What is temperature?

Peter Hänggi

Universität Augsburg

In collaboration with
Dr. Gerhard Schmid

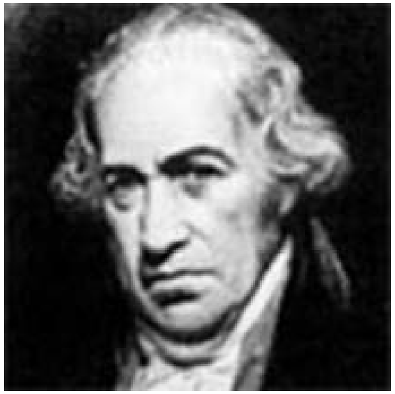
First thermometer & temperature scales

1638: Robert Fludd – air thermometer &scale
~1700: linseed oil thermometer by Newton
1701: red wine as temperature indicator by Rømer
1702: Guillaume Amontons: Absolute zero temperature?
1714: mercury and alcohol thermometer by Fahrenheit

Definition of temperature scales

Sir Isaac Newton
(1643 – 1727)

Olaf Christensen Römer
(1644 – 1710)



Daniel Gabriel Fahrenheit
(1686 – 1736)

René Antoine Ferchault de Réaumur
(1683 – 1757)

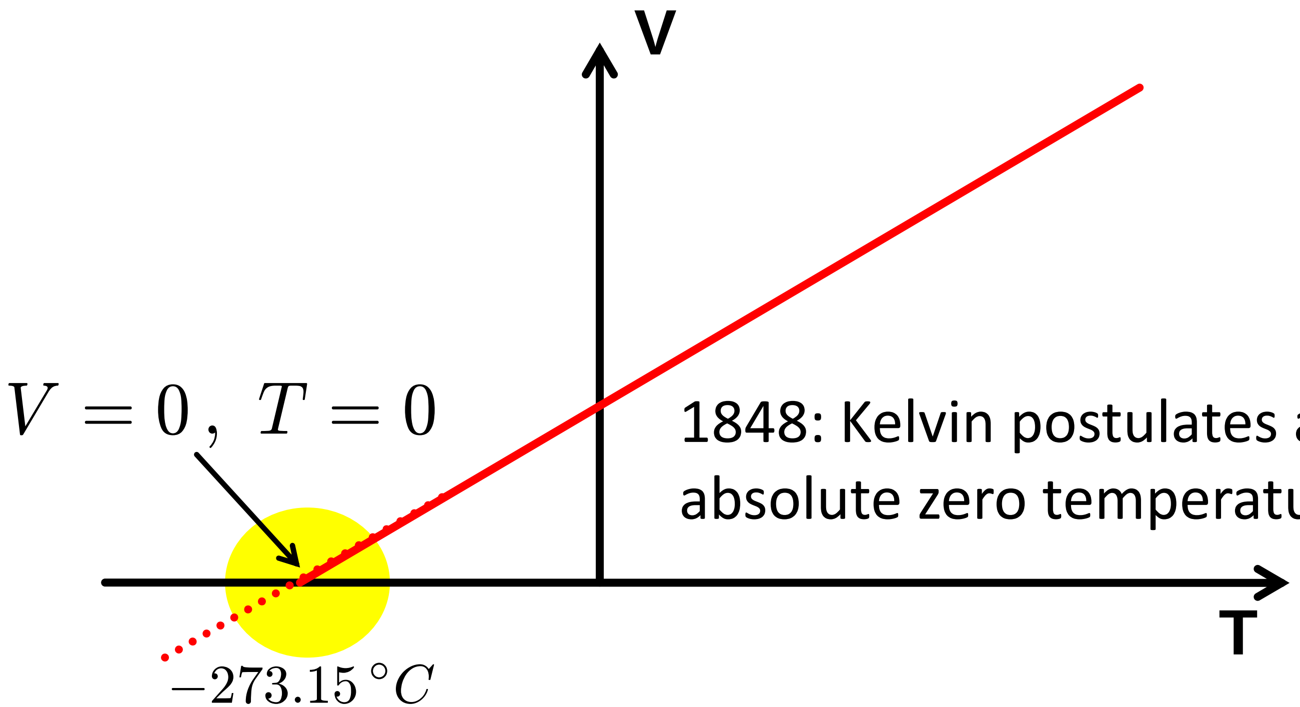
Anders Celsius
(1701 – 1744)

Typical temperature values [°C]

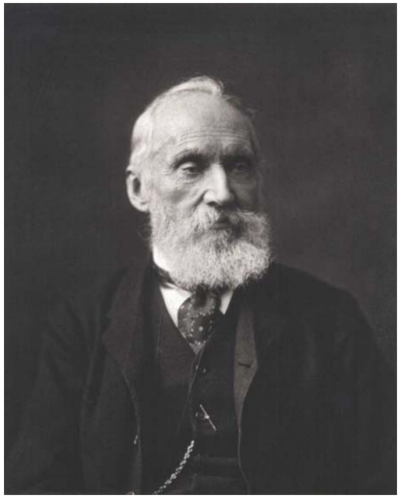
Boiling point of Nitrogen	-195.79
Lowest recorded surface temperature on Earth (Vostok, Antarctica – July 21, 1983)	-89
Highest recorded surface temperature on Earth (Al' Aziziyah, Libya – September 13, 1922)	58
Temperature in the Earth's Thermosphere (80 - 650 km above the surface)	~ 1500
Melting point of diamond	3547
Surface temperature of the sun (photosphere)	~ 5526
Temperature in the interior of the sun	~ $15 \cdot 10^6$

Absolute Zero

Ideal gas law: $p\,V = N\,k_{\mathrm{B}}\,T$



1848: Kelvin postulates an absolute zero temperature



William Thomson — Lord Kelvin
(1824 – 1907)

It is impossible by any procedure to reduce the temperature of a system to zero in a finite number of operations.

How to determine the absolute thermodynamic temperature

VORLESUNGEN

ÜBER

THERMODYNAMIK

VON

DR. MAX PLANCK,
PROFESSOR DER THEORETISCHEN PHYSIK
AN DER UNIVERSITÄT BERLIN.

VIERTE AUFLAGE.

MIT FÜNF FIGUREN IM TEXT.

LEIPZIG,
VERLAG VON VEIT & COMP.
1913

$$\log \frac{T}{T_0} = \int_{t_0}^{t} \frac{\left(\frac{\mathrm{d}v}{\mathrm{d}t}\right)_p \mathrm{d}t}{v + c_p' \left(\frac{\mathrm{d}t}{\mathrm{d}p}\right)}$$

t : arbitrary temperature scale

v : volume

c_p' : specific heat at constant pressure

" ... wo nun wieder unter dem Integralzeichen lauter direkt und verhältnismäßig bequem meßbare Größen stehen. ..."

M. Planck

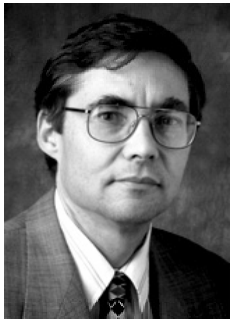
Low temperature milestones

1908: liquid helium; 5 K

Heike Kamerlingh Onnes
(1853 – 1926)

1995: Bose-Einstein-Condensate; 20 nK

Eric A. Cornell



Carl E. Wieman

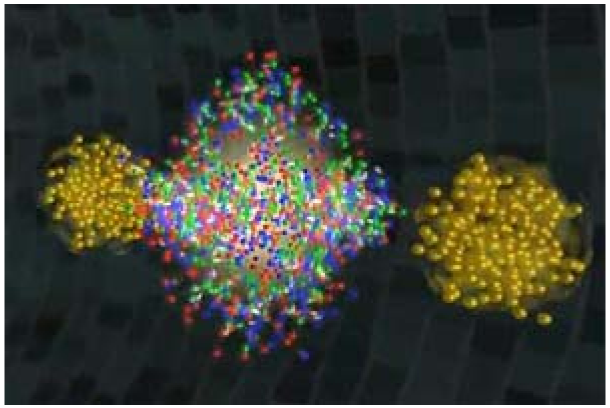
Wolfgang Ketterle

2003: BEC; 450 pK – W. Ketterle

Temperature Extrema

-89,2°C	21. Juli 1983	Wostok-Station	Antarktis	Gilt als der Kältepol der Erde; nicht offizielle bestätigter Wert: -91,5°C von 1997

70,7°C	2007	Iranische Wüste	Lut, Iran	Hitzeweltrekord übertroffen; Messung allerdings per Satellitenbeobachtung



p + n -> quark gluon plasma
with gold ion collisions in
Relativistic Heavy Ion Collider (RHIC)

4×10^{12} °C

Planck units

Name	Expression	SI equivalents
Planck temperature	$T_{\mathrm{P}} = \sqrt{\hbar c^5 G^{-1} k^{-2}}$	$1.41168 \cdot 10^{32}$ K
Planck length	$l_{\mathrm{P}} = \sqrt{\hbar G c^{-3}}$	$1.61625 \cdot 10^{-35}$ m
Planck mass	$m_{\mathrm{P}} = \sqrt{\hbar c G^{-1}}$	$2.17644 \cdot 10^{-8}$ kg
Planck time	$t_{\mathrm{P}} = \sqrt{\hbar G c^{-5}}$	$5.39124 \cdot 10^{-44}$ s

… ihre Bedeutung für alle Zeiten und für alle, auch außerirdische und außermenschliche Kulturen notwendig behalten unnd welche daher als natürliche Maßeinheiten bezeichnet werden können …

… These necessarily retain their meaning for all times and for all civilizations, even extraterrestrial and non-human ones, and can therefore be designated as natural units …

(Planck, 1899)

The highest temperature you can see

Lightning:

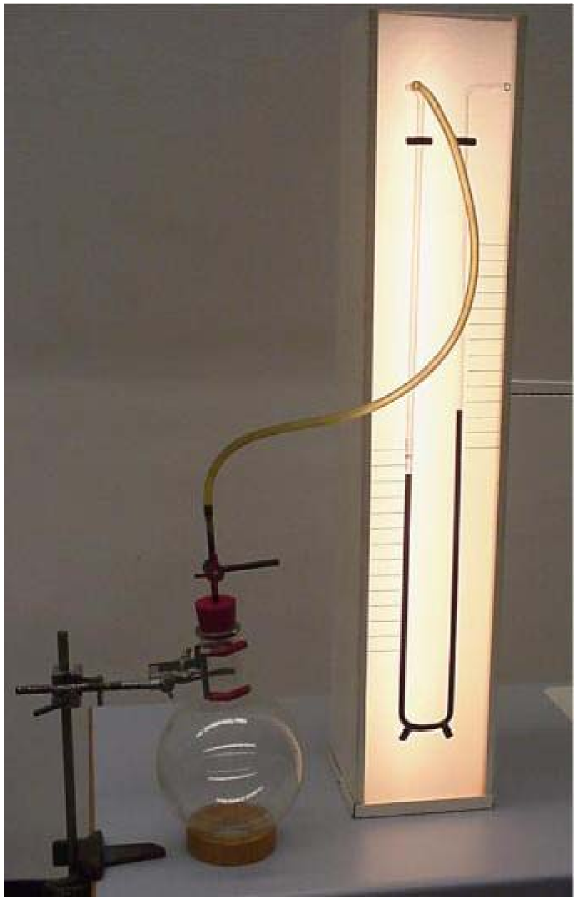
30 000 °C

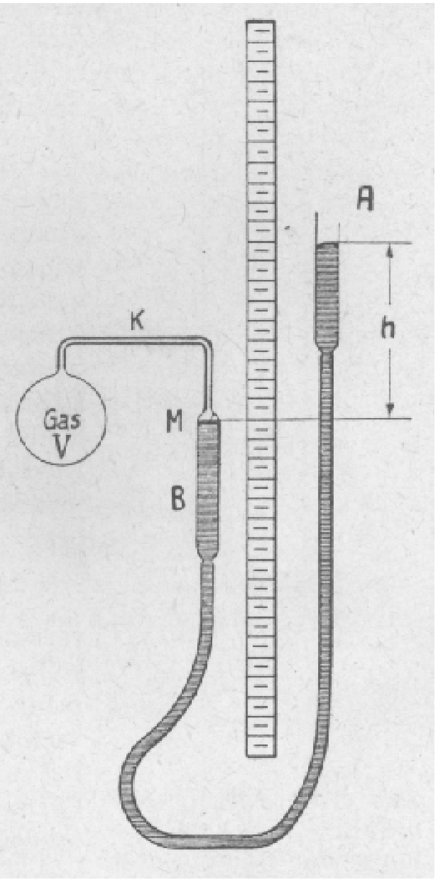
Woher weiß man …

… wie heiß ein Blitz ist?

Zuckt ein Blitz über den Gewitterhimmel, erwärmt sich sein Strahl auf bis zu 30 000 Grad Celsius. Das ist unglaubliche 20 Mal heißer als eine Kerzenflamme! Zu diesem Ergebnis kamen Physiker, indem sie Blitze mit einem sogenannten Spektrometer untersuchten. Dieses Gerät fängt alle Lichtwellen aus einem Blitz ein – auch die für uns unsichtbaren. Woher aber kommt das Licht des Blitzes? Wenn sich ein Blitz entlädt, fließen ungeheure Strommengen. Die Luftteilchen heizen sich auf und geraten in Schwingung. Einen Teil der zugeführten Energie geben sie als Licht wieder ab. Physiker messen nun nicht nur die Wellenlängen dieses Lichts, sondern auch deren Verteilung und Intensität. Anhand dieser Werte können sie auf die Temperatur schließen.

Gas Thermometers



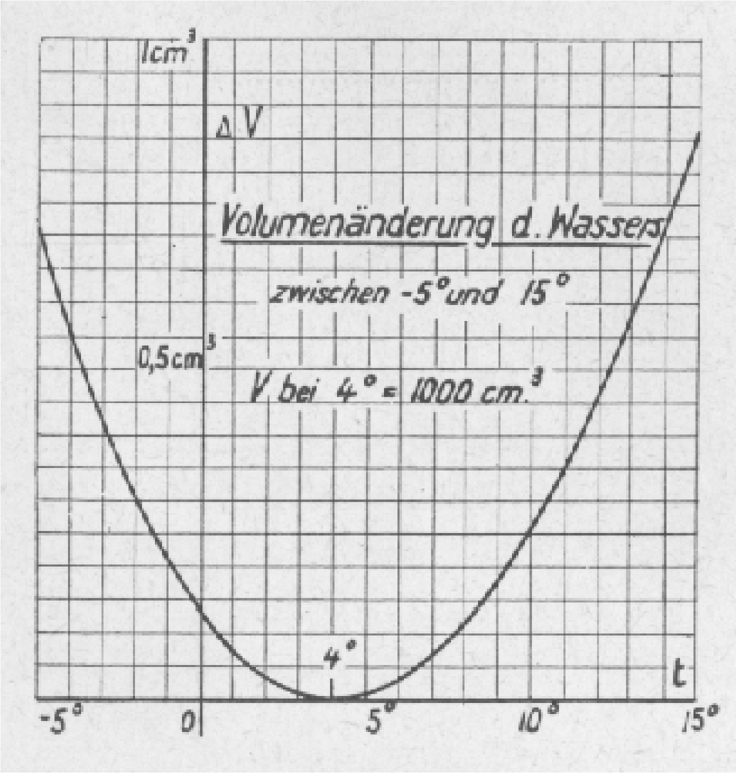


Ideal gas:

$$T = \left(\frac{V}{N\,k_{\mathrm{B}}} \right) p$$

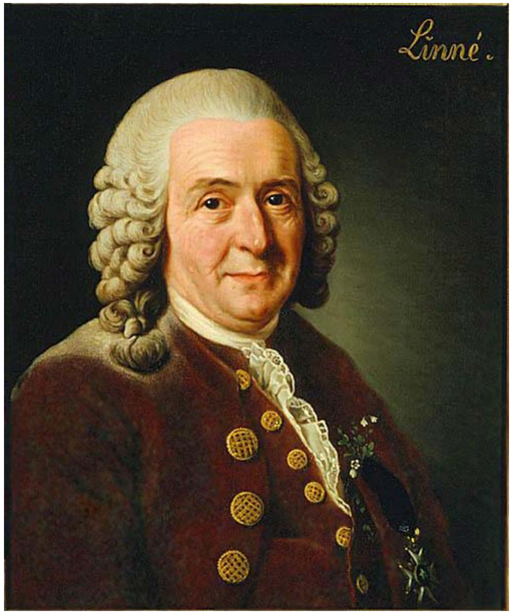
Galilei Thermometer

Volume change of water



Upon increasing T → 4°C ⟶ Water volume shrinks

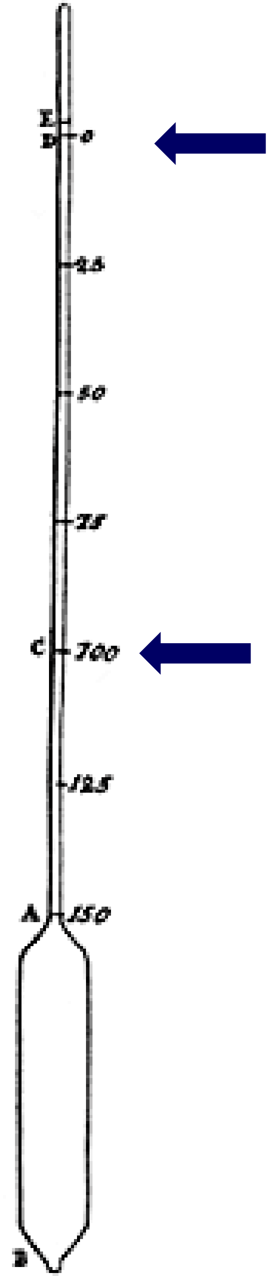
Linneaus thermometer



Carl von Linné
(1707 – 1778)

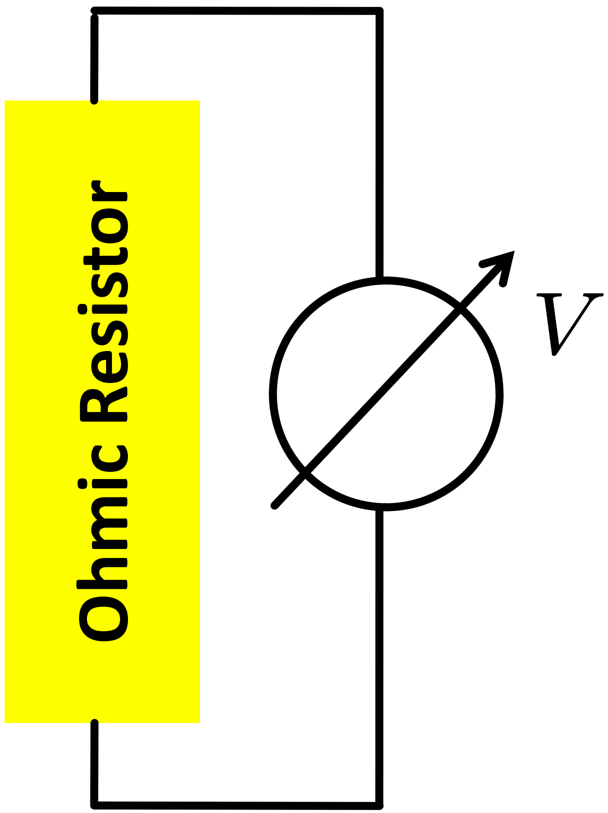
Reversed the Celsius scale

1744: broken on delivery
1745: botanical garden in Uppsala



Anders Celsius

Noise Thermometer



Johnson – Nyquist noise

$$\mathrm{PSD}_V(\omega) = 2k_\mathrm{B}TR$$

-- classical regime only --

PSD_V : power spectral density of the voltage signal

k_B : Boltzmann constant

R : resistance

Quantum fluctuation-dissipation theorem

$$PSD_I(\omega) = \hbar\omega \coth\left(\frac{\hbar\omega}{2k_\mathrm{B}T}\right) \mathrm{Re}Y(\omega)$$

$$= 2\left(\frac{\hbar\omega}{2} + \frac{\hbar\omega}{\exp(\beta\hbar\omega) - 1}\right) \mathrm{Re}Y(\omega)$$

$k_\mathrm{B}T \gg \hbar\omega$

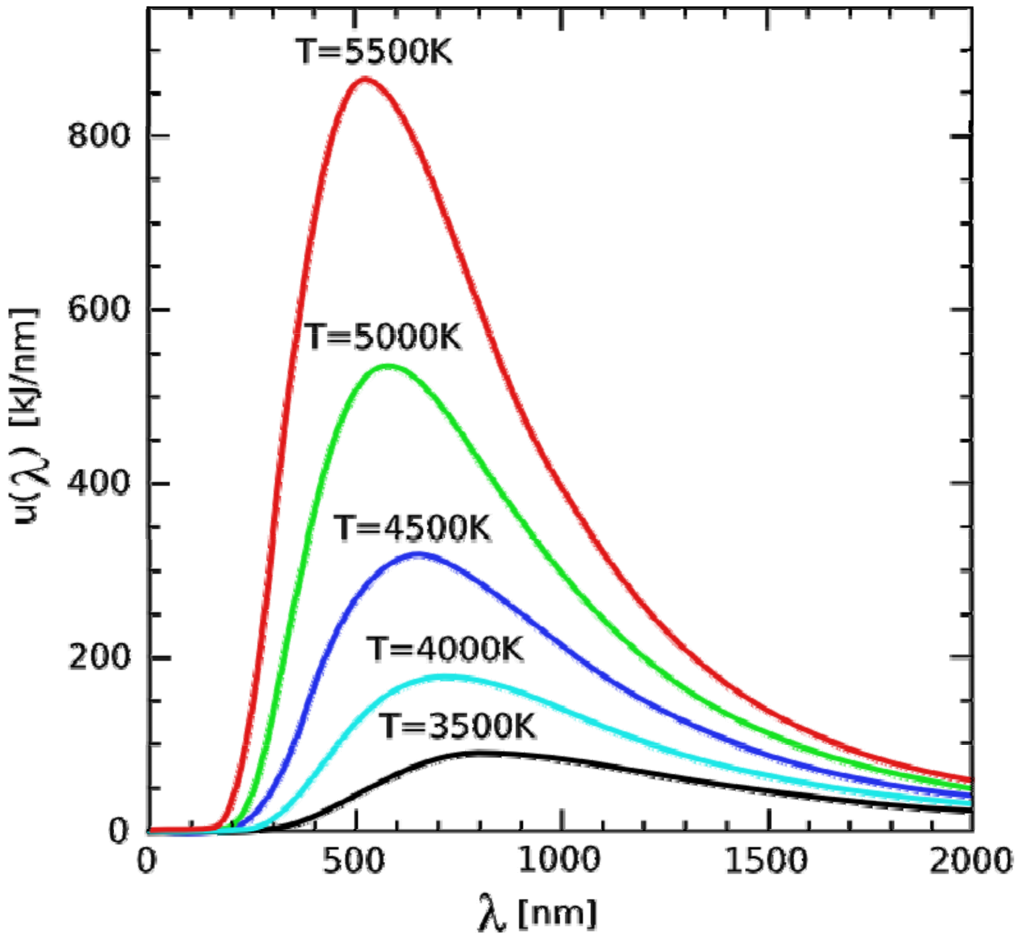
$k_\mathrm{B}T \ll \hbar\omega$

$$PSD_I(\omega) = 2k_\mathrm{B}T\,\mathrm{Re}Y(\omega)$$

$$PSD_I(\omega) = \hbar\omega\,\mathrm{Re}Y(\omega)$$

Black body radiation

Planck's law [1901]: $u(\lambda, T) = \frac{8\pi hc}{\lambda^5} \frac{1}{\exp(\frac{hc}{\lambda k_B T}) - 1}$



$u(\lambda, T)$: spectral energy density

λ : wavelength

h : Planck constant

c : speed of light

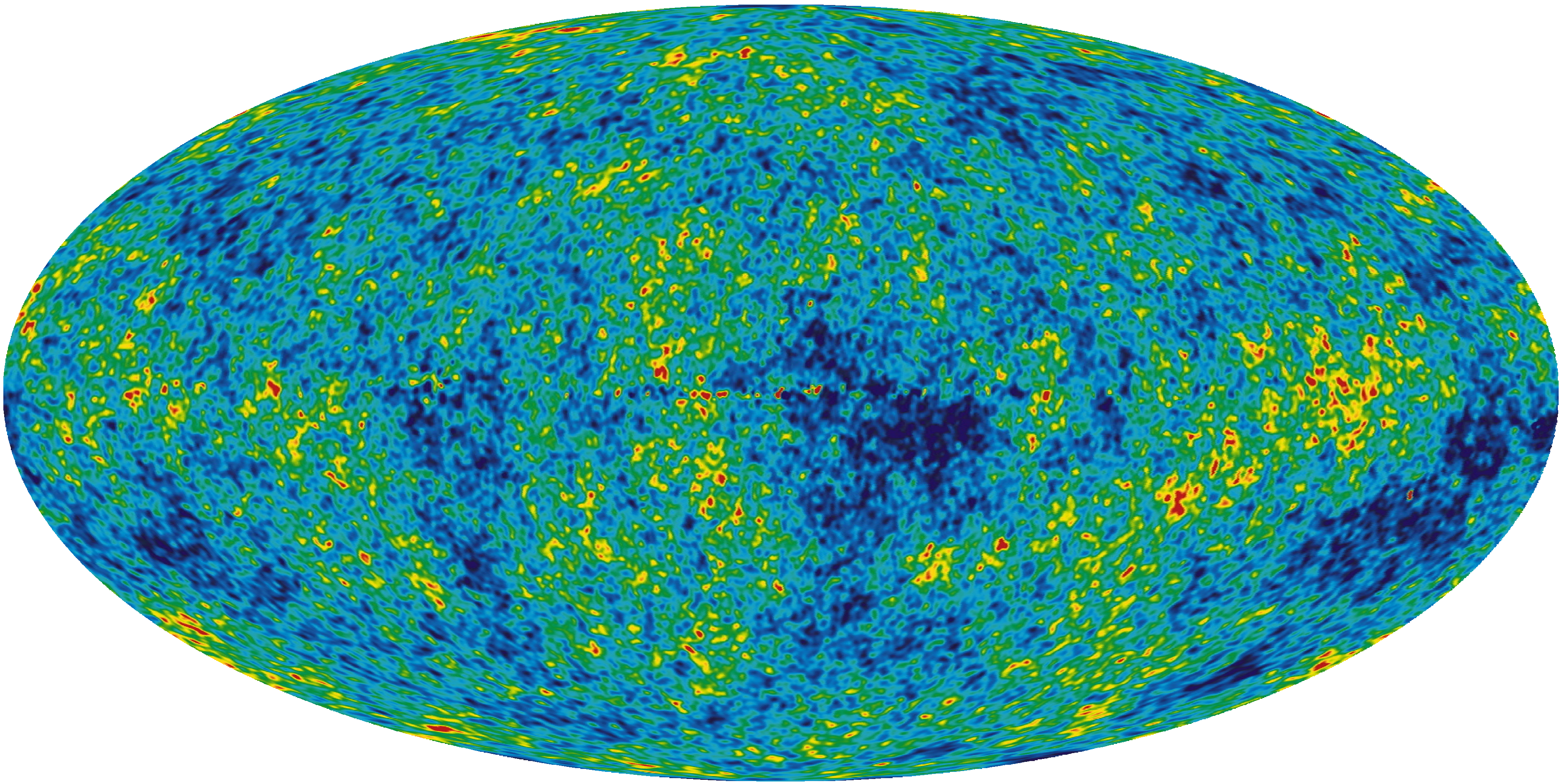
k_B : Boltzmann constant

Stefan – Boltzmann law:

$$E \propto T^4$$

Thermometer !

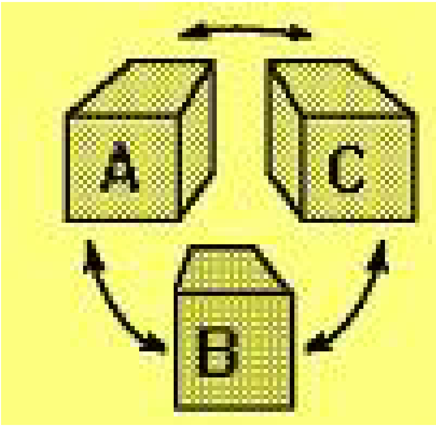
Cosmic background temperature



T = 2.725 ± …. K

Four Grand Laws of Thermodynamics

Zeroth Law



Transitivity !

$$\text{A in equilibrium with B:} \quad f_{\mathrm{AB}}(p_{\mathrm{A}}, V_{\mathrm{A}}; p_{\mathrm{B}}, V_{\mathrm{B}}, \ldots) = 0$$

$$\text{B in equilibrium with C:} \quad f_{\mathrm{BC}}(p_{\mathrm{B}}, V_{\mathrm{B}}; p_{\mathrm{C}}, V_{\mathrm{C}}, \ldots) = 0$$

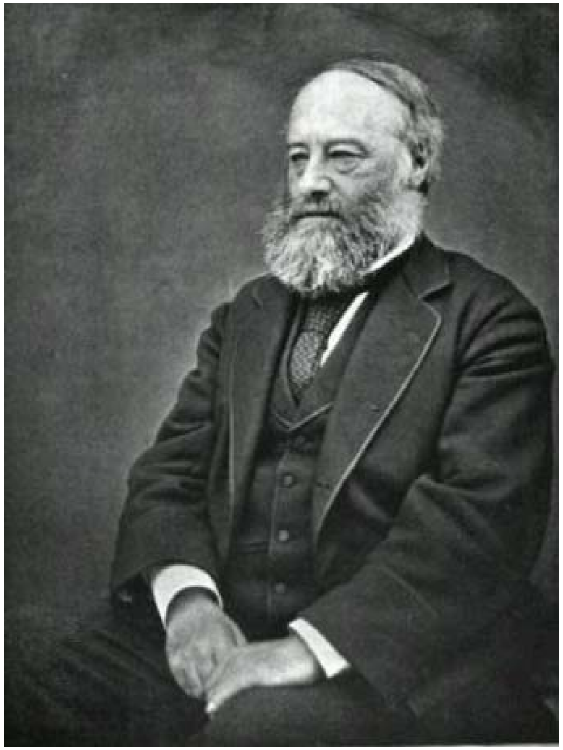
$$\Rightarrow \text{A in equilibrium with C} \Leftrightarrow f_{\mathrm{AC}}(p_{\mathrm{A}}, V_{\mathrm{A}}; p_{\mathrm{C}}, V_{\mathrm{C}}, \ldots) = 0$$

Allows the formal introduction of a temperature:

$$T = T_{\mathrm{A}}(p_{\mathrm{A}}, V_{\mathrm{A}}; \ldots) = T_{\mathrm{B}}(p_{\mathrm{B}}, V_{\mathrm{B}}; \ldots) = T_{\mathrm{C}}(p_{\mathrm{C}}, V_{\mathrm{C}}; \ldots)$$

First Law

Julius Robert von Mayer
(1814 – 1878)



James Prescott Joule
(1818 – 1889)

Hermann von Helmholtz
(1821 – 1894)

First Law – Energy Conservation

$$\Delta U = \Delta Q + \Delta W$$

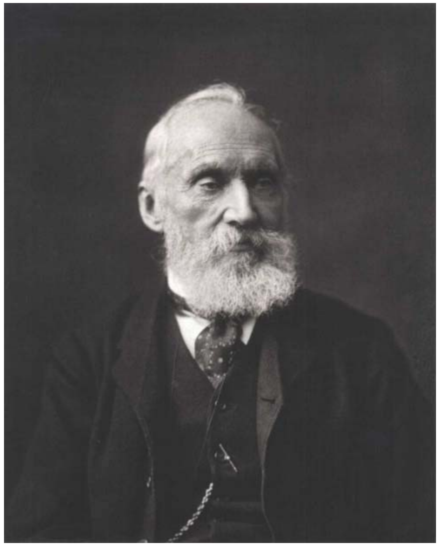
ΔU	change in internal energy
ΔQ	heat added on the system
ΔW	work done on the system

H. von Helmholtz: "Über die Erhaltung der Kraft" (1847)

$$\Delta U = (T\Delta S)_{\text{quasi-static}} - (p\Delta V)_{\text{quasi-static}}$$

Second Law

Rudolf Julius Emanuel Clausius
(1822 – 1888)



William Thomson alias Lord Kelvin
(1824 – 1907)

Heat generally cannot spontaneously flow from a material at lower temperature to a material at higher temperature.

No cyclic process exists whose sole effect is to extract heat from a single heat bath at temperature T and convert it entirely to work.

$$\delta Q = T\mathrm{d}S \quad \text{(Zürich, 1865)}$$

The famous Laws

Equilibrium Principle -- minus first Law

An isolated, macroscopic system which is placed in an arbitrary initial state within a finite fixed volume will attain a unique state of equilibrium.

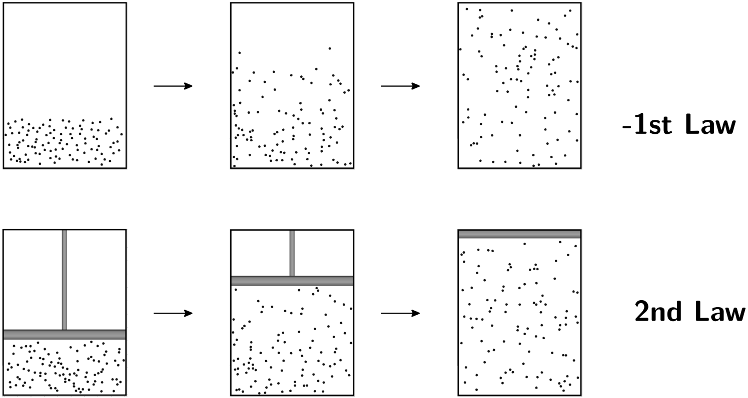
Second Law (Clausius)

For a non-quasi-static process occurring in a thermally isolated system, the entropy change between two equilibrium states is non-negative.

Second Law (Kelvin)

No work can be extracted from a closed equilibrium system during a cyclic variation of a parameter by an external source.

MINUS FIRST LAW vs. SECOND LAW



Thermodynamic Temperature

$$\delta Q^{\mathrm{rev}} = T\,dS \leftarrow \text{thermodynamic entropy}$$

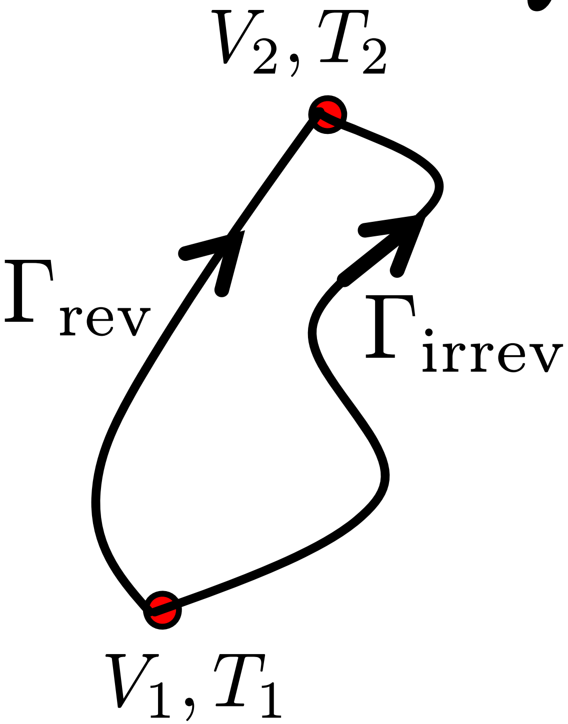
$$S = S(E, V, N_1, N_2, \ldots; M, P, \ldots)$$

$S(E, \ldots)$: (continuous) & differentiable and monotonic function of the internal energy E

$$\left(\frac{\partial S}{\partial E}\right)_{\ldots} = \frac{1}{T}$$

Entropy S – content of *transformation* „Verwandlungswert“

$$d\,S = \delta Q^{\mathrm{rev}} / T\,; \qquad \delta Q^{\mathrm{irrev}} < \delta Q^{\mathrm{rev}}$$



$$\oint_C \frac{\delta Q}{T} \leq 0$$

$$C = \Gamma_{\mathrm{rev}} + \Gamma_{\mathrm{irrev}}^{-1}$$

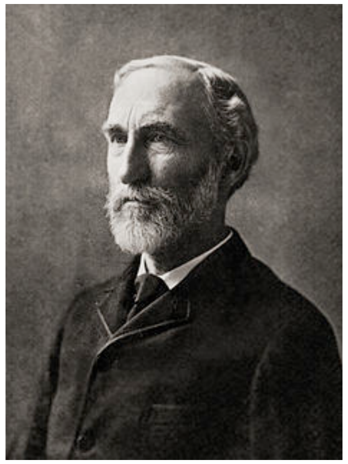
$$\left.\begin{aligned} S(V_2,T_2) - S(V_1,T_1) &\geq \int_{\Gamma_{\mathrm{irrev}}} \frac{\delta Q}{T} \\ S(V_2,T_2) - S(V_1,T_1) &= \int_{\Gamma_{\mathrm{rev}}} \frac{\delta Q^{\mathrm{rev}}}{T} \end{aligned}\right\} \quad \frac{\partial S}{\partial t} \geq 0 \quad \textbf{NO !}$$

GIBBS, JOSIAH WILLARD.

Elementary principles in statistical mechanics

Scribner's sons

New York 1902



CHAPTER VIII.

ON CERTAIN IMPORTANT FUNCTIONS OF THE ENERGIES OF A SYSTEM.

IN order to consider more particularly the distribution of a canonical ensemble in energy, and for other purposes, it will be convenient to use the following definitions and notations.

Let us denote by V the extension-in-phase below a certain limit of energy which we shall call ϵ. That is, let

$$V = \int \ldots \int dp_1 \ldots dq_n, \qquad (265)$$

the integration being extended (with constant values of the external coördinates) over all phases for which the energy is less than the limit ϵ. We shall suppose that the value of this integral is not infinite, except for an infinite value of the limiting energy. This will not exclude any kind of system to

CHAPTER XIV.

DISCUSSION OF THERMODYNAMIC ANALOGIES.

IF we wish to find in rational mechanics an *a priori* foundation for the principles of thermodynamics, we must seek mechanical definitions of temperature and entropy. The quantities thus defined must satisfy (under conditions and with limitations which again must be specified in the language of mechanics) the differential equation

$$d\epsilon = T d\eta - A_1\, da_1 - A_2\, da_2 - \text{etc.}, \qquad (482)$$

where ϵ, T, and η denote the energy, temperature, and entropy of the system considered, and $A_1\, da_1$, etc., the mechanical work (in the narrower sense in which the term is used in thermodynamics, *i. e.*, with exclusion of thermal action) done upon external bodies.

The quantity in the equation which corresponds to entropy is log V, the quantity V being defined as the extension-in-phase within which the energy is less than a certain limiting value (ϵ).

Entropy in Stat. Mech.

$$S = k_{\mathrm{B}} \ln \Omega(E, V, \ldots)$$

QM: $\Omega_{\mathrm{G}}(E, V, \ldots) = \sum_{0 \leq E_i \leq E} 1$

classical

Gibbs: $\Omega_{\mathrm{G}} = \left(\frac{1}{N!\, h^{\mathrm{DOF}}}\right) \int \mathrm{d}\Gamma\, \Theta\left(E - H(\underline{q}, \underline{p}; V, \ldots)\right)$

Boltzmann: $\Omega_{\mathrm{B}} = \epsilon_0 \frac{\partial\, \Omega_{\mathrm{G}}}{\partial E} \propto \int \mathrm{d}\Gamma\, \delta\left(E - H(\underline{q}, \underline{p}; V, \ldots)\right)$

density of states

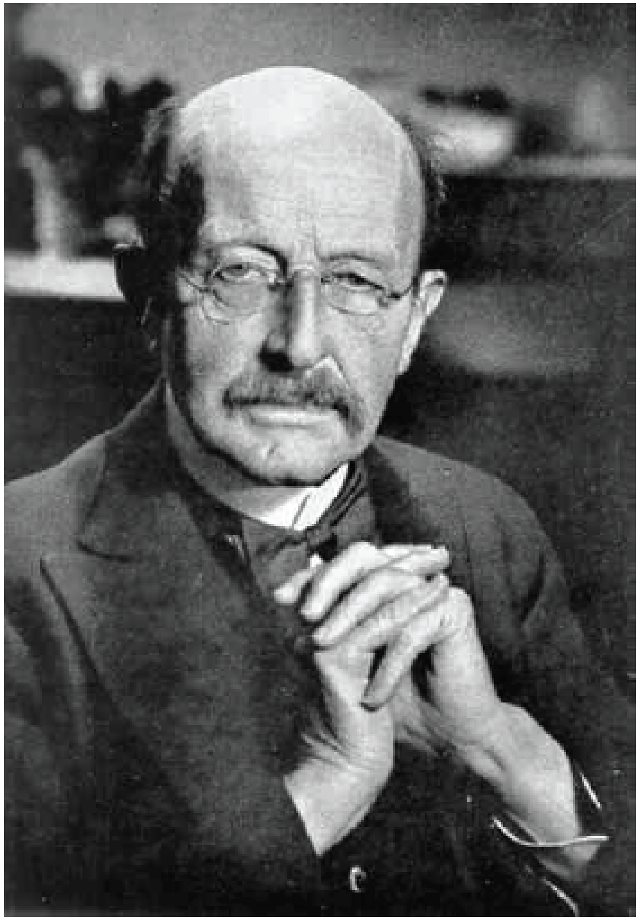
Third Law

Walter Hermann NERNST
(1864 - 1941)

„mein Wärmesatz"
(during his lecture August 15, 1905)

$$\frac{\Delta H - \Delta G}{T} = \Delta S \longrightarrow 0 \quad \text{as} \quad T \longrightarrow 0$$

… and Planck's version



Max PLANCK
(1858 - 1947)

The entropy $s = S/N$ per particle approaches at $T = 0$ a constant ($s_0 = k_B \ln g(N)/N$) value that possibly depends on the chemical composition of the system. This limiting value can generally be set to zero.

THIRD LAW AND PLANCK

VORLESUNGEN

ÜBER

THERMODYNAMIK

VON

DR. MAX PLANCK,
PROFESSOR DER THEORETISCHEN PHYSIK
AN DER UNIVERSITÄT BERLIN.

1913

Zunächst ist leicht einzusehen, daß man, da der Wert der Entropie eine willkürliche additive Konstante enthält, jenen für $T = 0$ eintretenden Wert unbeschadet der Allgemeinheit gleich Null setzen kann, so daß das NERNSTsche Wärmetheorem nun lautet:

Beim Nullpunkt der absoluten Temperatur besitzt die Entropie eines jeden chemisch homogenen festen oder flüssigen Körpers den Wert Null.

[2] Diese Fassung des Theorems ist inhaltlich etwas weitergehend als die von NERNST a. a. O. selber gegebene, nach welcher für $T=0$ die Differenz der Entropien eines solchen Körpers in zwei verschiedenen Modifikationen gleich Null ist. Letzterer Satz läßt nämlich noch die Möglichkeit offen, daß die Entropie selber für $T = 0$ negativ unendlich wird.

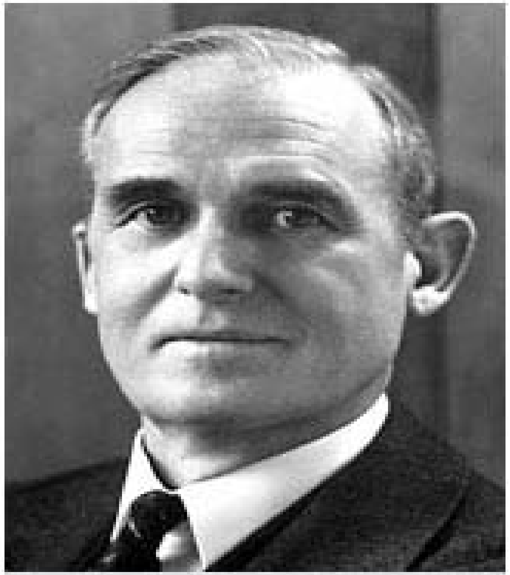
[1] Nach der von NERNST selber gegebenen Fassung (§ 282) tritt an die Stelle der Gleichung (256) die folgende:

$$S' - S = \int_0^T \frac{C_p' - C_p}{T} \, dT,$$

wobei $S' - S$ die Differenz der Entropien eines festen oder flüssigen Körpers in zwei verschiedenen Modifikationen bezeichnet. Dann kann man für $T = 0$ nur schließen, daß $C_p' = C_p$, aber nicht, daß $C_p' = C_p = 0$. Würden C_p und C_p' für $T = 0$ endlich bleiben, so wäre die Entropie S für $T = 0$ nicht gleich Null, sondern negativ unendlich. Es ist daher von Wichtigkeit zu bemerken, daß, wenn die Folgerung $C_p = 0$ durch die Erfahrung nicht bestätigt werden sollte, die NERNSTsche Fassung des Theorems deshalb doch aufrecht erhalten werden könnte.

The Nobel Prize in Chemistry 1949

"for his contributions in the field of chemical thermodynamics, particularly concerning the behaviour of substances at extremely low temperatures"



William Francis Giauque

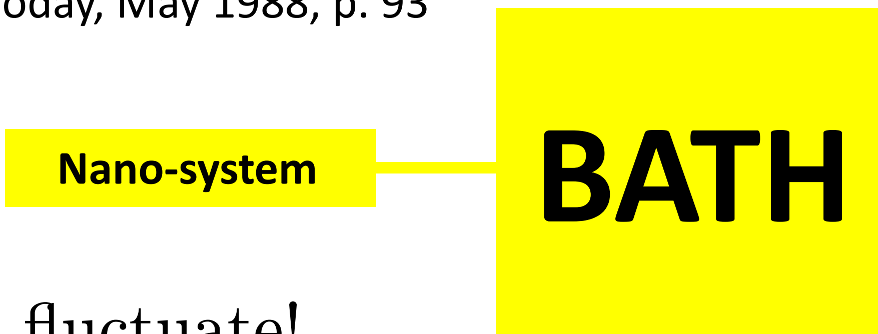
USA

University of California
Berkeley, CA, USA

b. 1895
d. 1982

Temperature **Fluctuations** – An Oxymoron

Ch. Kittel, Physics Today, May 1988, p. 93



$$\beta = \frac{1}{k_\mathrm{B} T}$$

T does NOT fluctuate!

$$|\Delta U|\,|\Delta\beta| = 1 \leftrightarrow |\Delta U|\,|\Delta T| = k_\mathrm{B} T^2 \quad \textbf{NO!}$$

"…Temperature is precisely defined only for a system in thermal equilibrium with a heat bath: The temperature of a system A, however small, is defined as equal to the temperature of a very large heat reservoir B with which the system is in equilibrium and in thermal contact. Thermal contact means that A and B can exchange energy, although insulated from the outer World. …"

DOES T FLUCTUATE?

I SAY **NO**

$$\left(\frac{\partial S}{\partial E}\right) = \frac{1}{T} \quad ; \quad \langle (\Delta E)^2 \rangle = k_B T^2 C$$

$$\left(\frac{\partial^2 S}{\partial E^2}\right) = -\frac{1}{T^2}\left(\frac{dT}{dE}\right) = \frac{-1}{C T^2} \qquad (*)$$

$$\Delta\left(\frac{1}{T}\right)\Delta\left(\frac{1}{T}\right) = -\frac{1}{T^2}(\Delta T) - \frac{1}{T^2}(\Delta T) = \frac{(\Delta T)^2}{T^4} \; ; \text{with } (*)$$

$$= \left(\frac{\partial^2 S}{\partial E^2}\right)\left(\frac{\partial^2 S}{\partial E^2}\right)(\Delta E)^2 = \frac{1}{C^2 T^4} \cdot k_B T^2 C$$

$$\Rightarrow \langle (\Delta T)^2 \rangle = \frac{k_B T^2 C}{C^2} = \boxed{\frac{k_B T^2}{C}}$$

C "ΔT" = "ΔE"

"$(\Delta E)^2$"$/C^2$

A 'SYMBOL' FOR "ΔE"'s

Estimate of temperature and its uncertainty in small systems

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The energy of a finite system thermally connected to a thermal reservoir may fluctuate, while the temperature is a constant representing a thermodynamic property of the reservoir. The finite system can also be used as a thermometer for the reservoir. From such a perspective, the temperature has an uncertainty, which can be treated within the framework of estimation theory. We review the main results of this theory and clarify some controversial issues regarding temperature fluctuations. We also offer a simple example of a thermometer with a small number of particles. We discuss the relevance of the total observation time, which must be much longer than the decorrelation time.

DOI: 10.1119/1.3563046

? Negative Temperature ?

Spin system: $|\vec{S}| = 1/2\,; \quad \vec{\mu} = \gamma \vec{S}\,; \quad H = -\sum \vec{\mu}_i \cdot \vec{B}$

$$\vec{S} \parallel \vec{B} \Rightarrow \text{ Two-State-System: } \quad \epsilon_g = -\frac{1}{2}\gamma B < \epsilon_e = +\frac{1}{2}\gamma B = \mu B$$

$$N = n_g + n_e \quad \& \; E = \mu B(n_e - n_g)\,, \text{ typically } \; E < 0$$

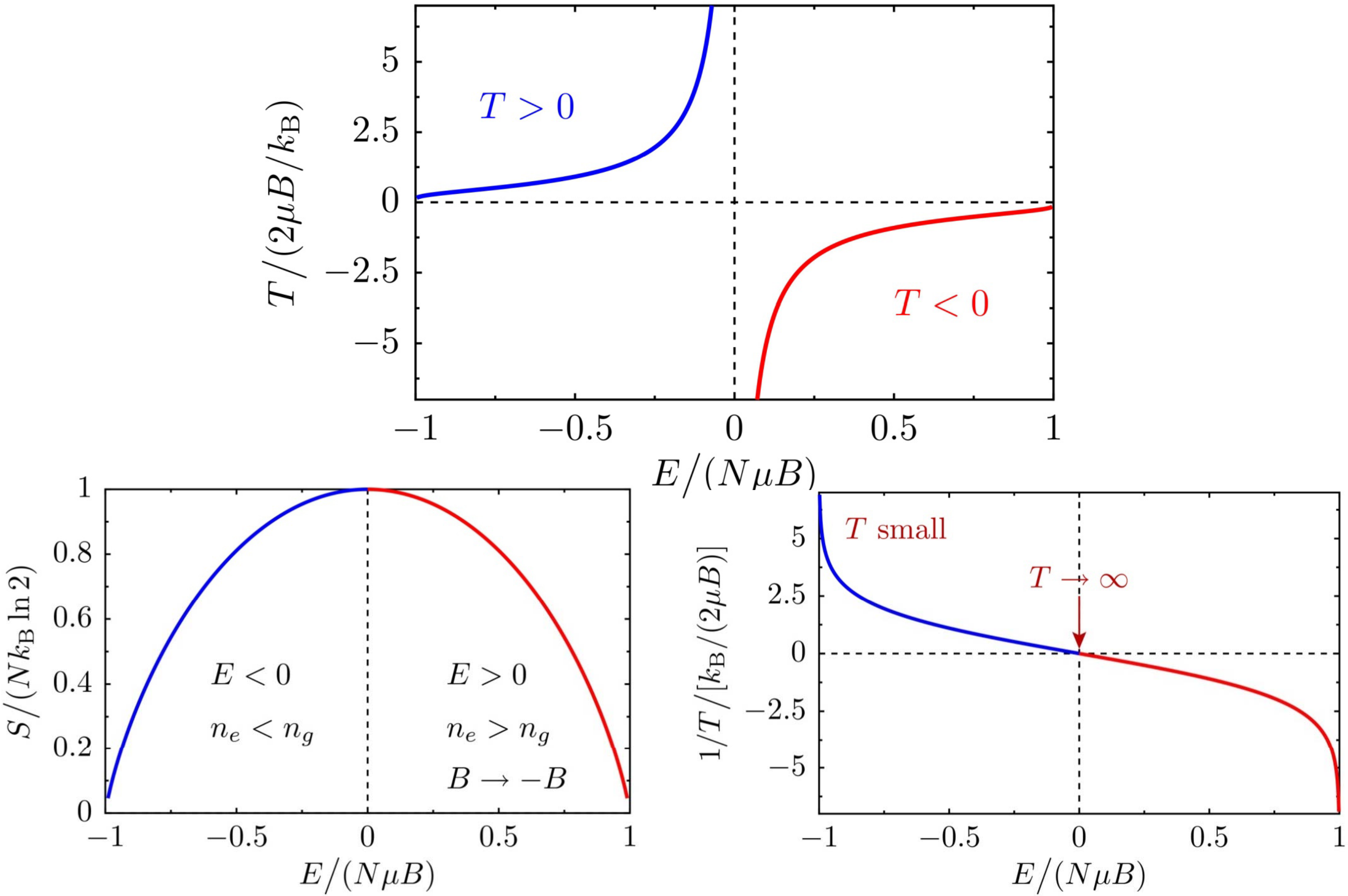
$$\Omega = \frac{N!}{n_g!\,n_e!} \Rightarrow S = k_{\mathrm{B}} \ln \Omega$$

$$\Rightarrow n_g = \frac{1}{2}\left(N - \frac{E}{\mu B}\right)$$

$$\Rightarrow n_e = \frac{1}{2}\left(N + \frac{E}{\mu B}\right)$$

$$\Rightarrow \frac{1}{T} = \frac{\partial S}{\partial E}$$

Negative (Spin)-Temperature!



Entropy in Stat. Mech.

$$S = k_\mathrm{B} \ln \Omega(E, V, \ldots)$$

Gibbs: $\Omega_\mathrm{G} = \left(\frac{1}{N!\, h^{\mathrm{DOF}}} \right) \int \mathrm{d}\Gamma\, \Theta \left(E - H(\underline{q}, \underline{p}; V, \ldots) \right)$

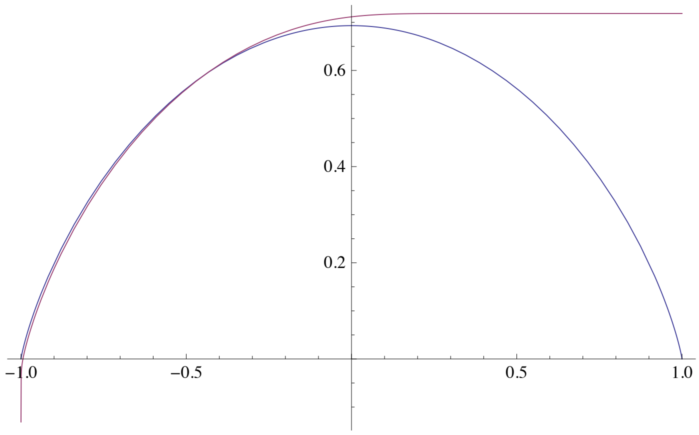
Boltzmann: $\Omega_\mathrm{B} = \epsilon_0 \frac{\partial\, \Omega_\mathrm{G}}{\partial E} \propto \int \mathrm{d}\Gamma\, \delta \left(E - H(\underline{q}, \underline{p}; V, \ldots) \right)$

density of states

```
In[1]:= SΩ[x_, n_, μ_, B_] :=
         n Log[2] - n / 2 (1 + x / (μ B n)) Log[1 + x / (μ B n)] - n / 2 (1 - x / (μ B n)) Log[1 - x / (μ B n)]
        W[x_, n_, μ_, B_] := Exp[SΩ[x, n, μ, B]]
        Ω[x_, n_, μ_, B_] := Exp[SΩ[x, n, μ, B]] / (2 μ B)
        Ωe[x_, n_, μ_, B_] := Derivative[1, 0, 0, 0][Ω][x, n, μ, B]
        ΩB[x_, n_, μ_, B_] := Derivative[0, 0, 0, B][Ω][x, n, μ, B]
        Φ[x_, n_, μ_, B_] := NIntegrate[Ω[y, n, μ, B], {y, -n μ B, x}]
        ΦB[x_, n_, μ_, B_] := NIntegrate[ΩB[y, n, μ, B], {y, -n μ B, x}]
        S[x_, n_, μ_, B_] := Log[Φ[x, n, μ, B]]
        T[x_, n_, μ_, B_] := Φ[x, n, μ, B] / Ω[x, n, μ, B]
        TΩ[x_, n_, μ_, B_] := Ω[x, n, μ, B] / Ωe[x, n, μ, B]
        MΩ[x_, n_, μ_, B_] := ΩB[x, n, μ, B] / Ωe[x, n, μ, B]
        M[x_, n_, μ_, B_] := -x / B

In[22]:= n = 10^2;
         m = 10^8;
         Plot[{SΩ[e n, n, 1, 1] / n, S[e n, n, 1, 1] / n}, {e, -1, 1}]
         Plot[{SΩ[e m, m, 1, 1] / m, S[e m, m, 1, 1] / m}, {e, -1, 1}]
         Plot[{TΩ[e n, n, 1, 1], T[e n, n, 1, 1]}, {e, -1, 1}, PlotRange → {-100, 100}]
         Plot[{TΩ[e m, m, 1, 1], T[e m, m, 1, 1]}, {e, -1, 1}, PlotRange → {-100, 100}]
         Plot[{MΩ[e n, n, 1, 1] / n, M[e n, n, 1, 1] / n}, {e, -1, 1}]
         Plot[{MΩ[e m, m, 1, 1] / m, M[e m, m, 1, 1] / m}, {e, -1, 1}]
         Clear[n, m]
```

Out[24]=

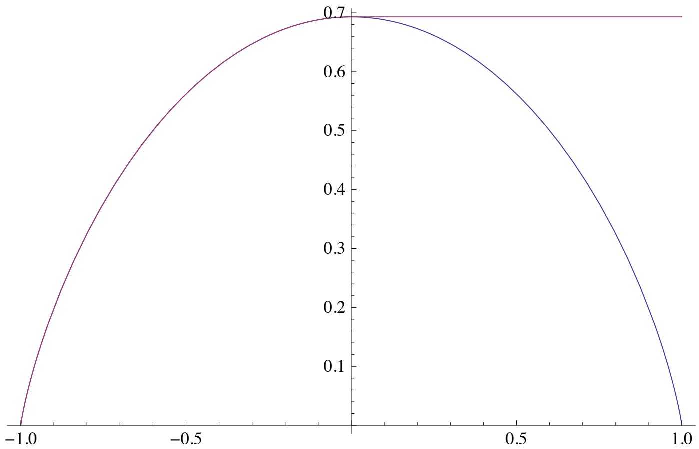


Purple: S_Phi /N
Blue: S_Omega/N

N=100

x-axis in all graphs is E/(2\mu N)

Out[25]=

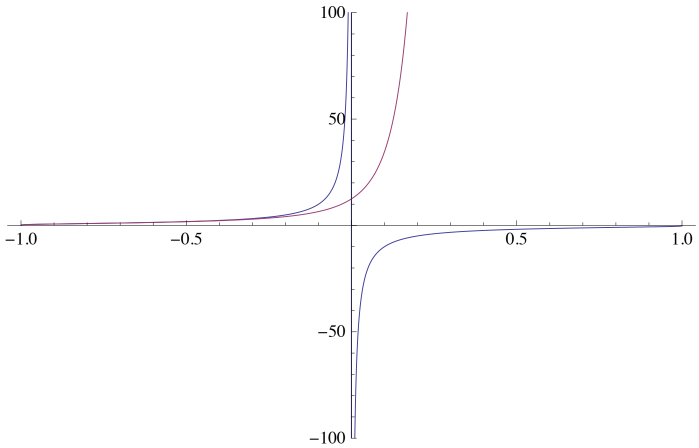


Purple: S_Phi /N
Blue: S_Omega/N

N=10^8

Limit Value = Log 2

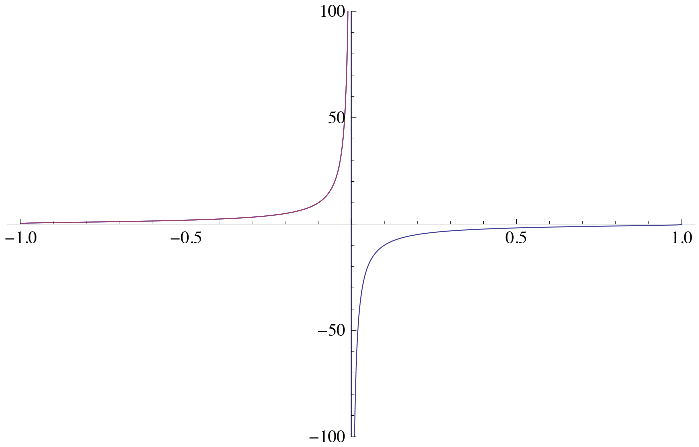
Out[26]=



Purple: T_Phi
Blue: T_Omega

N=100

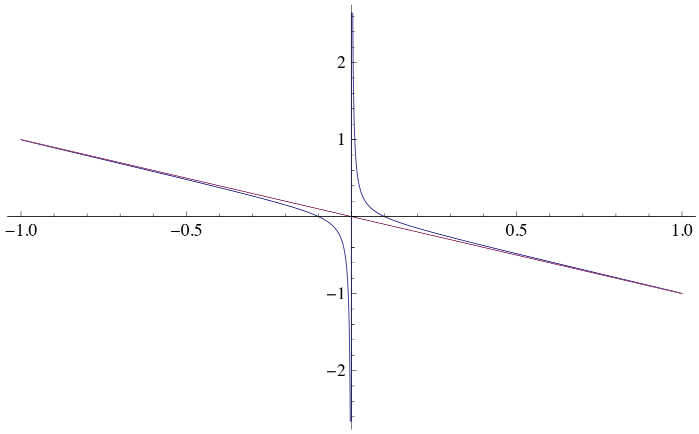
Out[27]=



Purple: T_Phi
Blue: T_Omega

N=10^8

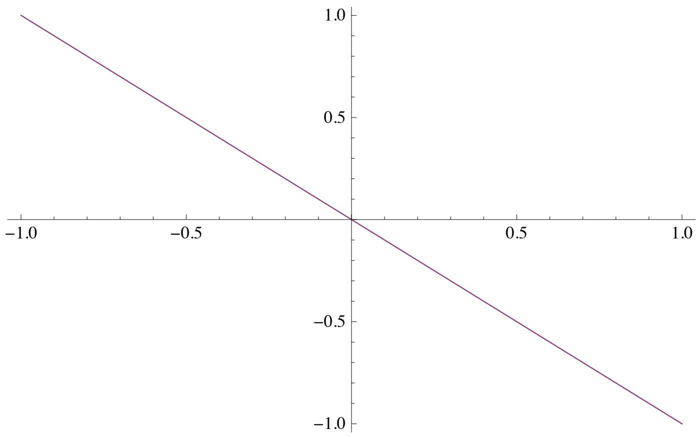
Out[28]=



Purple: M_Phi
Blue: M_Omega

N=100

Out[29]=



Purple: M_Phi
Blue: M_Omega

N=10^8

Inconsistent thermostatistics and negative absolute temperatures

Jorn Dunkel (DAMTP)

arxiv: 1304.2066

Example 1: Classical ideal gas

$$\Omega(E,V) = \alpha E^{dN/2} V^N, \qquad \alpha = \frac{(2\pi m)^{dN/2}}{N! h^d \Gamma(dN/2+1)}$$

$$S_\mathrm{B}(E,V,A) = k_\mathrm{B} \ln[\epsilon \omega(E)]$$

$$E = \left(\frac{dN}{2} - 1\right) k_\mathrm{B} T_\mathrm{B}$$

vs.

$$S_\mathrm{G}(E,V,A) = k_\mathrm{B} \ln[\Omega(E)]$$

$$E = \frac{dN}{2} k_\mathrm{B} T_\mathrm{G}$$

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Example 3: 1-dim 1-particle quantum gas

$$E_n = an^2/L^2, \qquad a = \hbar^2\pi^2/(2m), \qquad n = 1, 2, \ldots, \infty$$

$$\Omega = n = L\sqrt{E/a}$$

$$S_{\mathrm{B}}(E, V, A) = k_{\mathrm{B}} \ln[\epsilon\omega(E)]$$

$$k_{\mathrm{B}} T_{\mathrm{B}} = -2E < 0$$

$$p_{\mathrm{B}} \equiv T_{\mathrm{B}} \left(\frac{\partial S_{\mathrm{B}}}{\partial L}\right) = -\frac{2E}{L} \neq p$$

Dark energy ???

vs.

$$S_{\mathrm{G}}(E, V, A) = k_{\mathrm{B}} \ln[\Omega(E)]$$

$$k_{\mathrm{B}} T_{\mathrm{G}} = 2E, \qquad p_G \equiv T_{\mathrm{G}} \left(\frac{\partial S_{\mathrm{G}}}{\partial L}\right) = \frac{2E}{L}$$

$$p \equiv -\frac{\partial E}{\partial L} = \frac{2E}{L} = p_{\mathrm{G}}$$

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Dark energy ???

vs.

$$S_{\mathrm{G}}(E, V, A) = k_{\mathrm{B}} \ln[\Omega(E)]$$

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$$p \equiv -\frac{\partial E}{\partial L} = \frac{2E}{L} = p_{\mathrm{G}}$$

arxiv: 1304.2066

Consistency requirements

Consistent thermostatistical model (ρ, S) must fulfill

$$dS = \left(\frac{\partial S}{\partial E}\right) dE + \left(\frac{\partial S}{\partial V}\right) dV + \sum_i \left(\frac{\partial S}{\partial A_i}\right) dA_i \quad \equiv \frac{1}{T} dE + \frac{p}{T} dV + \sum_i \frac{a_i}{T} dA_i.$$

where

$$a_\mu \equiv T\left(\frac{\partial S}{\partial A_\mu}\right) \stackrel{!}{=} -\left\langle \frac{\partial H}{\partial A_\mu} \right\rangle \equiv -\mathrm{Tr}\left[\left(\frac{\partial H}{\partial A_\mu}\right)\rho\right]$$

Check

$$T_\mathrm{G}\left(\frac{\partial S_\mathrm{G}}{\partial A_\mu}\right) = \frac{1}{\omega}\frac{\partial}{\partial A_\mu}\mathrm{Tr}\Big[\Theta(E-H)\Big] = -\frac{1}{\omega}\mathrm{Tr}\left[-\frac{\partial}{\partial A_\mu}\Theta(E-H)\right]$$

$$= -\mathrm{Tr}\left[\left(\frac{\partial H}{\partial A_\mu}\right)\frac{\delta(E-H)}{\omega}\right] = -\left\langle \frac{\partial H}{\partial A_\mu}\right\rangle$$

$$\boxed{\Longrightarrow \quad \text{Only} \quad (\rho, S_\mathrm{G}) \quad \text{consistent model}}$$

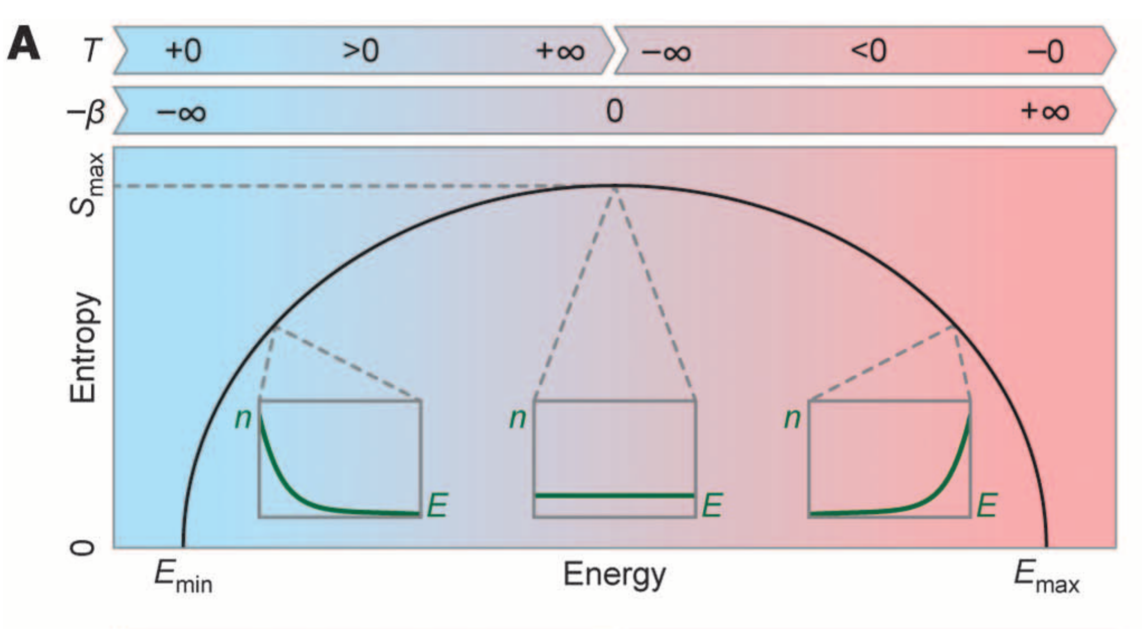
see also Campisi, Physica A 2007

Experimental 'evidence' for 'negative absolute temperature' ?

SCIENCE VOL 339 4 JANUARY 2013

Negative Absolute Temperature for Motional Degrees of Freedom

S. Braun,[1,2] J. P. Ronzheimer,[1,2] M. Schreiber,[1,2] S. S. Hodgman,[1,2] T. Rom,[1,2] I. Bloch,[1,2] U. Schneider[1,2]*



$$S_{\mathrm{B}}(E,V,A) = k_{\mathrm{B}} \ln[\epsilon\omega(E)],$$

$$T_{\mathrm{B}}(E,V,A) = \left(\frac{\partial S_{\mathrm{B}}}{\partial E}\right)^{-1} = \frac{1}{k_{\mathrm{B}}}\frac{\omega}{\omega'}$$

SCIENCE VOL 339 4 JANUARY 2013

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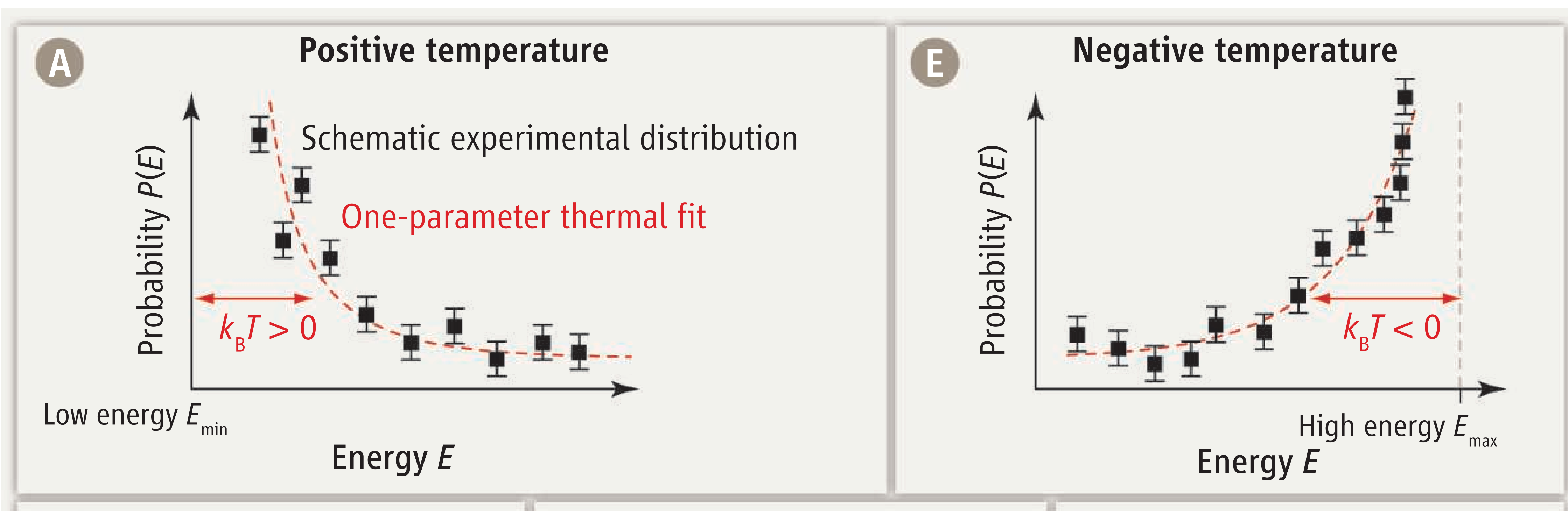
Because negative temperature systems can absorb entropy while releasing energy, they give rise to several counterintuitive effects, such as Carnot engines with an efficiency greater than unity (*4*). Through a stability analysis for thermodynamic equilibrium, we showed that negative temperature states of motional degrees of freedom necessarily possess negative pressure (*9*) and are thus of fundamental interest to the description of dark energy in cosmology, where negative pressure is required to account for the accelerating expansion of the universe (*10*).

✓ Carnot efficiencies >1

✓ Dark Energy

Crucial question:

- is the exponential fit parameter the thermodynamic temperature ?
- if not, what happens to the other claims ?



L. D. Carr. Negative temperatures? *Science*, 339:42–43, 2013.

arxiv: 1304.2066

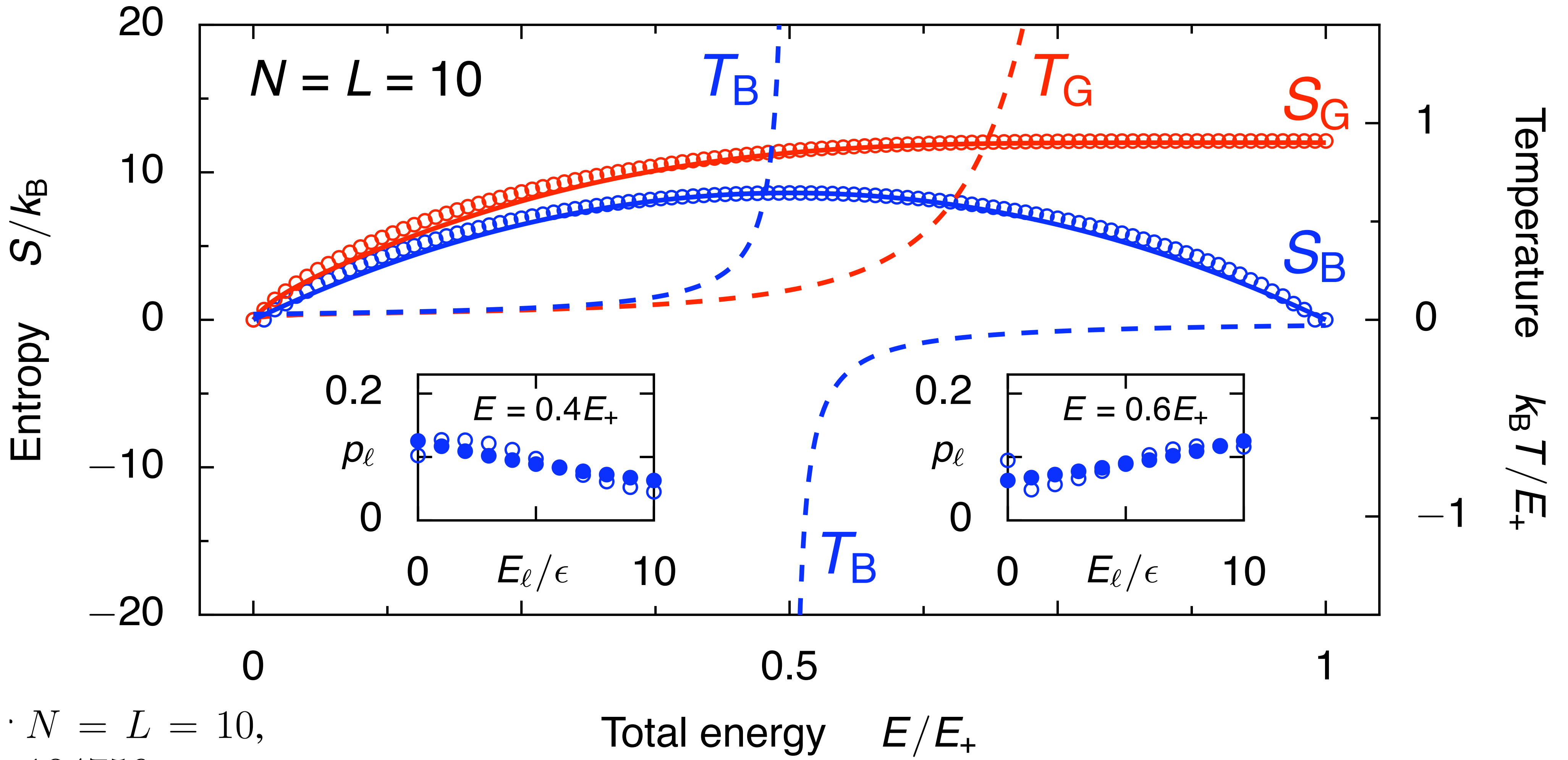
Generic spin or oscillator model

$$H_N \simeq \sum_{n=1}^{N} h_n, \qquad E_{\ell_n} = \epsilon \ell_n \qquad \ell_n = 0, 1 \ldots, L$$

$$E_\Lambda = \epsilon(\ell_1 + \ldots + \ell_N) \qquad 0 \leq E_\Lambda \leq E_+ = \epsilon L N$$

$$\omega(E) \simeq \omega_* \exp[-(E - E_*)^2/\sigma^2]$$

$$\Omega(E) \simeq 1 + \frac{\omega_* \sqrt{\pi}\sigma}{2}\left[\mathrm{erf}\left(\frac{E - E_*}{\sigma}\right) + \mathrm{erf}\left(\frac{E_*}{\sigma}\right)\right]$$



$N = L = 10$,
184756 **states**

$$k_B T_B = \frac{\sigma^2}{E_+ - 2E}$$

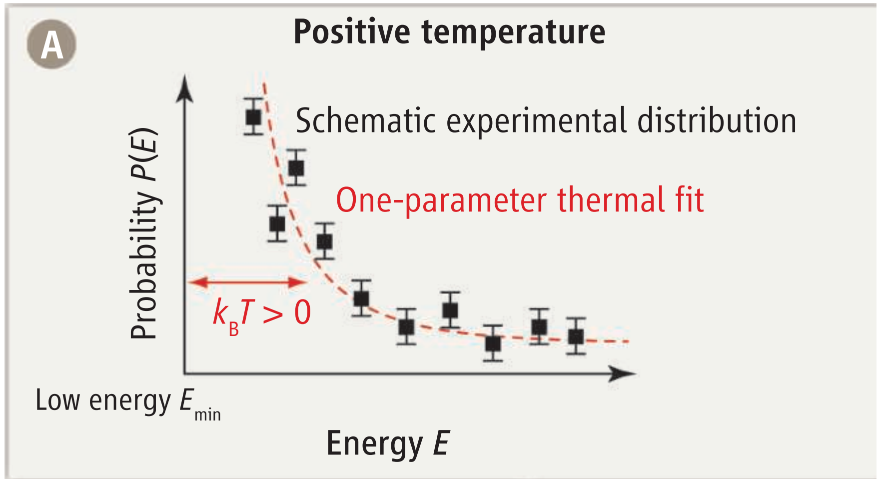
but

$$T_G > 0$$

Measuring T_{B} *vs.* T_{G}

arxiv: 1304.2066

One-particle distribution



$$\rho_1 = \mathrm{Tr}_{N-1}[\rho_N] = \frac{\mathrm{Tr}_{N-1}[\delta(E - H_N)]}{\omega_N}$$

Steepest-descent approximation

$$\rho_1 = \exp[\ln \rho_1] \quad \Rightarrow \quad p_\ell \simeq \frac{e^{-E_\ell/(k_{\mathrm{B}} T_{\mathrm{B}})}}{Z}, \qquad Z = \sum_\ell e^{-E_\ell/(k_{\mathrm{B}} T_{\mathrm{B}})}.$$

see e.g. Huang's textbook

features T_{B} and not T_{G}

$\Rightarrow$ one-particle thermal fit does not give absolute $T = T_{\mathrm{G}}$

Generally

$$\boxed{T_{\mathrm{B}} = \frac{T_{\mathrm{G}}}{1 - k_{\mathrm{B}}/C}}$$

Relativistic Regime

$$\Sigma(u = 0) \longrightarrow \Sigma'(u \neq 0)$$

$$x' = \gamma(u)\,(x - u \cdot t)$$

$$t' = \gamma(u)\left(t - ux/c^2\right)$$

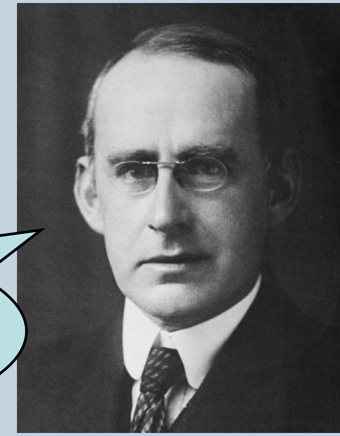
$$\text{with } \gamma(u) = \left(1 - \frac{u^2}{c^2}\right)^{-1/2}$$

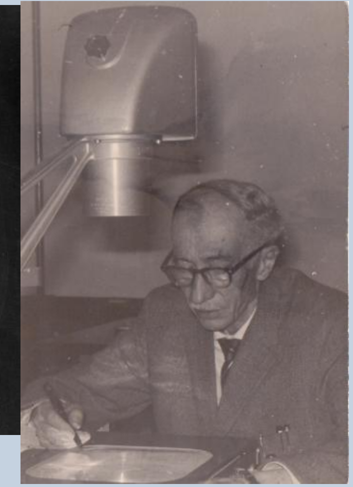
$$x^2 - c^2t^2 = (x')^2 - c^2(t')^2$$

Note: thermodynamic observables are **NONLOCAL**

J. Dunkel & P.H., *Relativistic Brownian motion*, Phys. Rep. **471**, 1 - 73 (2009)

"Temperature" problem in RTD?





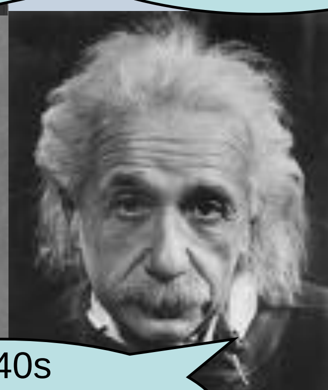
1923/1963

.. hotter!

1907/08

moving bodies appear cooler

$$T'(w) = T\,(1-w^2)^{\alpha/2} \qquad \alpha = \begin{cases} +1 & \text{Planck, Einstein} \\ 0 & \text{Landsberg, van Kampen} \\ -1 & \text{Ott} \end{cases}$$



1940s

maybe ... not

T=T' 1966-69

CK Yuen, Amer. J. Phys. 38:246 (1970)

Heat, second law & temperature

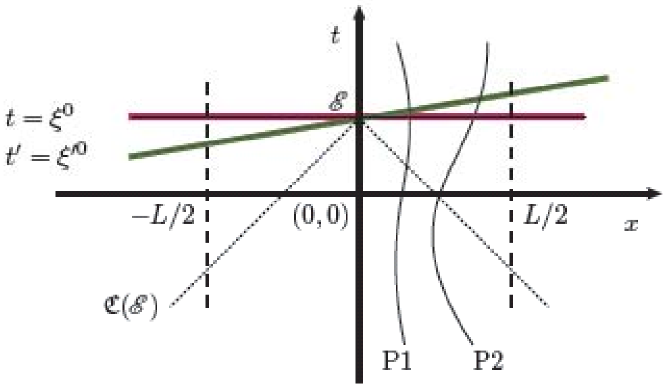
Planck-Einstein

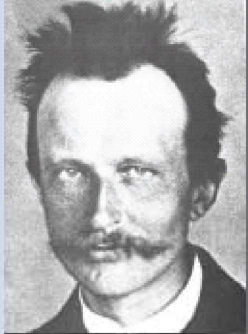
$$\text{đ}\mathcal{Q}'[\mathfrak{I}'] := \mathcal{T}'\mathrm{d}\mathcal{S}' := \mathrm{d}\mathcal{U}'^0[\mathfrak{I}'] - w'\mathrm{d}\mathcal{U}'^1[\mathfrak{I}'] + \mathcal{P}'\mathrm{d}V'$$

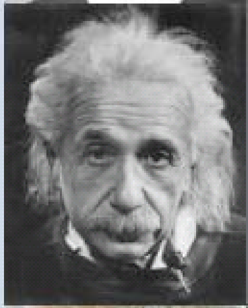
$$\gamma = (1 - w'^2)^{-1/2}$$

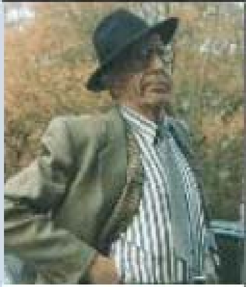
$$\mathcal{T}'\,\mathrm{d}\mathcal{S}' := \text{đ}\mathcal{Q}'^0[\mathfrak{I}'] = \gamma^{-1}\text{đ}\mathcal{Q}^0[\mathfrak{I}] = \gamma^{-1}\,\mathcal{T}\,\mathrm{d}\mathcal{S}$$

cooler









Ott

$$\text{đ}\mathcal{Q}^\mu[\mathfrak{I}] := \mathrm{d}\mathcal{U}^\mu[\mathfrak{I}] - \text{đ}\mathcal{A}^\mu[\mathfrak{I}],$$

$$(\text{đ}\mathcal{A}^\mu[\mathfrak{I}]) := (-\mathcal{P}\mathrm{d}V, \mathbf{0}).$$

$$\mathcal{T}'\,\mathrm{d}\mathcal{S}' := \text{đ}\mathcal{Q}'^0 = \gamma\text{đ}\mathcal{Q}^0 = \gamma\,\mathcal{T}\,\mathrm{d}\mathcal{S}.$$

hotter

van Kampen / Landsberg

$$\text{đ}\mathcal{Q}^\mu[\mathfrak{I}] := \mathrm{d}\mathcal{U}^\mu[\mathfrak{I}] - \text{đ}\mathcal{A}^\mu[\mathfrak{I}],$$

$$\text{đ}\mathcal{Q}' := -w'_\mu\text{đ}\mathcal{Q}'^\mu = -w_\mu\text{đ}\mathcal{Q}^\mu = \text{đ}\mathcal{Q} = \text{đ}\mathcal{Q}^0.$$

$$\mathcal{T}'\mathrm{d}\mathcal{S}' := \text{đ}\mathcal{Q}' = \text{đ}\mathcal{Q} = \mathcal{T}\mathrm{d}\mathcal{S},$$

T'=T

“Isochronous” RTD useful at all?

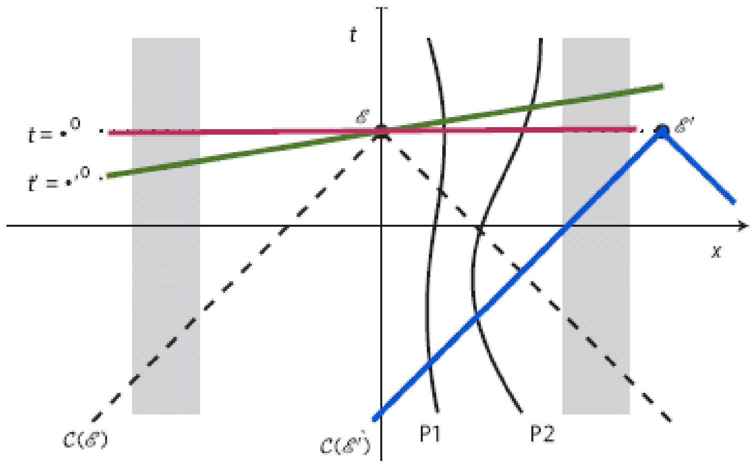
shortcomings

(i) not feasible experimentally
(ii) extension to General Relativity problematic

SOLUTION: replace isochronous hyperplanes by lightcones

Why?

✓ photographic measurements
✓ equivalent for moving observers
✓ GR extension
✓ nonrelativistic limit



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Thermodynamic variables

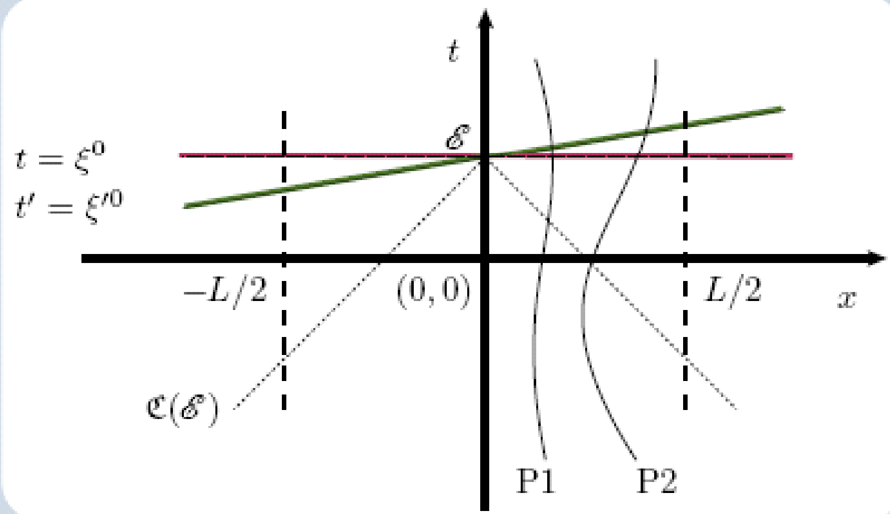
$$\partial_\mu j^\mu \equiv 0 \qquad \partial_\nu s^\nu \equiv 0 \qquad \boxed{\partial_\mu \theta^{\mu i} \not\equiv 0}$$

non-local TD variables $\Leftrightarrow$ surface integrals in space-time

$$\mathcal{N}[\mathfrak{H}] := \int_{\mathfrak{H}} d\sigma_\nu \, j^\nu = \mathcal{N}[\mathfrak{H}'] \qquad \text{scalar}$$

$$\mathcal{S}[\mathfrak{H}] := \int_{\mathfrak{H}} d\sigma_\nu \, s^\nu = \mathcal{S}[\mathfrak{H}'] \qquad \text{scalar}$$

$$\mathfrak{U}^\nu[\mathfrak{H}] := \int_{\mathfrak{H}} d\sigma_\mu \, \theta^{\mu\nu} \boxed{\neq \mathfrak{U}^\nu[\mathfrak{H}']} \qquad \text{4-vector}$$



$$\mathcal{N}[\mathfrak{H}] = \mathcal{N}'[\mathfrak{H}] = \mathcal{N}'[\mathfrak{H}'] = \mathcal{N}[\mathfrak{H}'] \qquad \mathcal{S}[\mathfrak{H}] = \mathcal{S}'[\mathfrak{H}] = \mathcal{S}'[\mathfrak{H}'] = \mathcal{S}[\mathfrak{H}'] \qquad \Lambda^\nu{}_\mu \mathfrak{U}^\mu[\mathfrak{H}] = \boxed{\mathfrak{U}'^\nu[\mathfrak{H}] \neq \mathfrak{U}'^\nu[\mathfrak{H}']} = \Lambda^\nu{}_\mu \mathfrak{U}^\mu[\mathfrak{H}']$$

"Photographic" thermodynamics

light-cone averaging

$$\mathfrak{C}(\mathscr{E}) \;:=\; \{\, (t, \boldsymbol{x}) \mid t = \xi^0 - |\boldsymbol{x} - \boldsymbol{\xi}| \,\}$$

photographic state variables

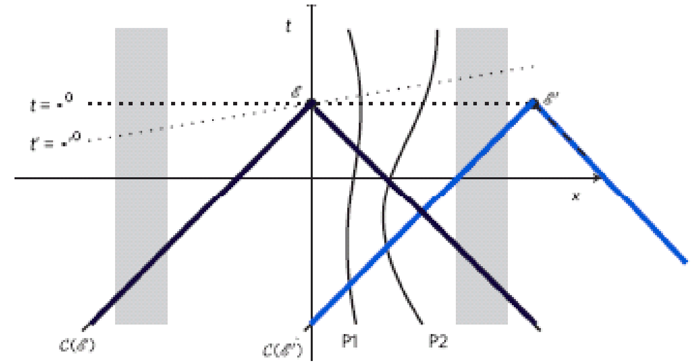
$$\mathcal{U}^0[\mathfrak{C}] \;=\; N \langle p^0 \rangle$$

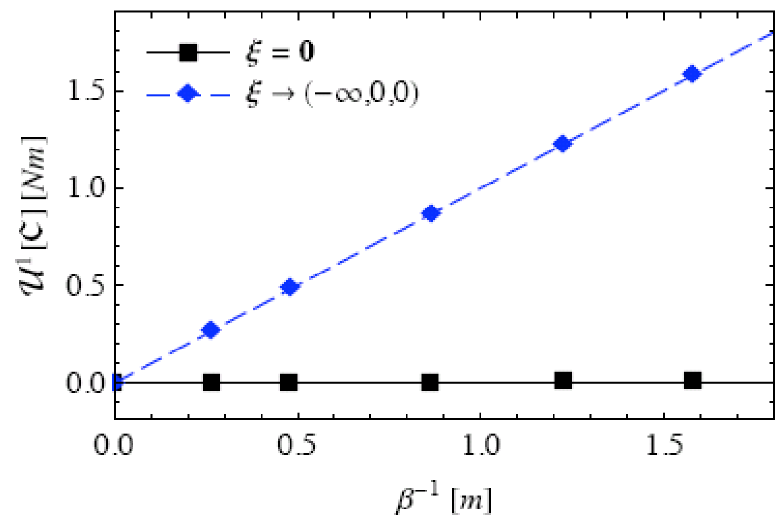
$$\mathcal{U}^i[\mathfrak{C}] \;=\; \frac{N}{\beta} \int \mathrm{d}^3 x \, \frac{x^i - \xi^i}{|\boldsymbol{x} - \boldsymbol{\xi}|} \, \varrho(\boldsymbol{x})$$

distant observer (at rest !)

$$\mathcal{U}^i[\mathfrak{C}] = -\frac{\xi^i}{|\boldsymbol{\xi}|} N k_\mathrm{B} \mathcal{T}$$

apparent drift !





JD, Peter Hanggi & Stefan Hilbert, Nature Physics 5:741, 2009

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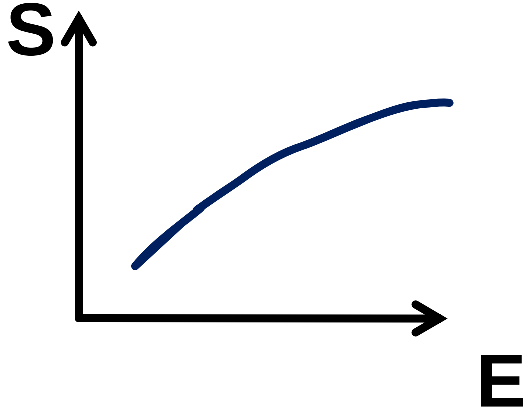
Take Home Messages

- $\exists$ absolute temperature $T \geq 0$



- $T = \frac{\partial E}{\partial S}$ ...

  with $S(E)$ a concave function of E !

- $S(E)$: microcanonical NOT always $=$ $S(E)$: canonical (long range, non-ergodic parts)

- T does **NOT** fluctuate

- quantum mechanics: no virial theorem; no equipartion

- relativistic statistical thermometer

$$\mathcal{T}_\Sigma = \mathcal{T}_{\Sigma'}$$

Conclusions

- population inversion $\Longrightarrow$ microcanonical
- bounded spectrum $\Longrightarrow$ ensembles not equivalent
- consistent thermostatistics $\Longrightarrow$ Gibbs entropy
- temperature always positive ('by construction')
- no Carnot efficiencies > 1
- please correct textbooks & lecture notes

arxiv: 1304.2066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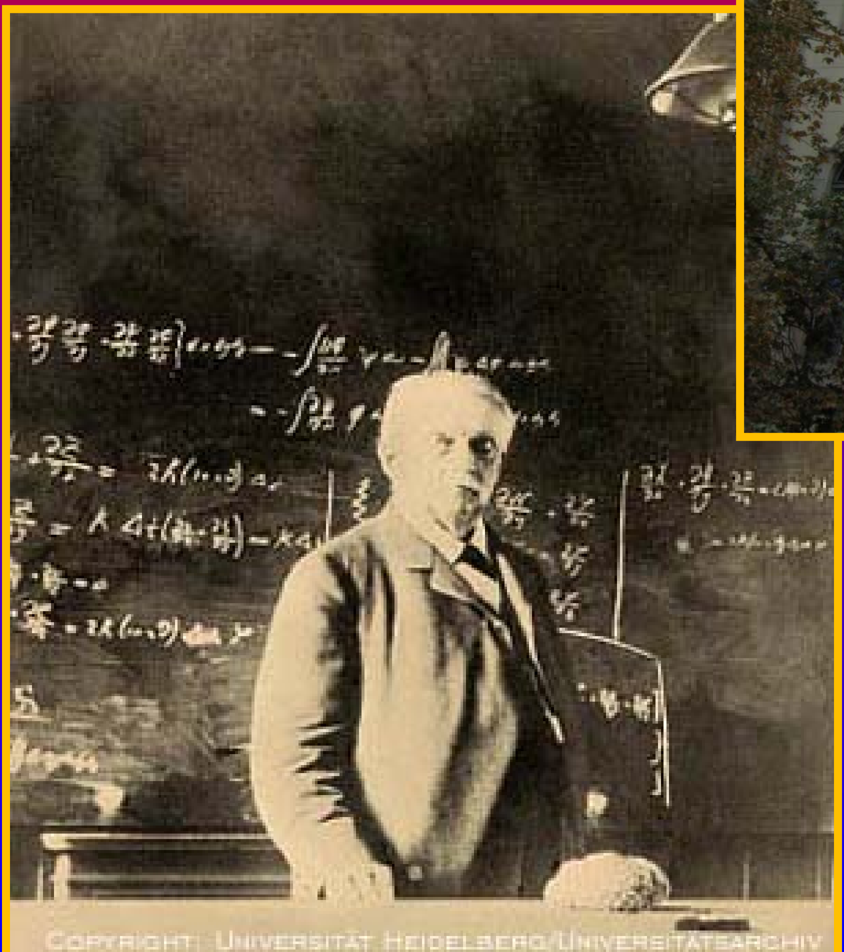
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