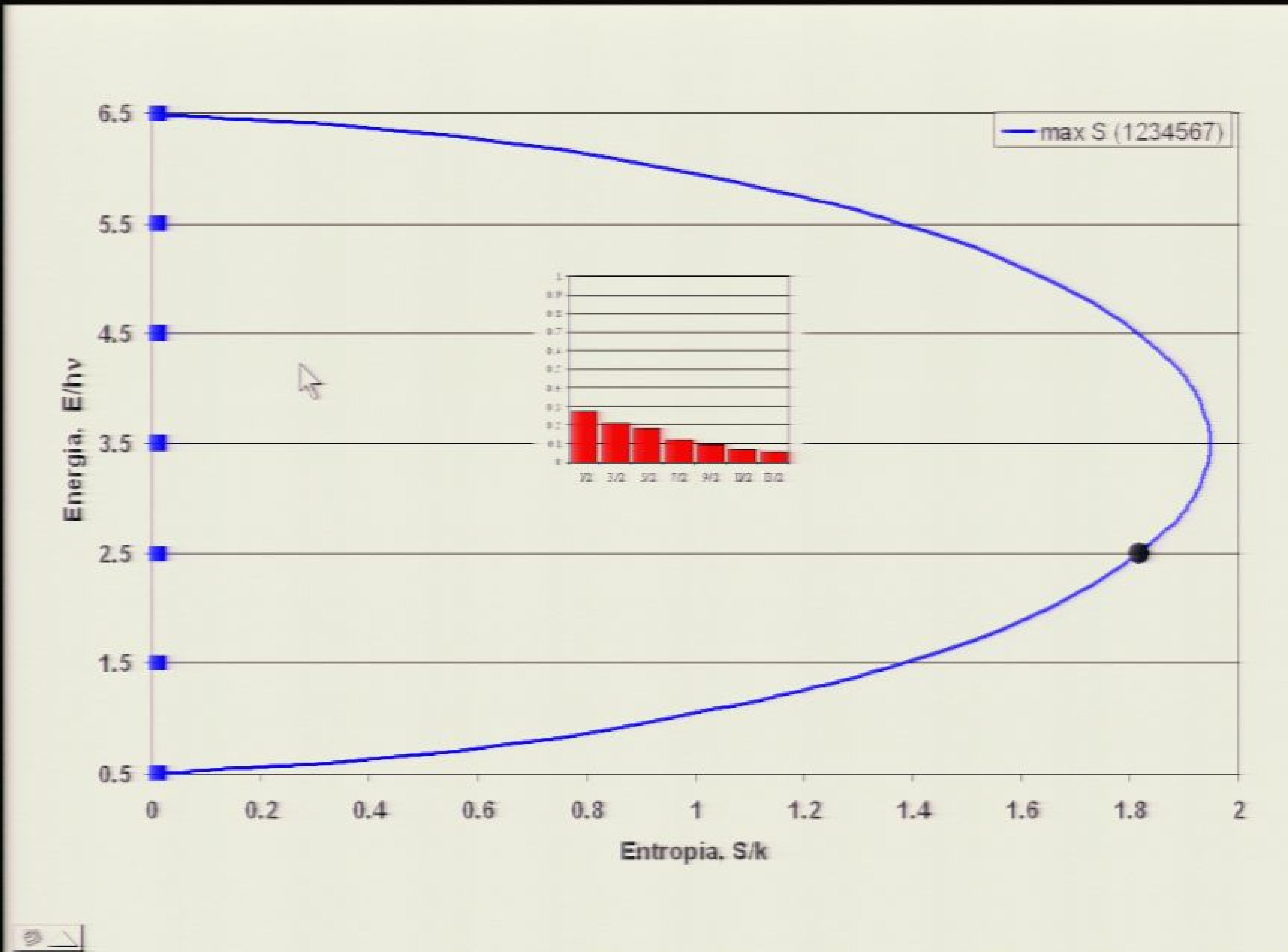
Entropia, S/k



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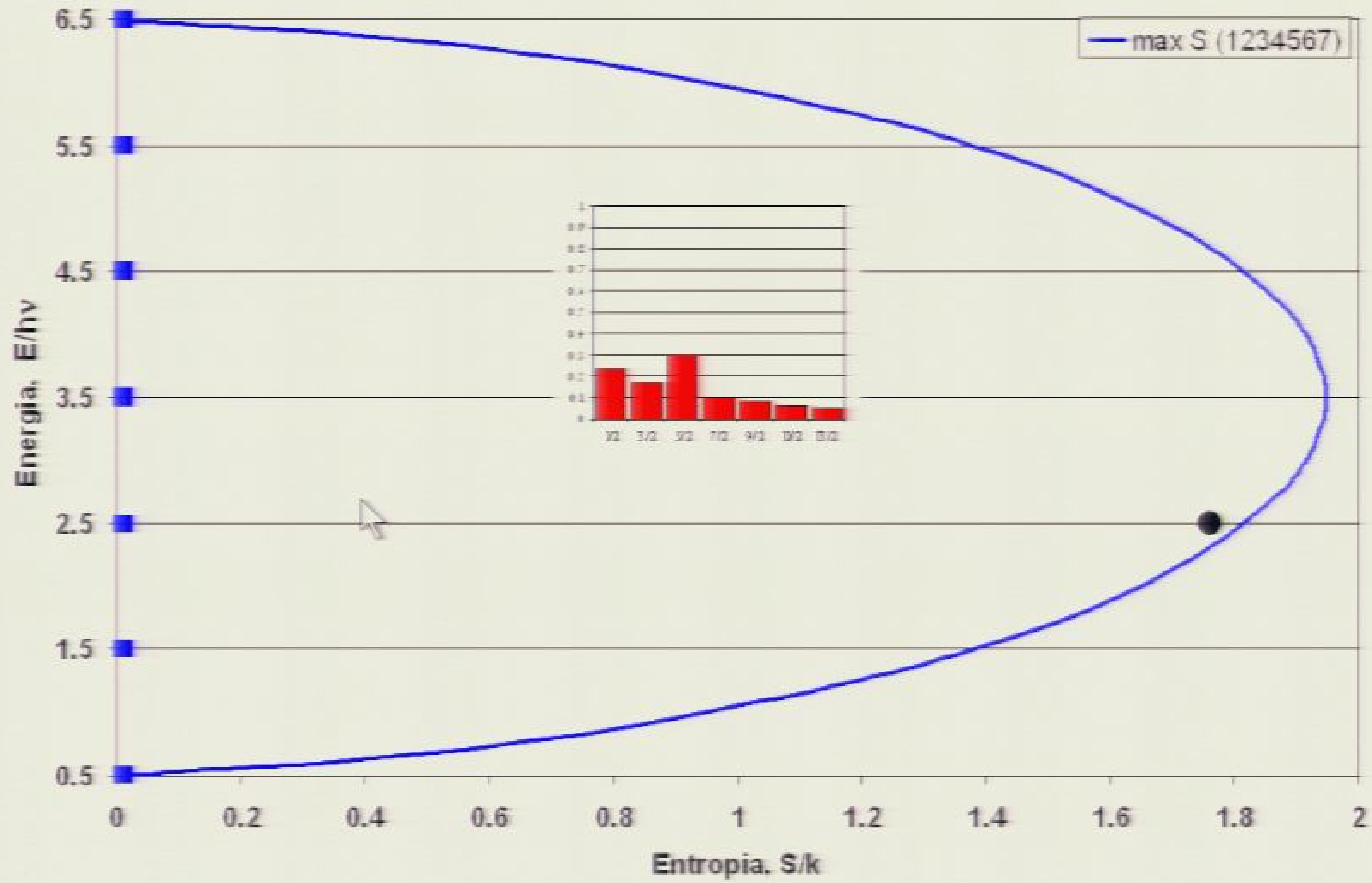
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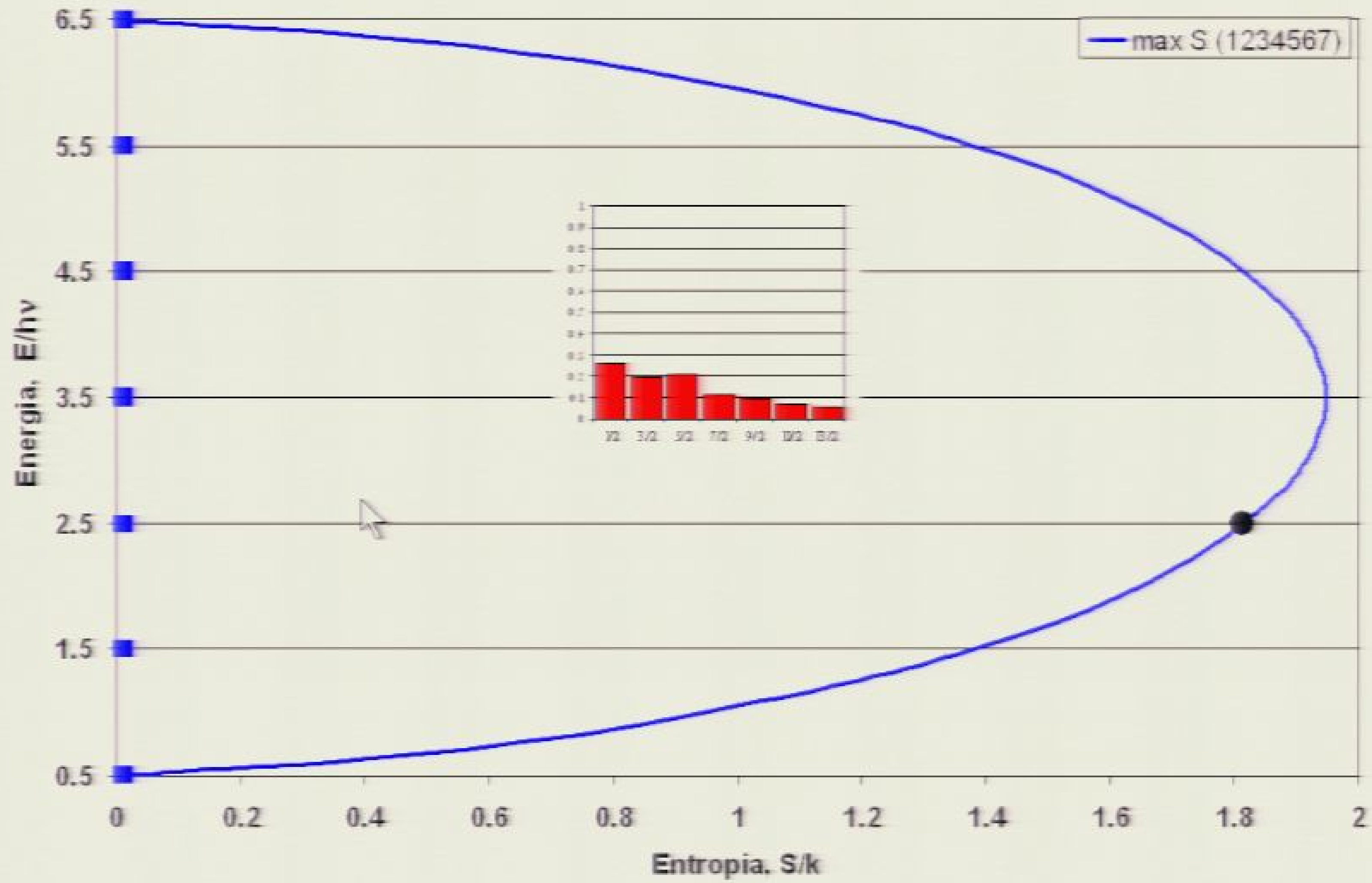
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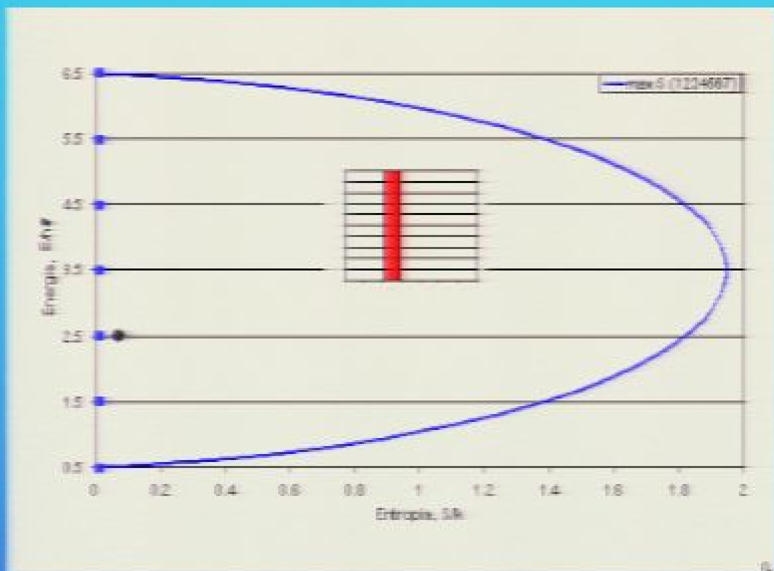

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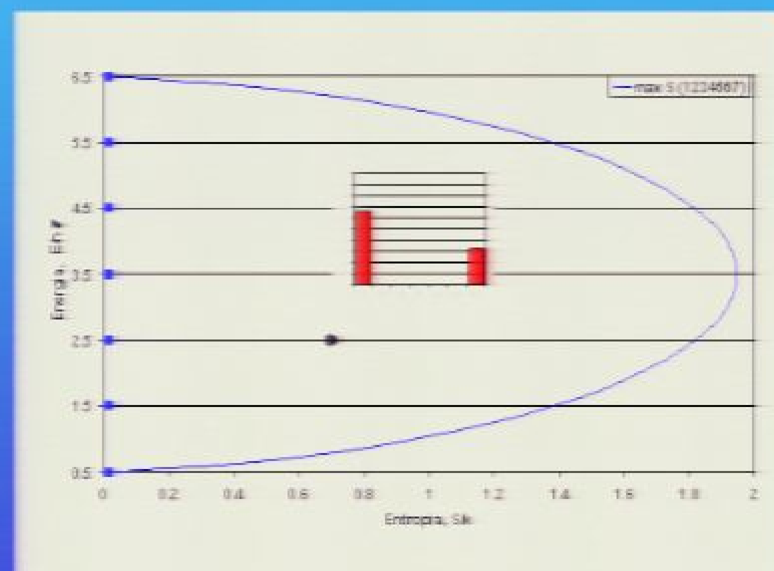

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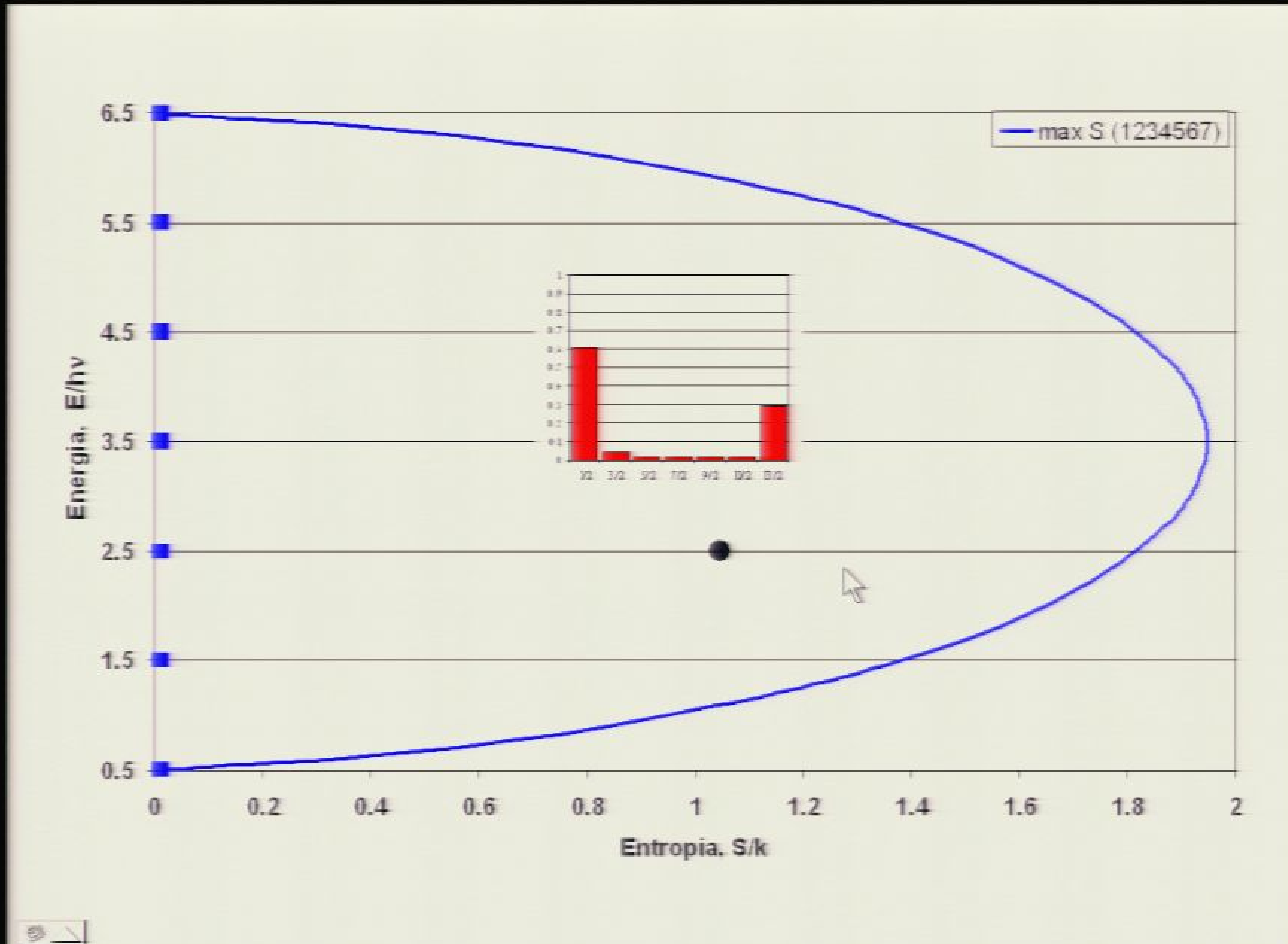
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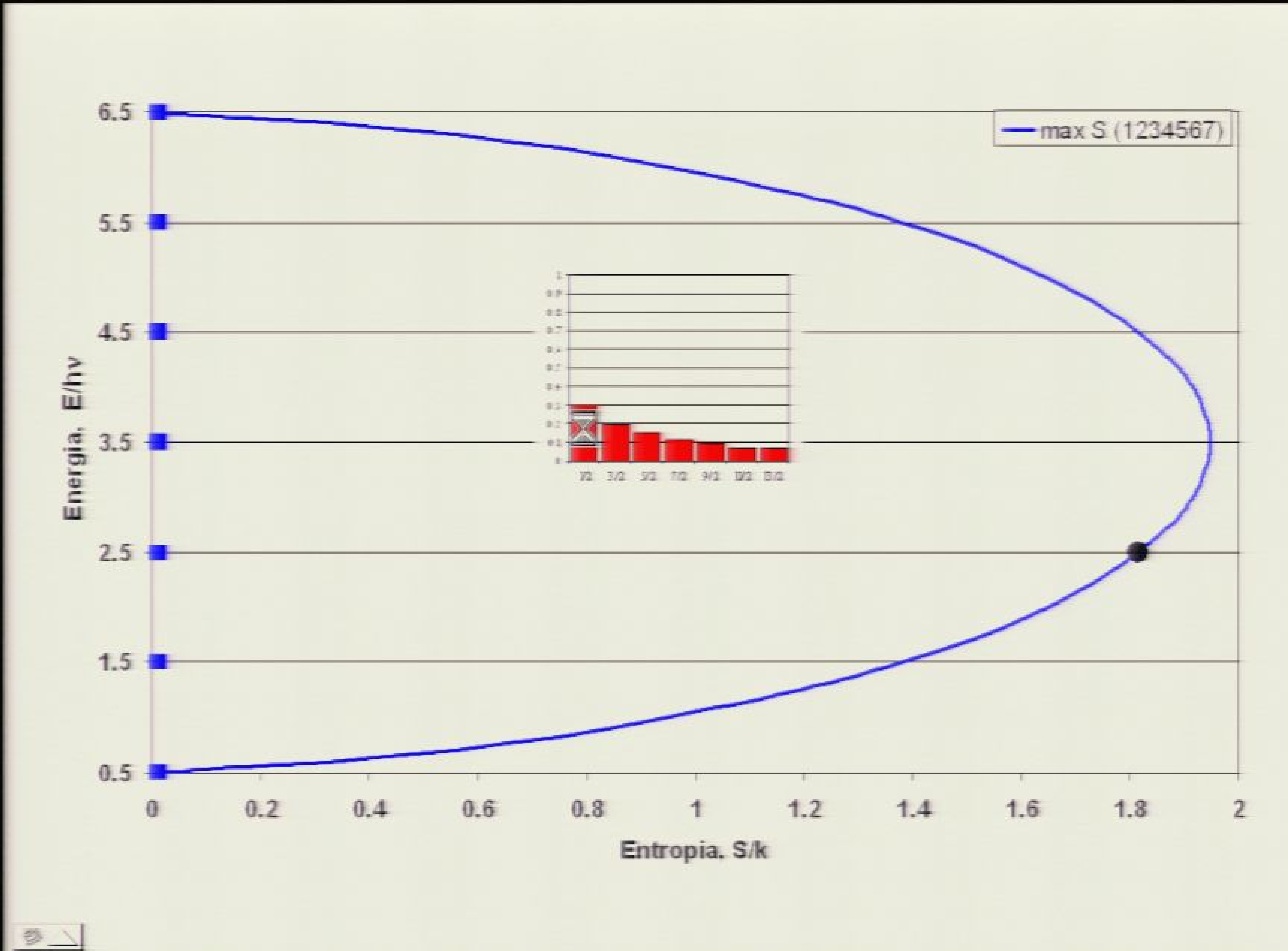
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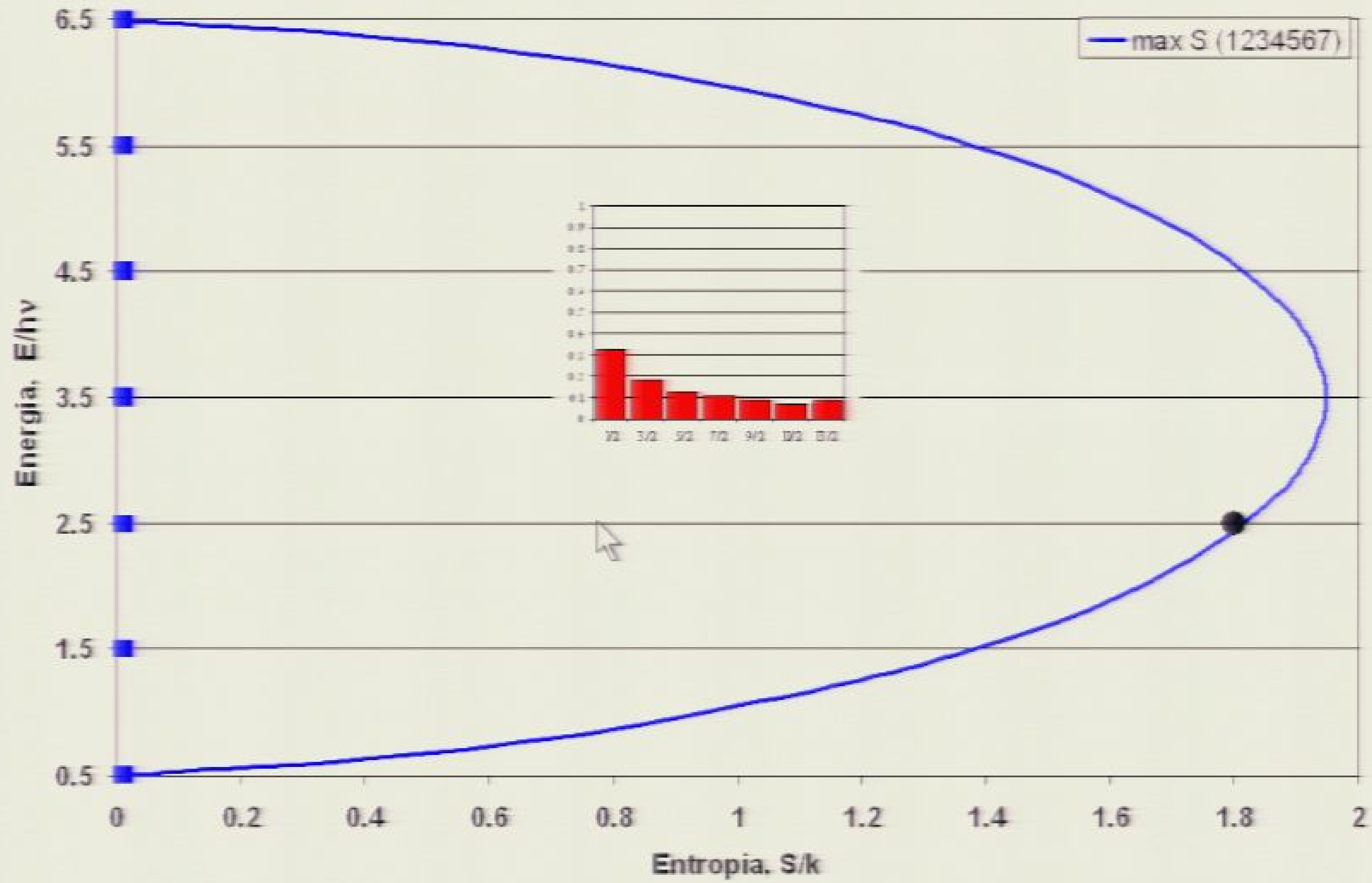
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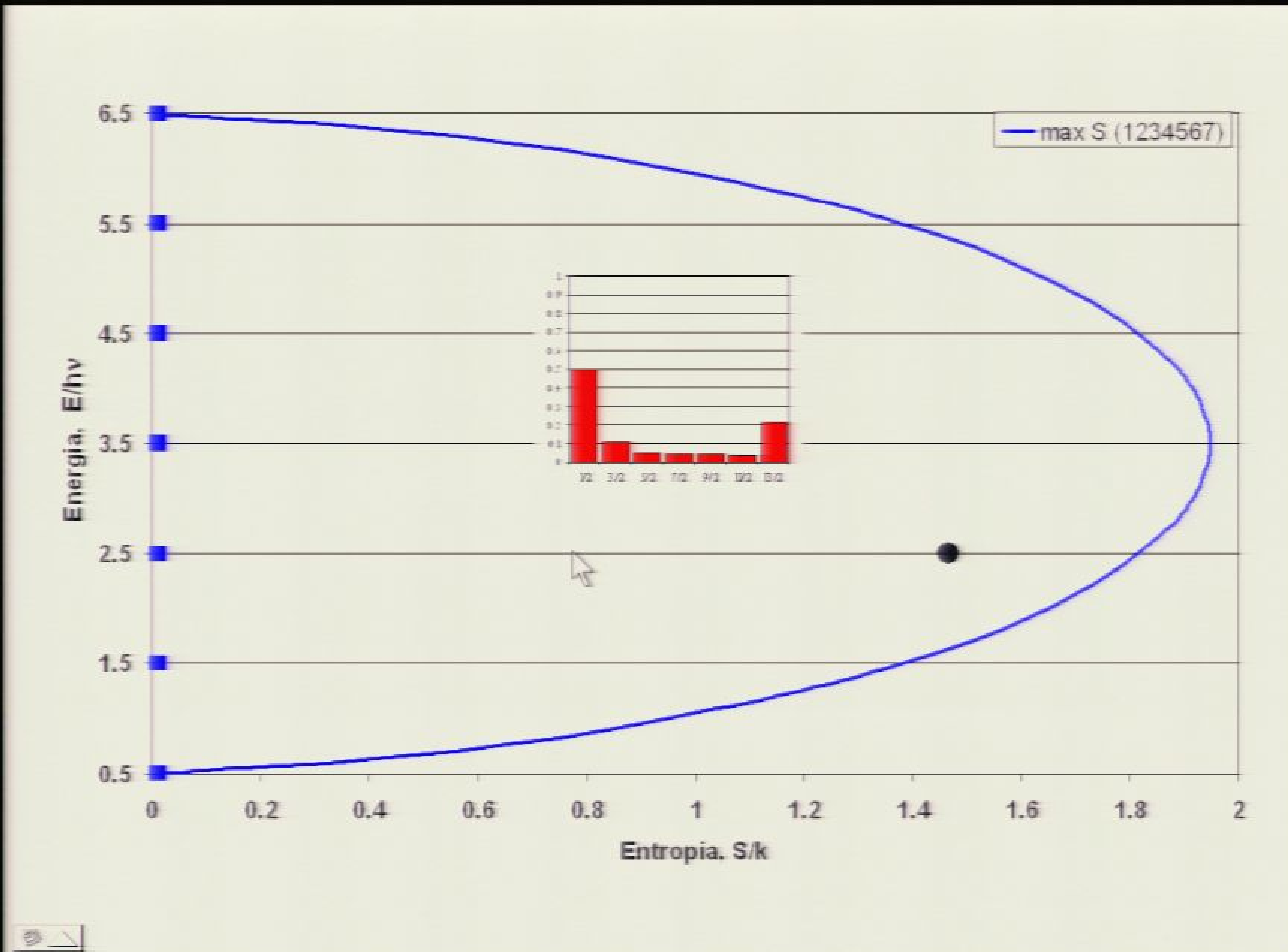
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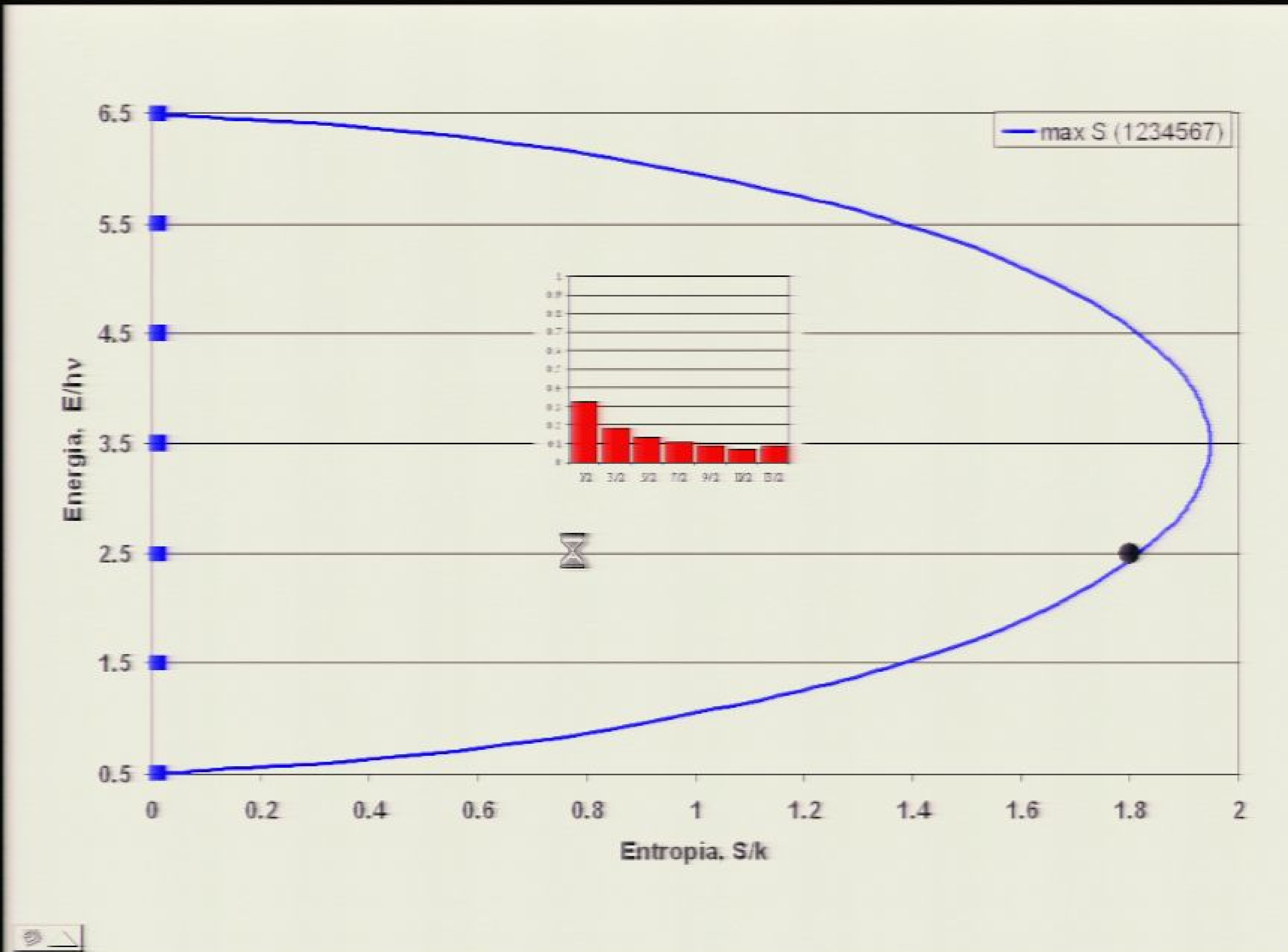
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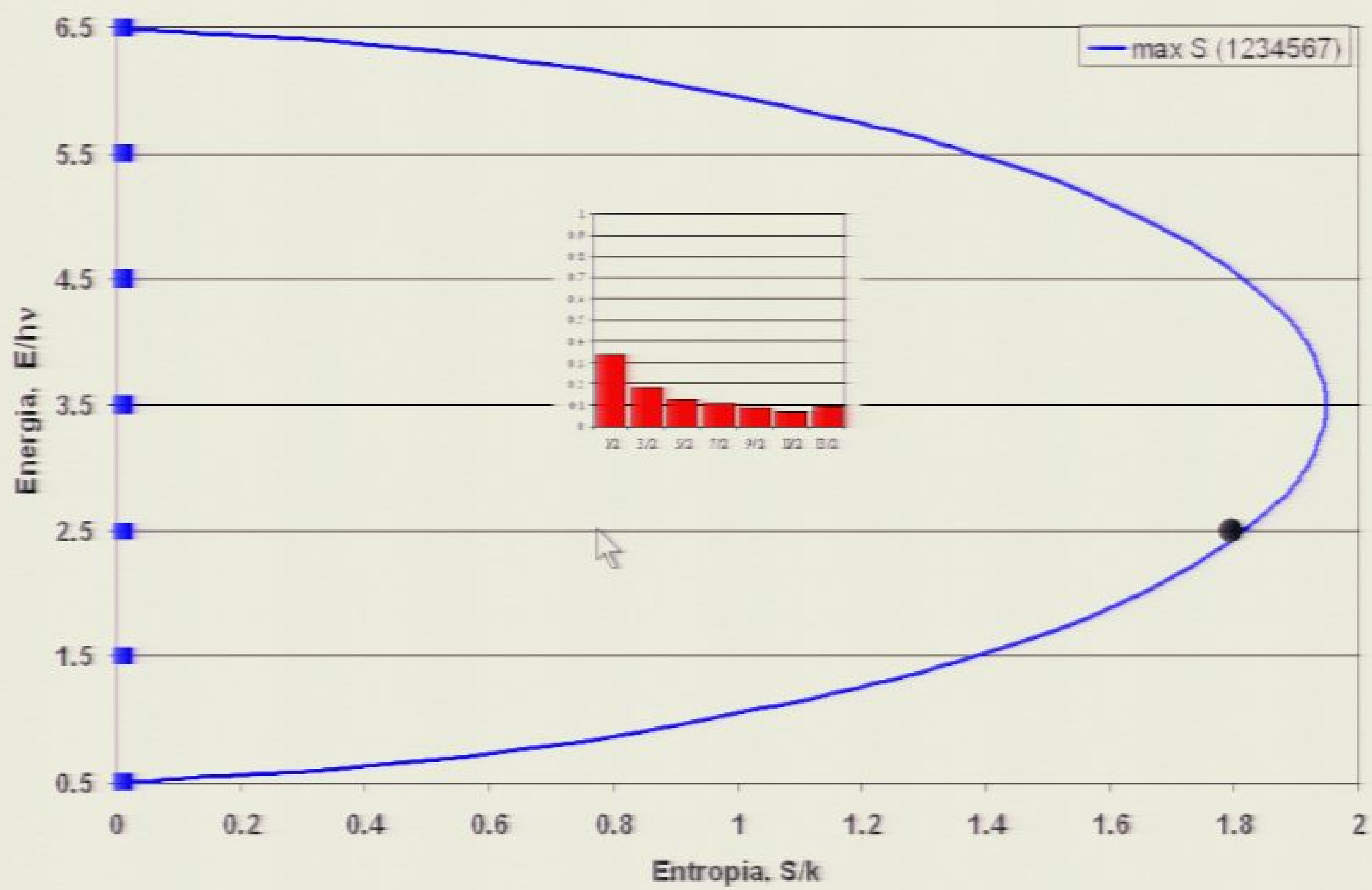

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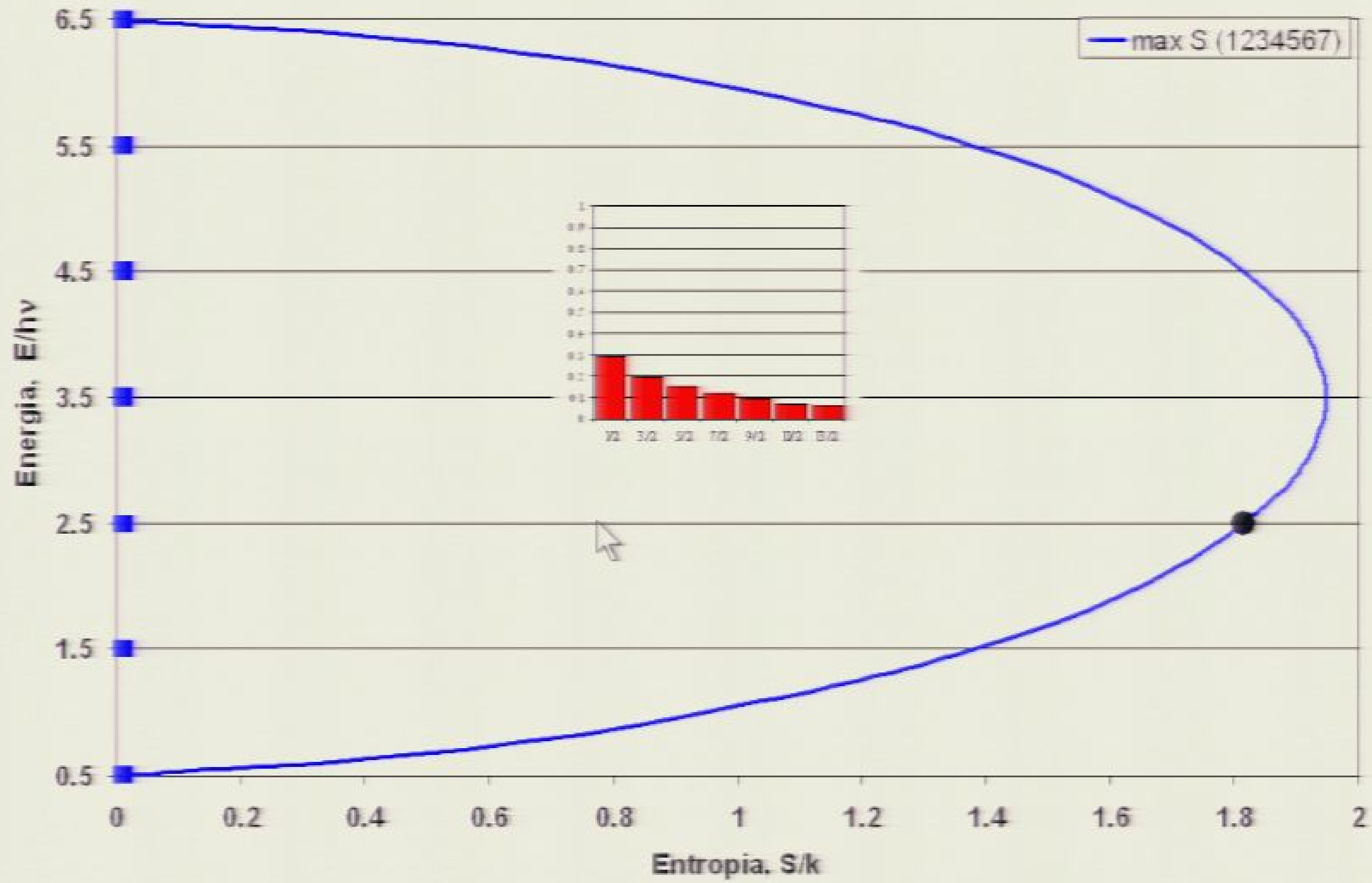
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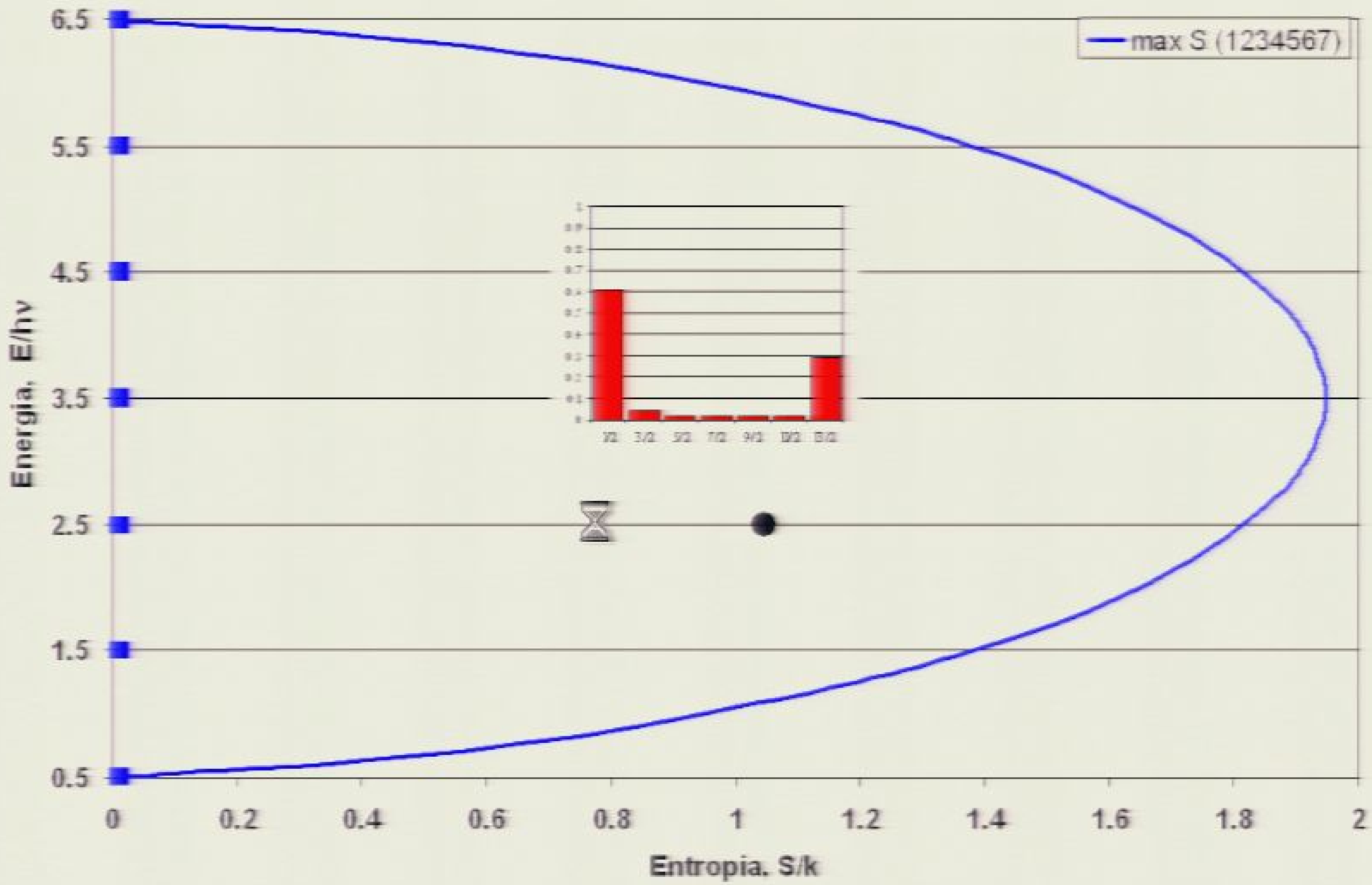
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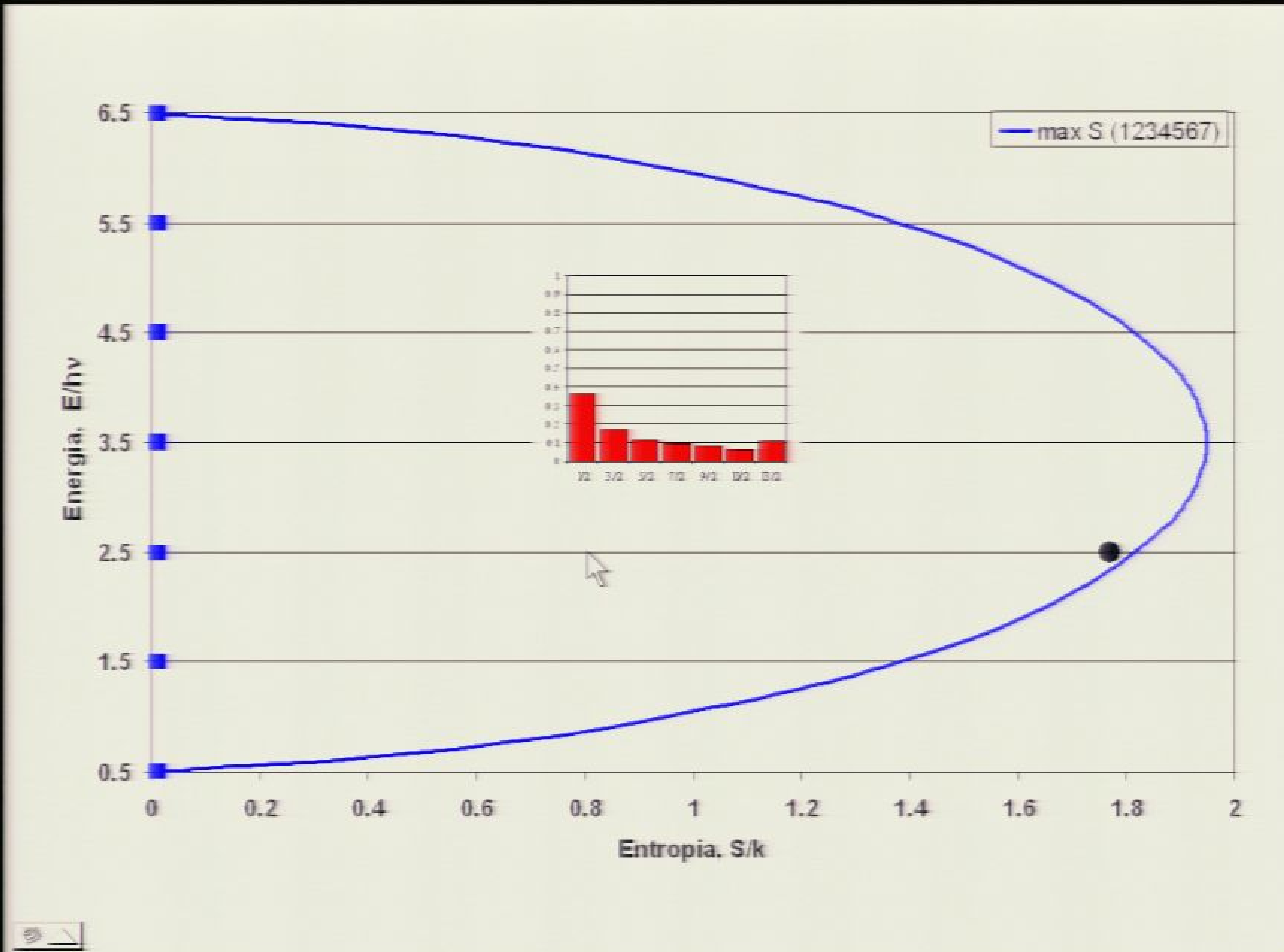
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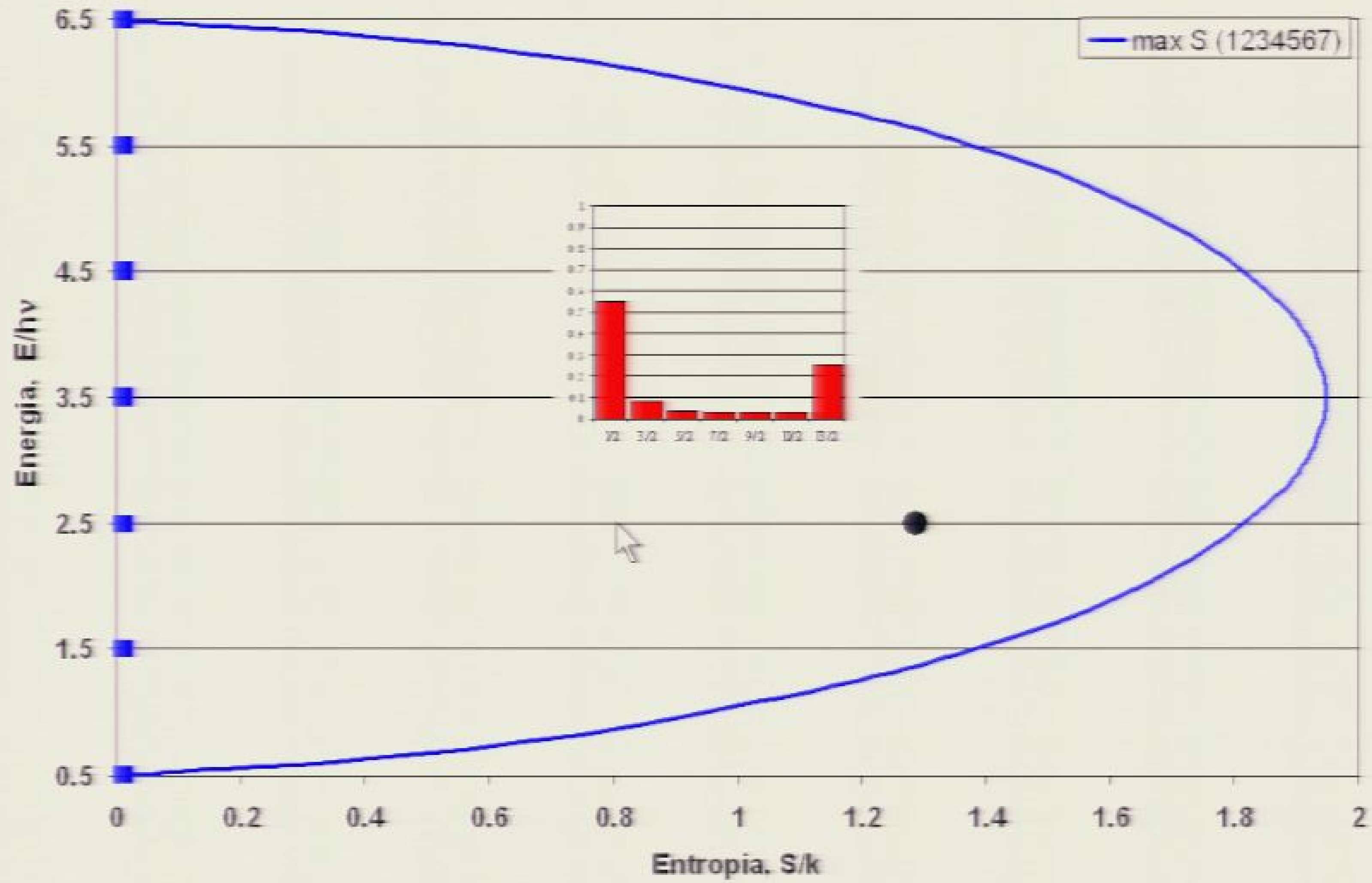
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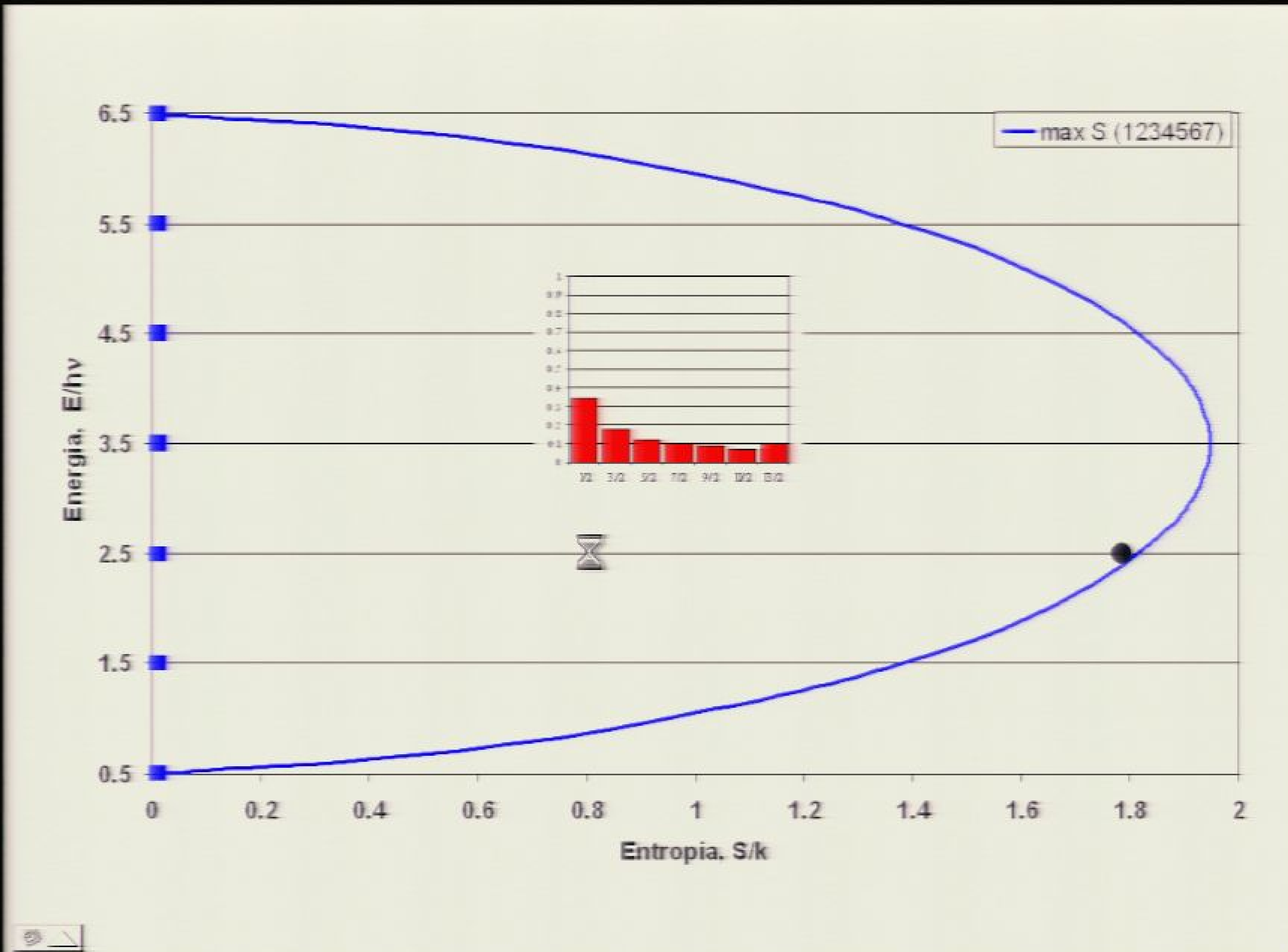
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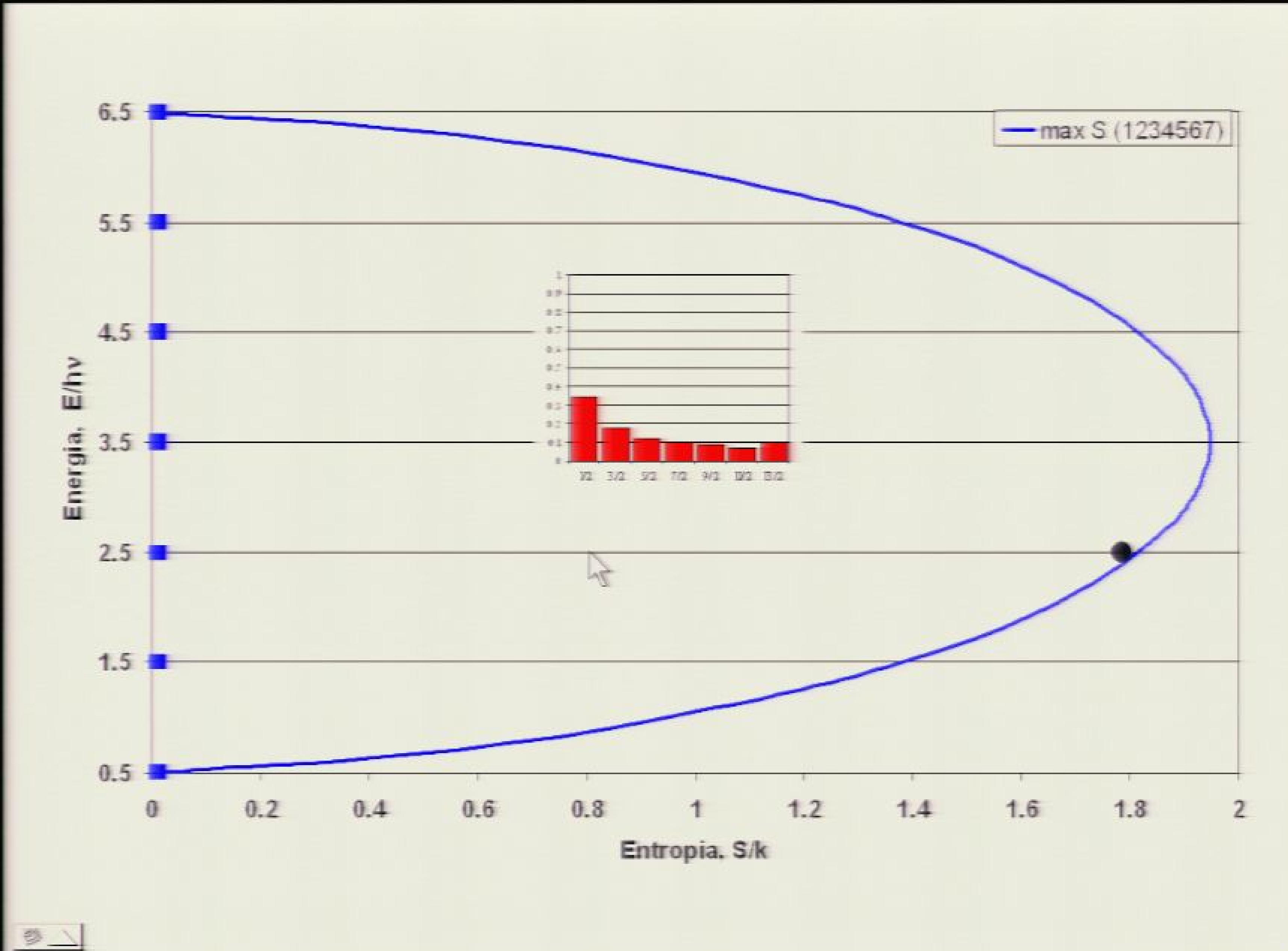

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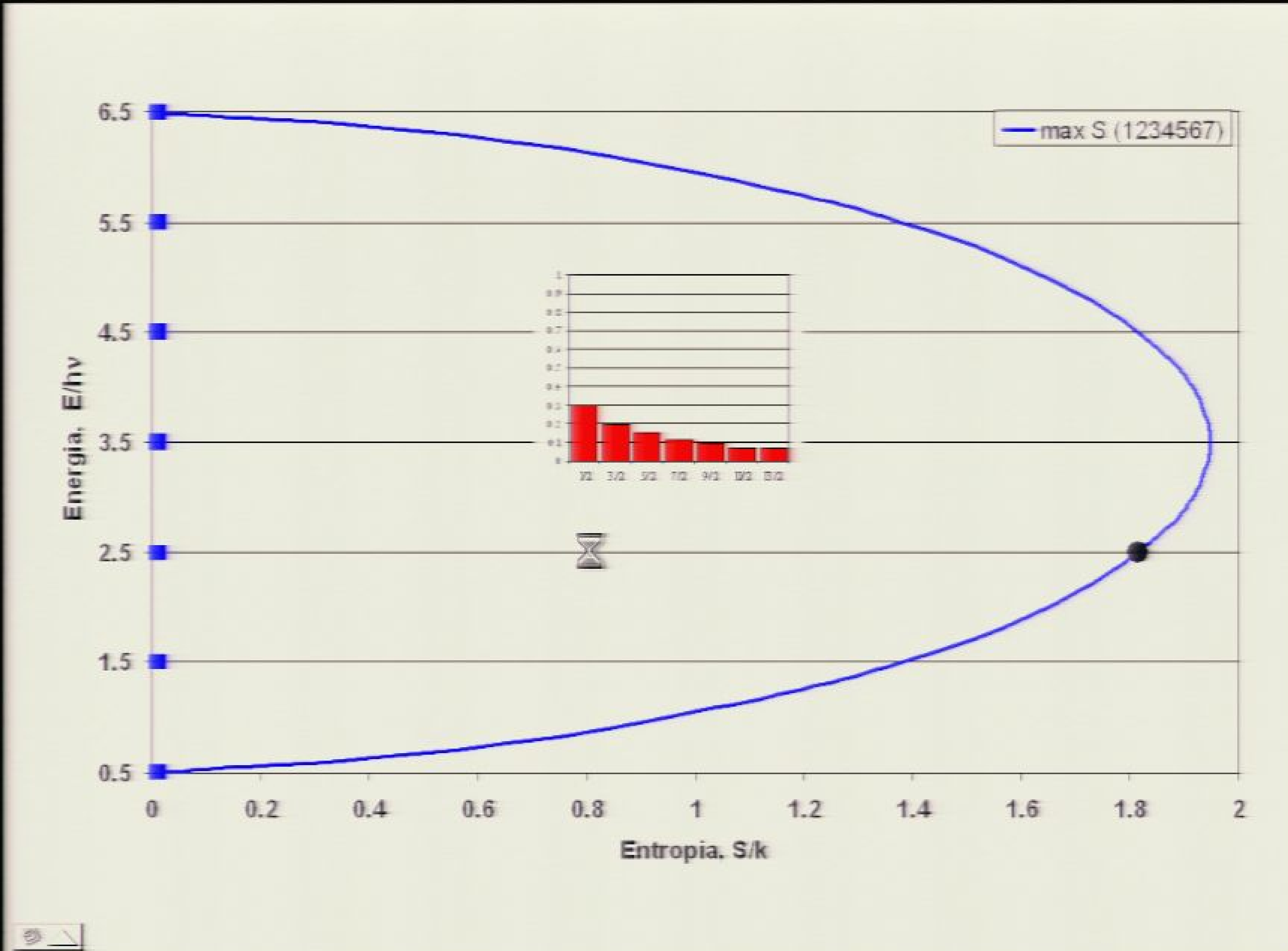
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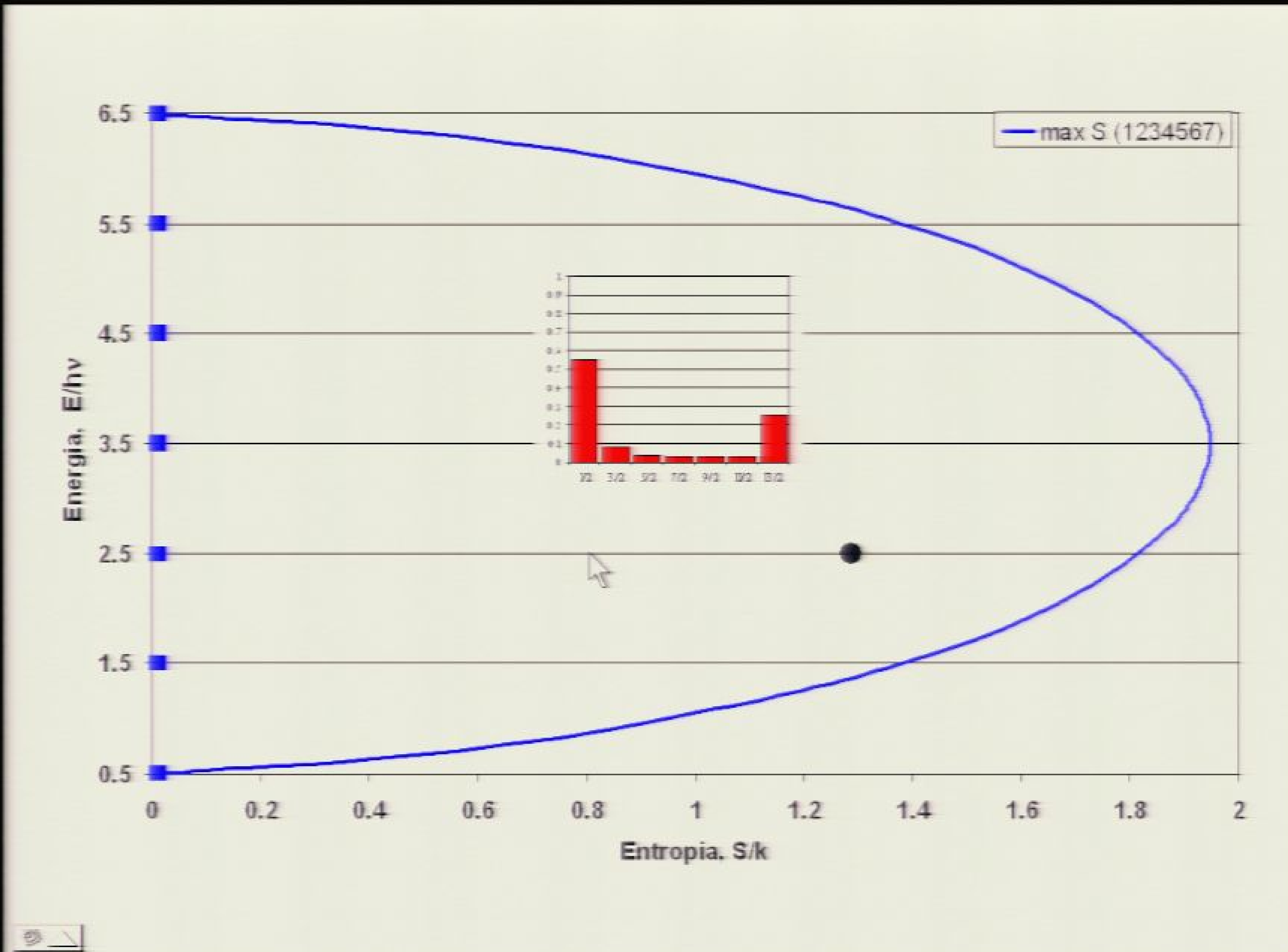

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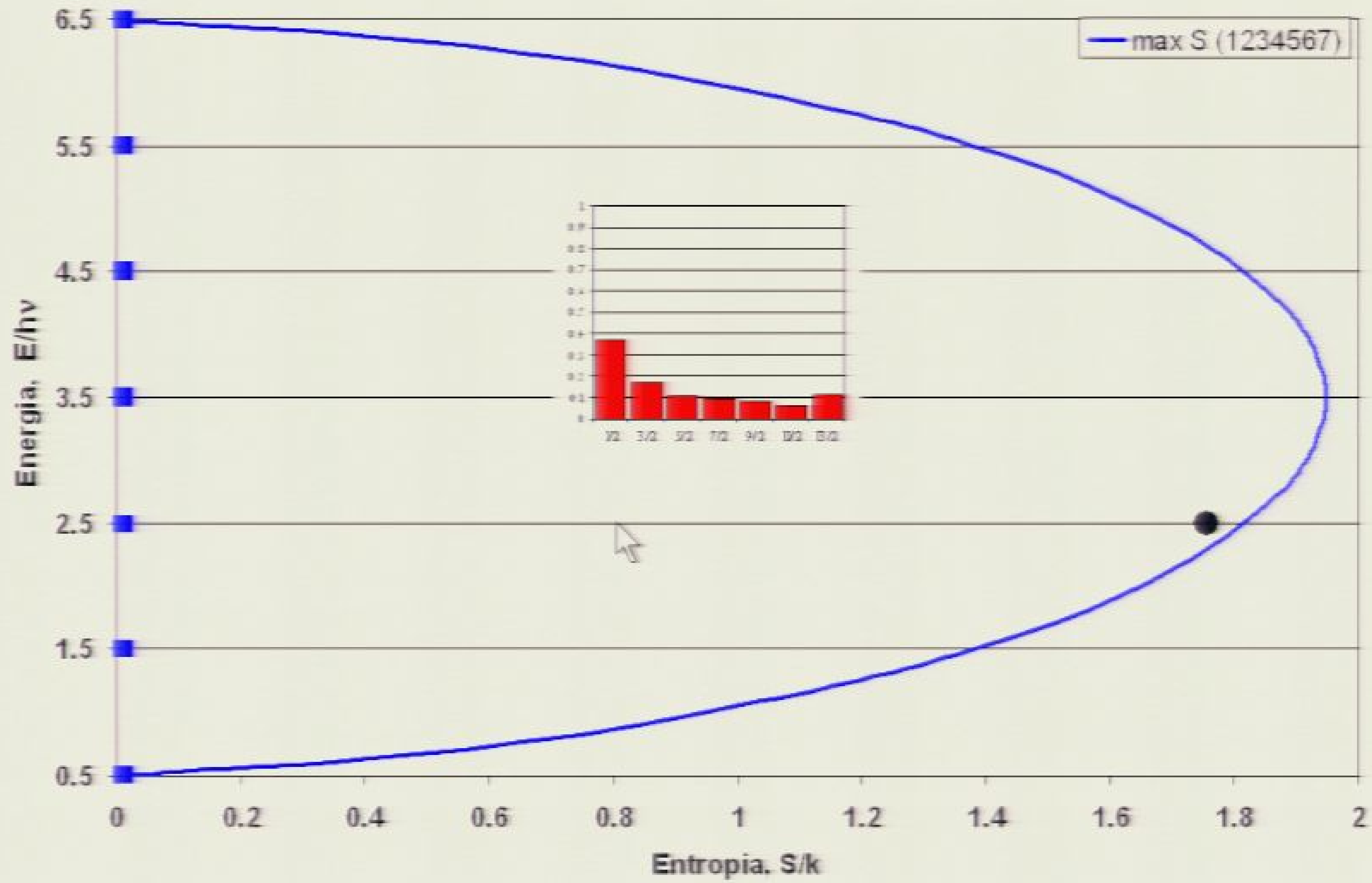
Entropia, S/k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Energia, E/hv
Entropia, S/k
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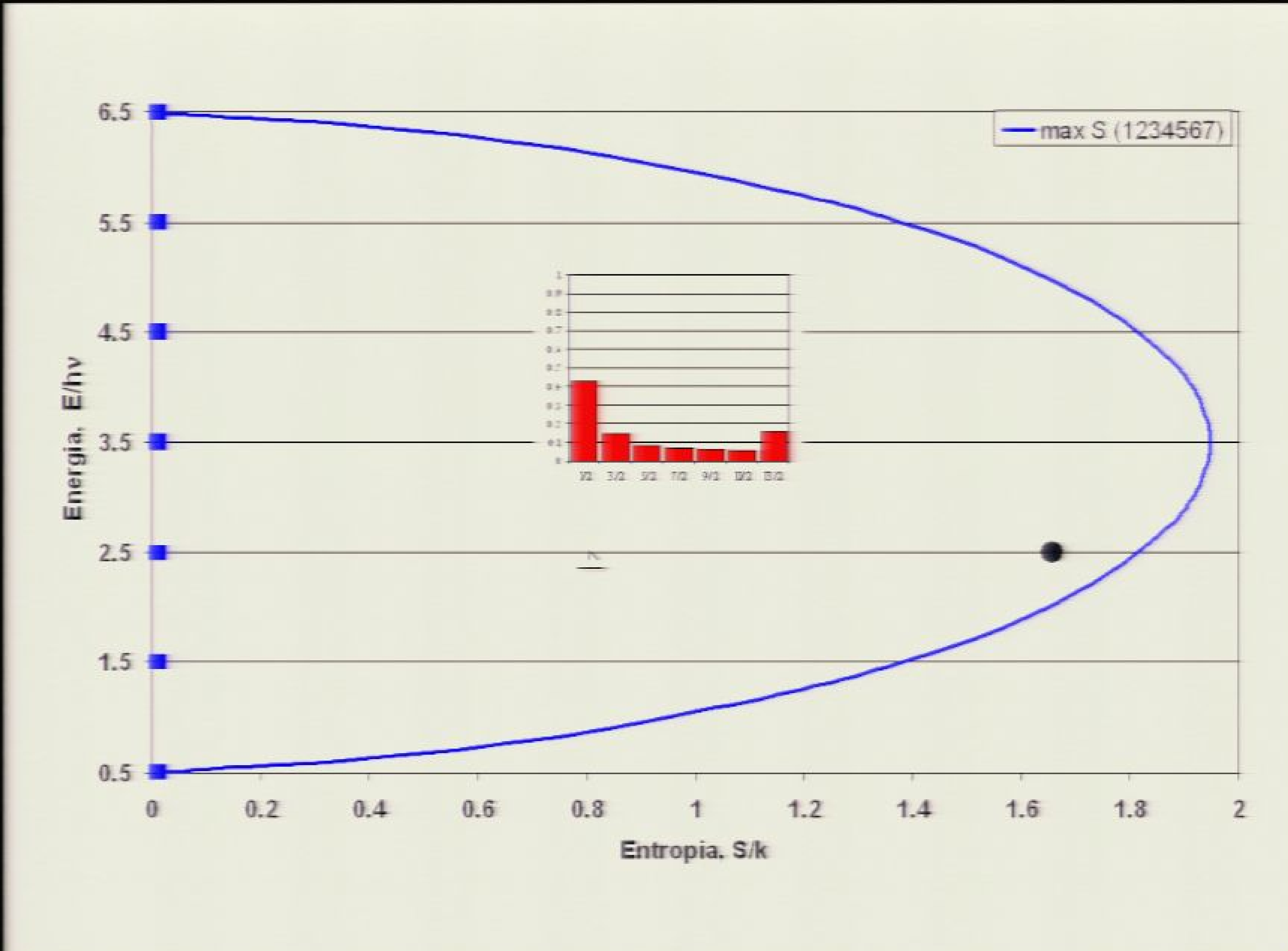

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6.5
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2.5
1.5
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Energia, E/hν
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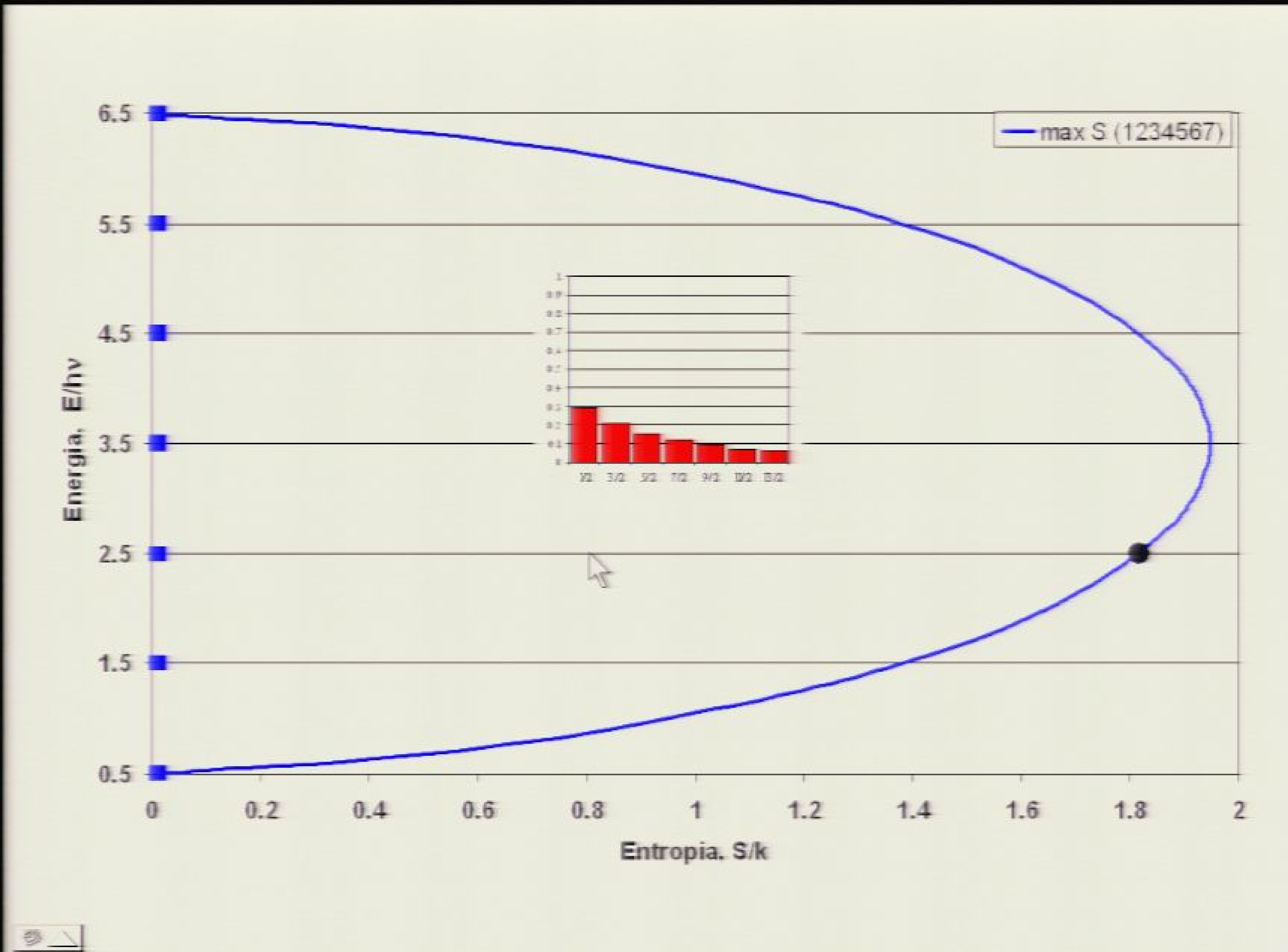
2
Entropia, S/k



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Energia, E/hv
Entropia, S/k
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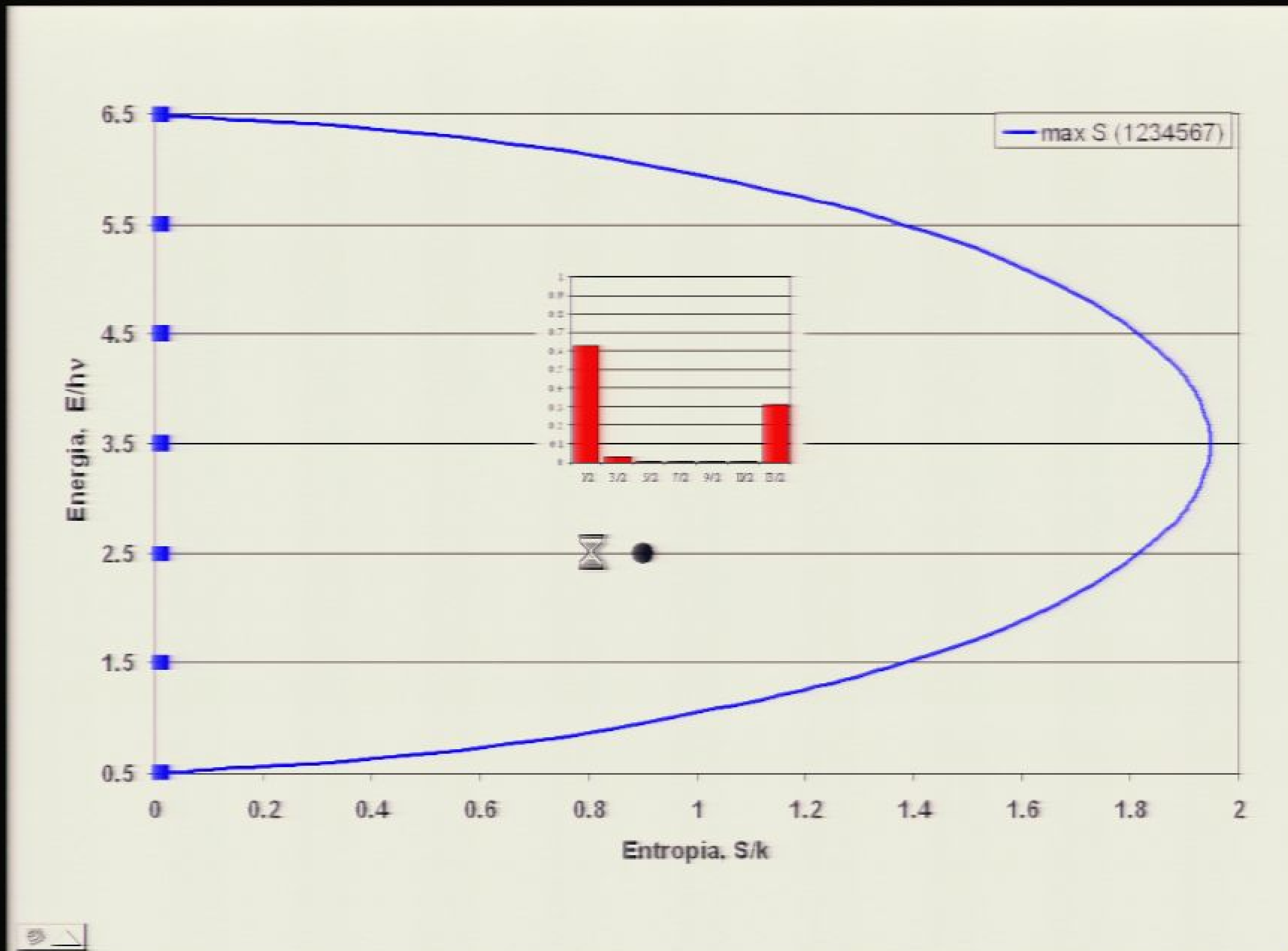
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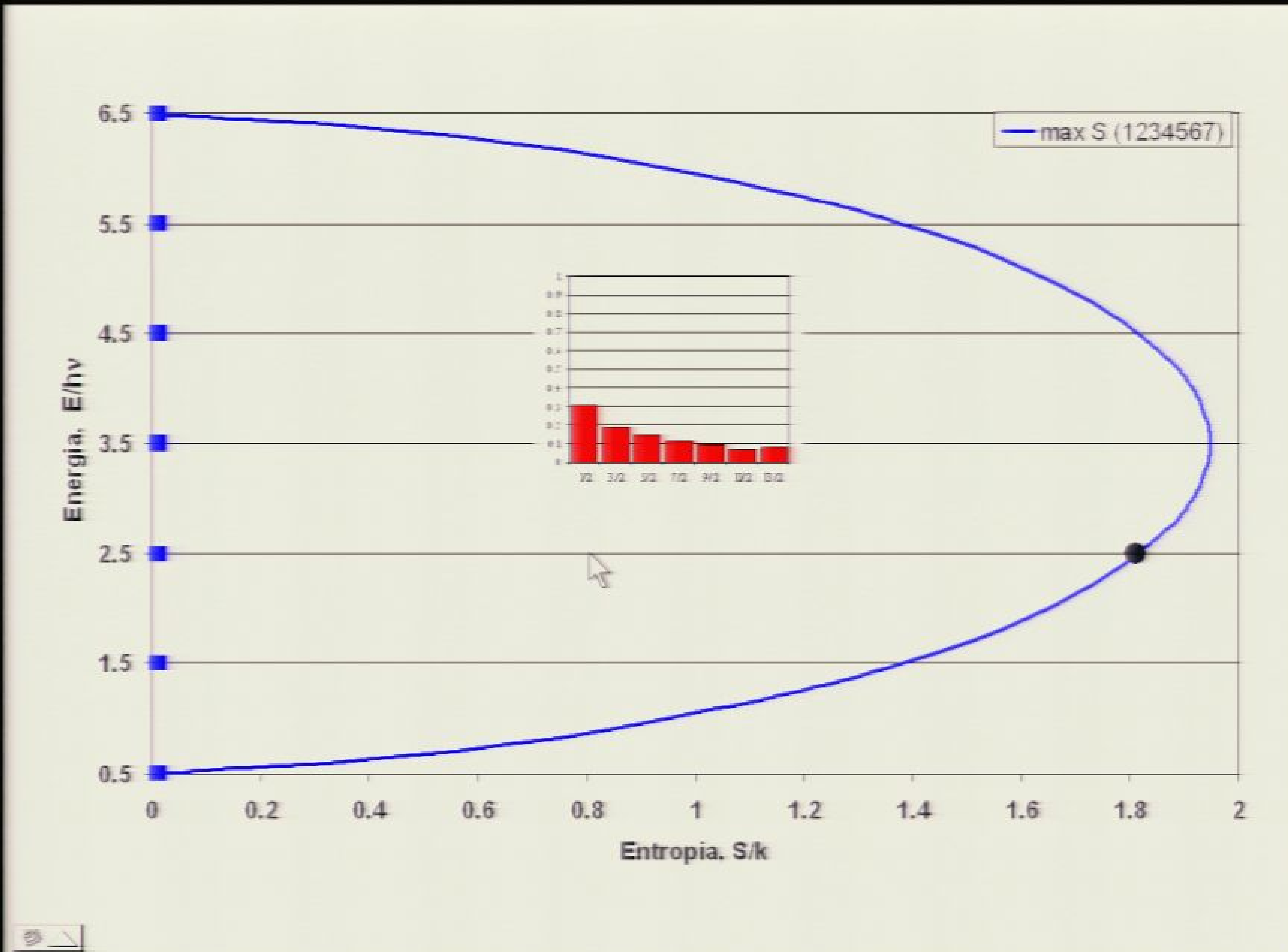
Entropia, S/k



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Energia. E/hν
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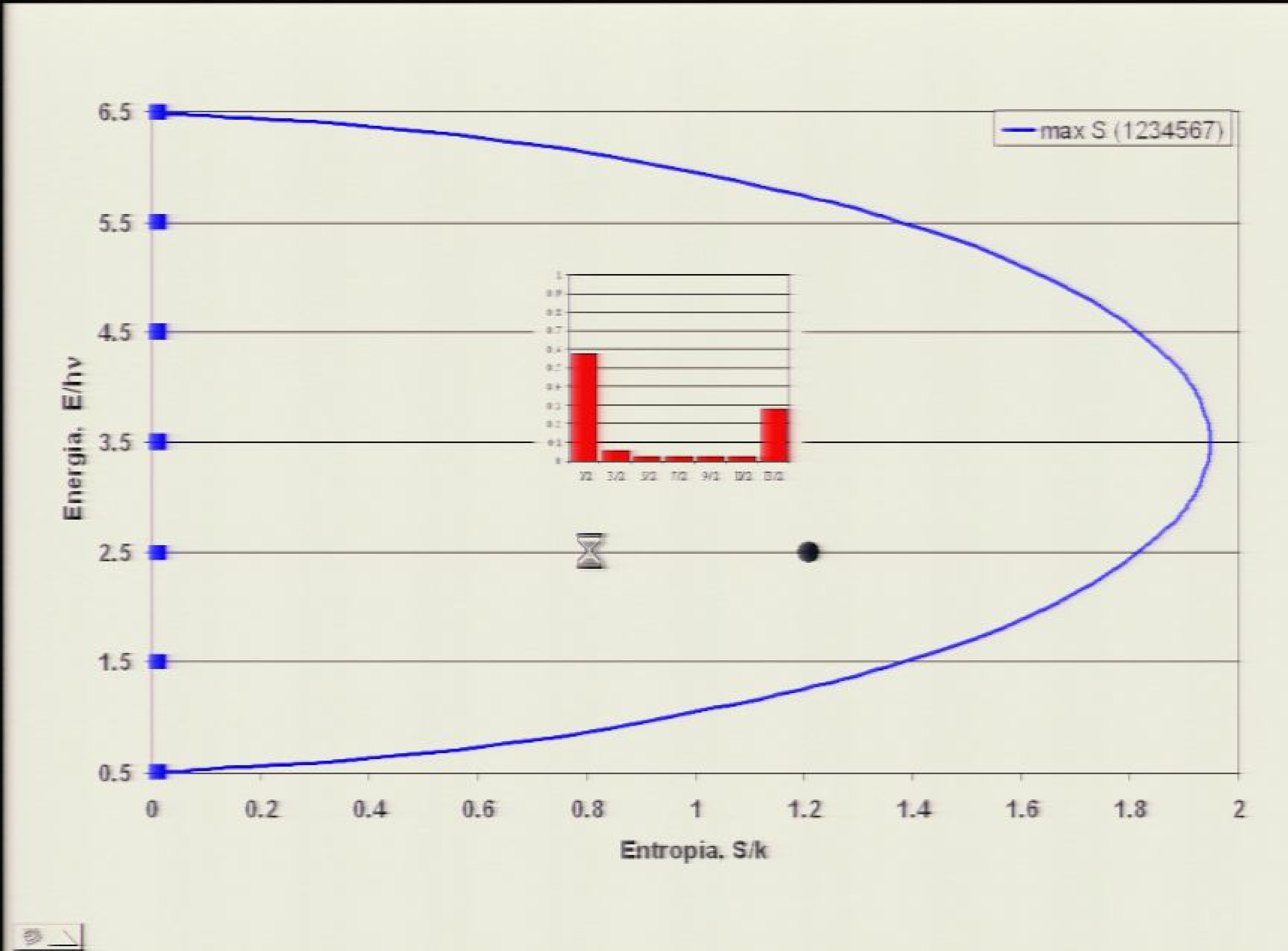
Entropia. S/k



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Energia. E/hv
Entropia. S/k
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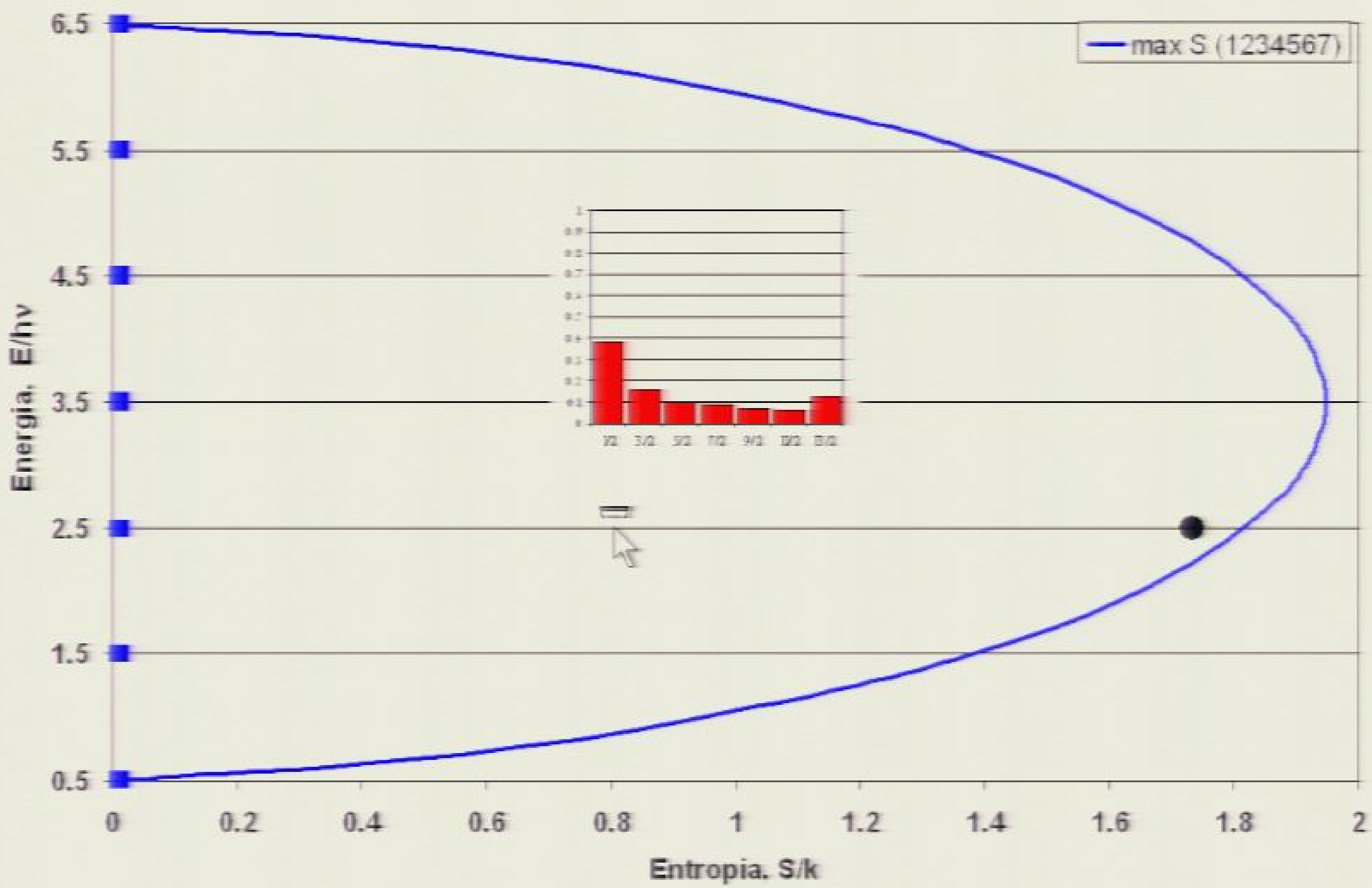
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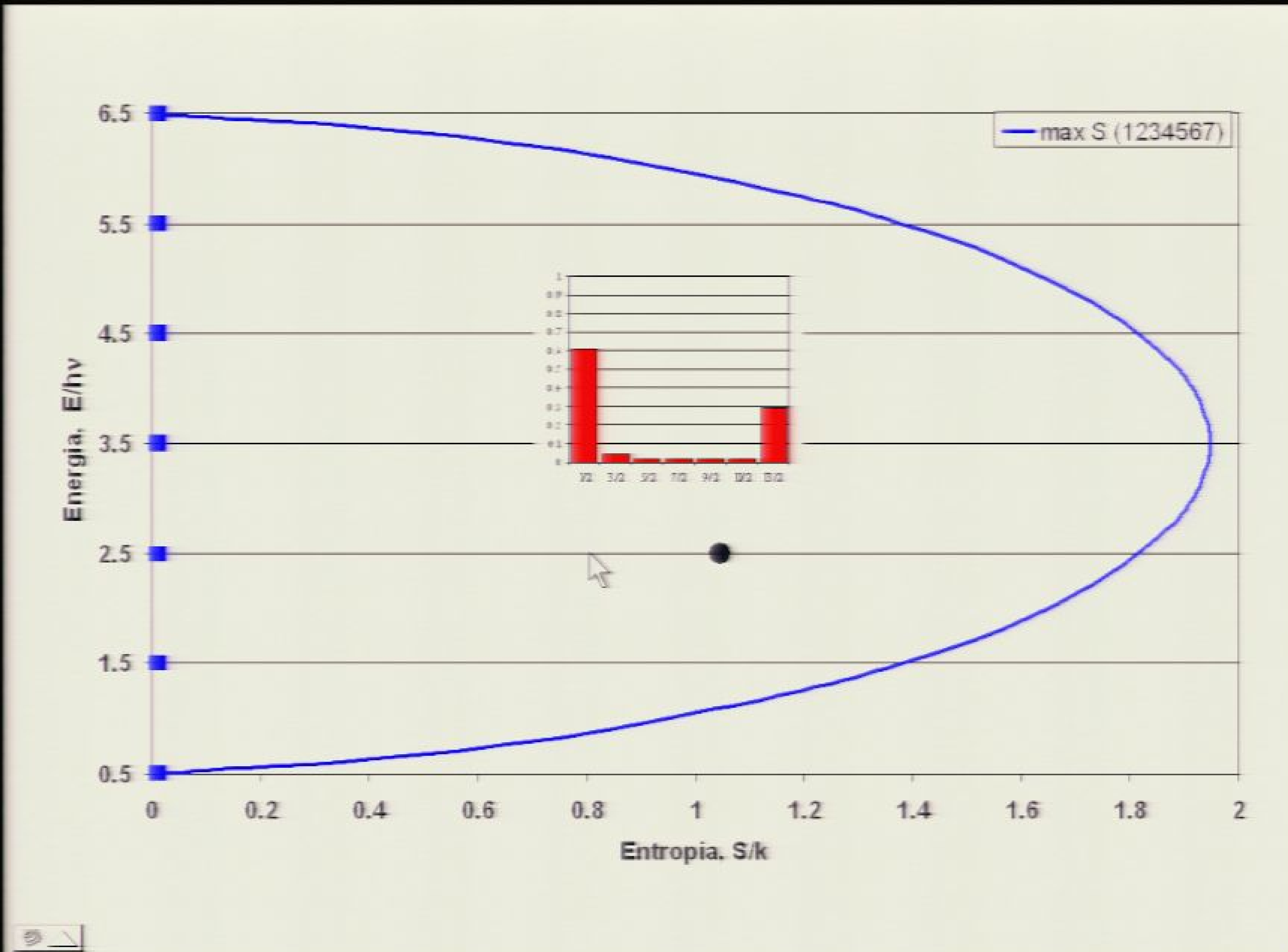
Entropia. S/k



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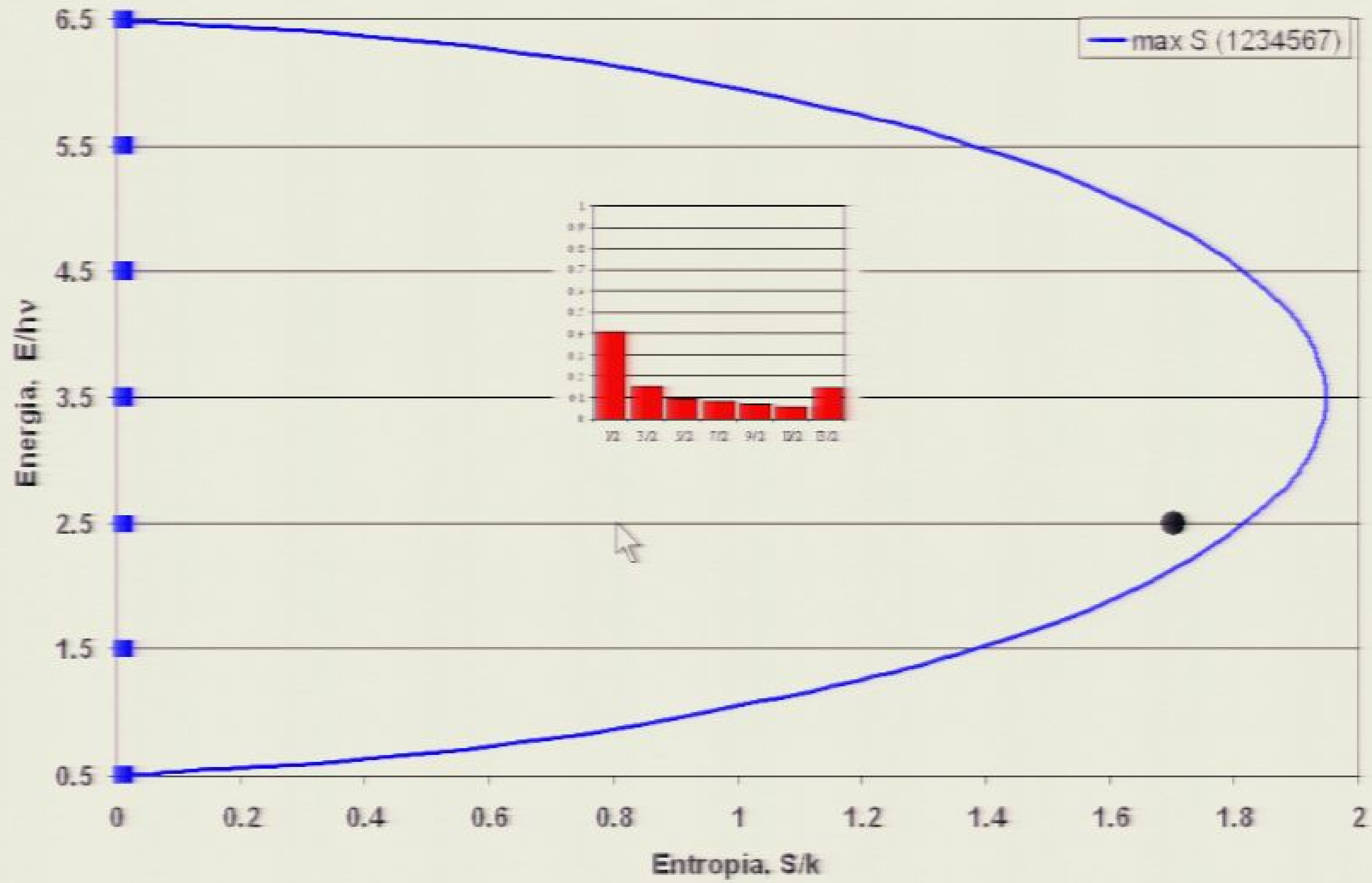
Entropia, S/k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Energia, E/hν
Entropia, S/k
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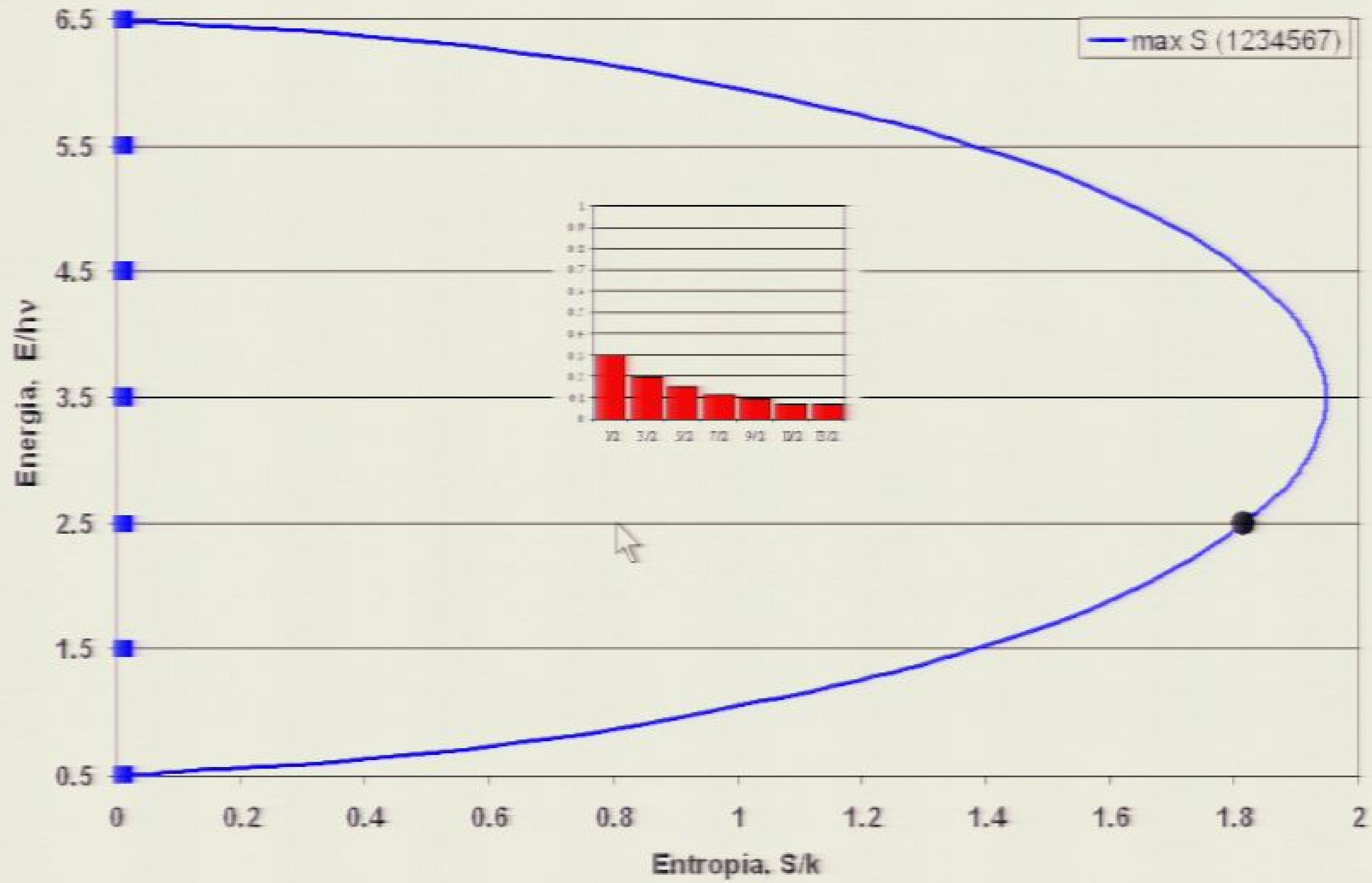
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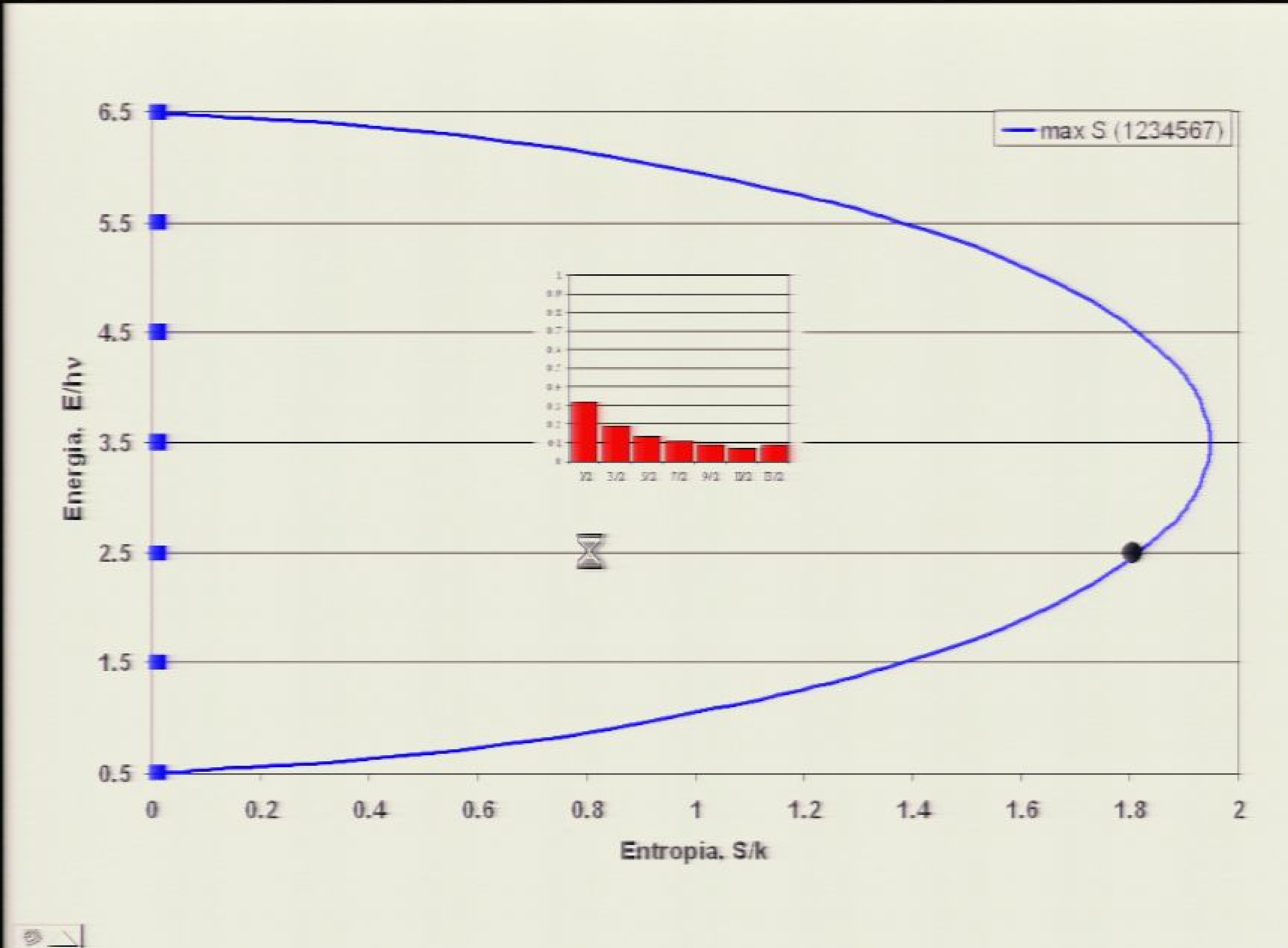
Entropia, S/k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Energia. E/hv
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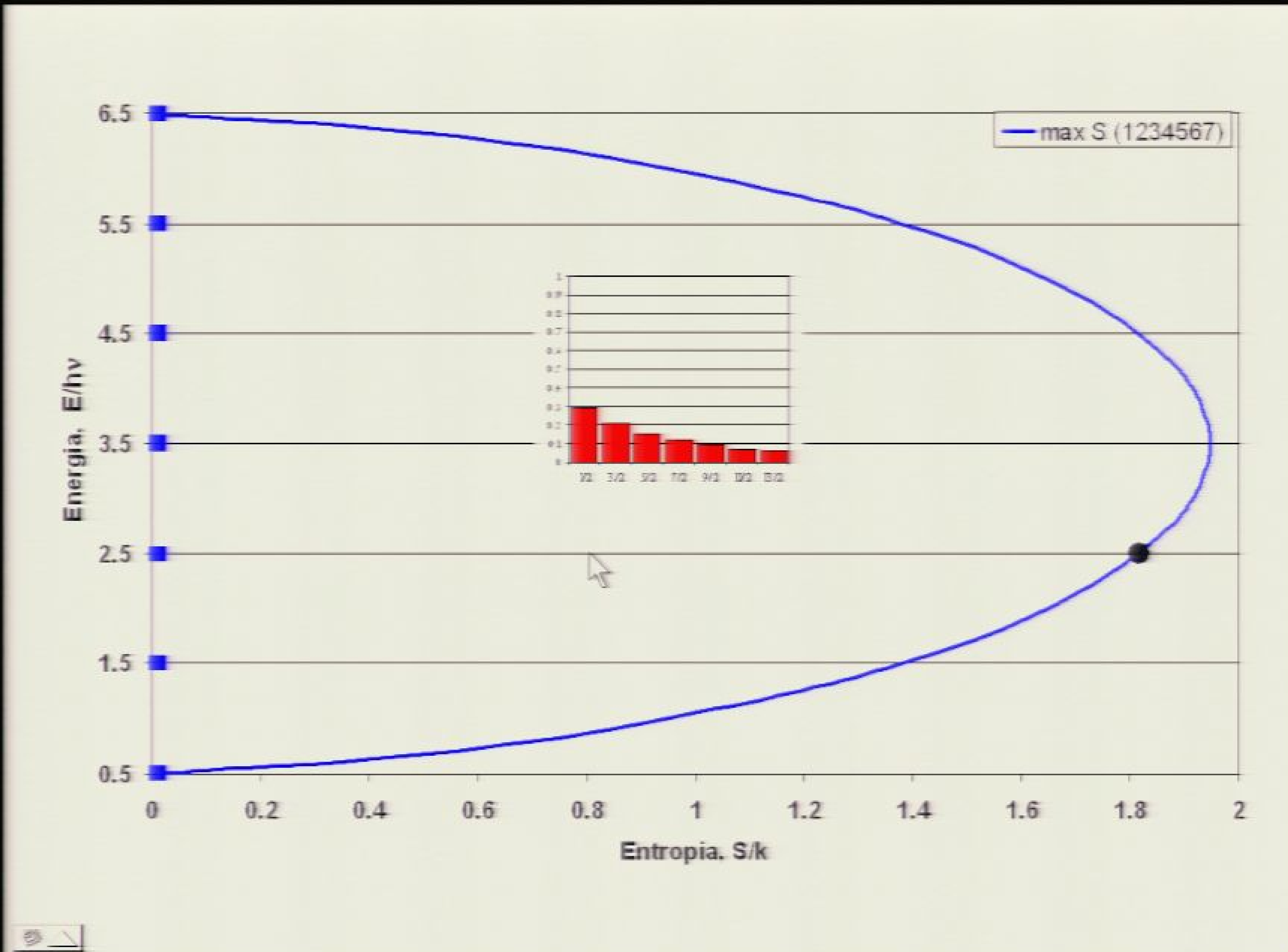
Entropia. S/k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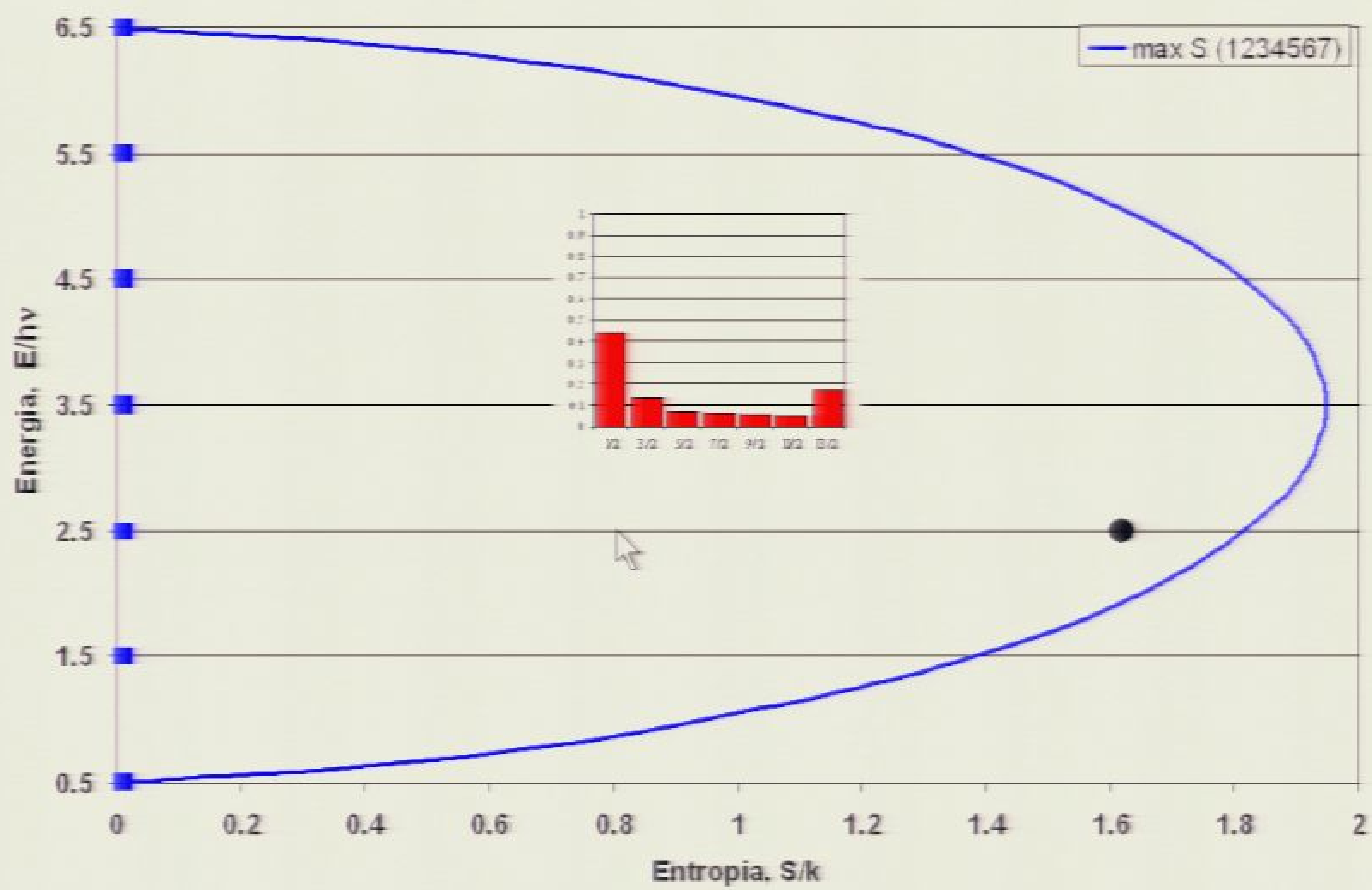
Entropia. S/k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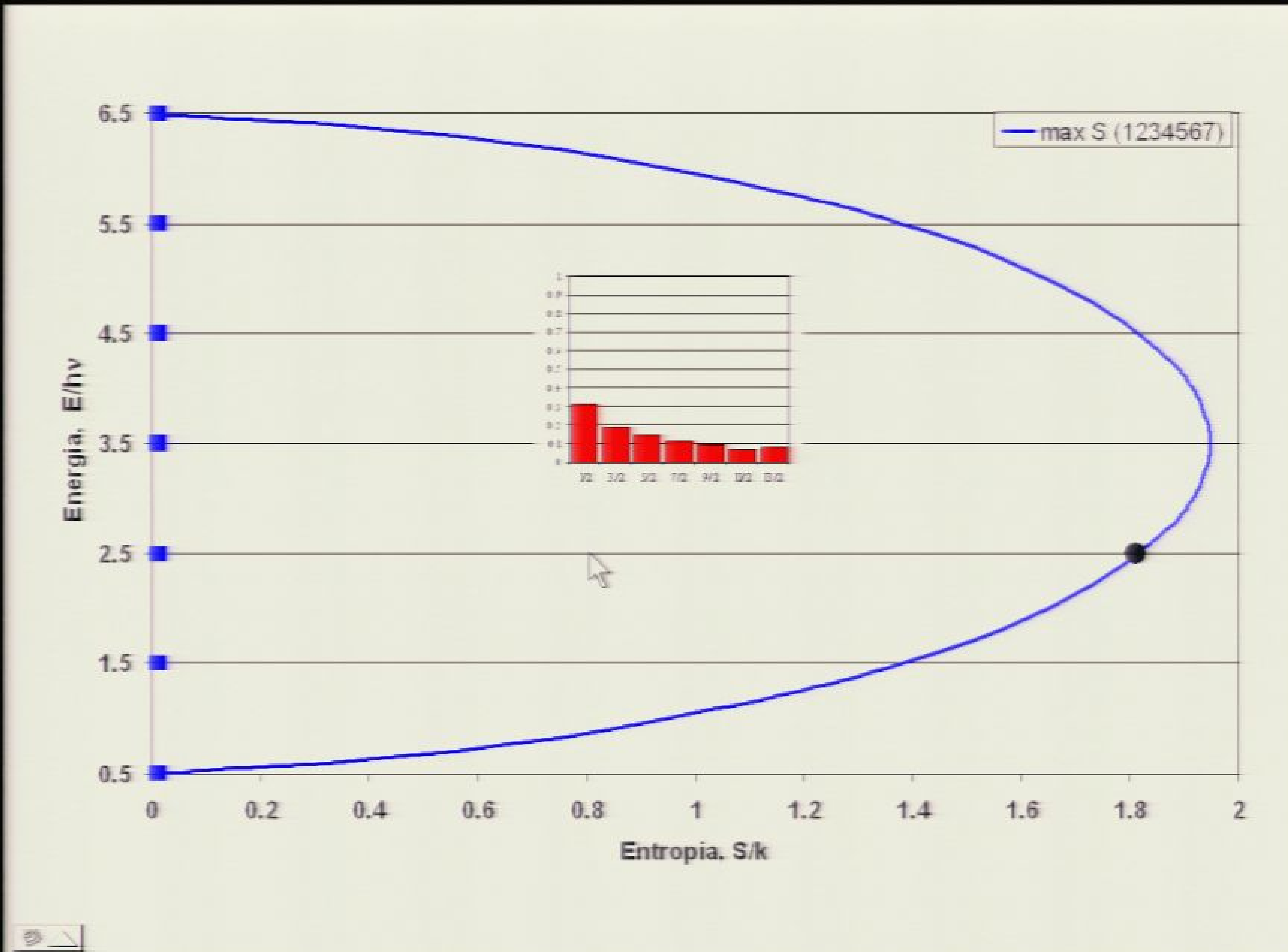
Entropia, S/k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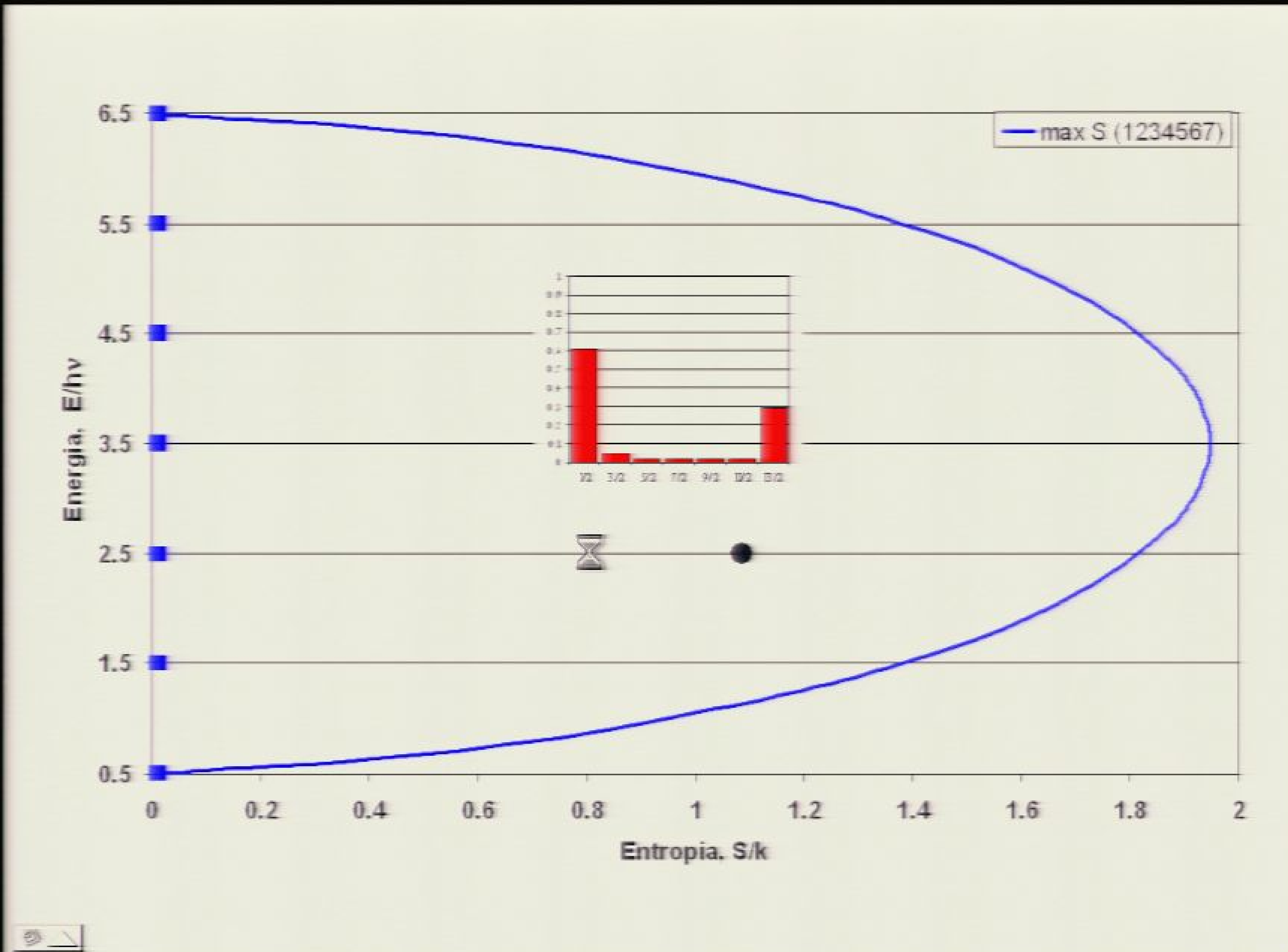
Entropia, S/k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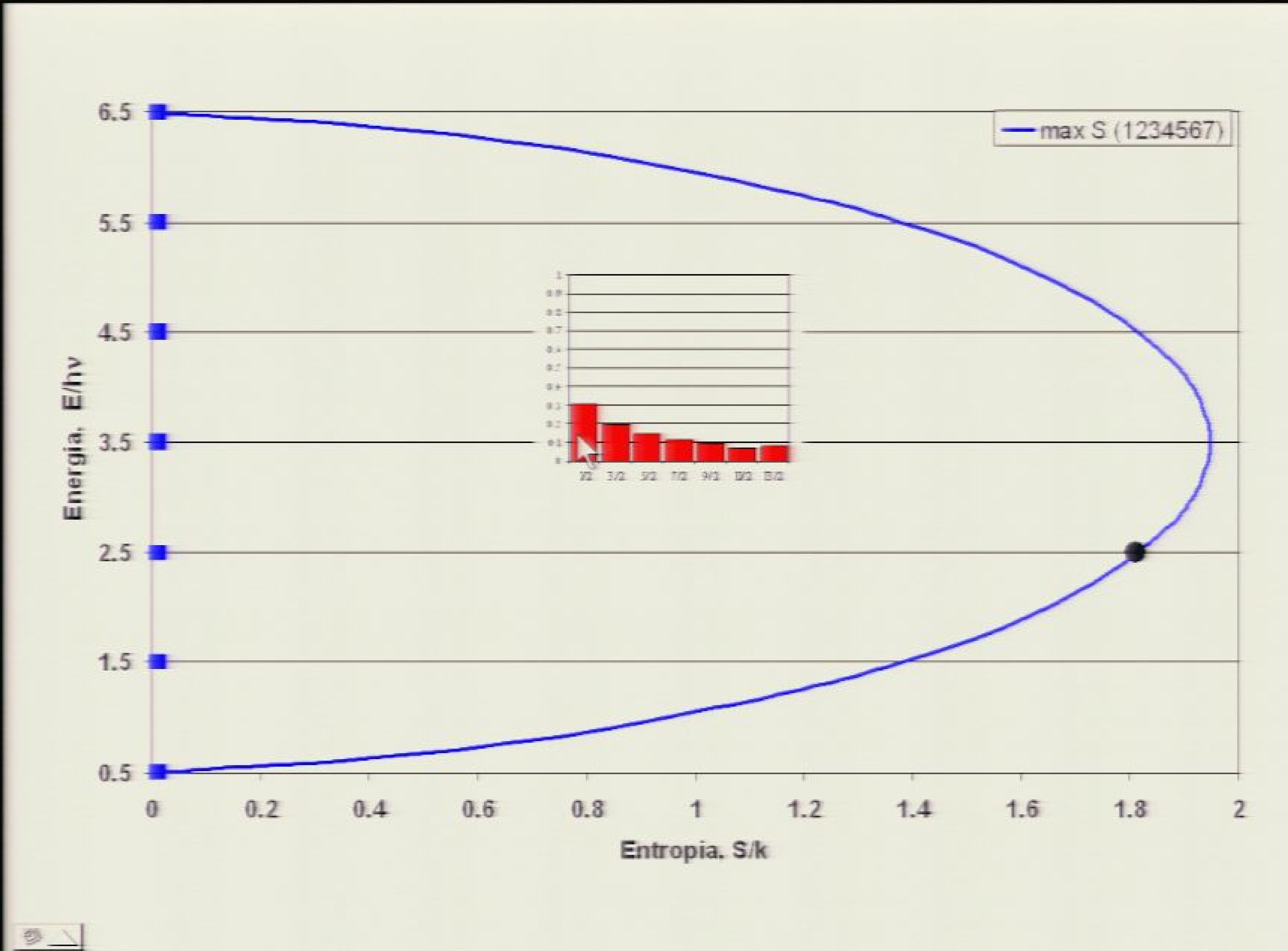
Entropia, S/k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Energia. E/hv
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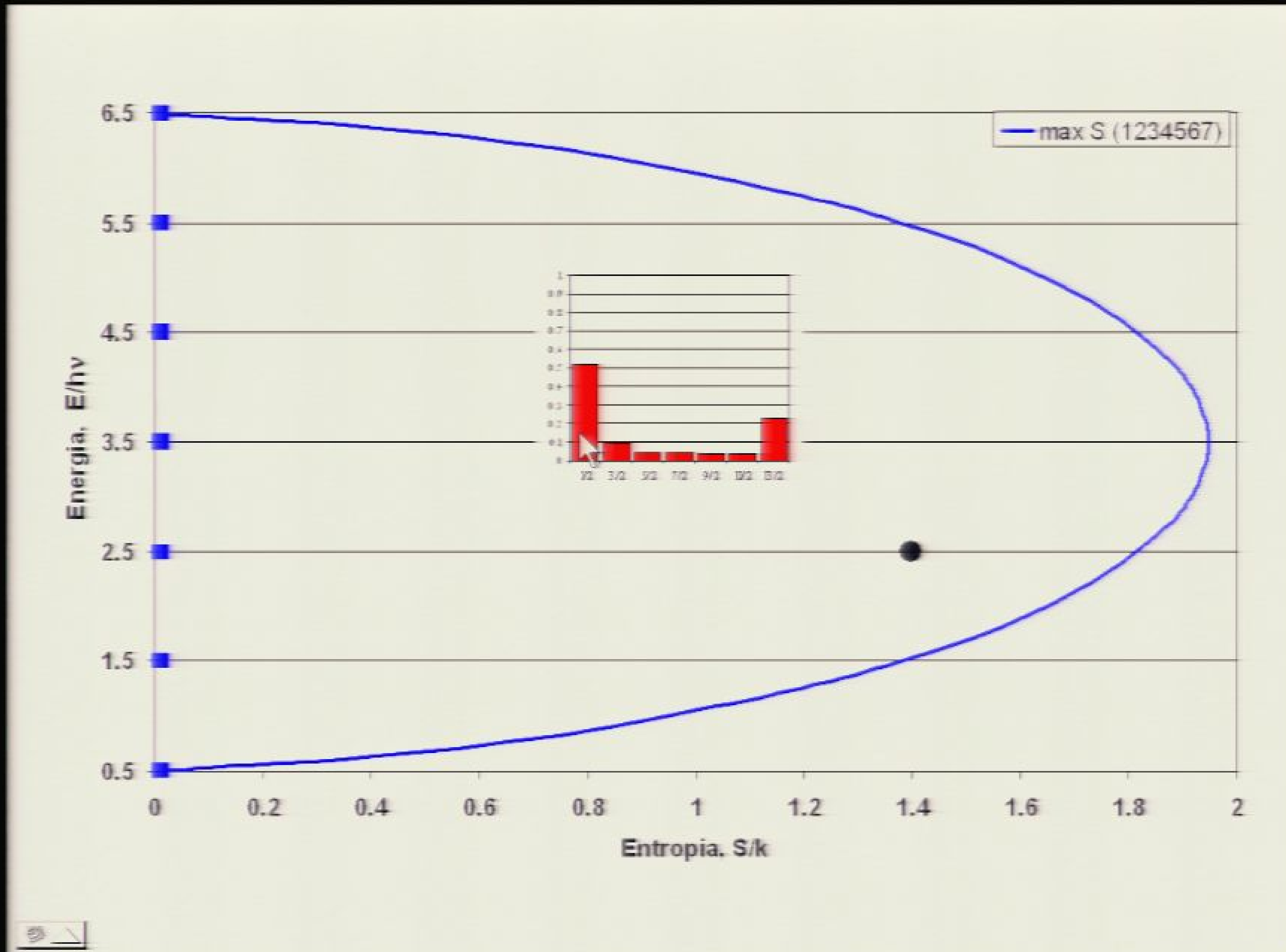
Entropia. S/k
max S (1234567)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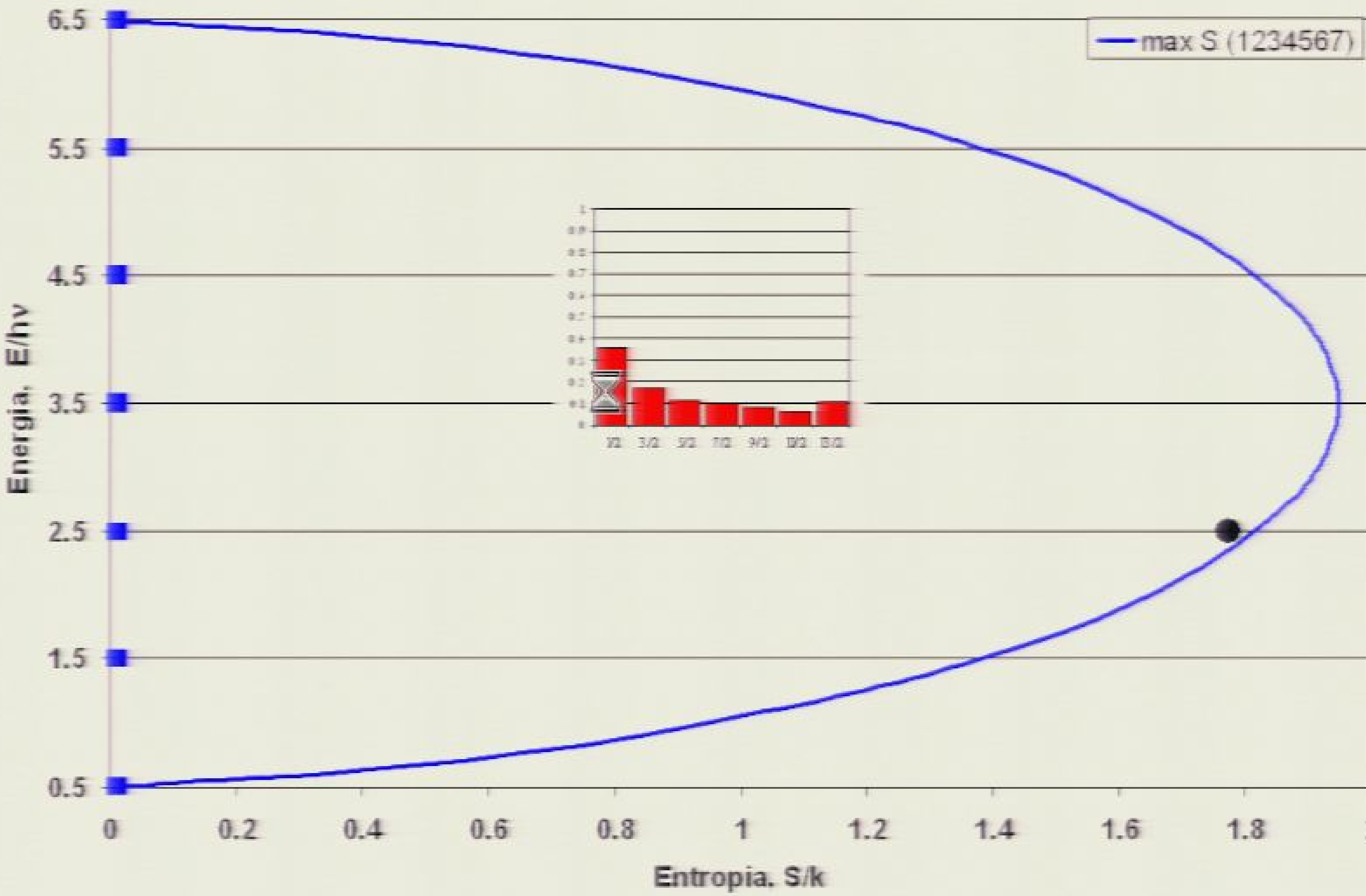
Entropia, S/k



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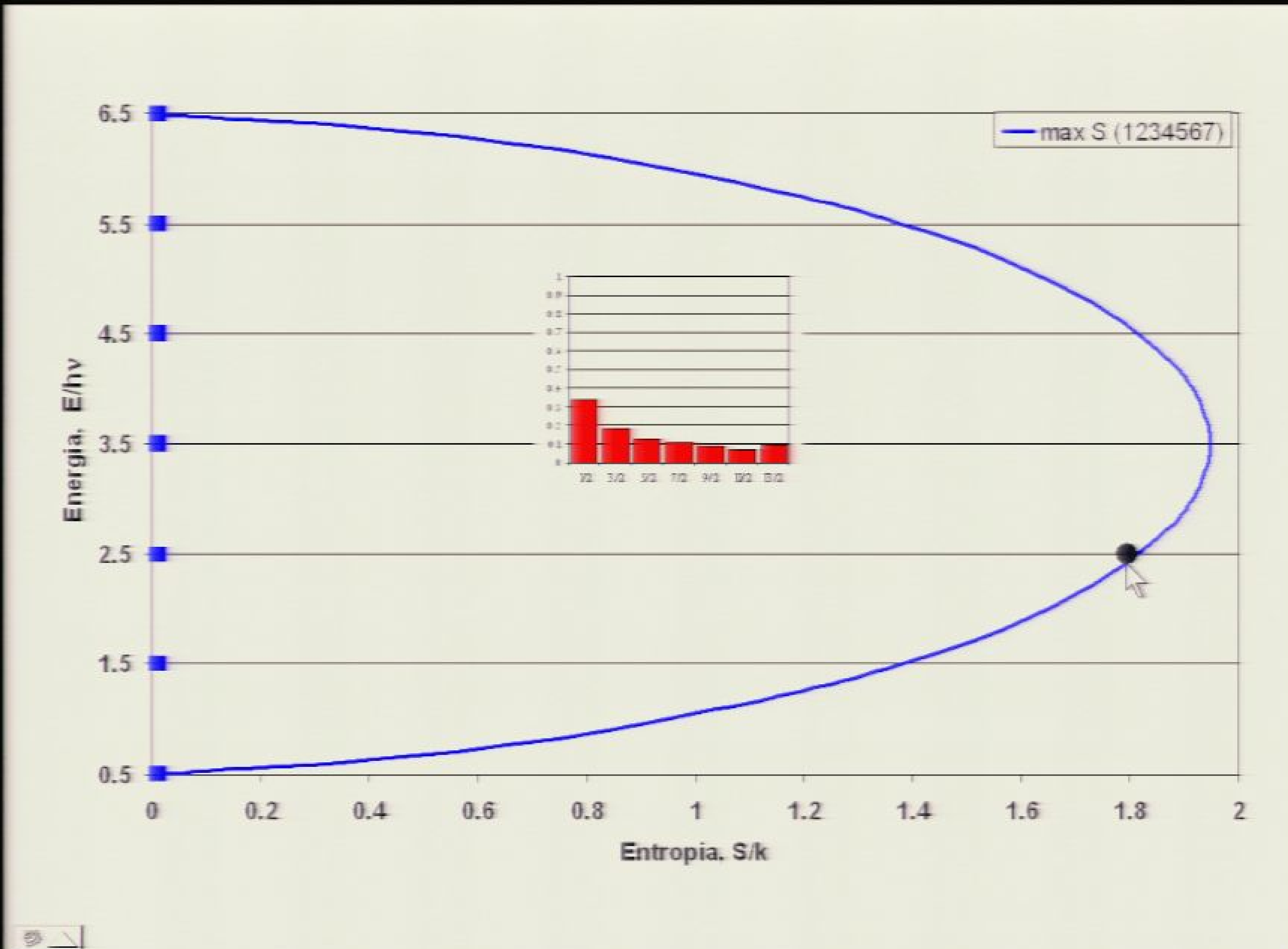
Entropia, S/k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0.5
Energia, E/hv
max S (1234567)
1/2 3/2 5/2 7/2 9/2 11/2 13/2
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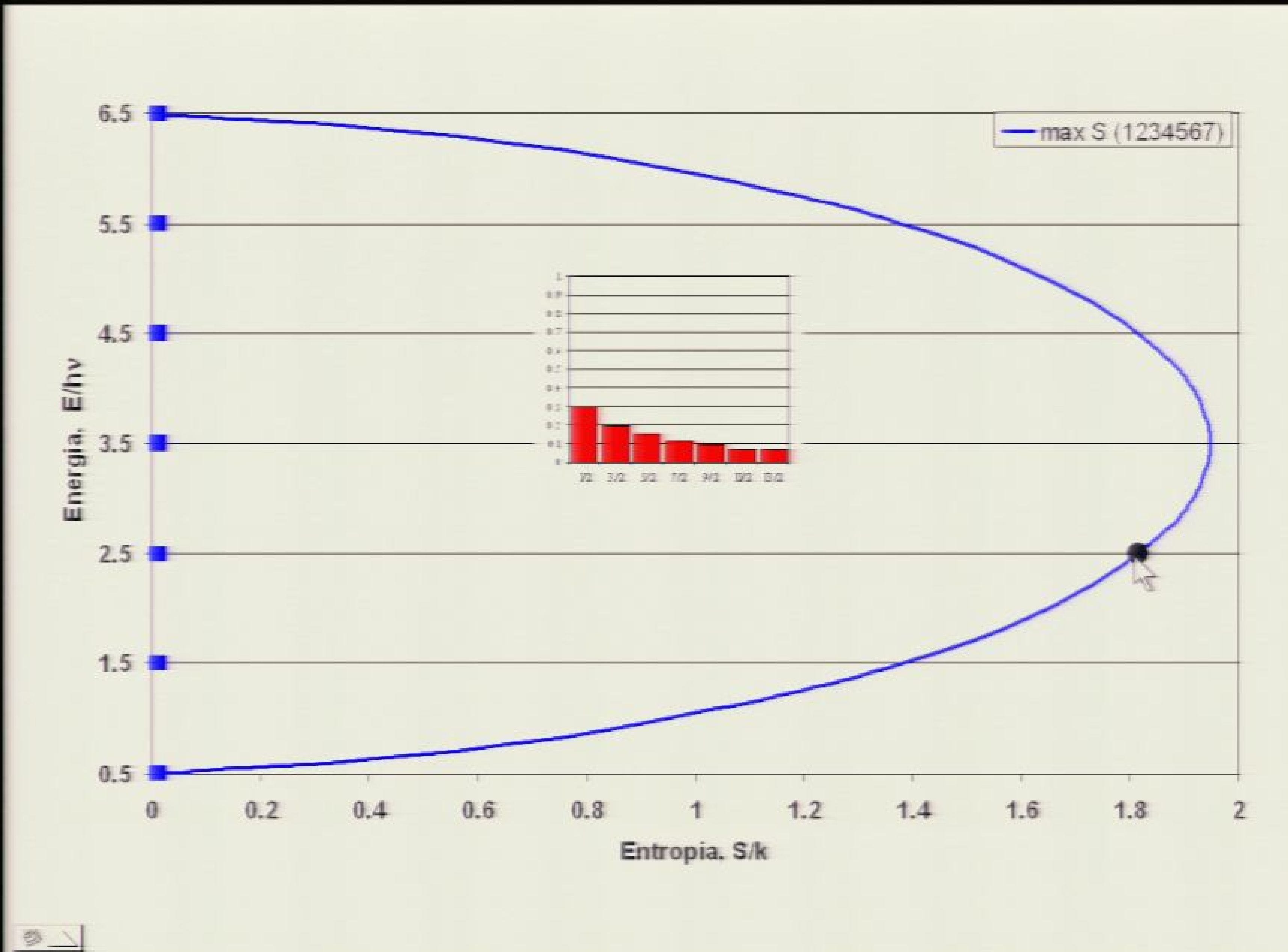
Entropia, S/k



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1.5
0.5
Energia, E/hv
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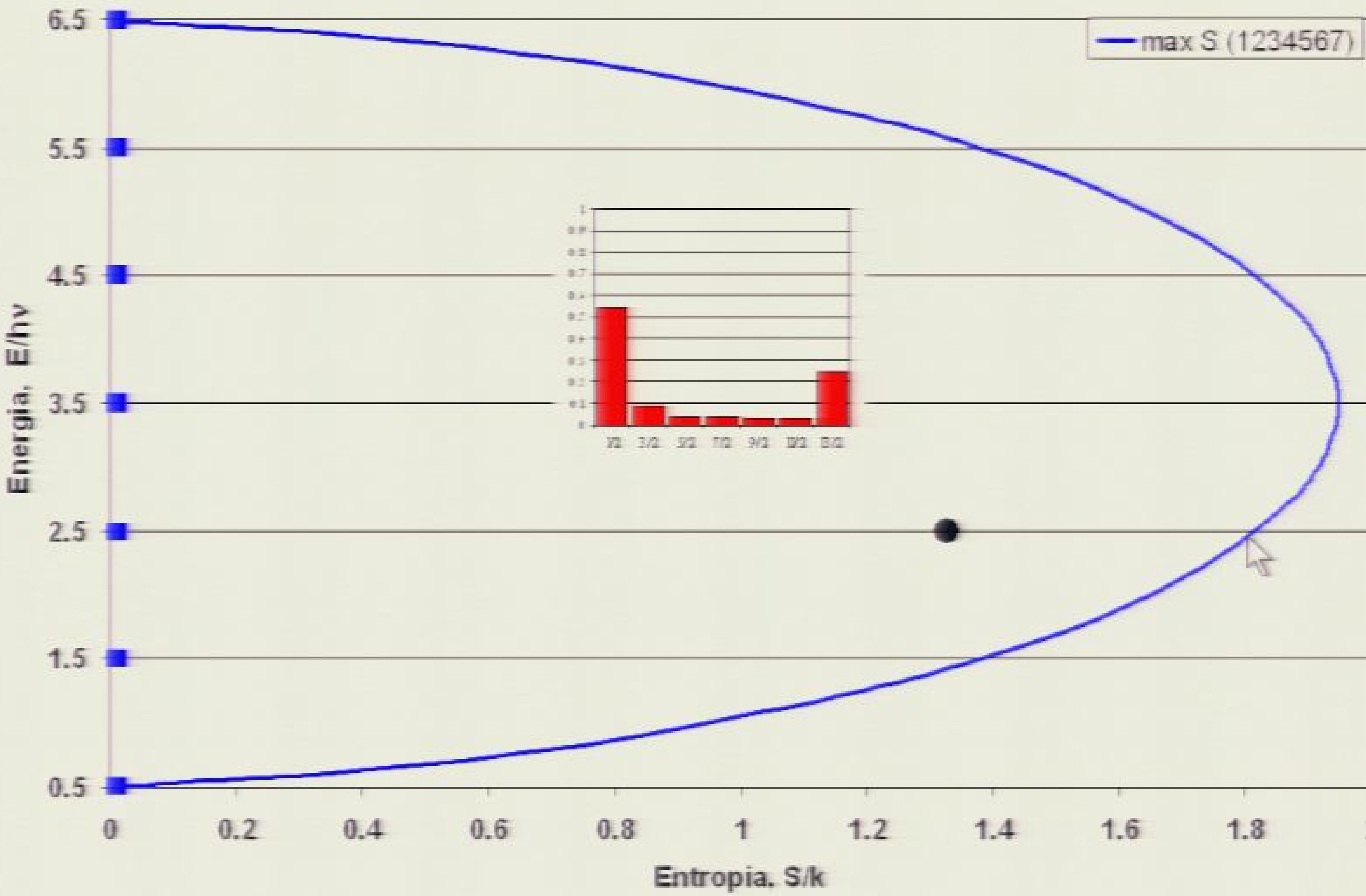
Entropia, S/k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Energia, E/hv
0
0.2
0.4
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1
1.2
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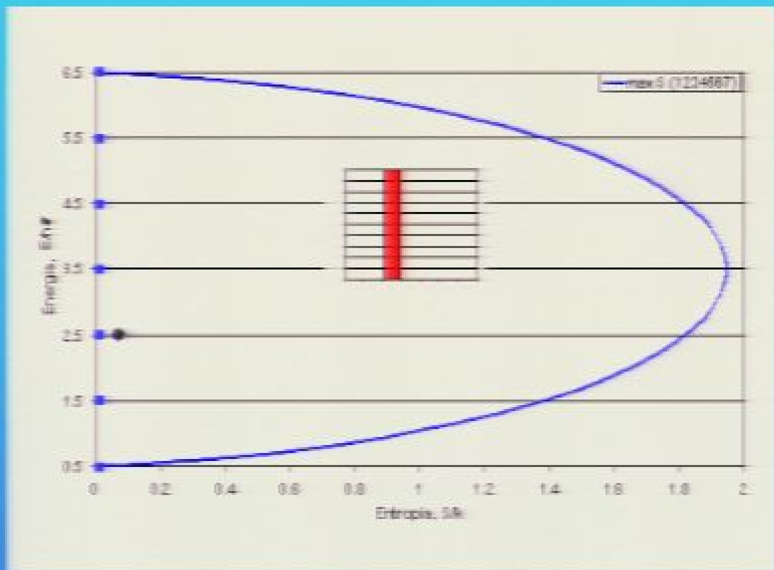
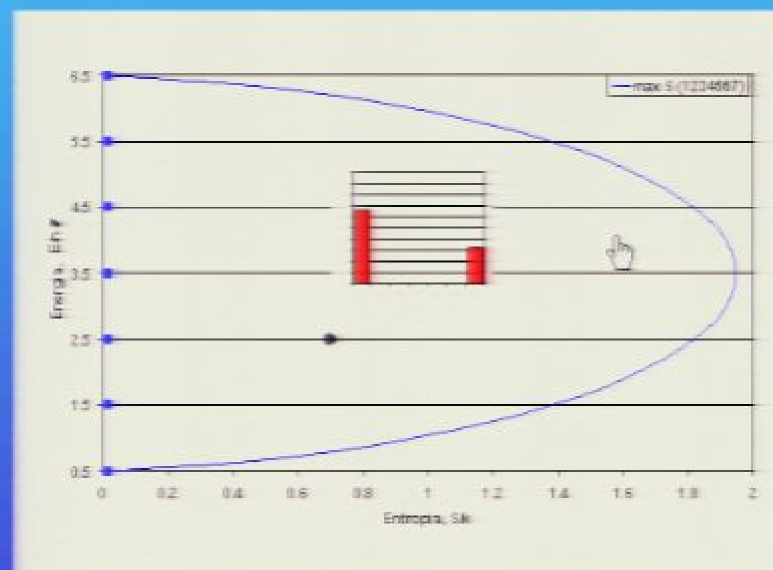
1.8
2
Entropia, S/k

Giving an "ontic" status to irreversibility



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 ?



In **Quantum Thermodynamics**, irreversible time evolution, for **ρH=Hρ,** can be interpreted as the internal **redistribution of energy** among all the eigenmodes of energy storage that are acecssible to the particle

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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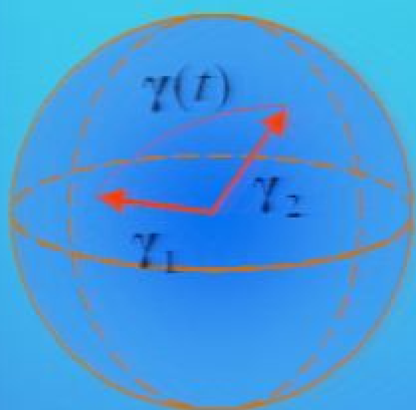
- Ontic status of density operators and microscopic entropy

3) Geometrical construction (1981) of a 'maximal entropy generation' dynamics
- Ontic and microscopic status to the second law and to irreversibility

- "Design of the equation" using square-root density operator

Geometrical setting: 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, $\boldsymbol{p}(t) = \{p_i(t)\}$, where t is a parameter, the distance between distributions $\boldsymbol{p}(t+dt)$ and $\boldsymbol{p}(t)$ 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)

Geometrical setting: square-root density operator

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

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

be the *real* scalar product. Then,

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

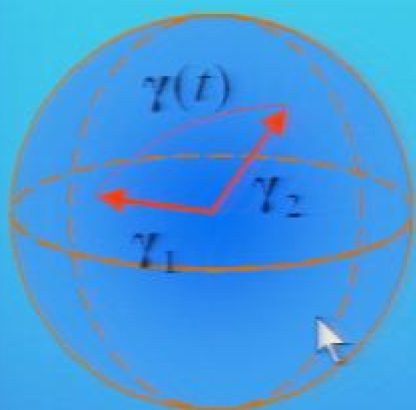
$$1 = \mathrm{Tr}\rho = \gamma \cdot \gamma$$

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)
Rep.Math.Phys. (2009)

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

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

Geometrical setting: square-root density operator



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

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

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

$$\langle S \rangle = -k_{\mathrm{B}} \mathrm{Tr}\rho \ln \rho = \gamma \cdot S'/2 \qquad \text{where } S' = -4k_{\mathrm{B}}\gamma \ln \gamma$$

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

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

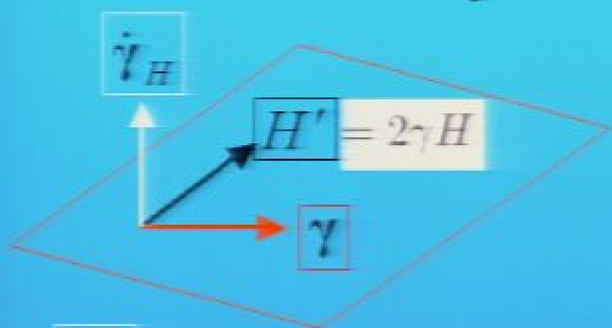
$$\dot\rho = \dot\gamma^\dagger \gamma + \gamma^\dagger \dot\gamma$$

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

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

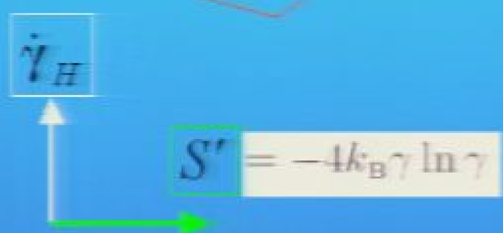
$$d\langle S \rangle/dt = \dot\gamma \cdot S'$$

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

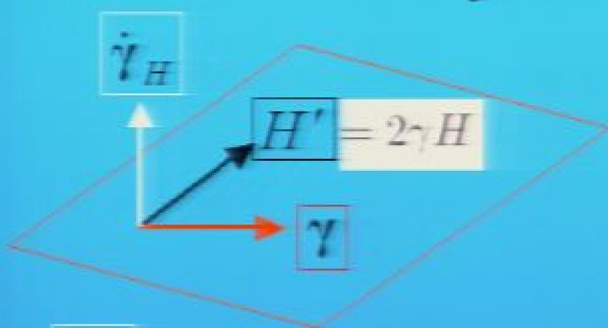
Phys.Rev.E, 73, 026113 (2006)

Entropy, 10, 160 (2008)

Rep.Math.Phys. (2009)

quant-ph/0907.1977

Hamiltonian dynamics: Schroedinger-von Neumann eq.



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

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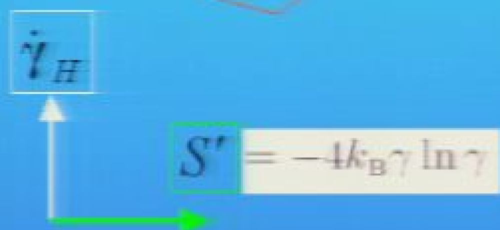


Note: since $\gamma\Delta H \cdot \gamma\Delta H = \mathrm{Tr}\rho(\Delta H)^2 = \langle\Delta H\Delta H\rangle$ and

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

the Fischer-Rao metric is

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

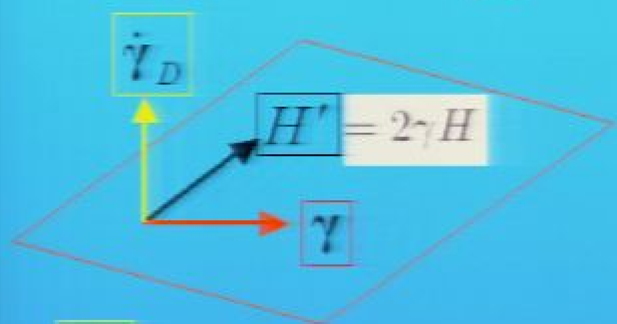
which defines the intrinsic Hamiltonian time τ_H such that

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

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

Exact time-energy uncertainty relation

Steepest-entropy-ascent: non-Hamiltonian contribution



$$\dot\gamma_H = i\gamma\Delta H/\hbar \quad \Rightarrow \quad \dot\rho_H = -i[H,\rho]/\hbar$$

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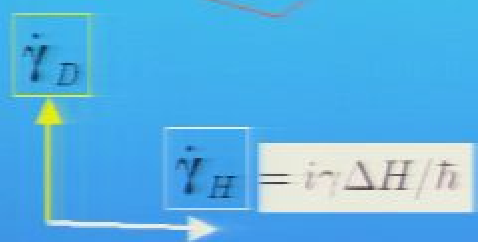


Instead, let us assume

$$\dot\gamma = \dot\gamma_H + \dot\gamma_D$$

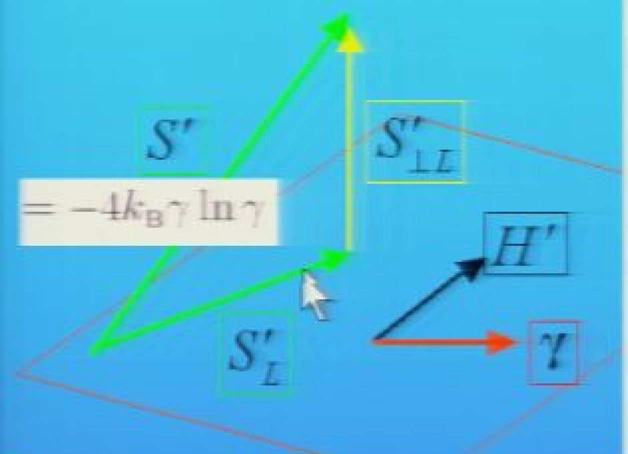
with $\dot\gamma_D$ in the direction of steepest entropy ascent compatible with the constraints

$$\dot\gamma_D \cdot \gamma = 0 \qquad (\text{conservation of } \mathrm{Tr}\rho = 1)$$
$$\dot\gamma_D \cdot H' = 0 \qquad (\text{conservation of } \langle H\rangle)$$

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

Steepest-entropy-ascent: finding the "direction"



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

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

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

quant-ph/0509116

quant-ph/0511091

quant-ph/0612215

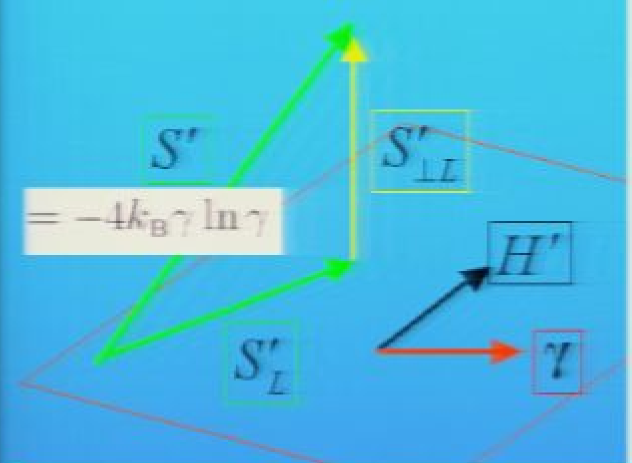
Phys.Rev.E, 73, 026113 (2006)

Entropy, 10, 160 (2008)

Rep.Math.Phys. (2009)

quant-ph/0907.1977

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

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

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

quant-ph/0509116

quant-ph/0511091

quant-ph/0612215

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

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

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

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

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

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

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

quant-ph/0509116

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or, equivalently, for the density operator

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

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

where M ("non-equilibrium Massieu operator") is

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

where $S = -k_{\rm B}\ln(\rho + P_{{\rm Ker}\,\rho})$ and

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

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

quant-ph/0509116
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Phys.Rev.E, 73, 026113 (2006)
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Steepest-entropy-ascent: dynamical law (single isolated particle)

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

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

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

Steepest-entropy-ascent: rate of entropy increase

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

where

$$M = S - \frac{H}{\theta} \qquad S = -k_{\rm B}\ln(\rho + P_{{\rm Ker}\rho}) \qquad \theta = \frac{\langle\Delta H\Delta H\rangle}{\langle\Delta S\Delta H\rangle}$$

The rate of entropy generation is (nonnnegative)

$$\frac{d\langle S\rangle}{dt} = \frac{d(-k_{\rm B}\,{\rm Tr}\rho\ln\rho)}{dt} = \dot\gamma\cdot S' = \frac{1}{k_{\rm B}\tau}\langle\Delta M\Delta M\rangle$$

$$= \frac{1}{k_{\rm B}\tau}\left(\langle\Delta S\Delta S\rangle - \frac{\langle\Delta H\Delta H\rangle}{\theta^2}\right)$$

$$= \frac{1}{4k_{\rm B}\tau}S'_{\perp L}\cdot S'_{\perp L} = 4k_{\rm B}\tau\,\dot\gamma_D\cdot\dot\gamma_D$$

quant-ph/0509116

quant-ph/0511091

quant-ph/0612215

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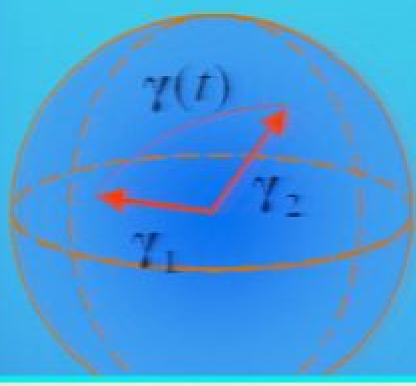
Entropy increase, metric, and time-entropy uncertainty



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

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

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

which defines also the intrinsic dissipative time τ_D such that

$$\langle \Delta S \Delta S\rangle\, \tau_D^2 \geq \langle \Delta M \Delta M\rangle\, \tau_D^2 = (k_{\rm B}\tau)^2$$

(a general time-entropy uncertainty relation).

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: 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, spontanueous 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 $p_j > 0$).

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

for i, j = 1, 2, ..., N

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

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

Existence and uniqueness of solutions ρ(t) for any ρ(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!

Existence and uniqueness of solutions ρ(t) for any ρ(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 $u : \Re^+ \times \mathcal{G} \longrightarrow \mathcal{G}$ such that, for all t, s in $\Re^+$ and all γ in $\mathcal{G}$:

- $u(\cdot, \gamma)$: $\Re^+ \longrightarrow \mathcal{G}$ 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 $\Re^+$ 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

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

Steepest-entropy-ascent: Onsager reciprocity everywhere

Any nonequilibrium ρ can be written as

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

where the set $\{I, X_j\}$ spans the real space of hermitian operators on $(\mathcal{H})$, and $B = B^2$. Hence,

$$\langle X_j \rangle = \mathrm{Tr}(\rho X_j)$$

$$\langle S \rangle = k_{\mathrm{B}} f_0 + k_{\mathrm{B}} \sum_j f_j \langle X_j \rangle$$

$$\text{where} \quad k_{\mathrm{B}} f_j = \left. \frac{\partial \langle S \rangle}{\partial \langle X_j \rangle} \right|_{\langle X_{i \neq j} \rangle}$$

may be interpreted as a "generalized affinity" or force, and

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

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

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

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

Linear interrelations between rates and affinities.

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

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

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

Found.Phys., 17, 365 (1987)

quant-ph-0112046

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

..and
the Second Law
as a theorem!

quant-ph-0112046
quant-ph-0612215
quant-ph-0511091
Phys.Rev.E, 73, 026113 (2006)

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,

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

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 $\mathrm{Tr}B > 1$, then $B(t) = U(t)B(0)U^{-1}(t)$;
- pure limit cycles if $[B, H] \neq 0$ and $\mathrm{Tr}B = 1$ (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.*

Equilibrium states for a 4-level isolated particle

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

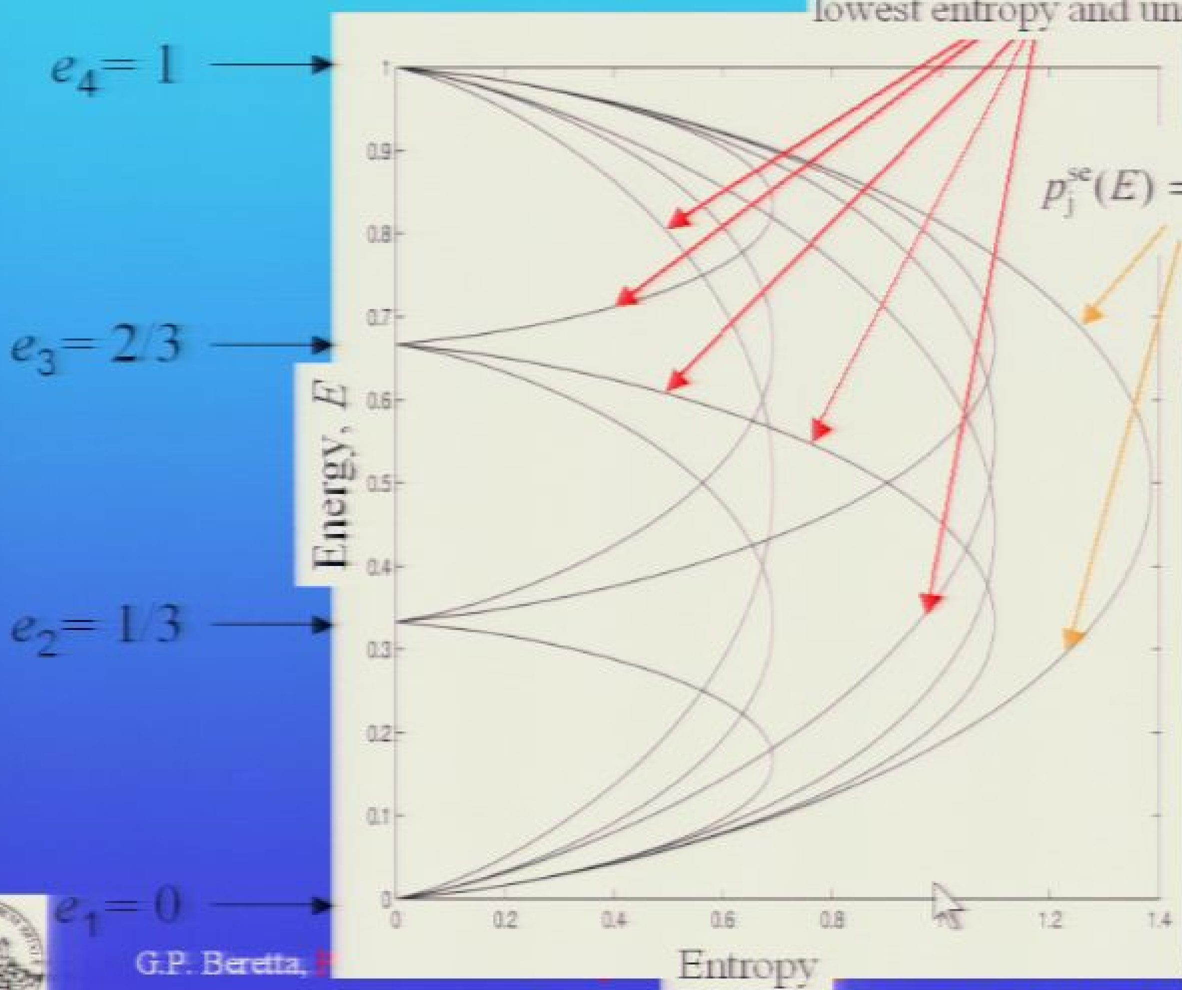
$$p_j^{pe}(E,\boldsymbol{\delta}) = \frac{\delta_j \exp(-\beta^{pe}(E,\boldsymbol{\delta})\, e_j)}{\sum_{i=1}^{N} \delta_i \exp(-\beta^{pe}(E,\boldsymbol{\delta})\, e_i)}$$

lowest entropy and unstable equilibrium states

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

(canonical distribution)

stable equilirium states

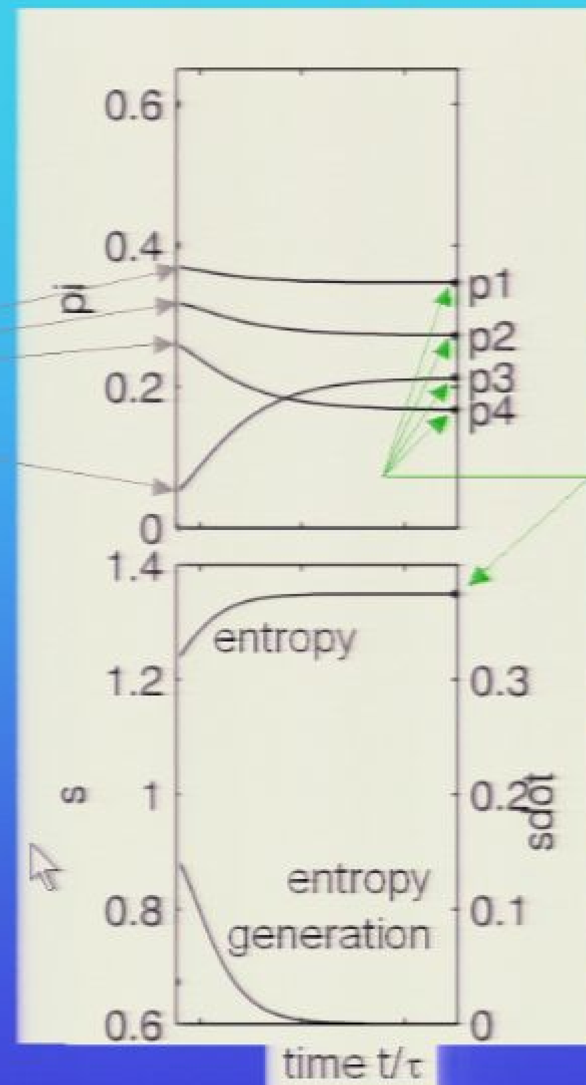


Relaxation to equilibrium for a 4-level isolated particle

$N = 4$

$[H,\rho]=0$

An arbitrary initial distribution (state)



Stable equilibrium state (highest entropy)

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

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

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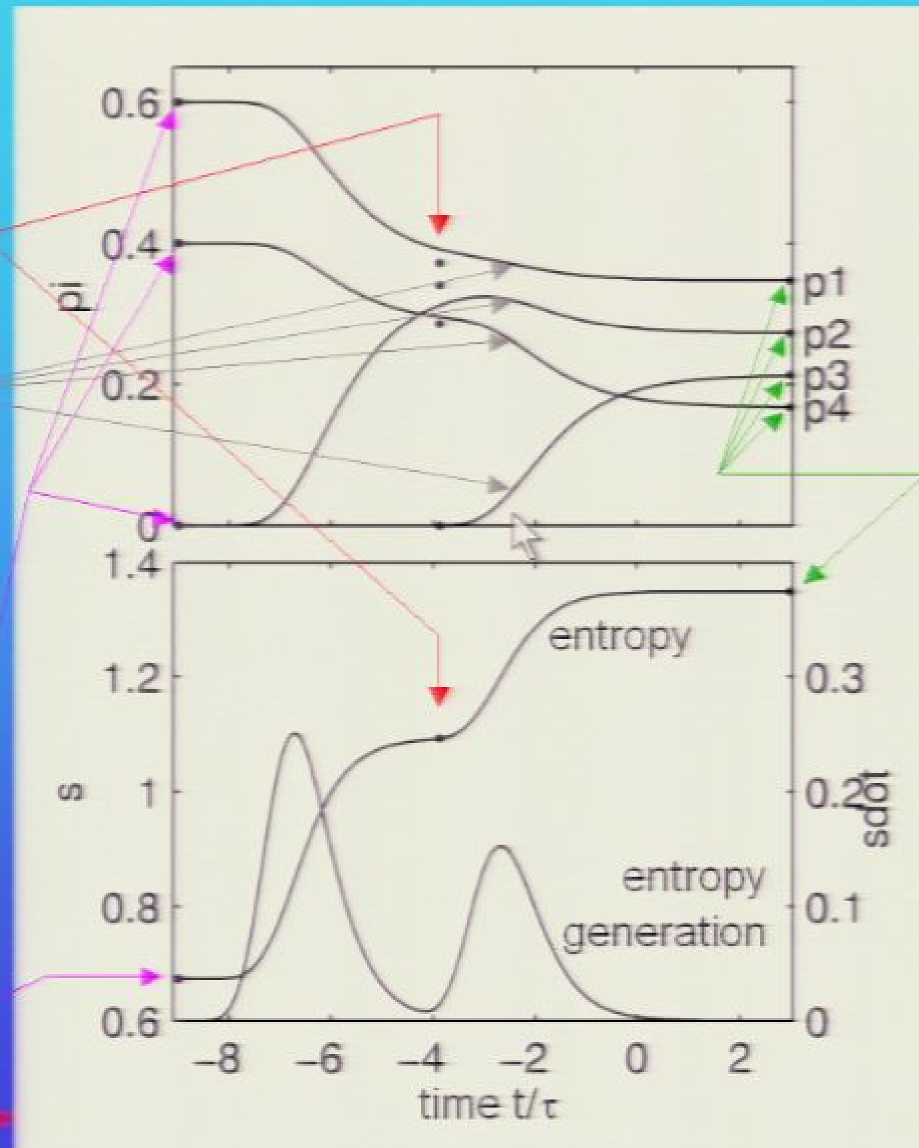
Relaxation to equilibrium for a 4-level isolated particle

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

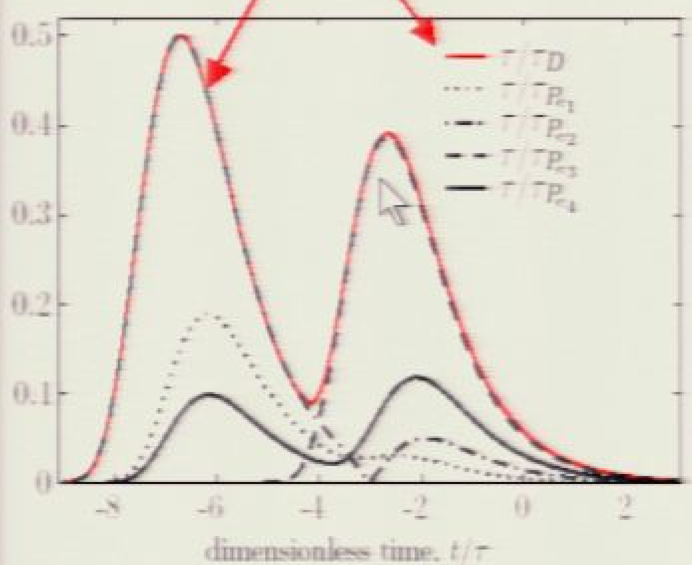


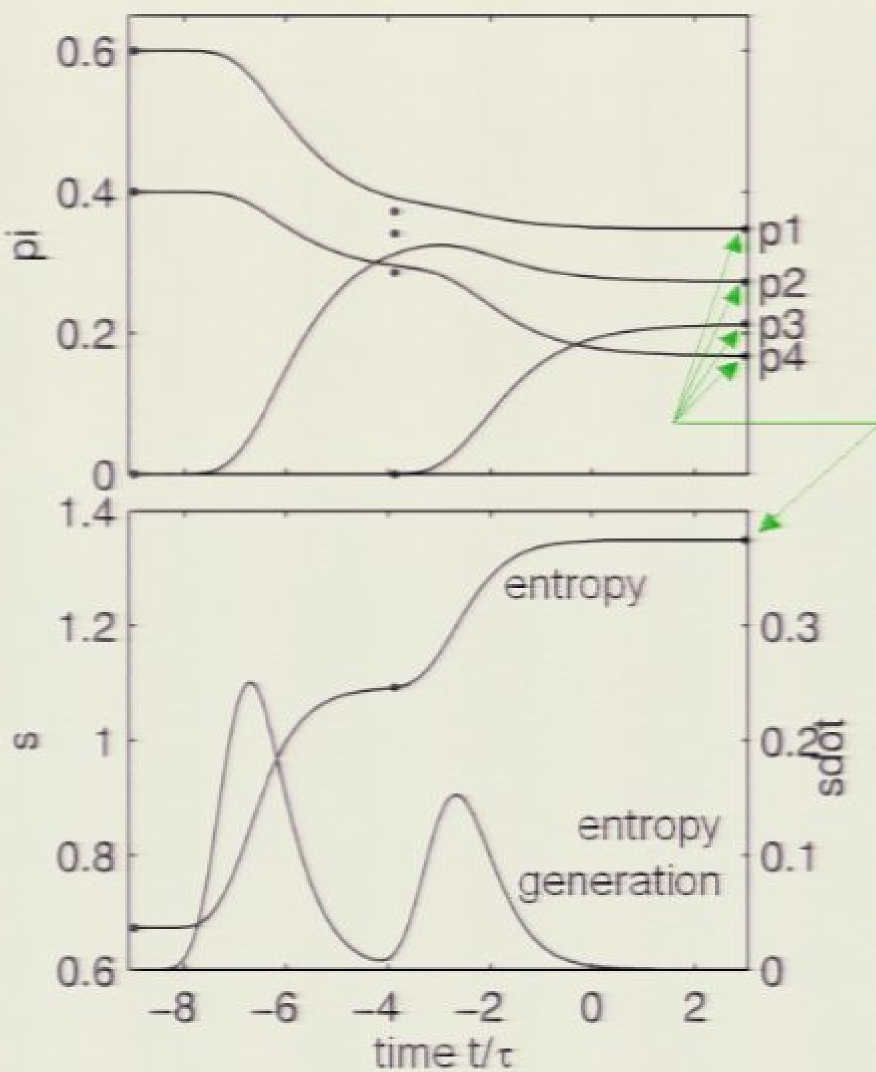
Stable equilibrium state (highest entropy)

Phys.Rev.E, 73, 026113 (2006)
G.P. Beretta, PIAF '09 "New Perspe... 2009
References ... www.quantumthermodynamics.org

Relaxation to equilibrium for a 4-level isolated particle

time-entropy uncertainty bound





Stable equilibrium state (highest entropy)

2009

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Part IV

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

- Structure of the nonlinear dynamical law for composite systems
- Locality and separability

No free lunch! Dealing with composite systems

A = Alice

B = Bob

Nuovo Cimento B, 87, 77 (1985)

quant-ph-0112046

Rep.Math.Phys. (2009)

In linear dynamics, the equation of motion remains

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

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:

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

Simply taking

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -\frac{i}{\hbar}[H,\rho] + \frac{1}{2k_{\mathrm{B}}\tau}\{\Delta M,\rho\}$$

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

G.P. Beretta, PIAF

Steepest-locally-perceived-entropy-ascent

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

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

$$(\Delta H)^A = \mathrm{Tr}_B[(I_A\otimes\rho_B)\Delta H]$$
$$(\Delta H)^B = \mathrm{Tr}_A[(\rho_A\otimes I_B)\Delta H]$$
$$(\Delta S)^A = \mathrm{Tr}_B[(I_A\otimes\rho_B)\Delta S]$$
$$(\Delta S)^B = \mathrm{Tr}_A[(\rho_A\otimes I_B)\Delta S]$$

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

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

Nuovo Cimento B, 87, 77 (1985)

quant-ph-0112046

Rep.Math.Phys. (2009)

G.P. Beretta, PIAF '09

Steepest-locally-perceived-entropy-ascent

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

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

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$$(\Delta S)^A = \mathrm{Tr}_B[(I_A\otimes\rho_B)\Delta S]$$
$$(\Delta S)^B = \mathrm{Tr}_A[(\rho_A\otimes I_B)\Delta S]$$

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

~~$\frac{\mathrm{d}\rho_A}{\mathrm{d}t} = f(\rho_A)$~~

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

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

Nuovo Cimento B, 87, 77 (1985)
quant-ph-0112046
Rep.Math.Phys. (2009)

G.P. Beretta, PIAF '09 "?"

Conclusions

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
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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

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

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

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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 AND VIEWS

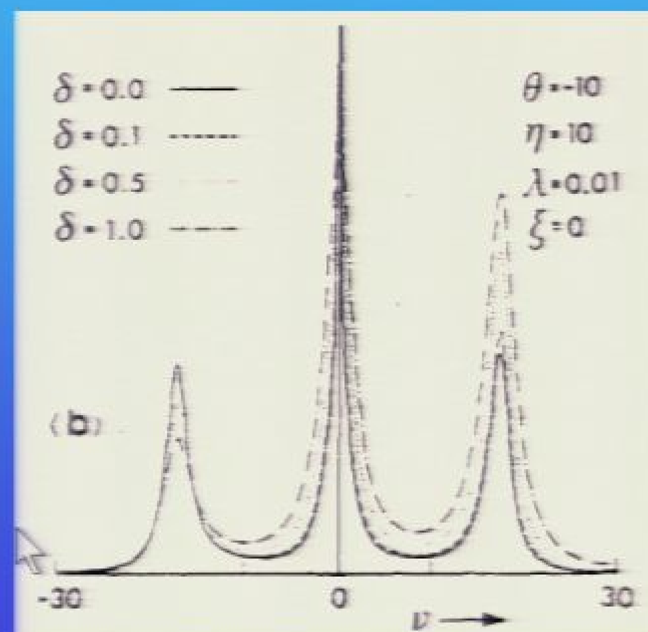
Uniting mechanics and statistics

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

Measurable effects?

Irreversible internal redistribution
implies
asymmetries
in the spectral distribution



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

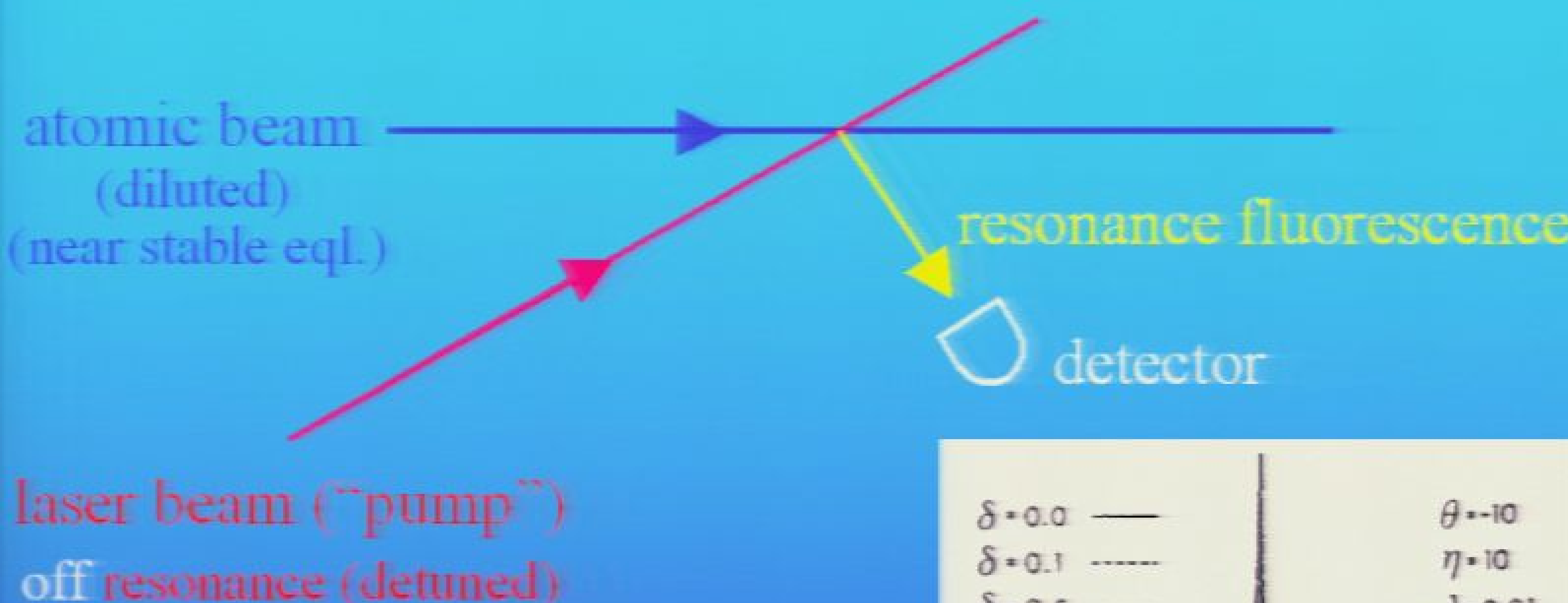
Conclusions

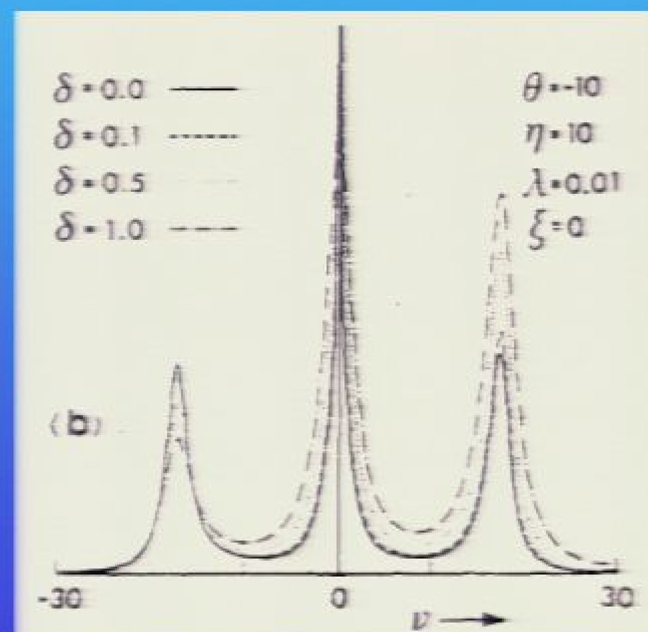
- The second law is forced directly into the microscopic laws and emerges as a theorem of the constrained steepest-entropy-ascent (or maximal entropy generation) dynamical law (stability of equilibrium states)
- Entropy emerges from the microscopic level as a measure of the degree of “load sharing” among 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 philosophycal scrutiny.
- An ontic role of the density operator makes Quantum Thermodynamics fundamental.

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?





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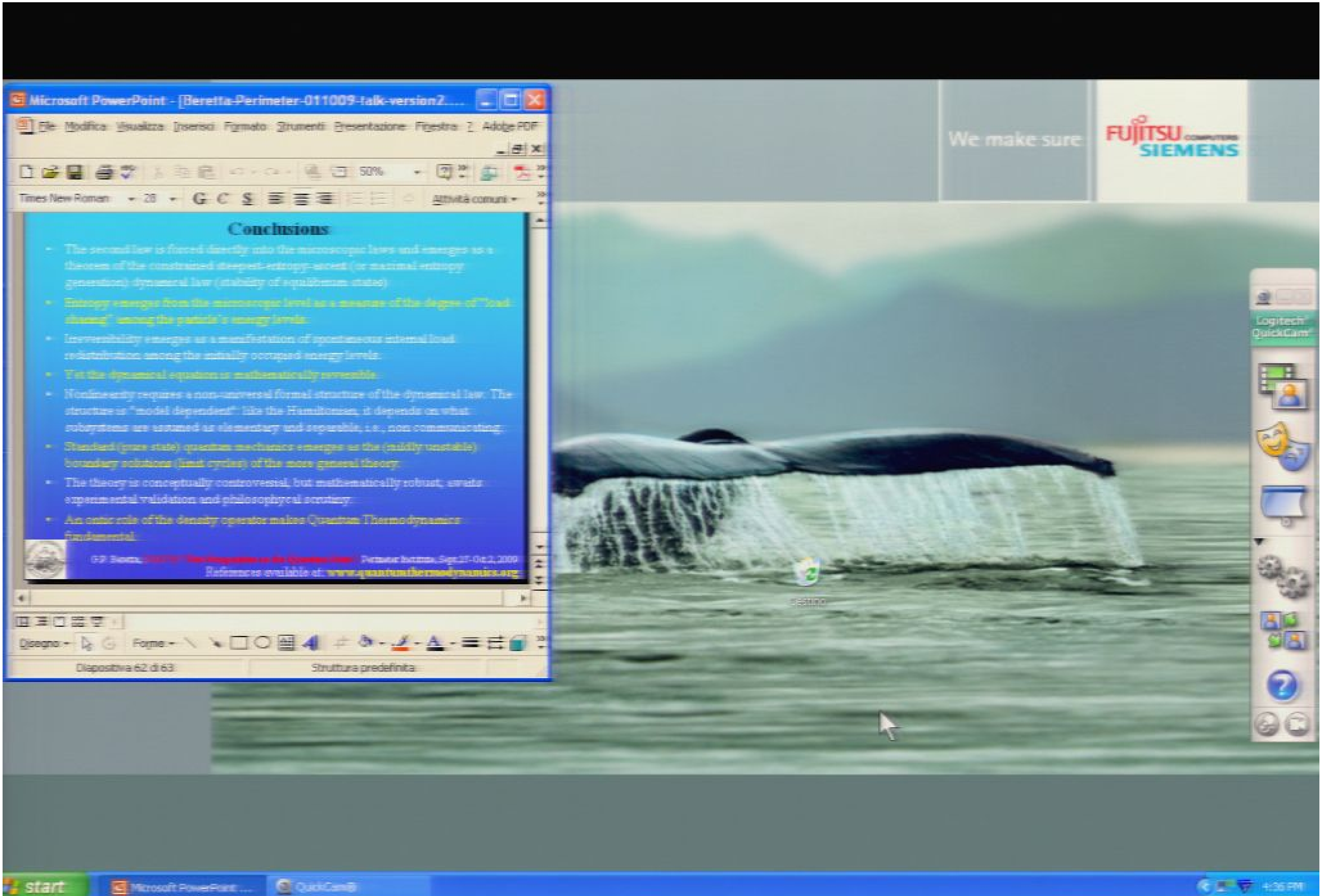
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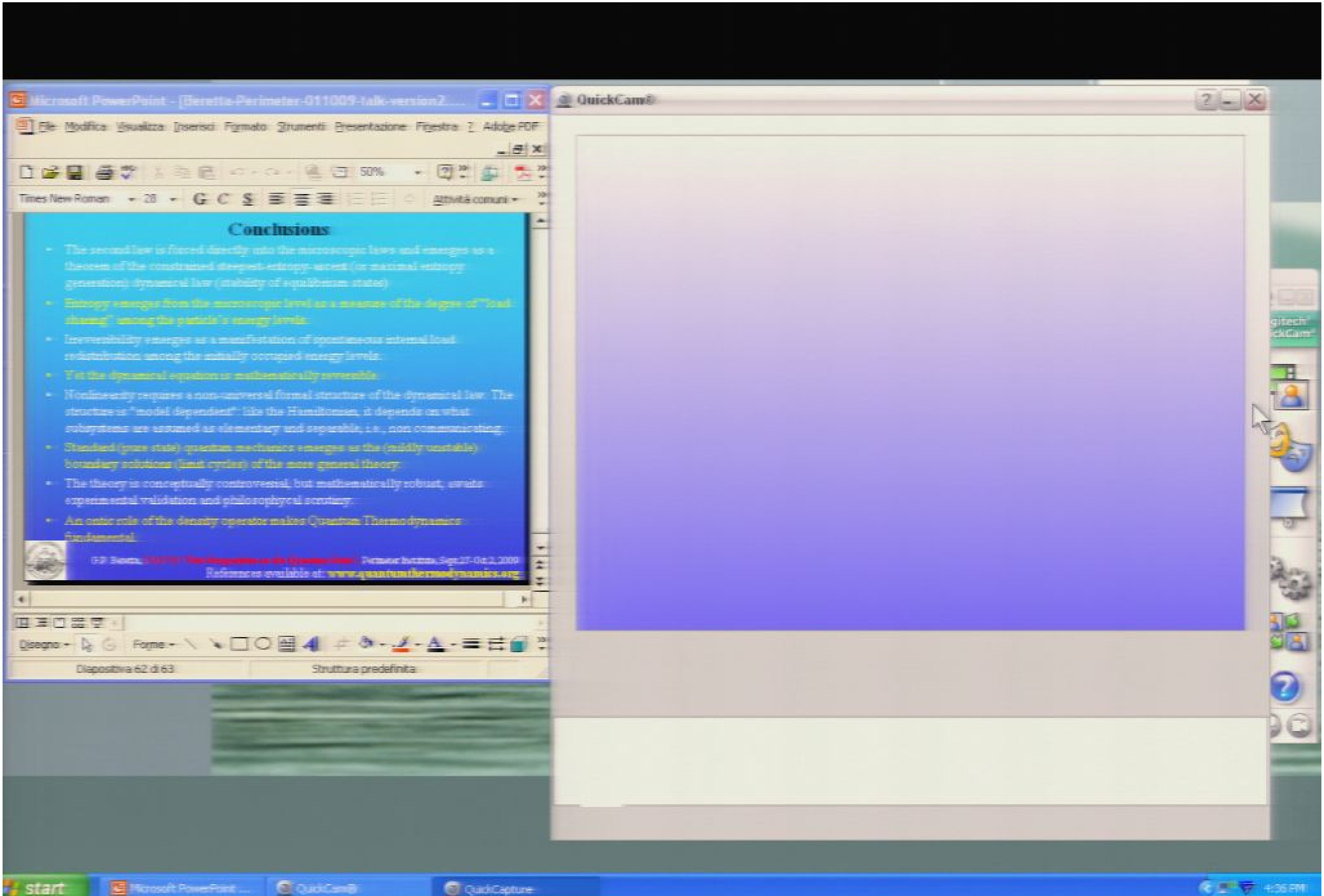
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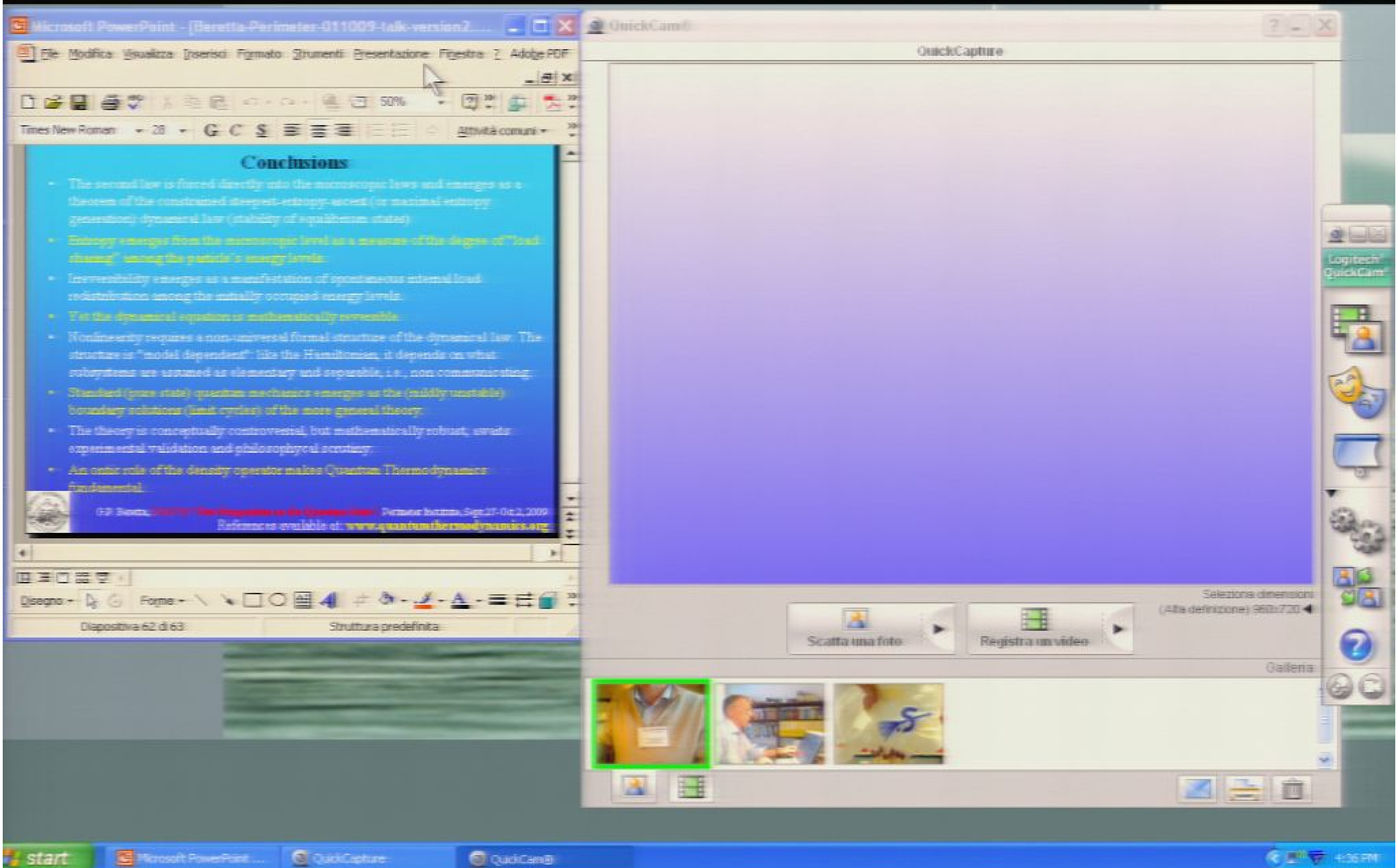
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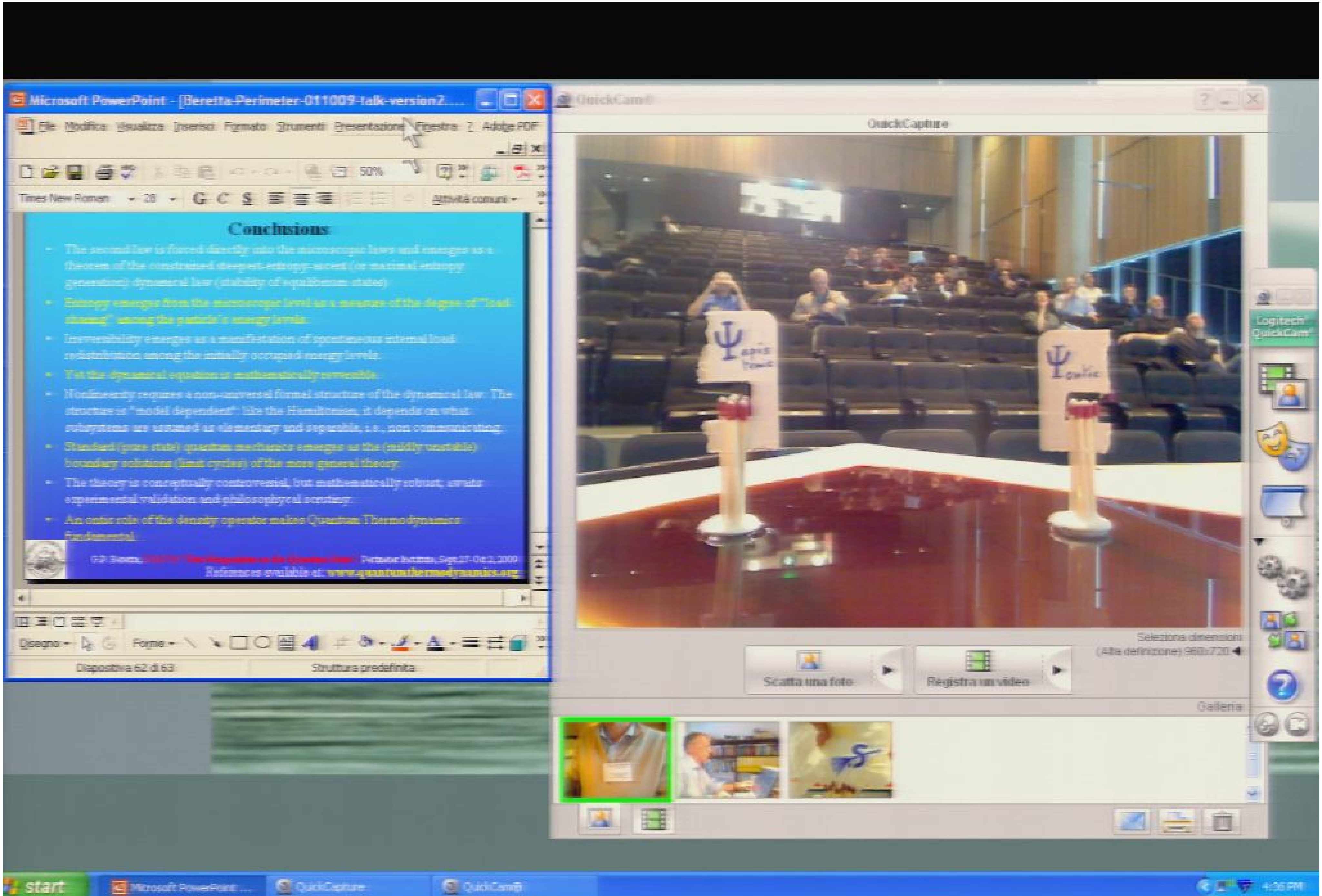
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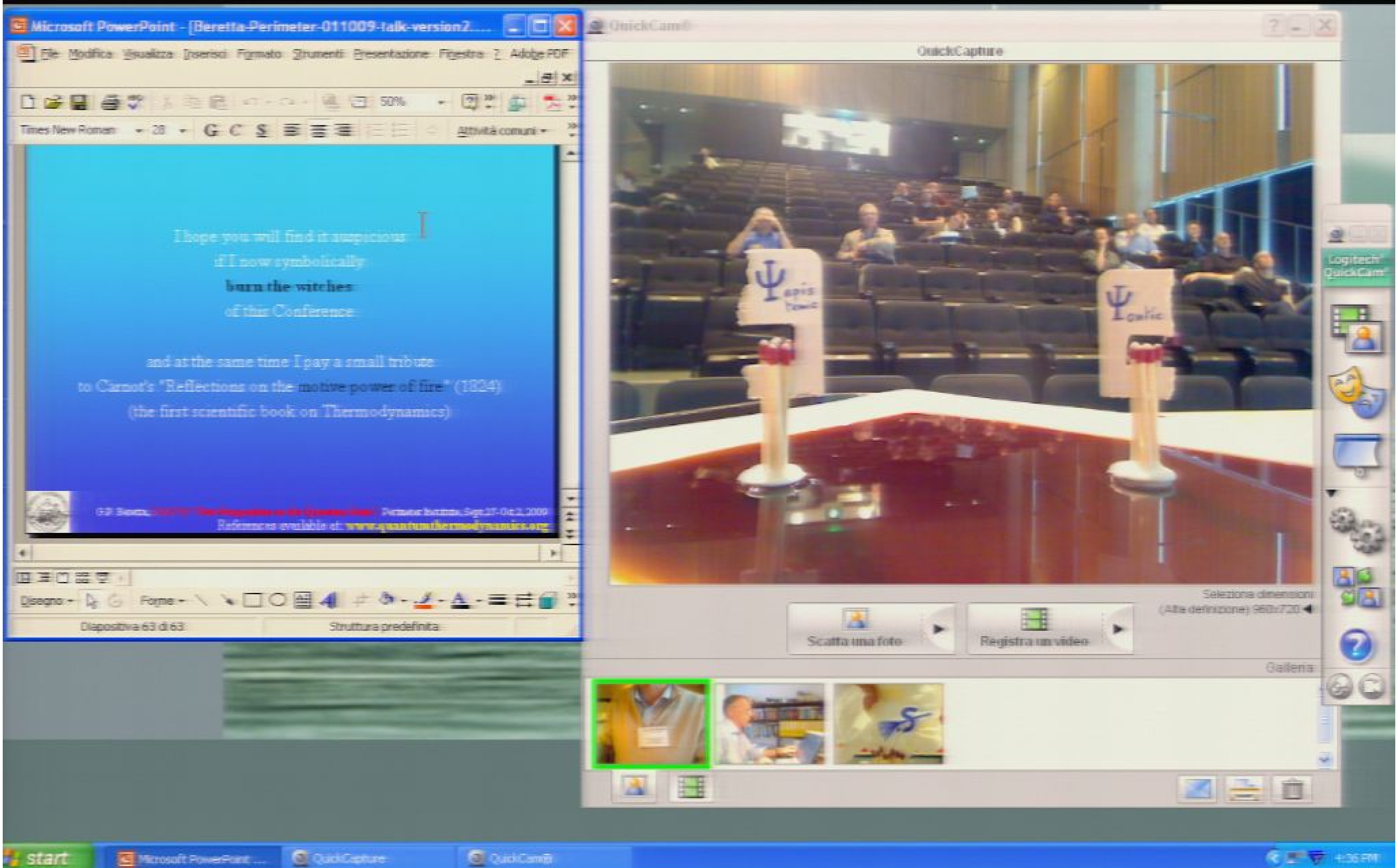
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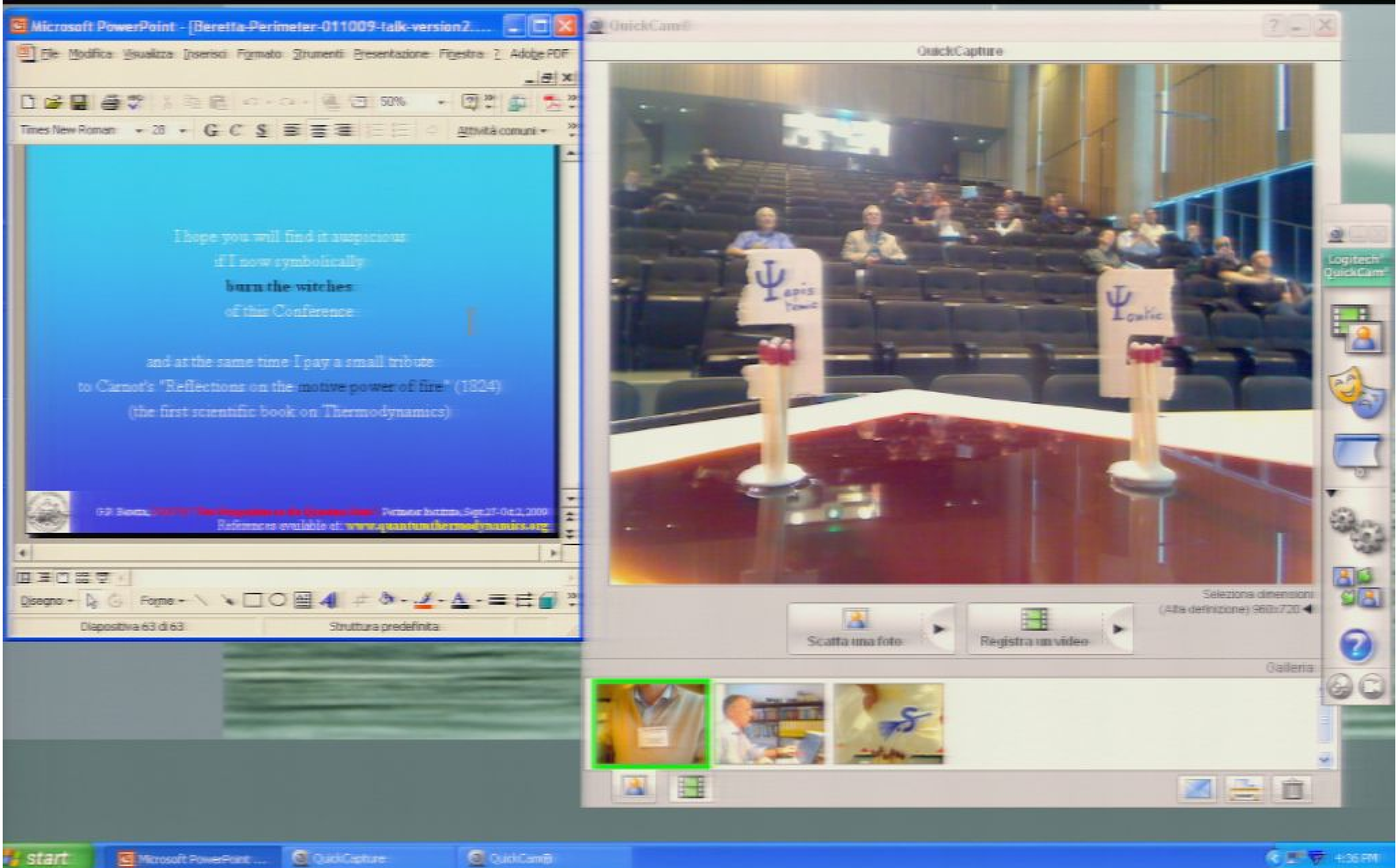
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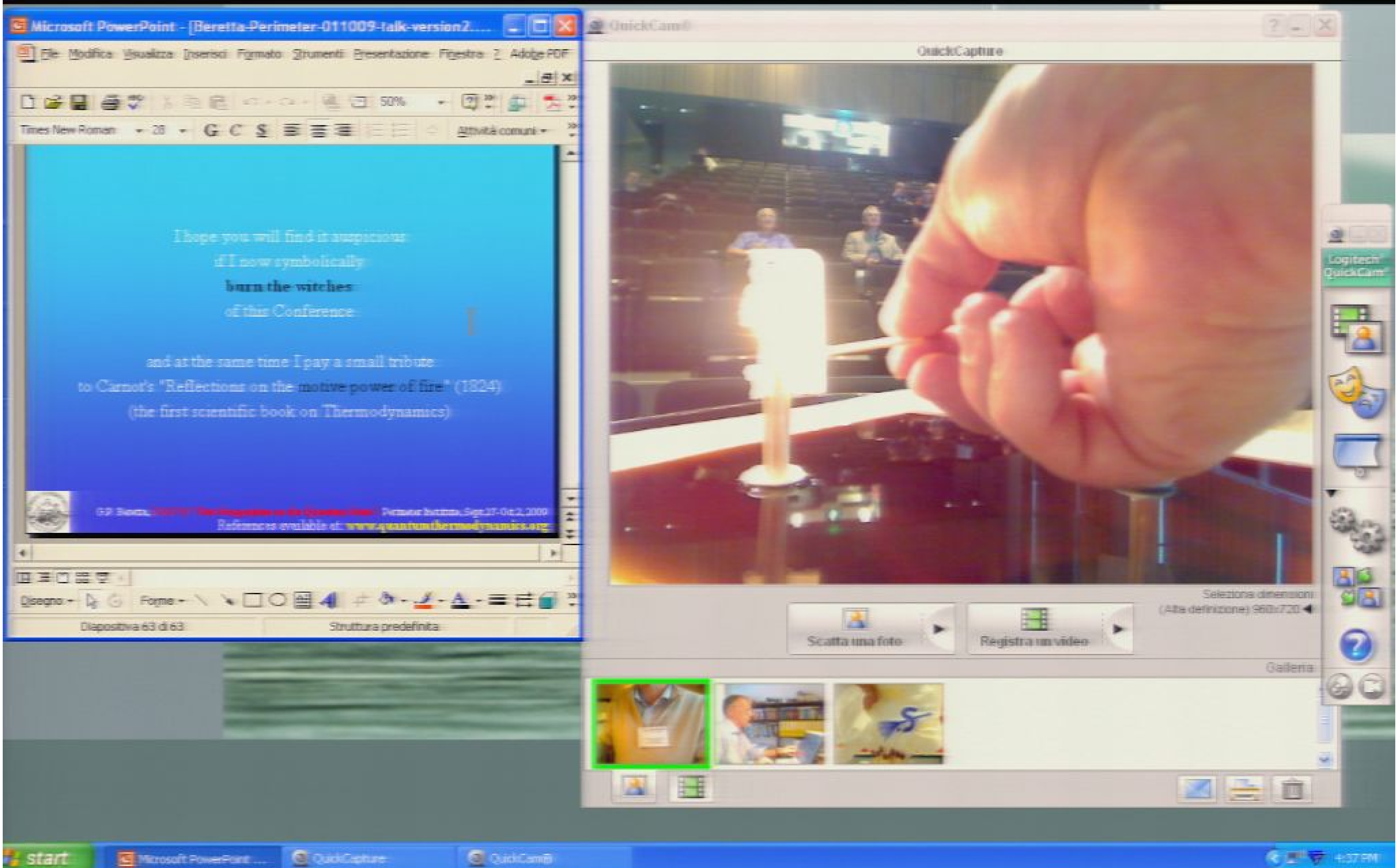
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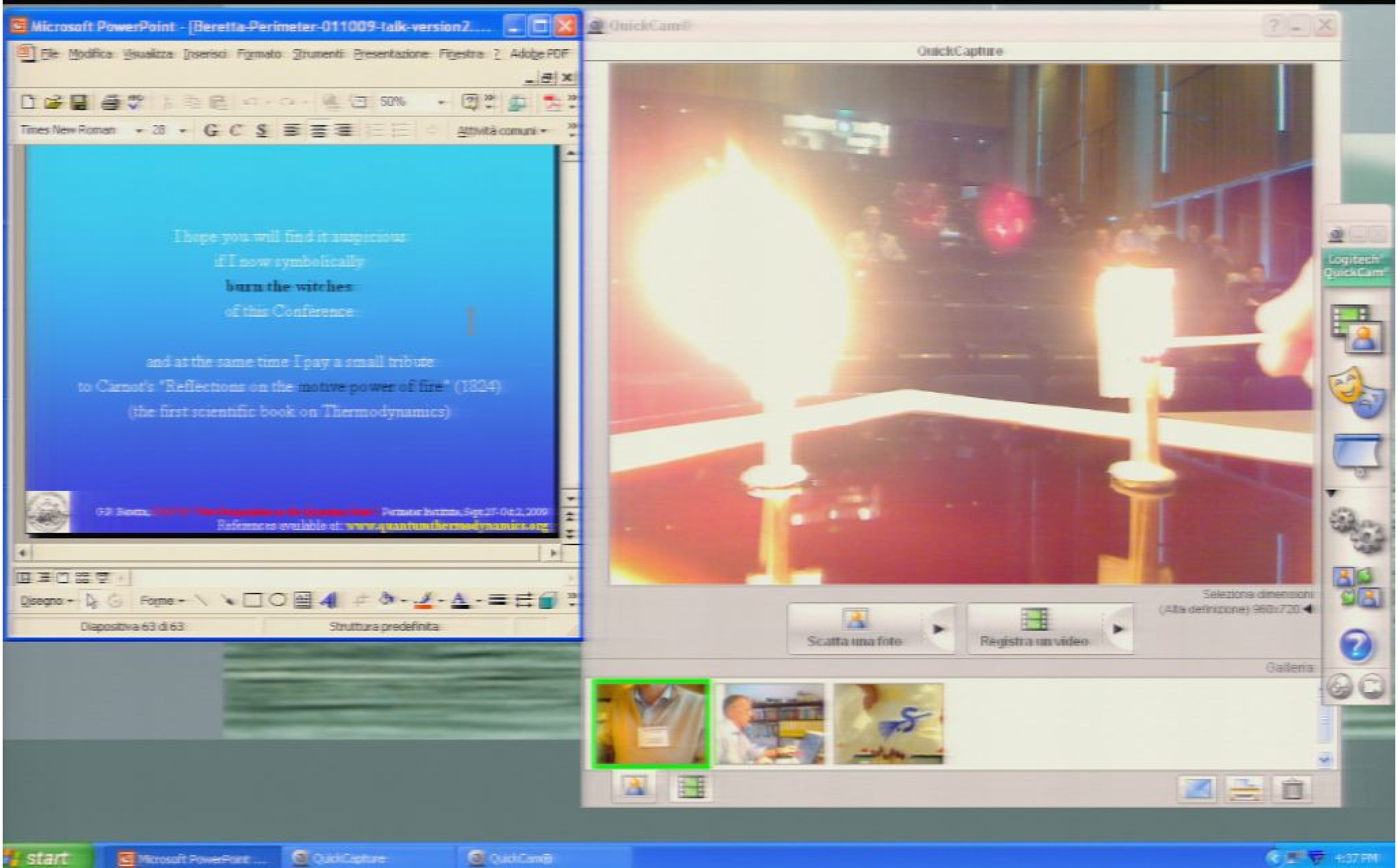
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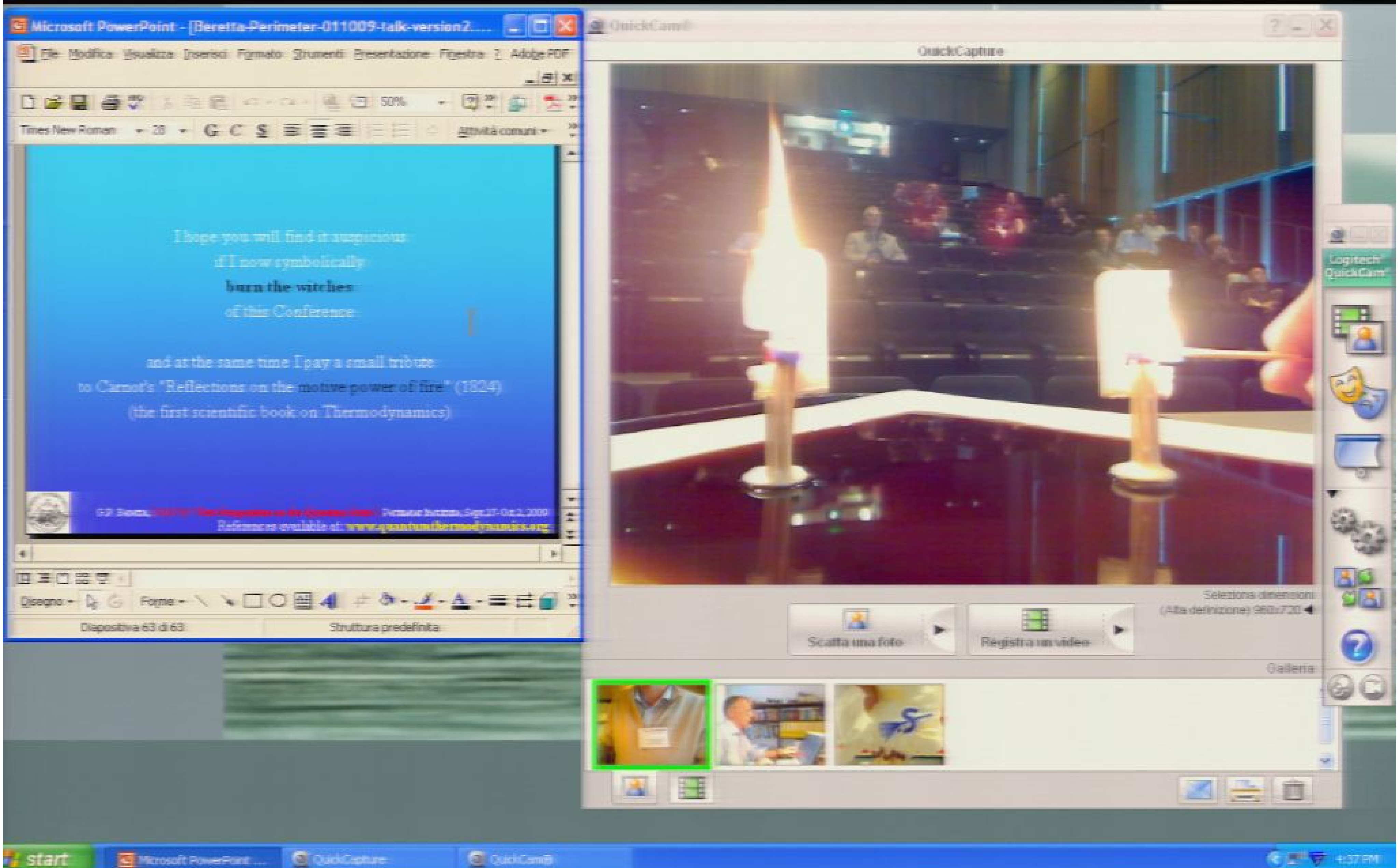
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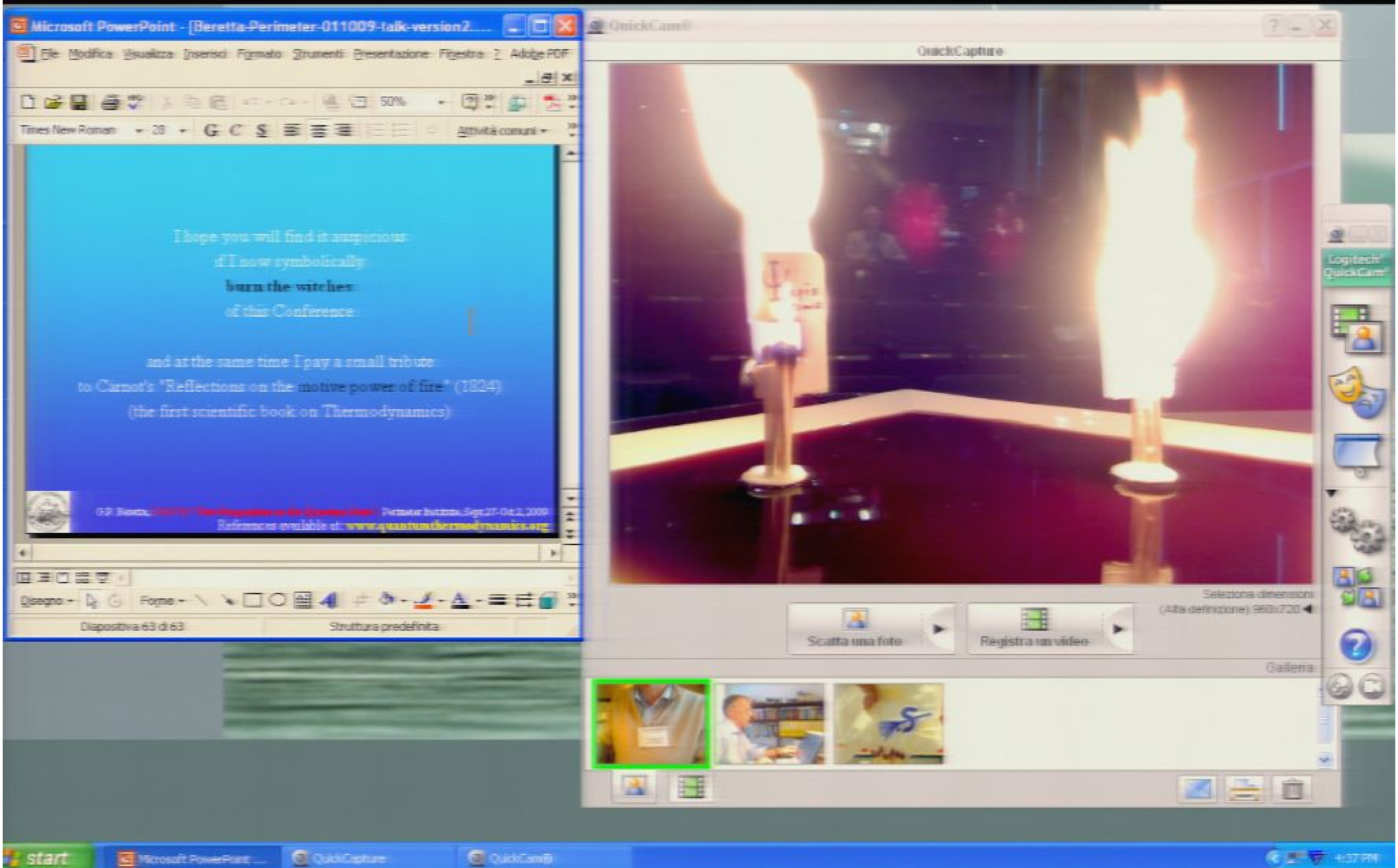
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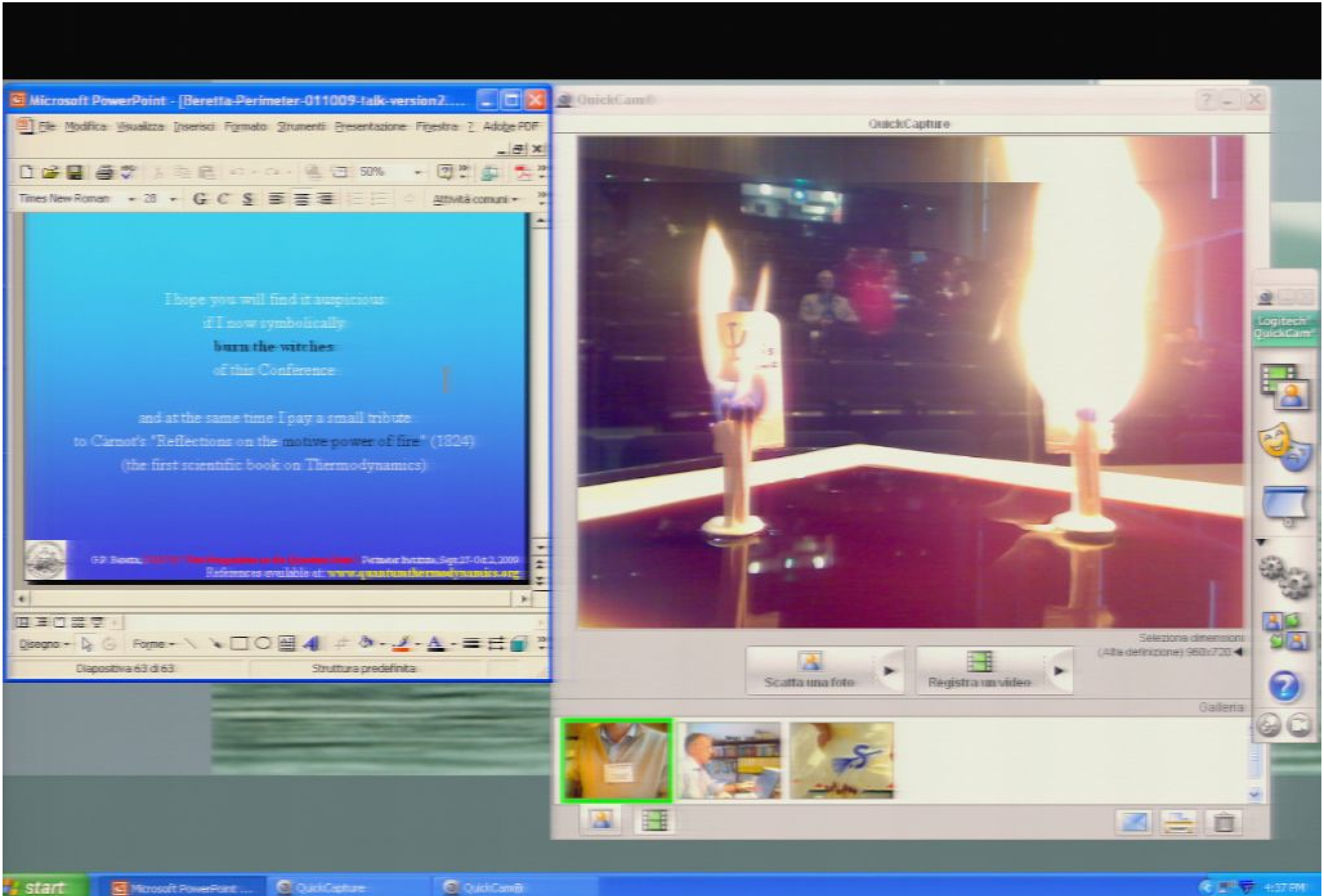
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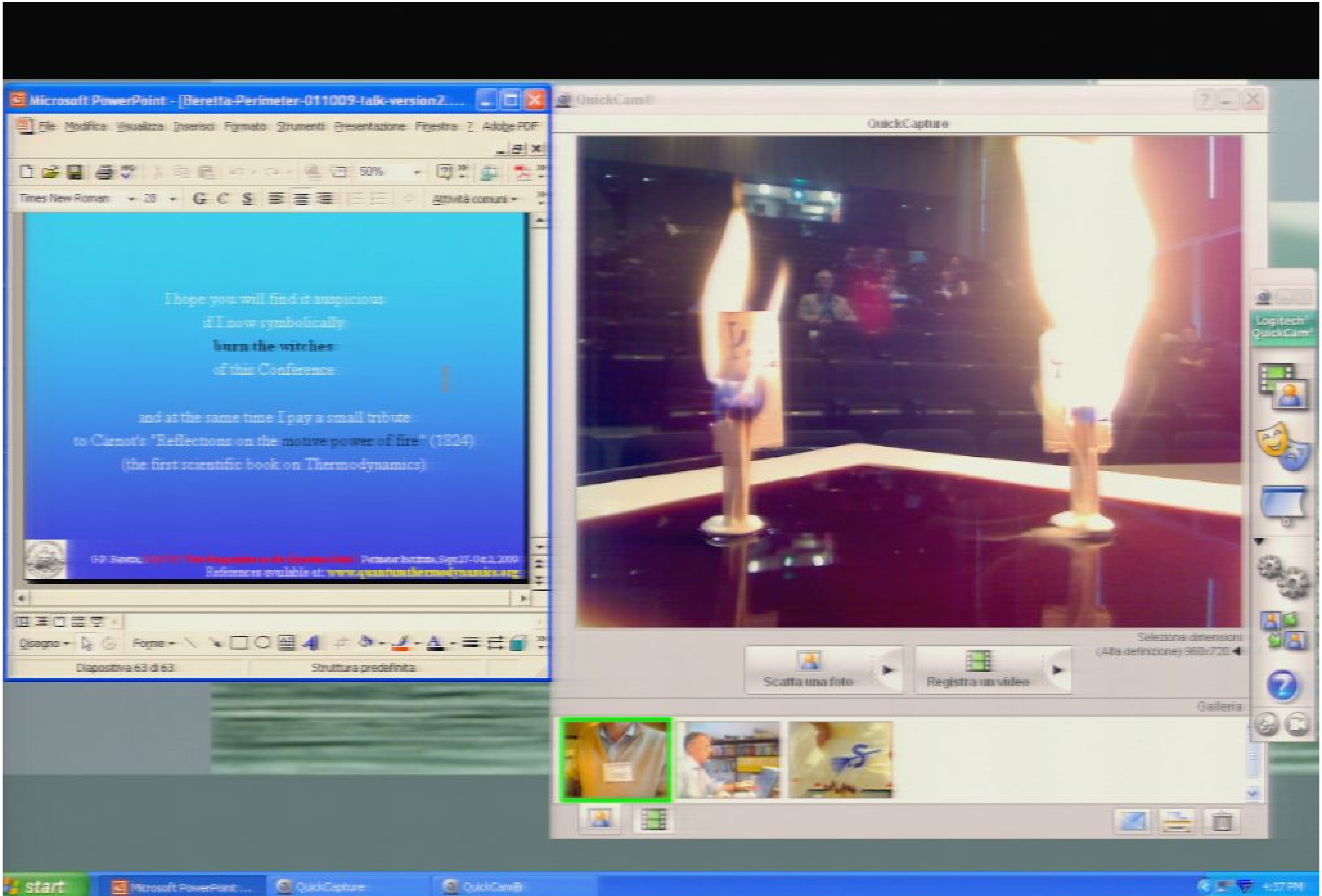
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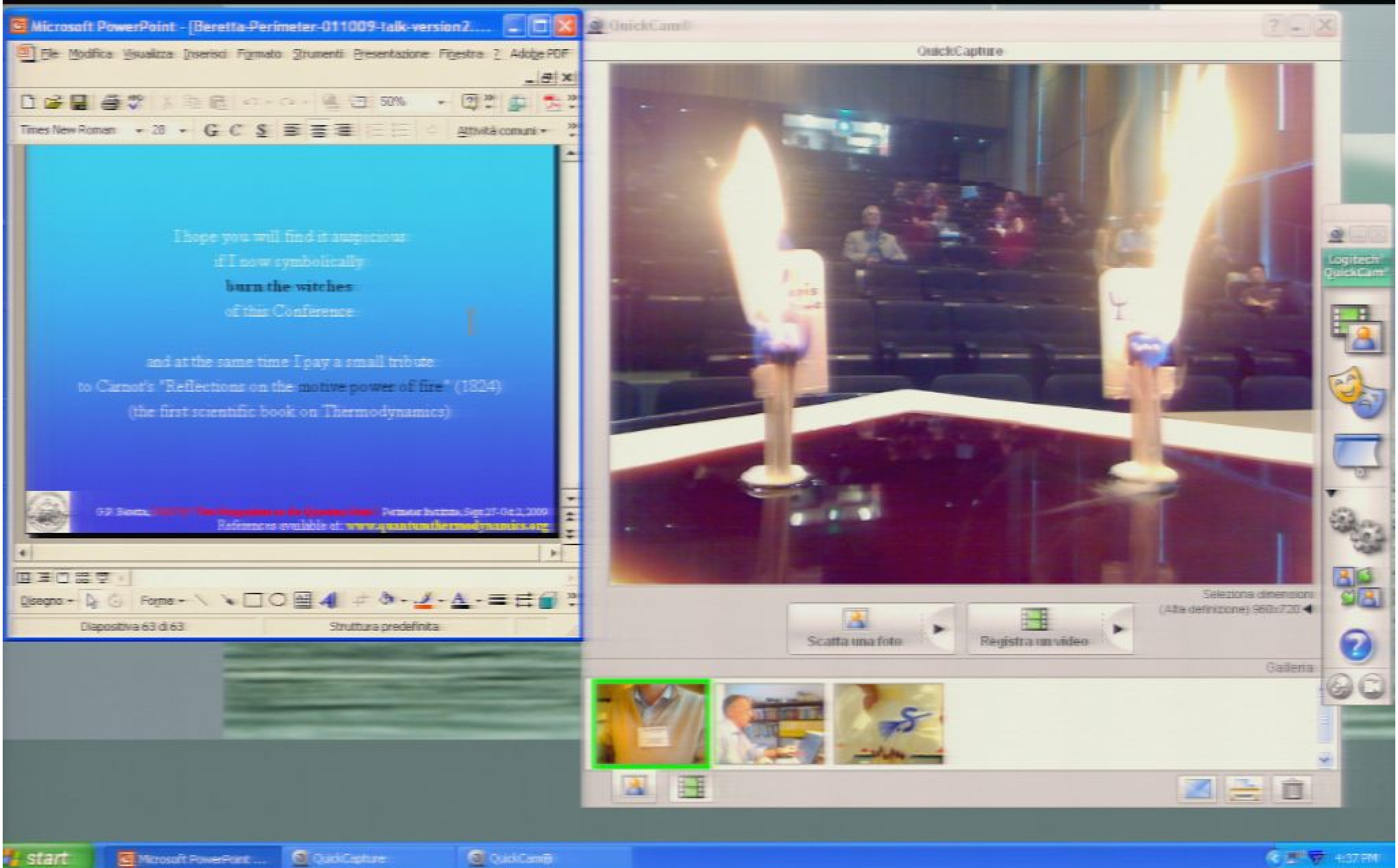
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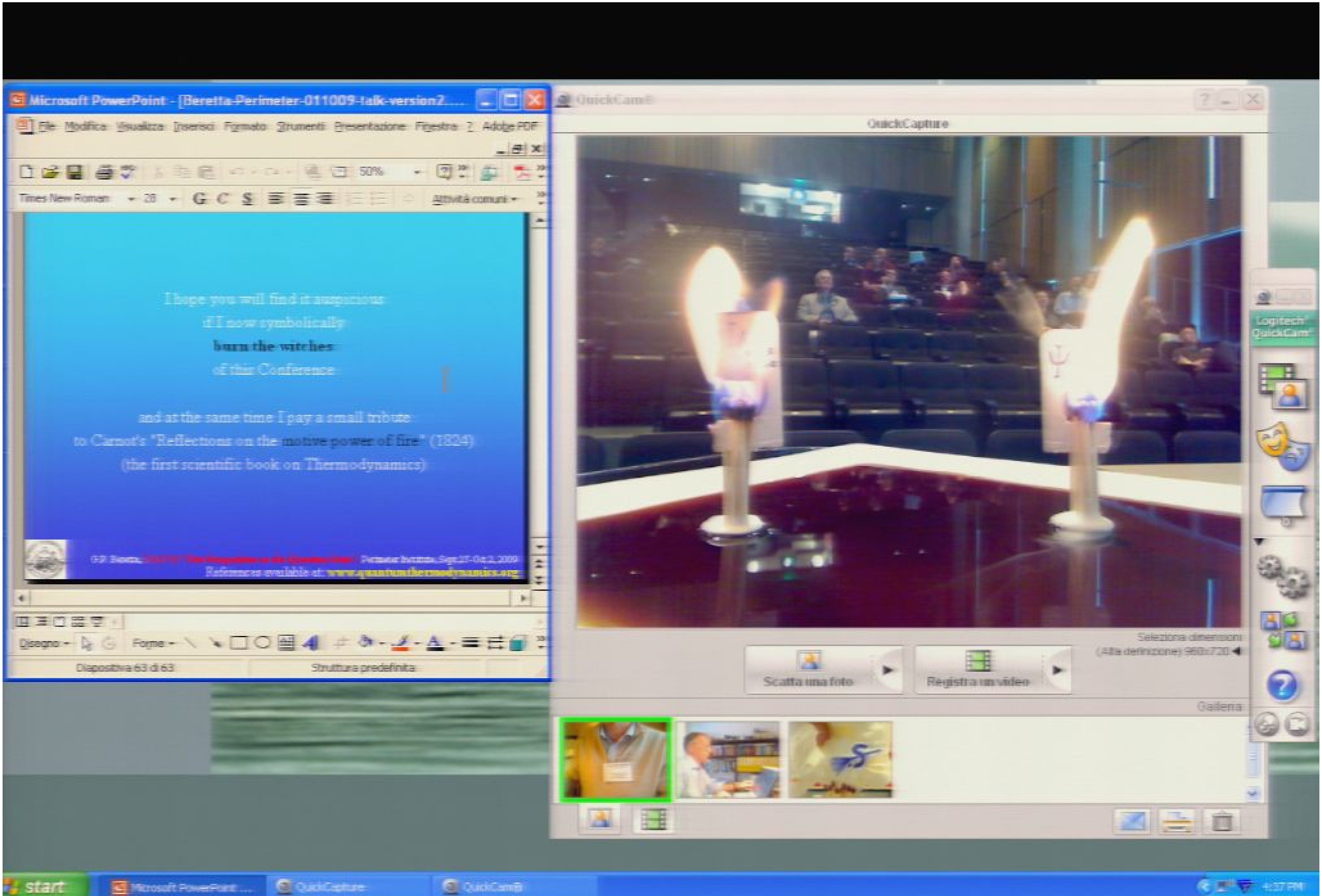
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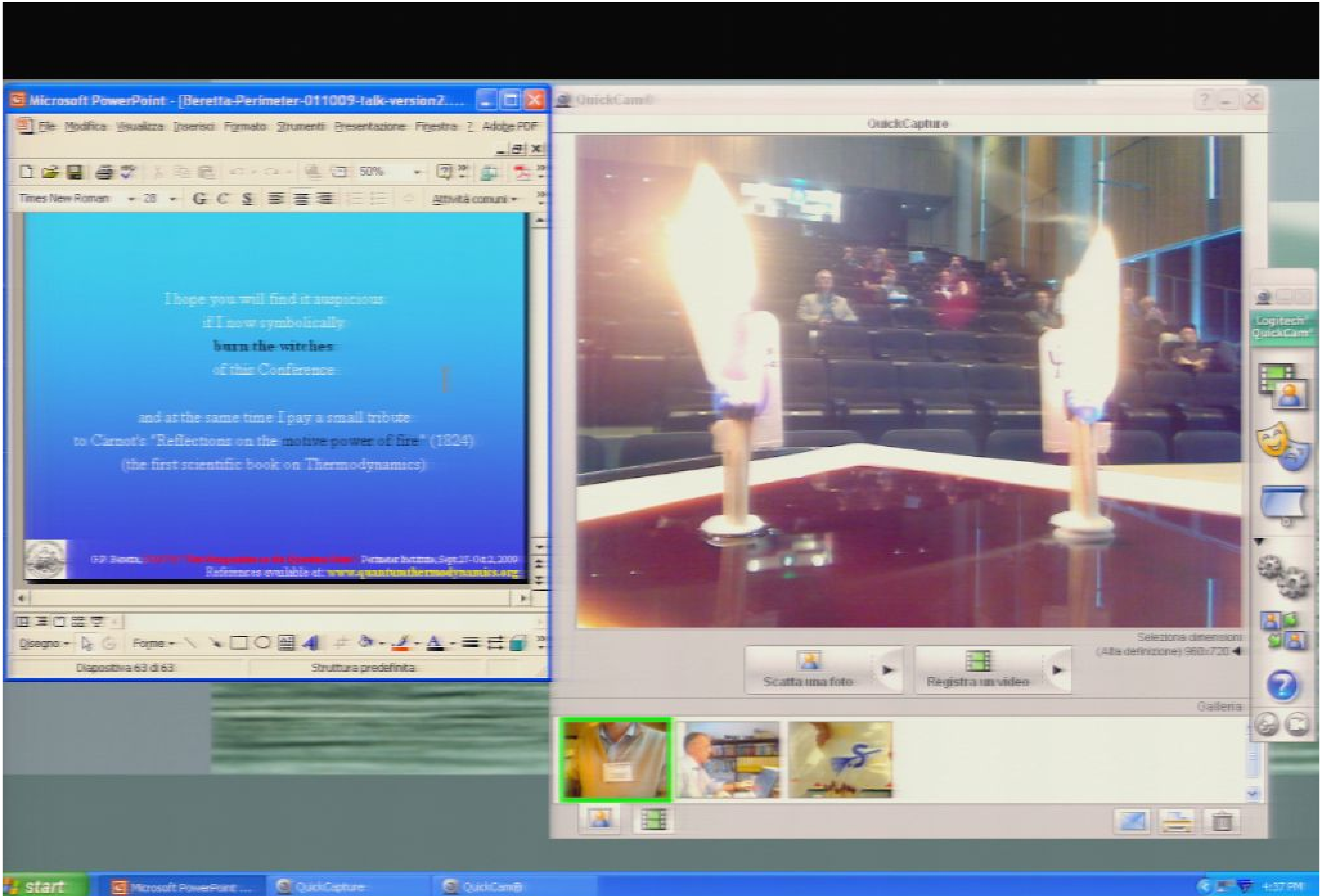
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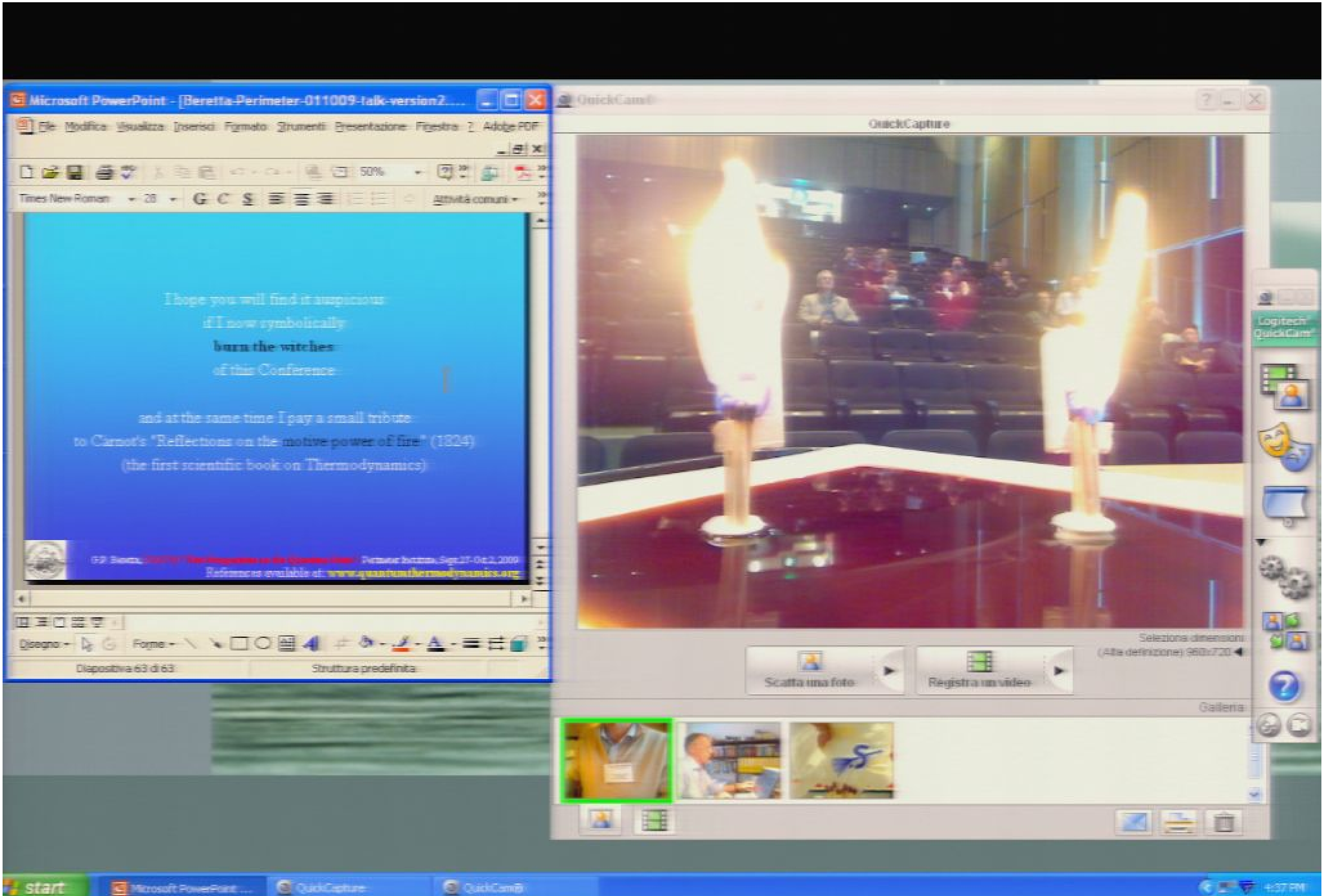
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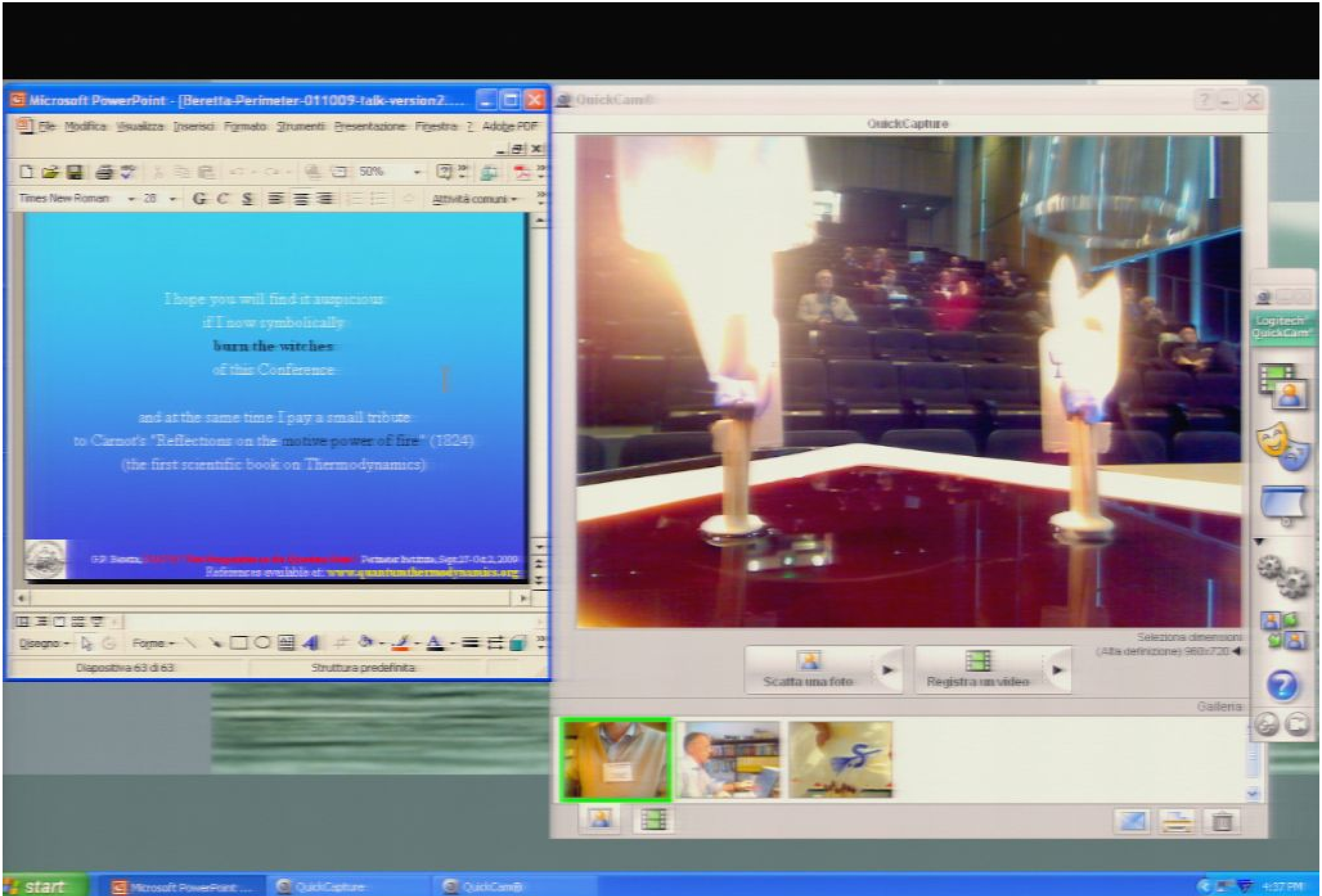
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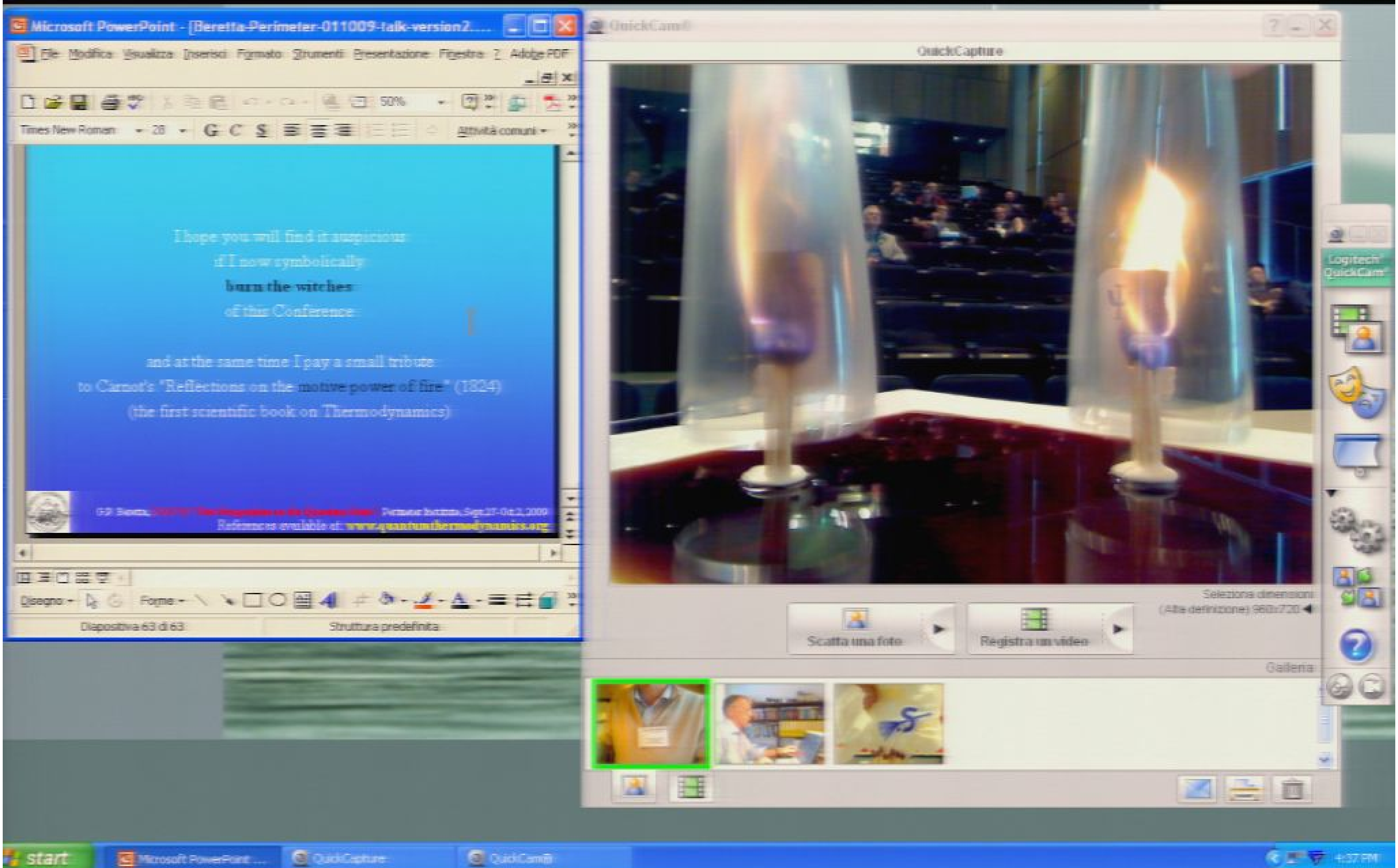
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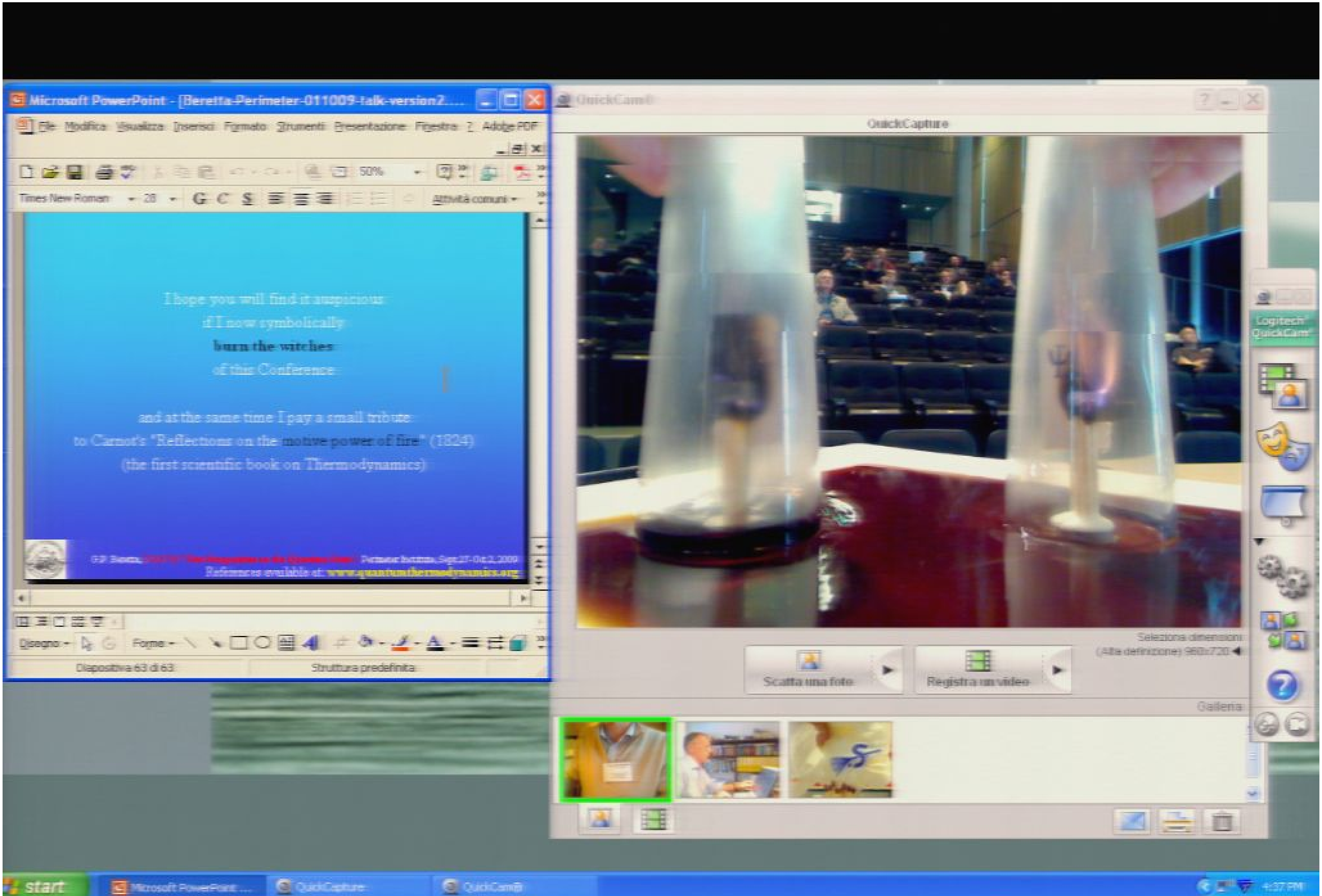
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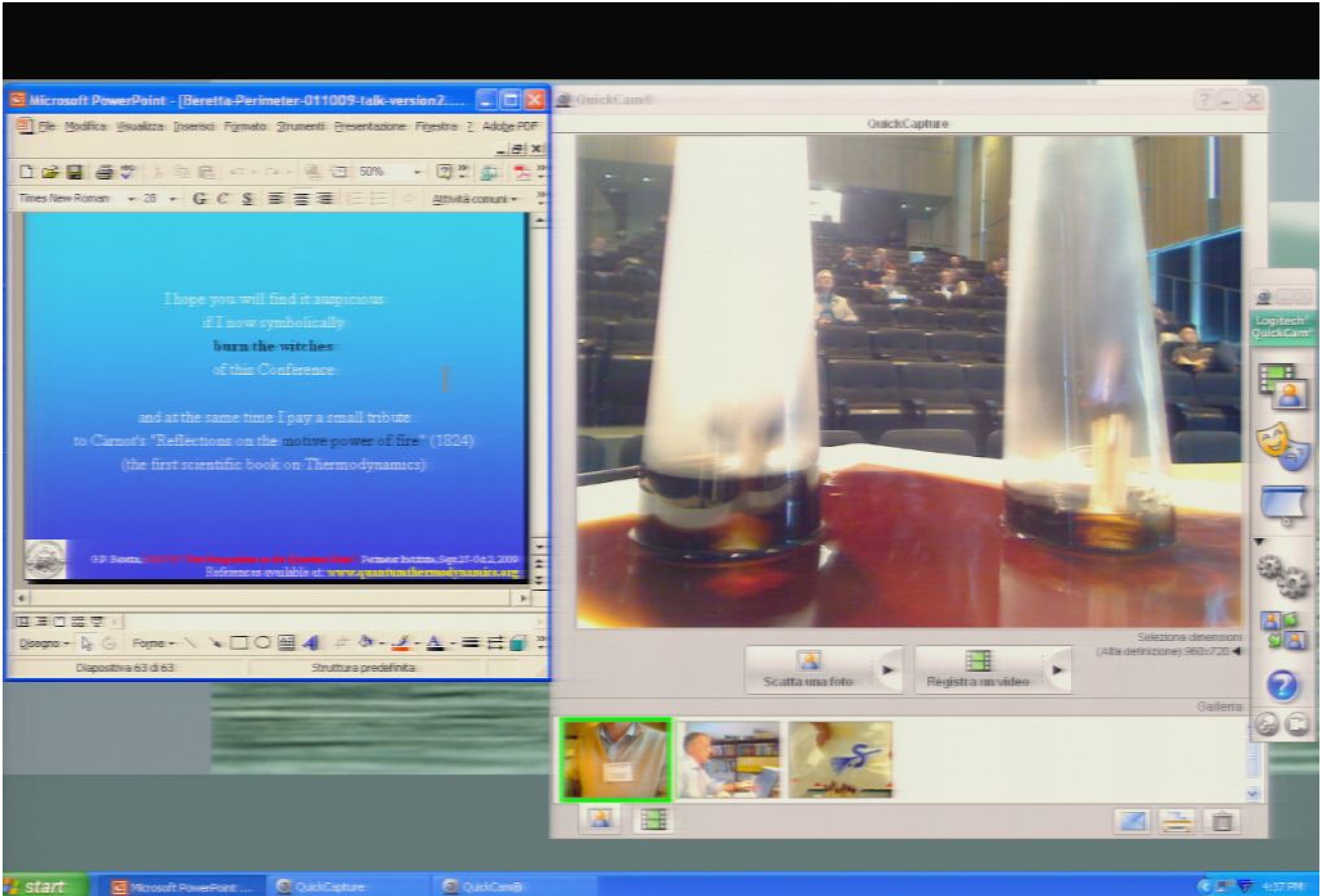
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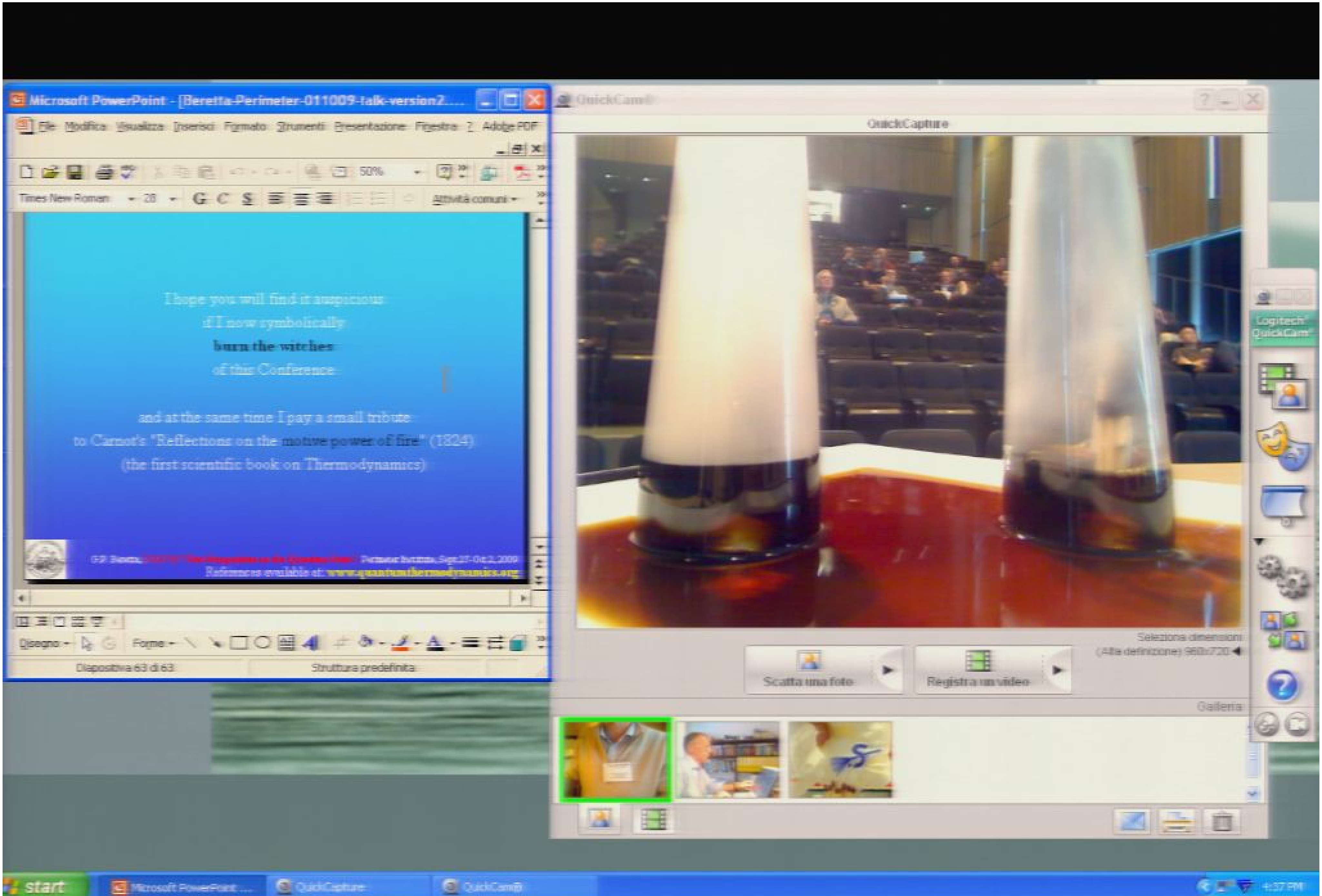
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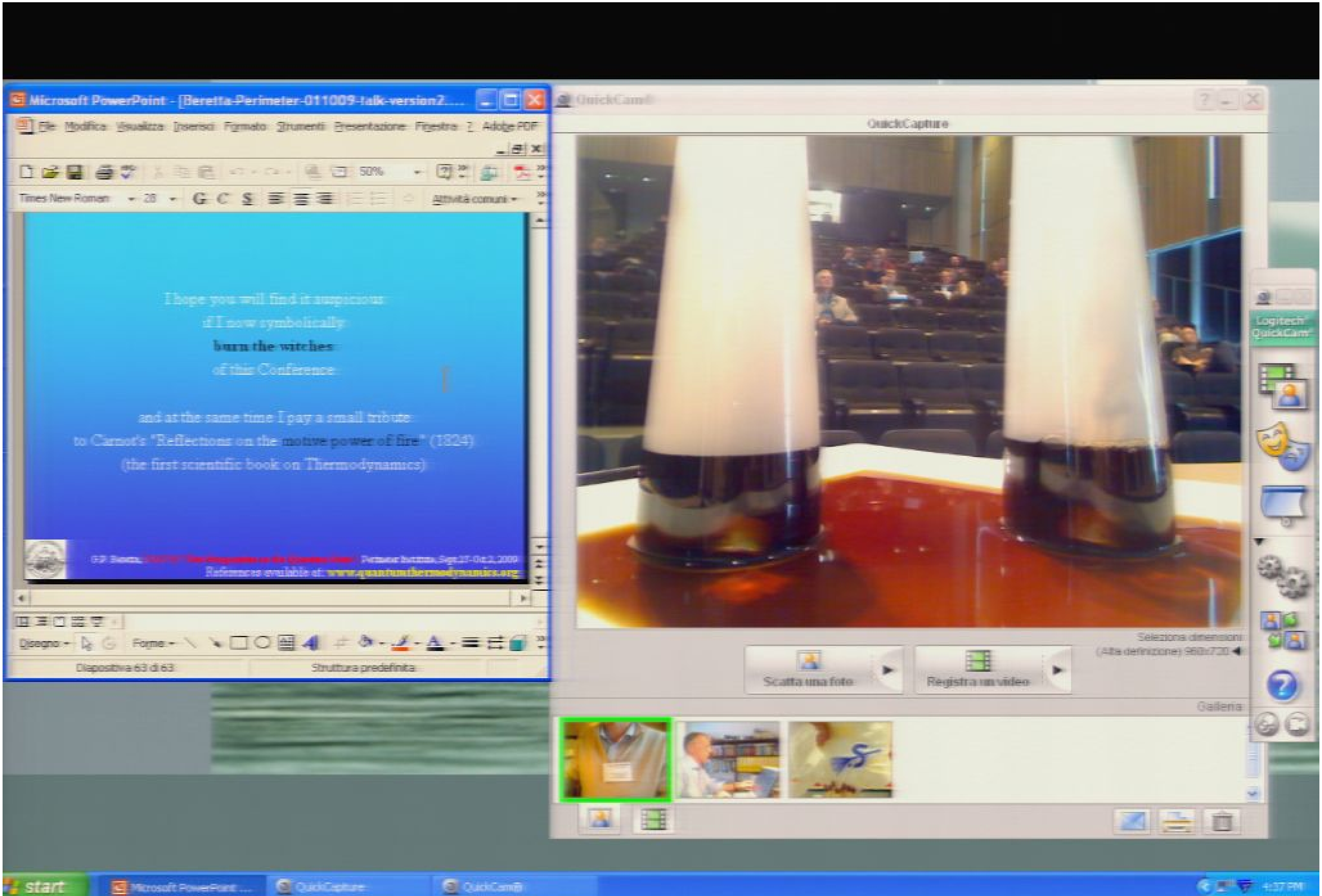
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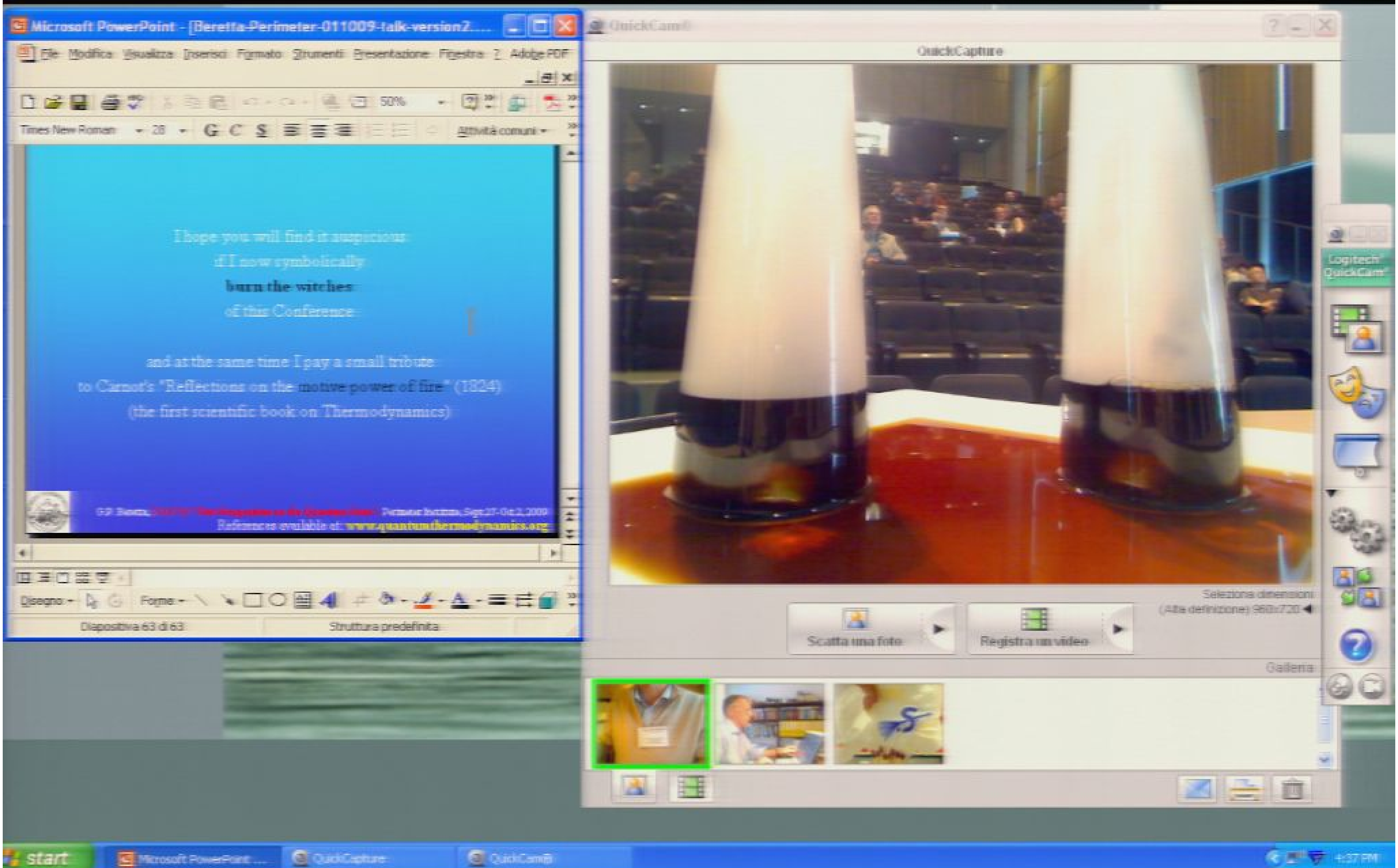
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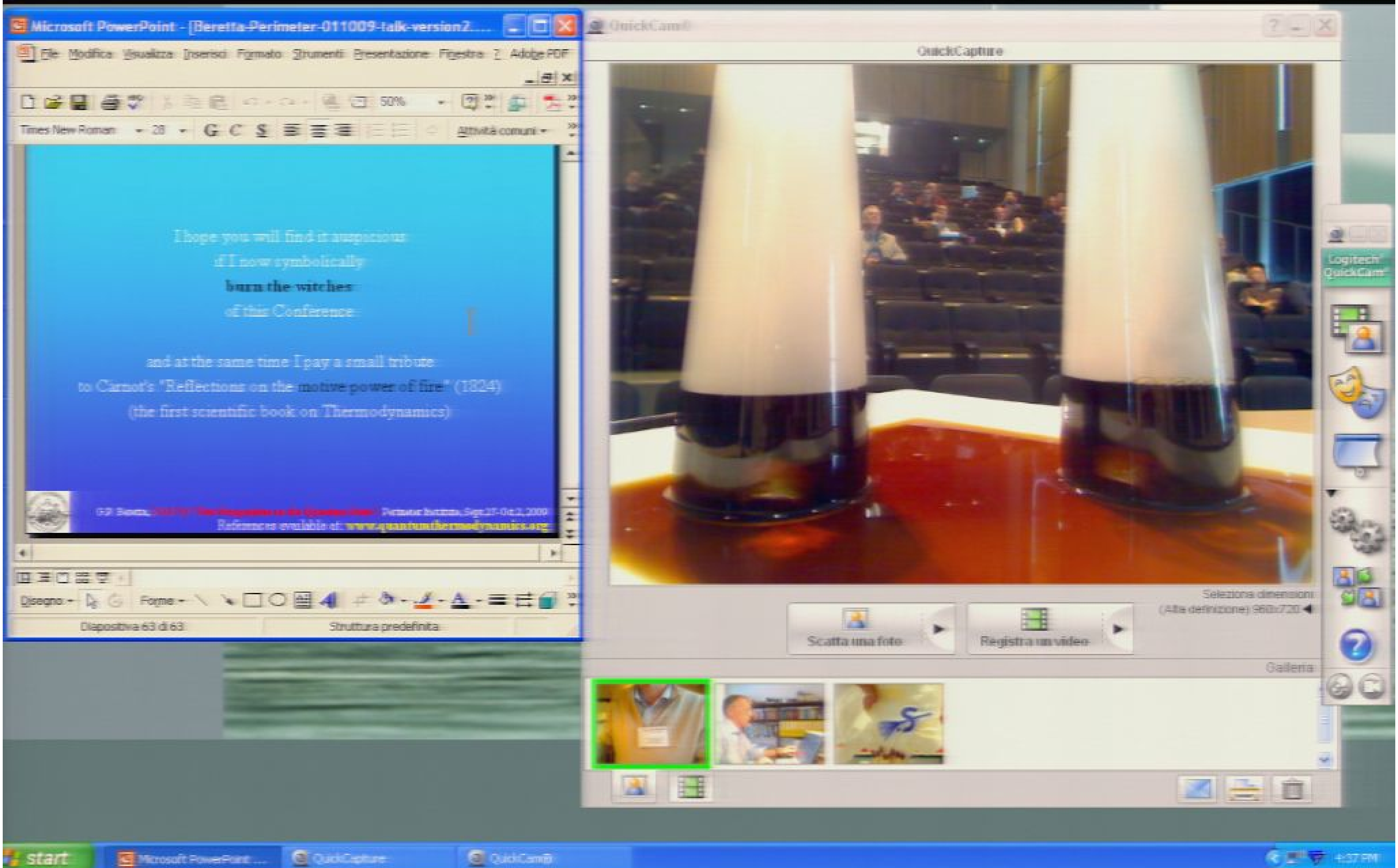
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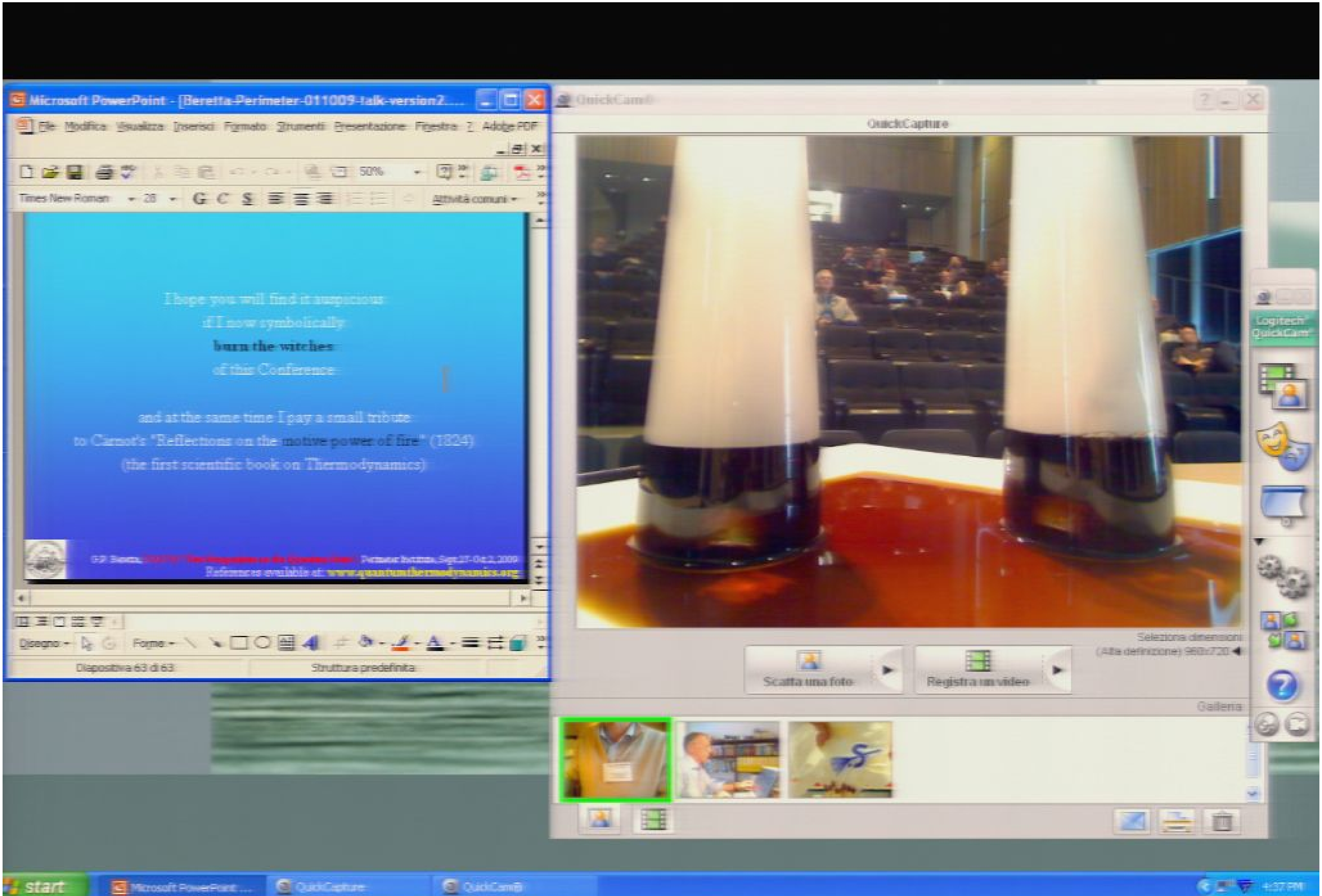
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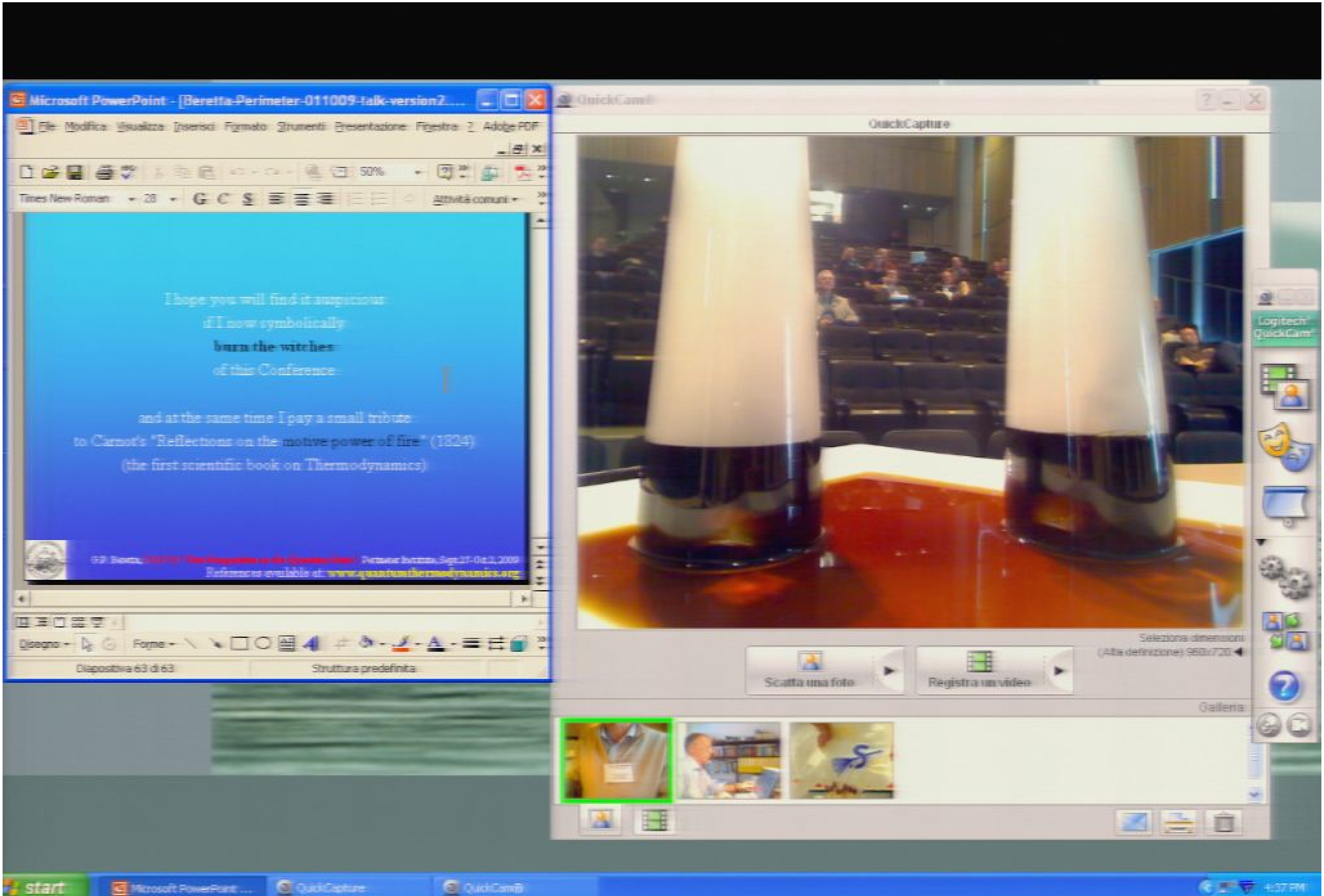
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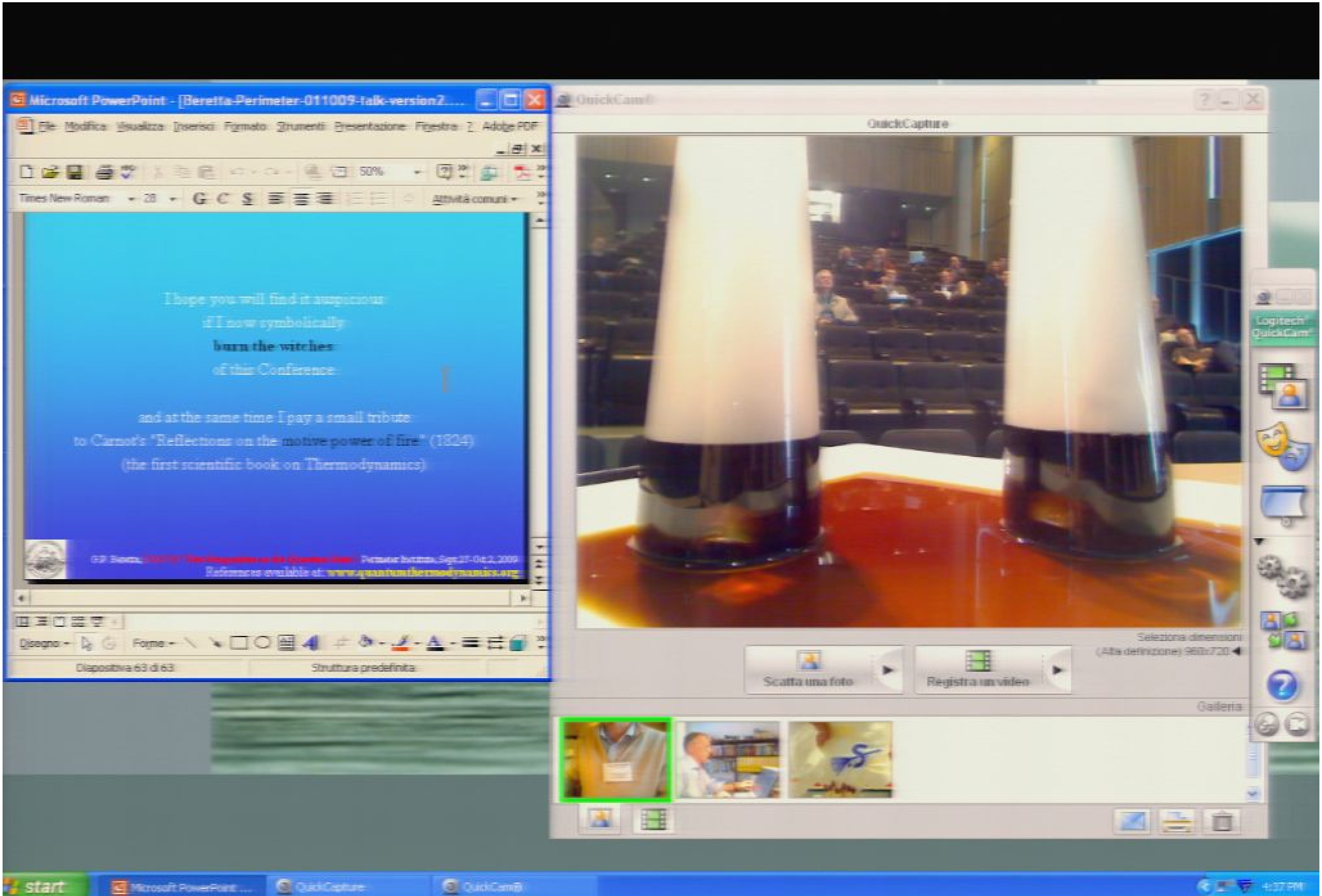

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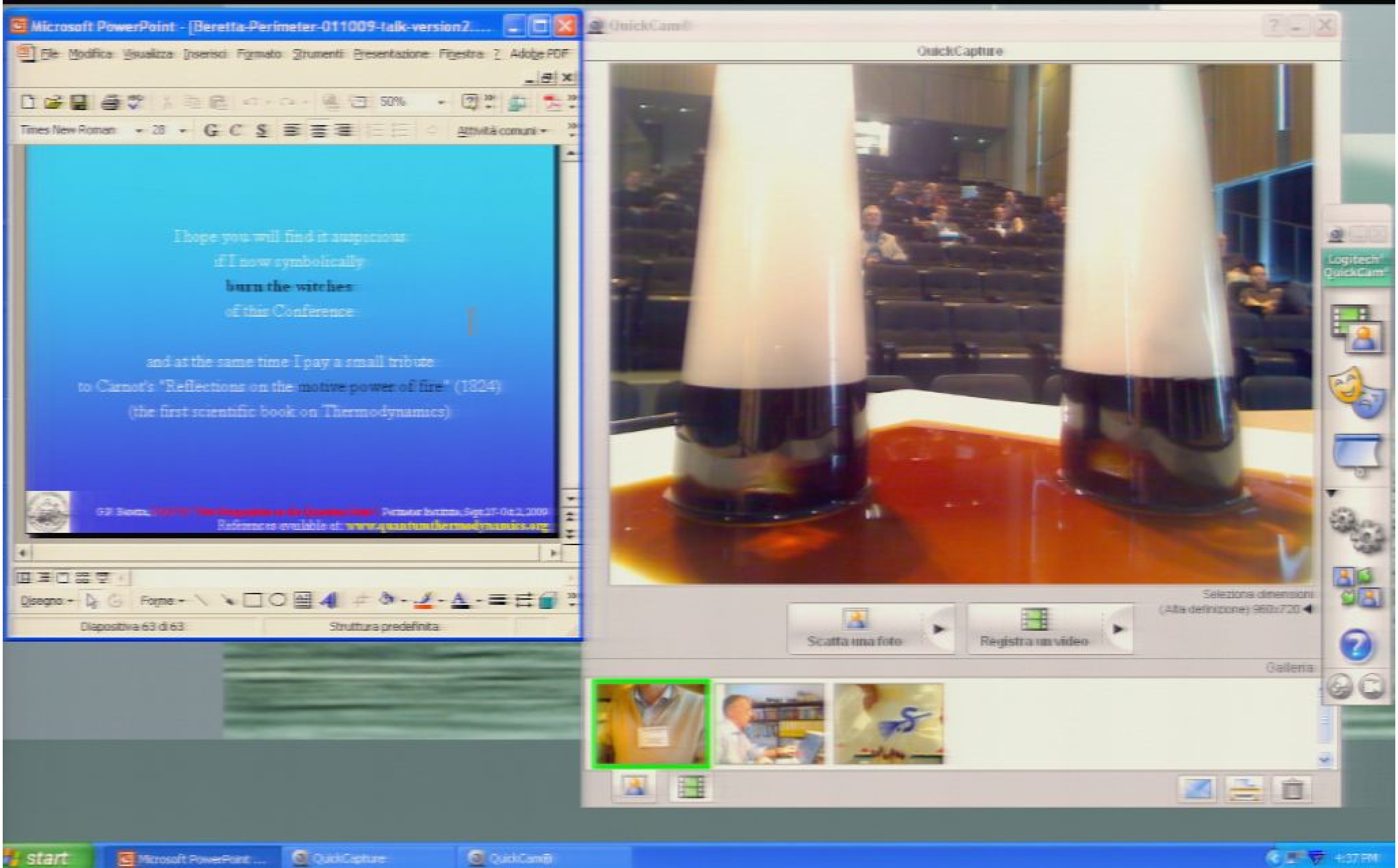
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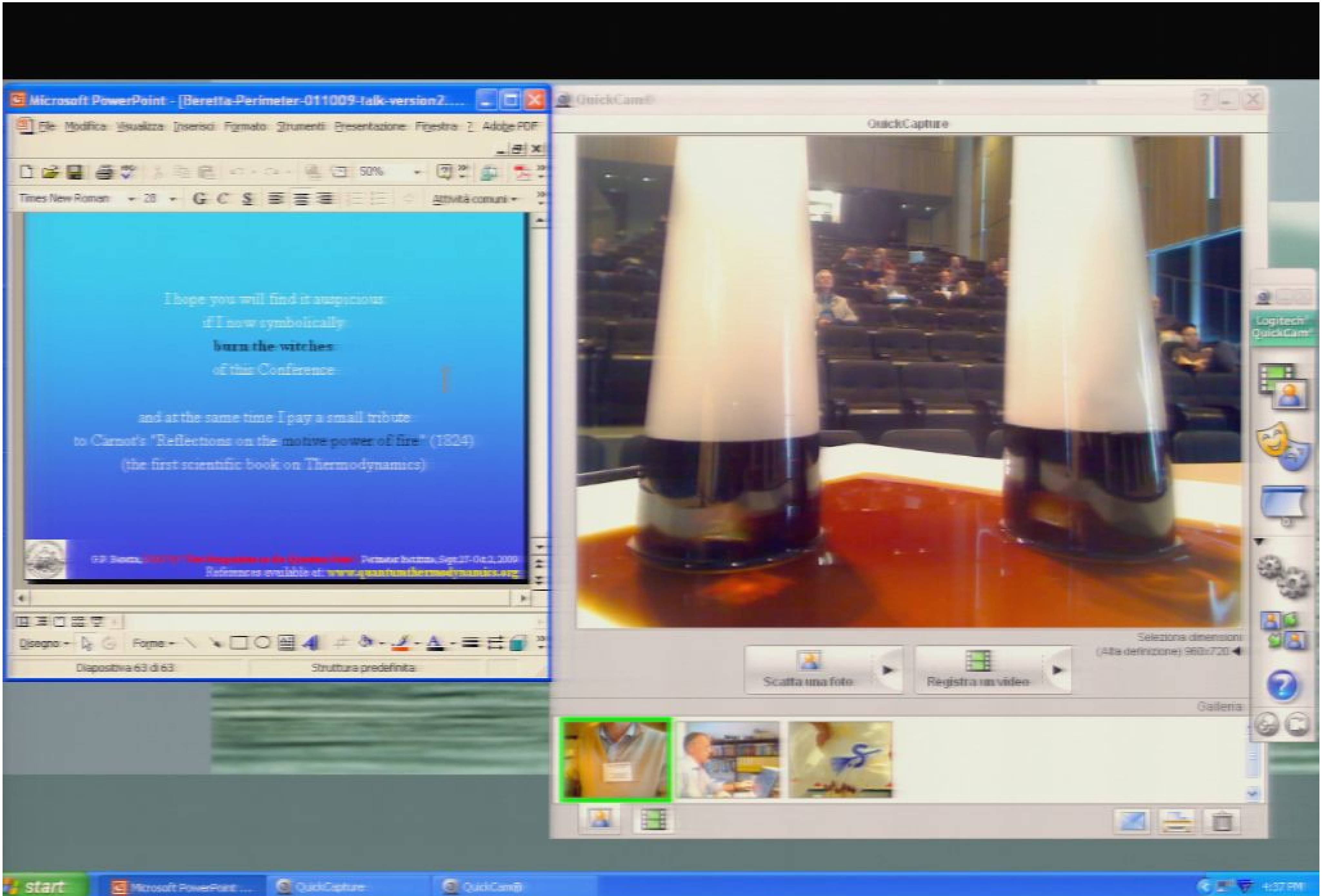
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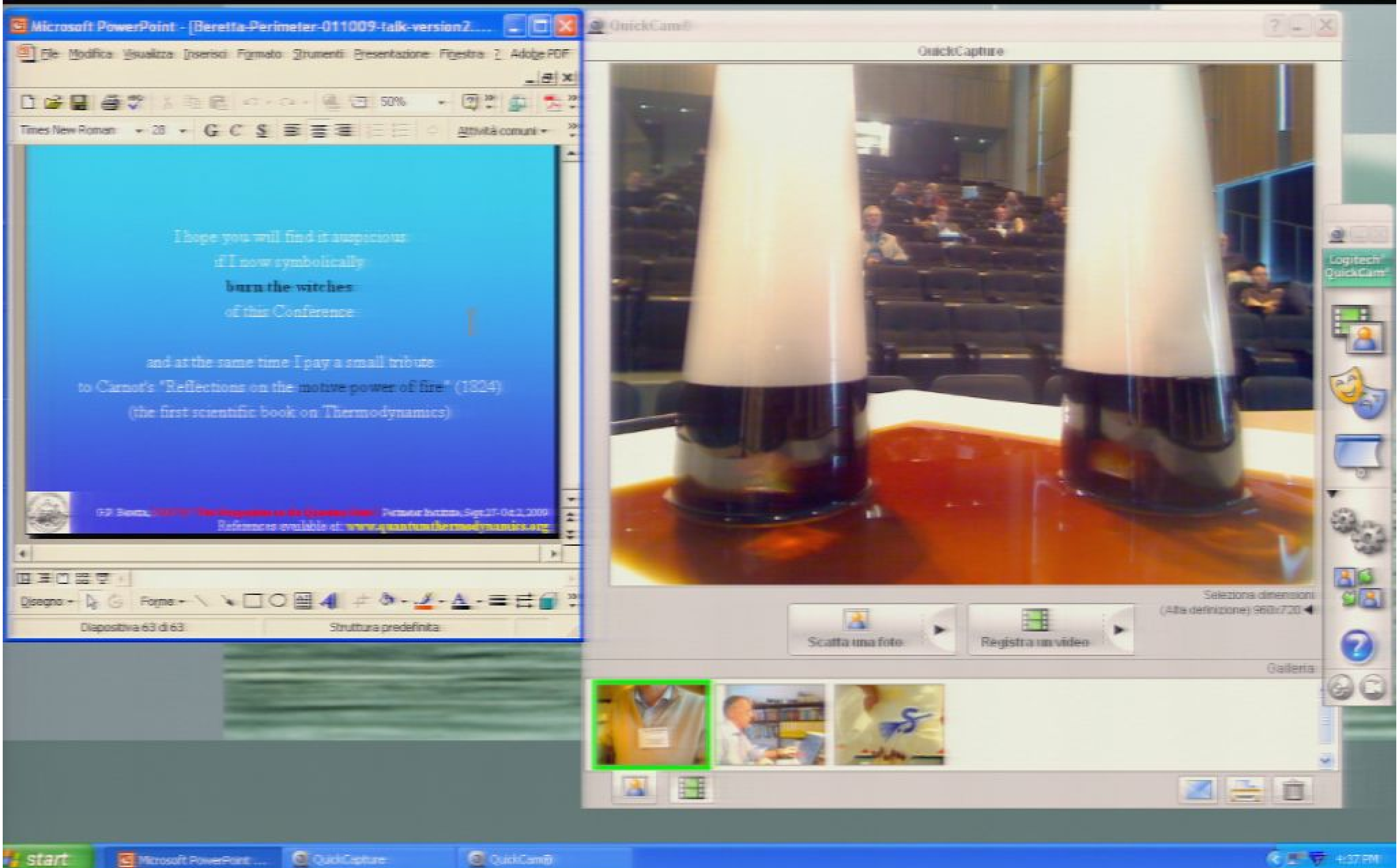
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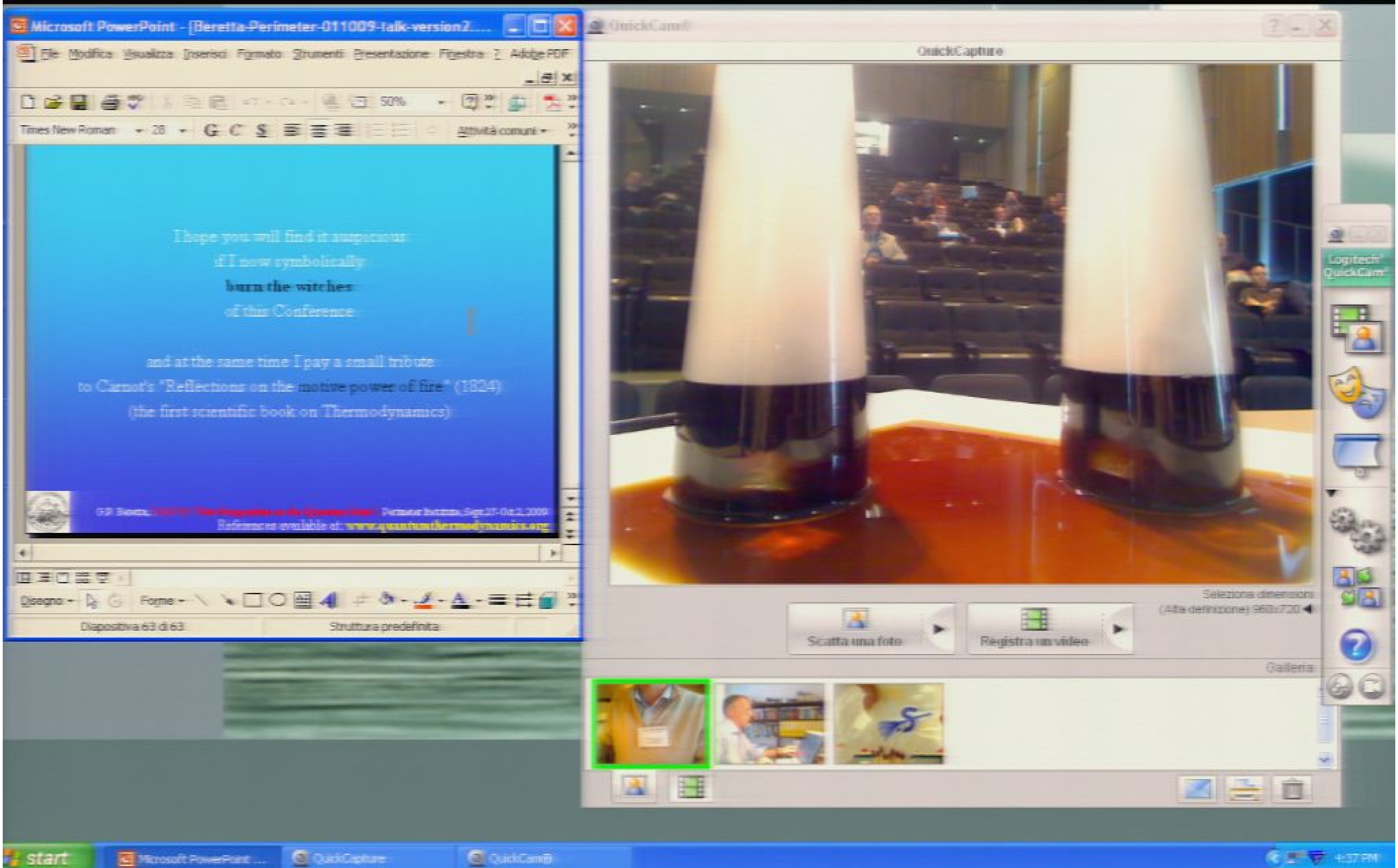

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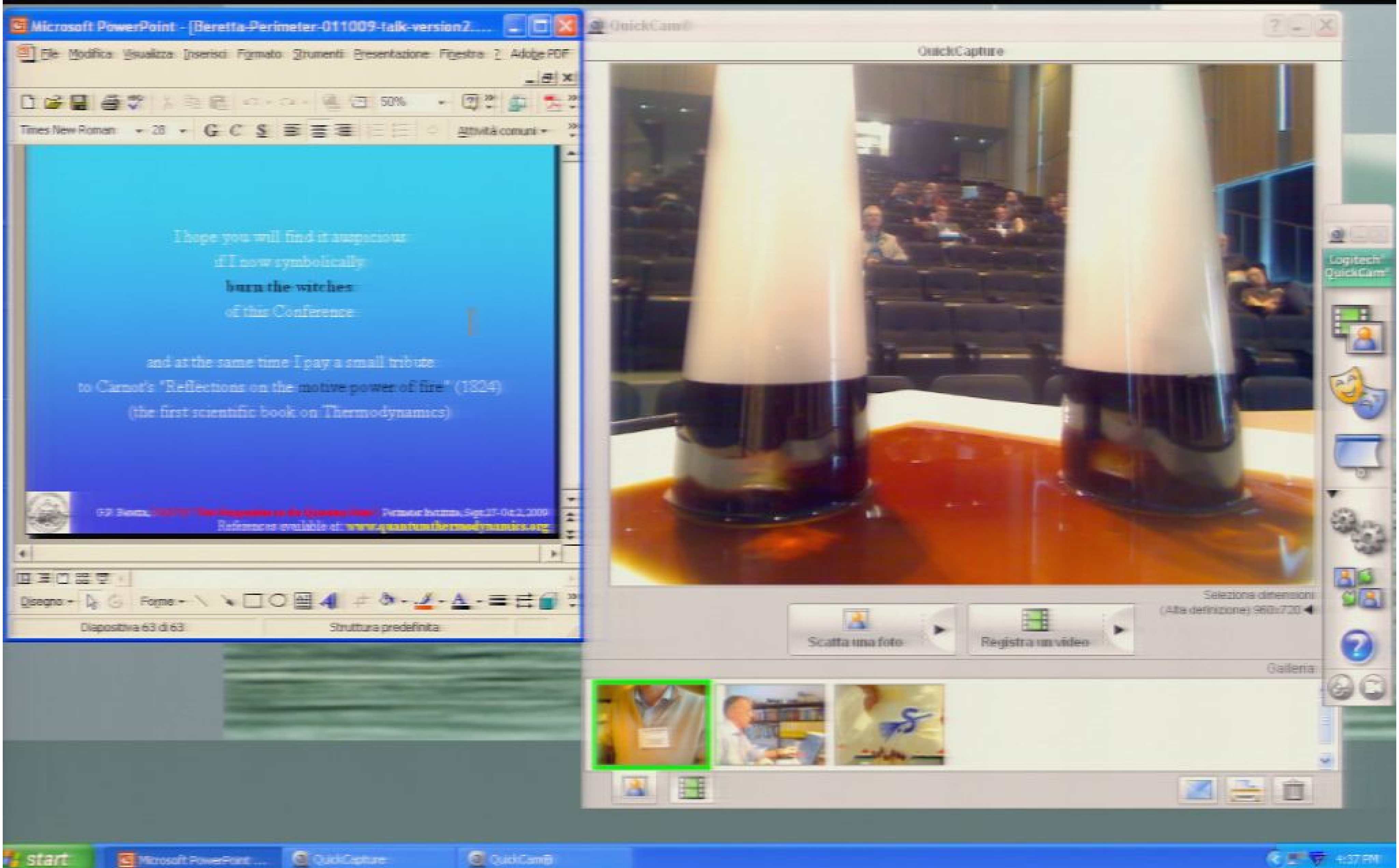
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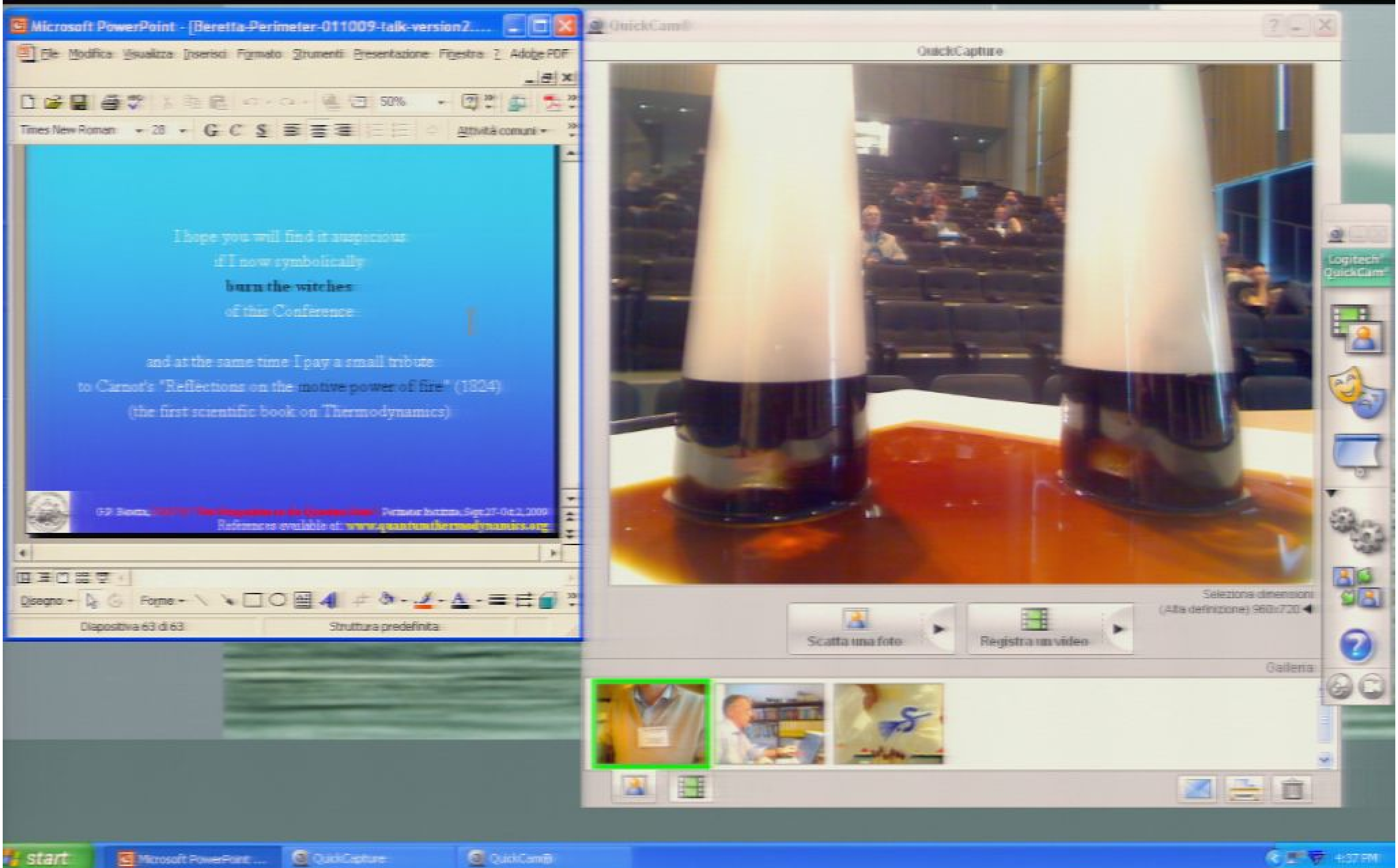
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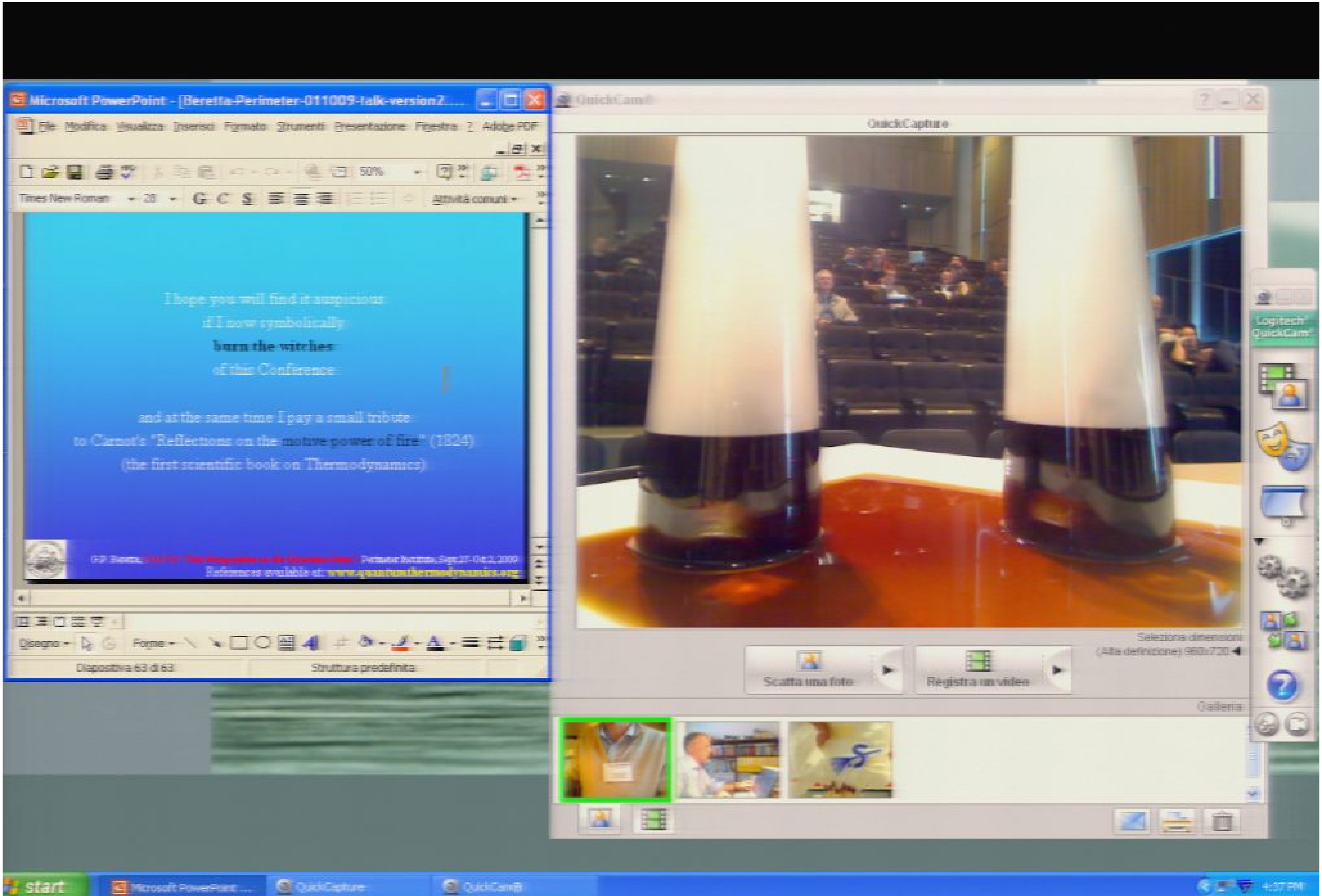
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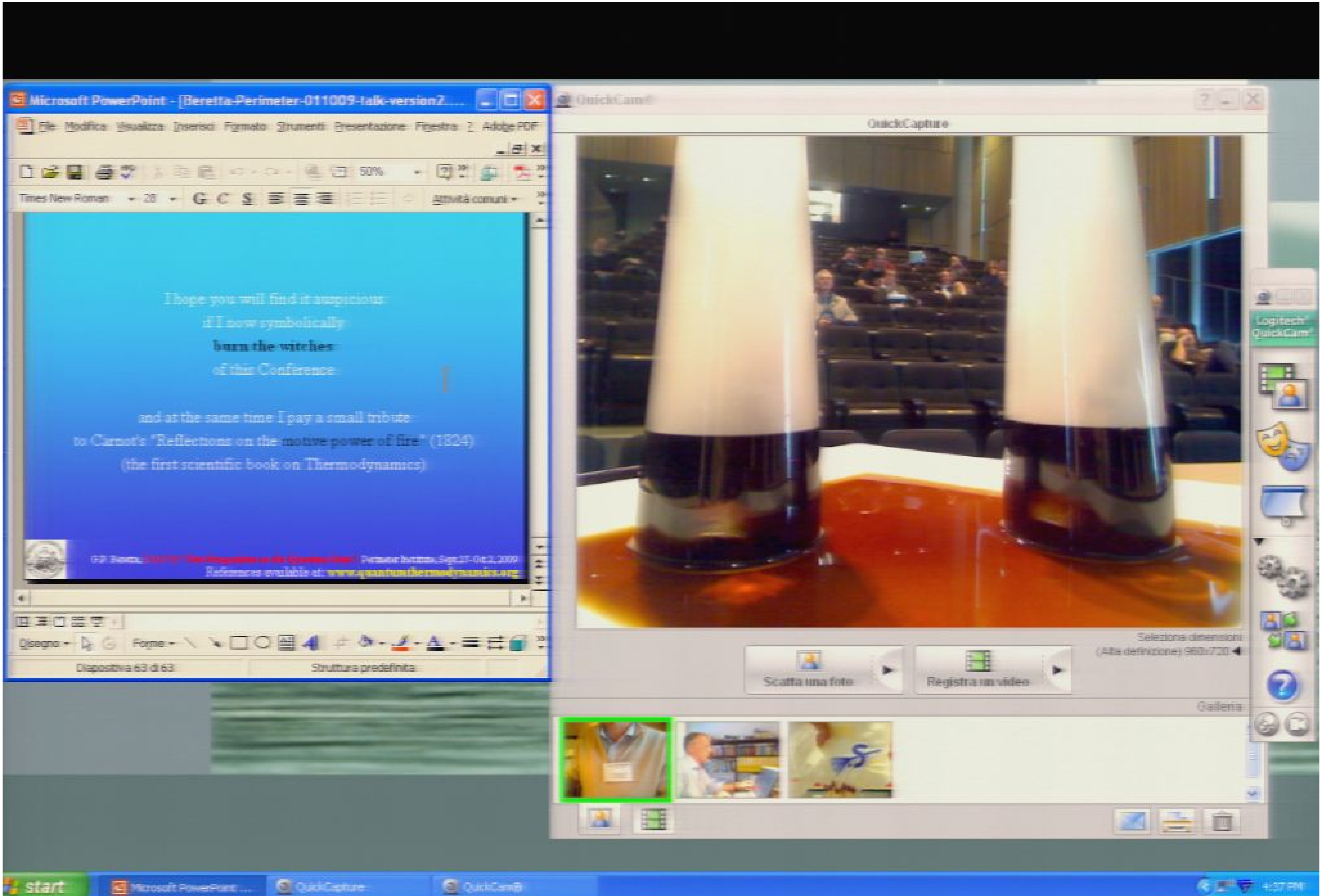
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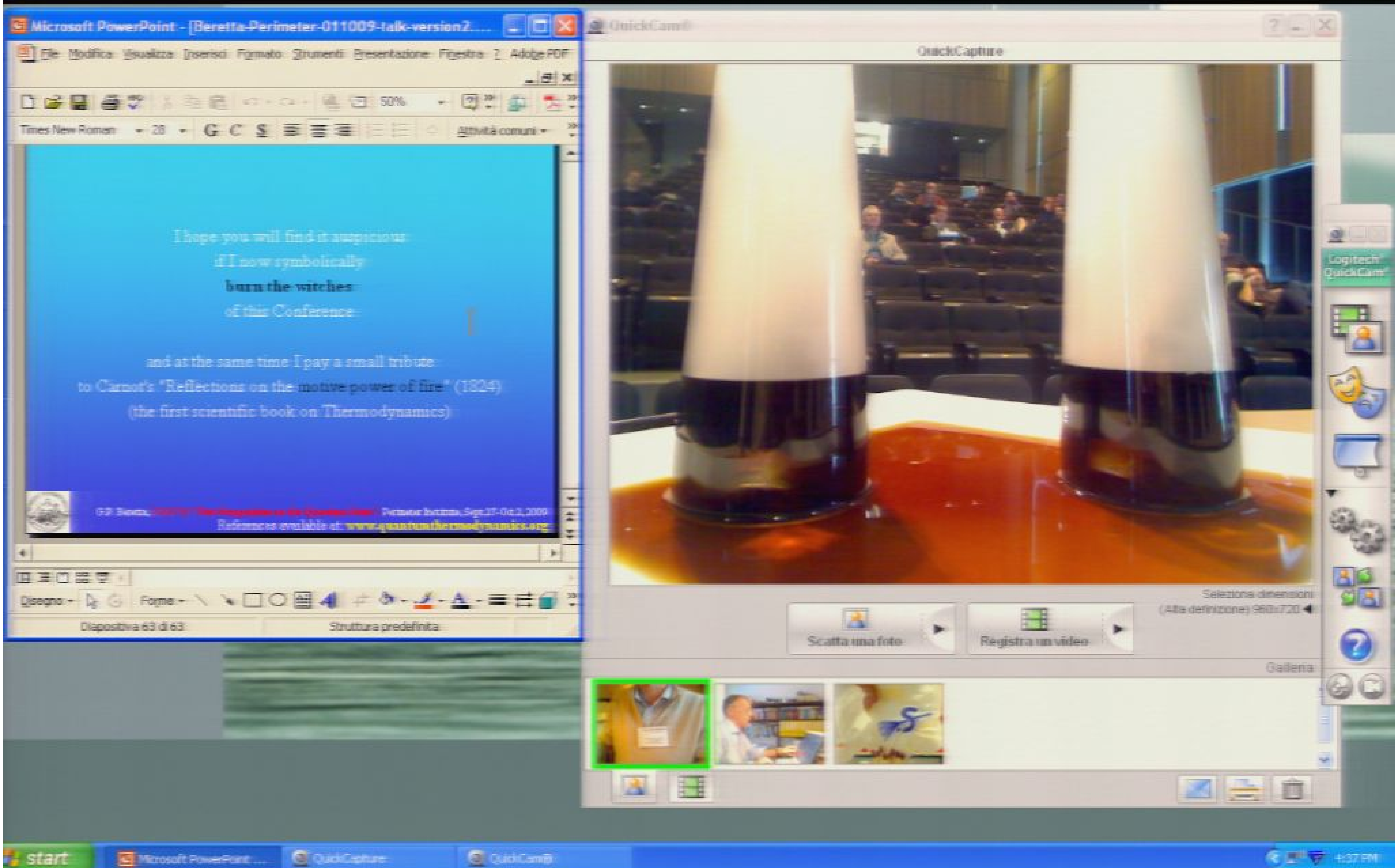
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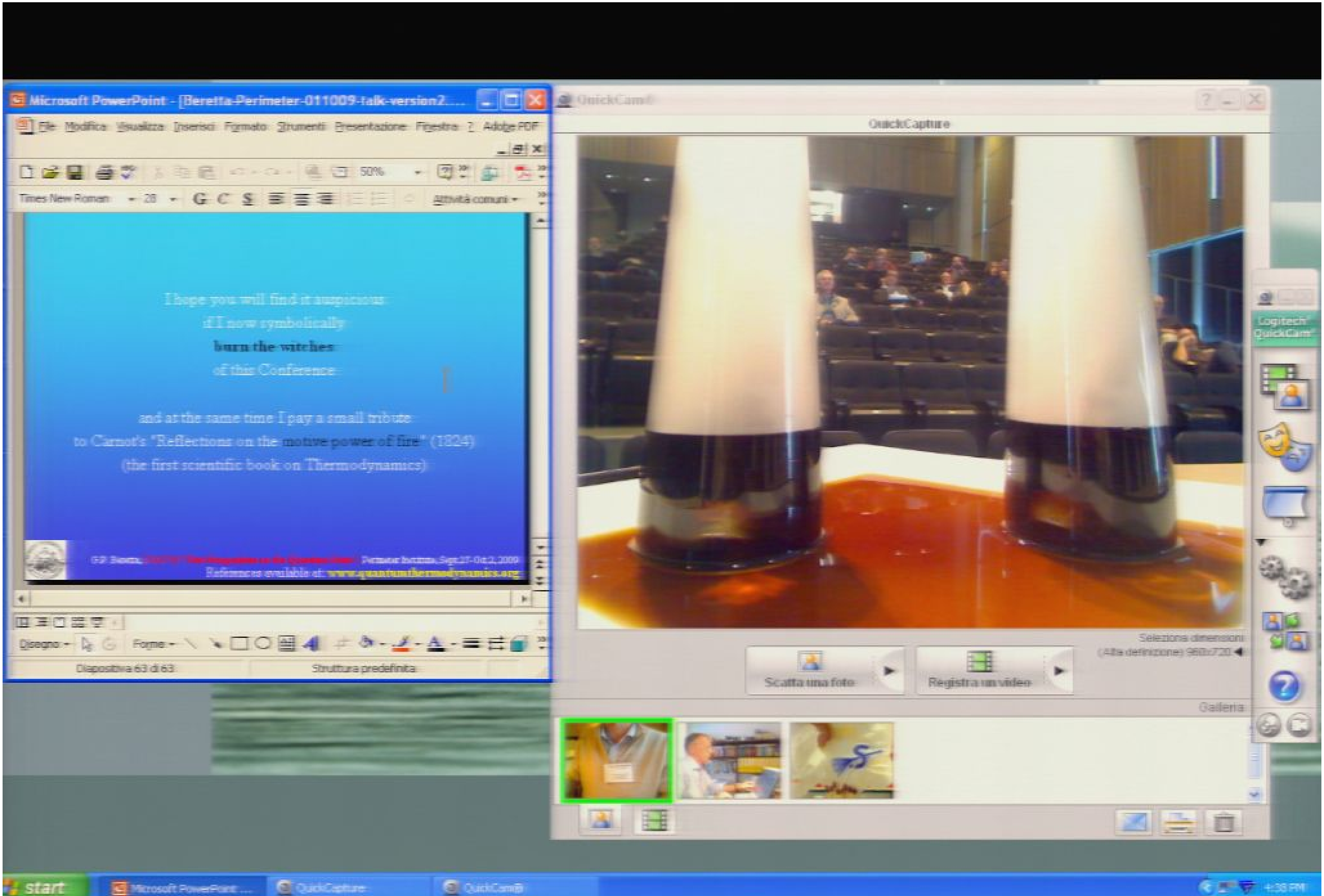
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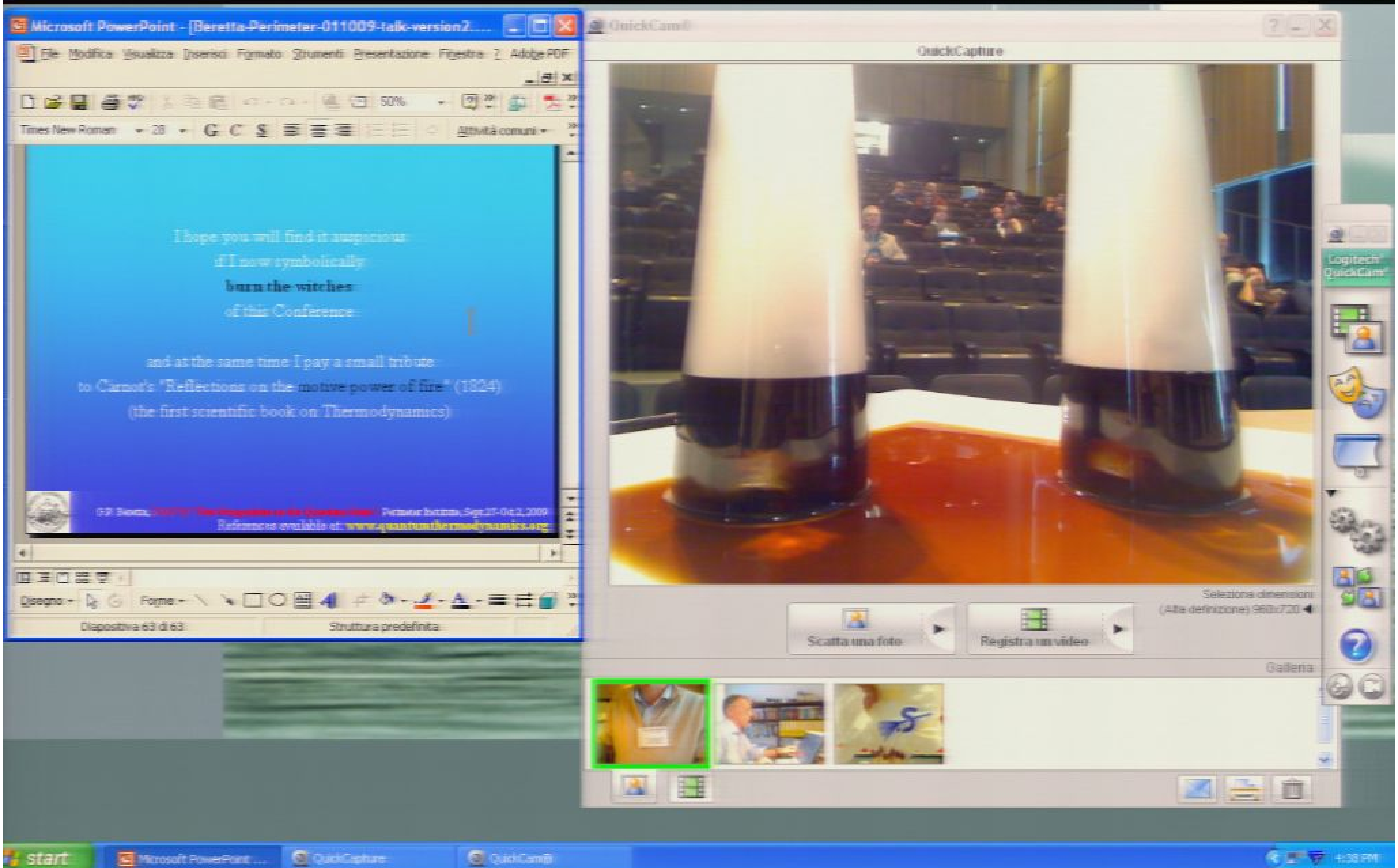
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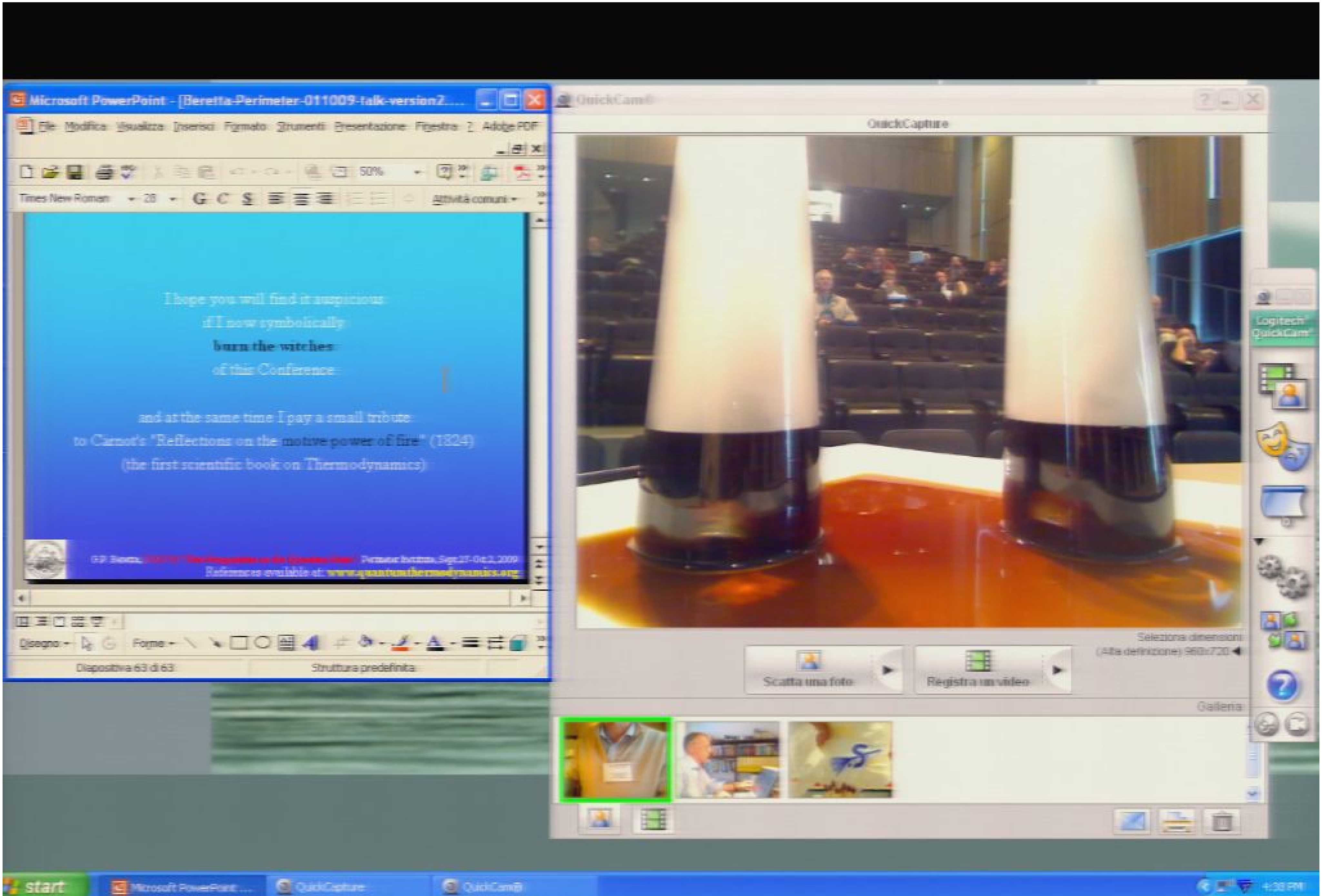
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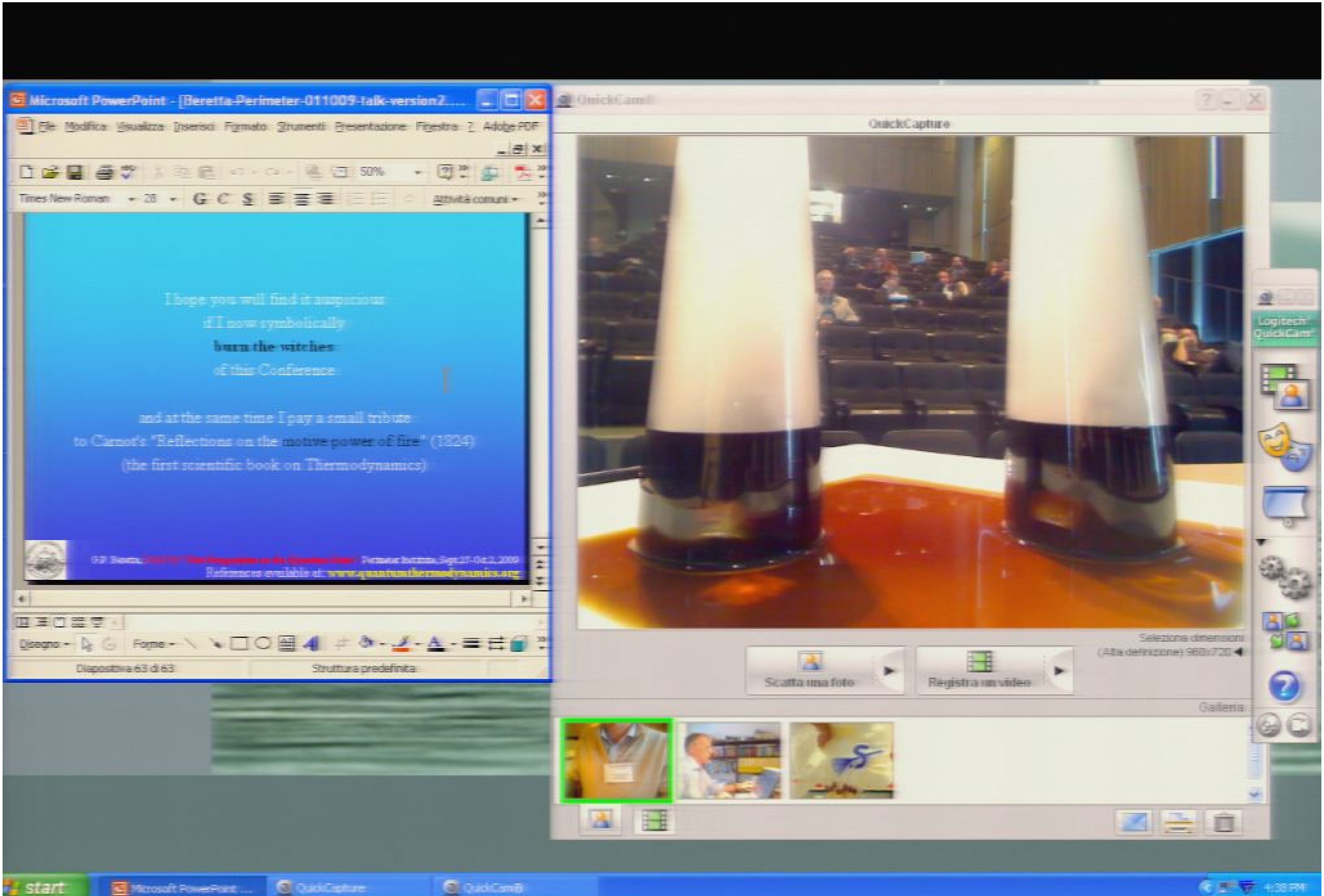
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