On the Use and Abuse of THERMODYNAMIC Entropy

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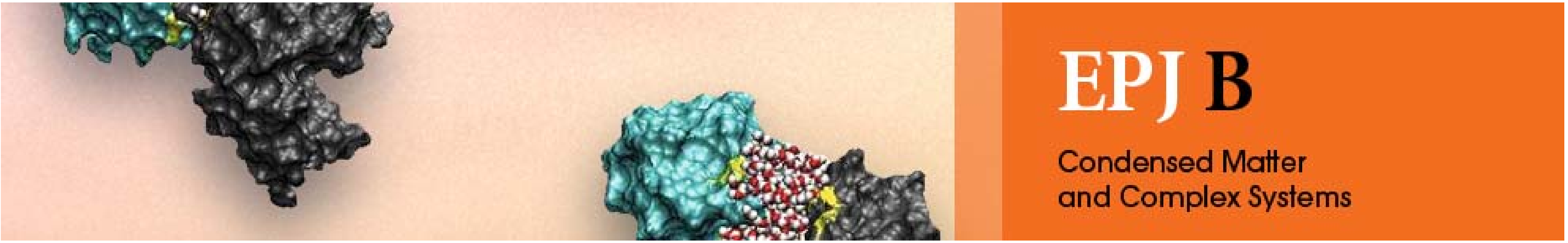

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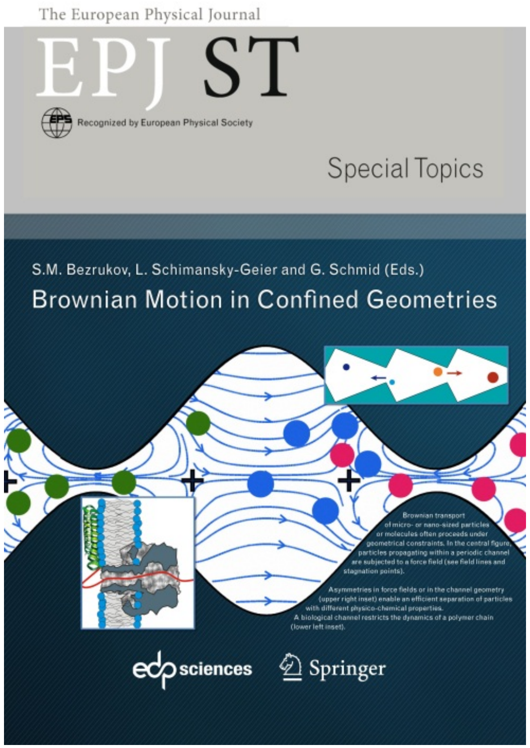

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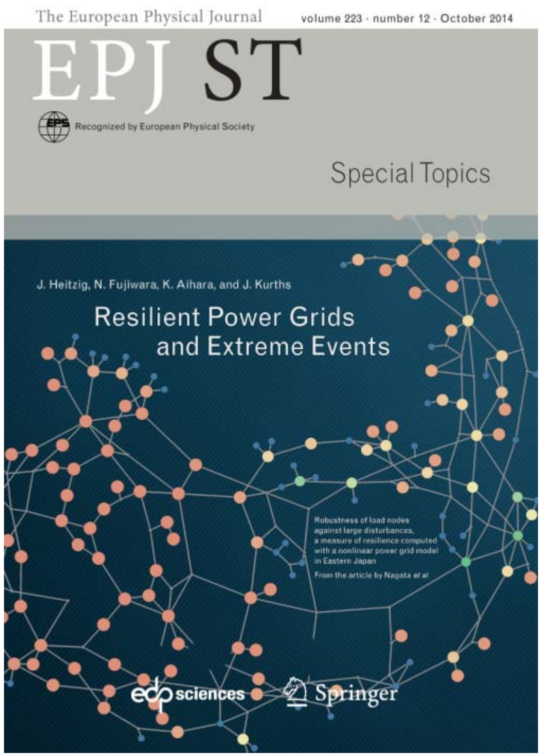

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Thermodynamic laws in isolated systems

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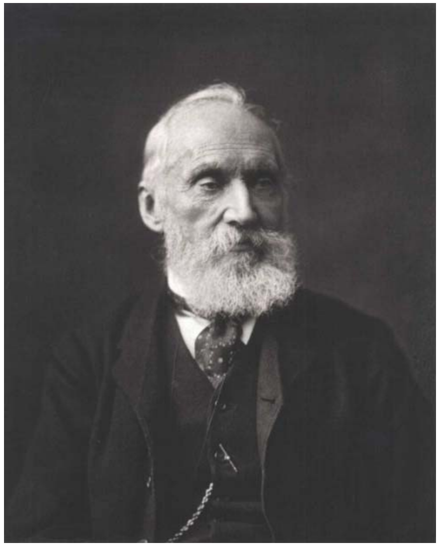
**** 23 pages ****

Second Law

Rudolf Julius Emanuel Clausius
(1822 – 1888)

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

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

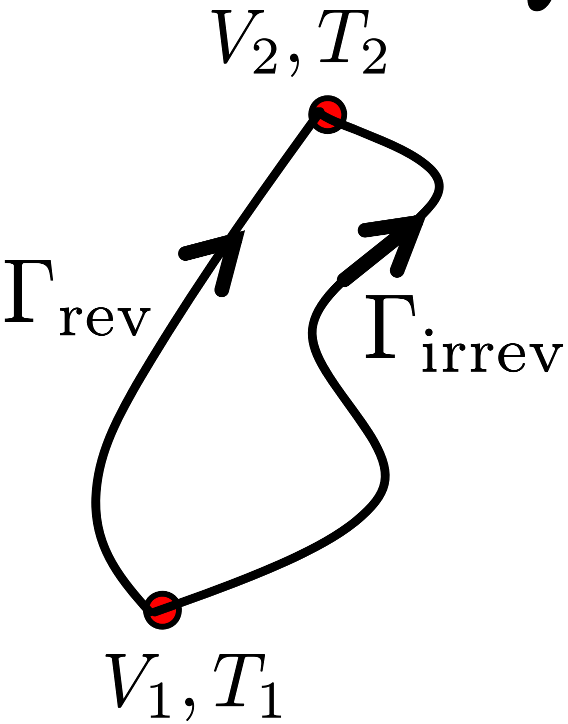


William Thomson alias Lord Kelvin
(1824 – 1907)

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.

Entropy S – content of *transformation* „Verwandlungswert“

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



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

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

$$S(V_2, T_2) - S(V_1, T_1) \geq \int_{\Gamma_{\text{irrev}}} \frac{\delta Q}{T}$$

$$S(V_2, T_2) - S(V_1, T_1) = \int_{\Gamma_{\text{rev}}} \frac{\delta Q^{\text{rev}}}{T}$$

$$\frac{\partial S}{\partial t} \geq 0$$

NO !

SECOND LAW

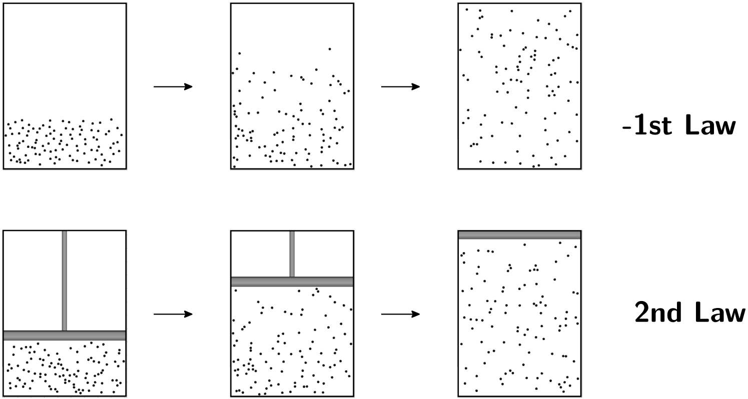
Quote by Sir Arthur Stanley Eddington:

“If someone points out to you that your pet theory of the universe is in disagreement with Maxwell’s equations – then so much the worse for Maxwell’s equations. If it is found to be contradicted by observation – well, these experimentalists do bungle things sometimes. But if your theory is found to be against the second law of thermodynamics I can give you no hope; there is nothing for it but to collapse in deepest humiliation.“

Freely translated into German:

Falls Ihnen jemand zeigt, dass Ihre Lieblingstheorie des Universums nicht mit den Maxwellgleichungen übereinstimmt - Pech für die Maxwellgleichungen. Falls die Beobachtungen ihr widersprechen - nun ja, diese Experimentatoren bauen manchmal Mist. -- Aber wenn Ihre Theorie nicht mit dem zweiten Hauptsatz der Thermodynamik übereinstimmt, dann kann ich Ihnen keine Hoffnung machen; ihr bleibt nichts übrig als in tiefster Schande aufzugeben.

MINUS FIRST LAW vs. SECOND LAW

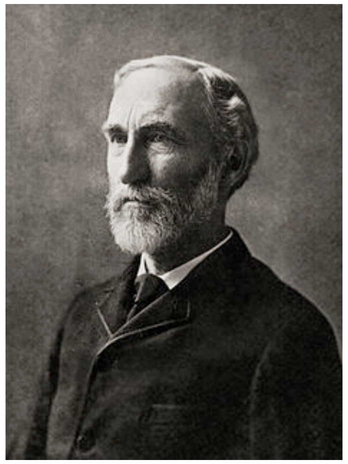


GIBBS, JOSIAH WILLARD.

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.

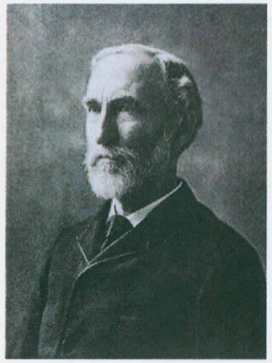
DISCUSSION OF THERMODYNAMIC ANALOGIES.

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

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

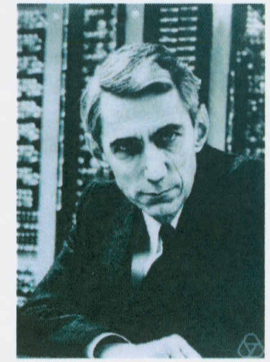
where ϵ, T, and η denote the energy, temperature, and entropy of the system considered, and $A_1\,da_1$, etc., the mechanical work (in the narrower sense in which the term is used in thermodynamics, *i. e.*, with exclusion of thermal action) done upon external bodies.

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).



J. W. Gibbs

L. Boltzmann



C. E. Shannon

$$H_G = \int W_N \ln W_N \, d\Gamma_N$$

$$S_G = k_B \ln \Omega_G$$

$$H_B = N \int w_1 \ln w_1 \, d\Gamma_1$$

$$S_B = k_B \ln \left(\frac{\partial \Omega_G}{\partial E}\right) \delta E$$

$$S_S = - \sum_i p_i \log_2 p_i$$

+ 200

Renyi

Relative-

Kullback-Leibler

v. NEUMANN

KOLMOGOROV-SINAI

CONDITIONAL

CLAUSIUS

FISHER

Daroczy-Harvda-Charvat-Tsallis

WEHRL

Hartley-chaitin

ETC.

Entropy in Stat. Mech.

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

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

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

Thermodynamic Temperature

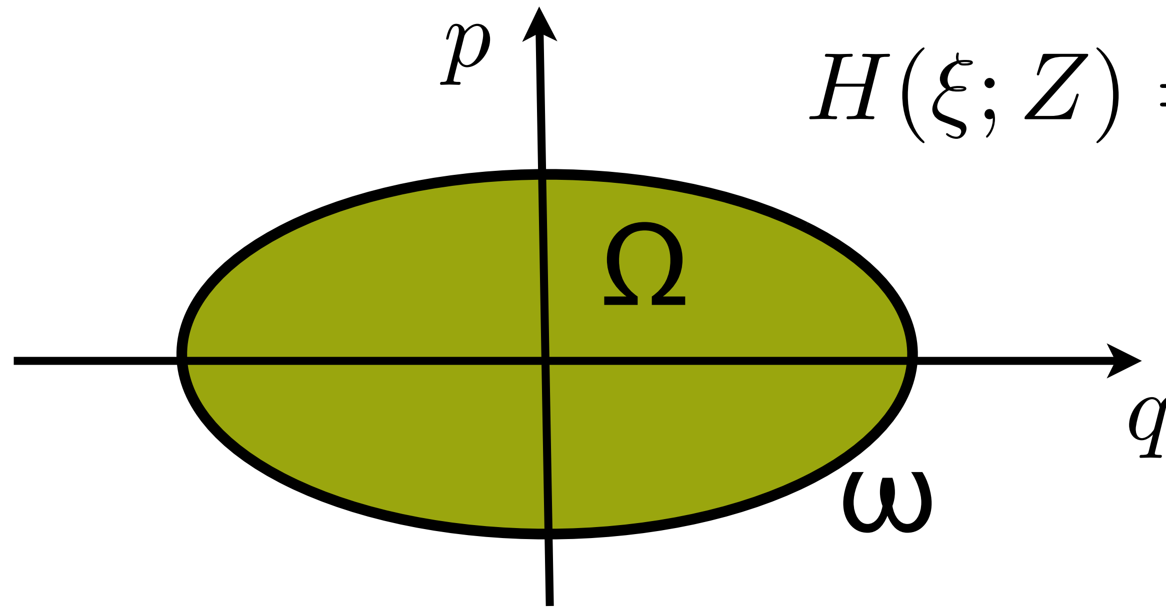
$$\delta Q^{\mathrm{rev}} = T\, dS \leftarrow \text{thermodynamic entropy}$$

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

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

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

Microcanonical thermostatistics



$$H(\xi; Z) = E$$

D-Operator

$$\rho(\boldsymbol{\xi}|E, Z) = \frac{\delta(E - H)}{\omega}$$

DoS

$$\omega(E, Z) = \mathrm{Tr}[\delta(E - H)] \geq 0$$

$$\Omega(E, Z) = \mathrm{Tr}[\Theta(E - H)]$$

IntDoS

Thermodynamic Entropy ?

$$S_{\mathrm{B}}(E) = \ln(\epsilon\,\omega)$$

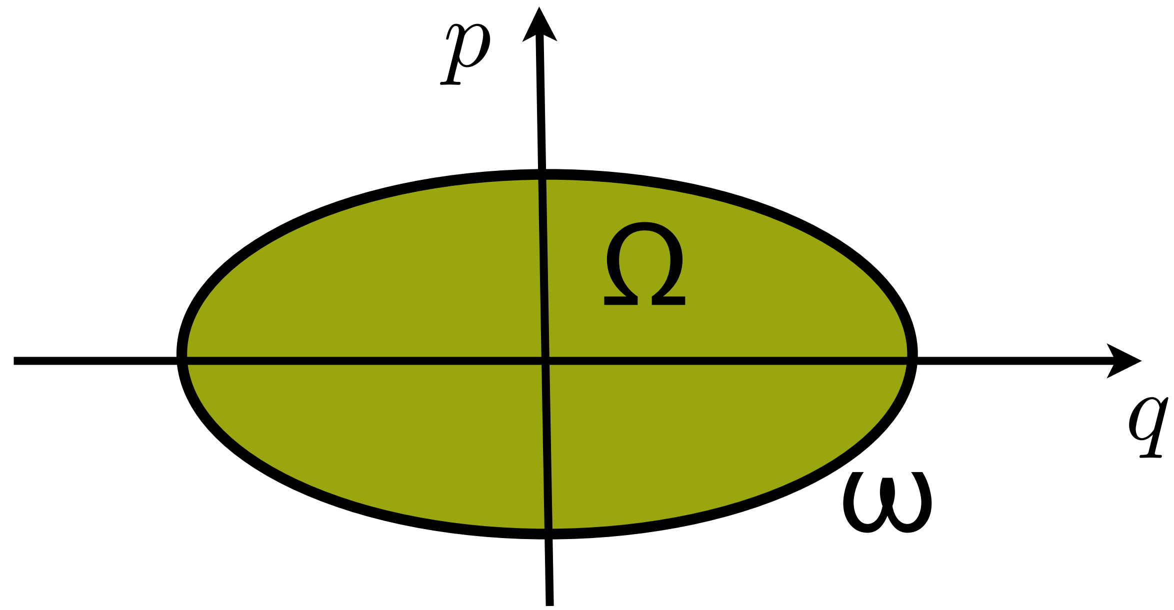
Boltzmann (?)

vs.

$$S_{\mathrm{G}}(E) = \ln \Omega$$

Gibbs (1902), Hertz (1910)

Boltzmann *vs.* Gibbs



$$S_{\mathrm{B}}(E) = \ln(\epsilon\,\omega) \qquad\qquad S_{\mathrm{G}}(E) = \ln\Omega$$

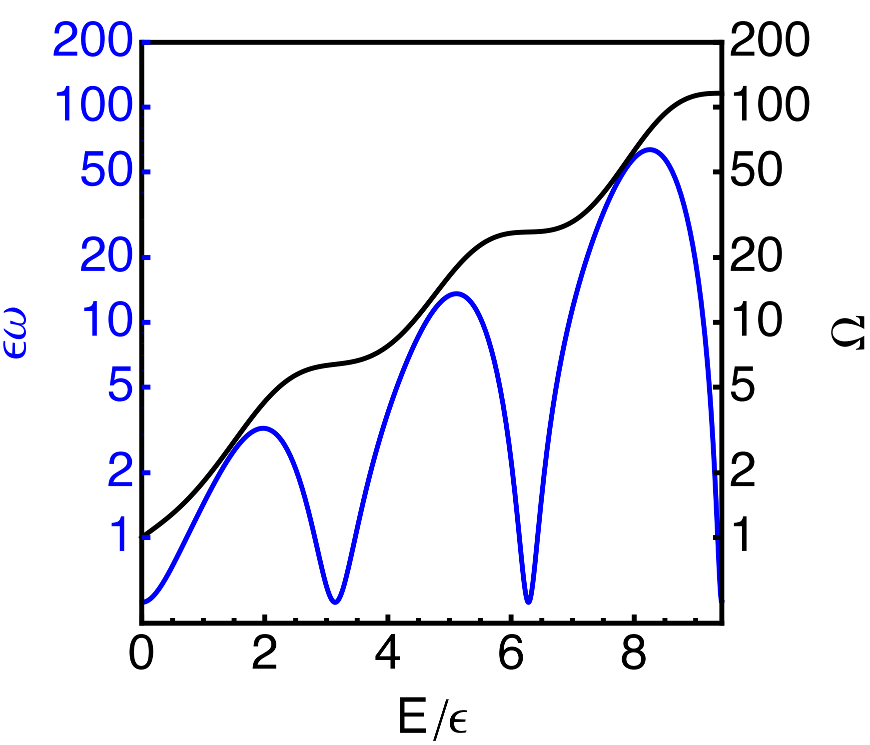
$$T(E,Z) \equiv \left(\frac{\partial S}{\partial E}\right)^{-1}$$

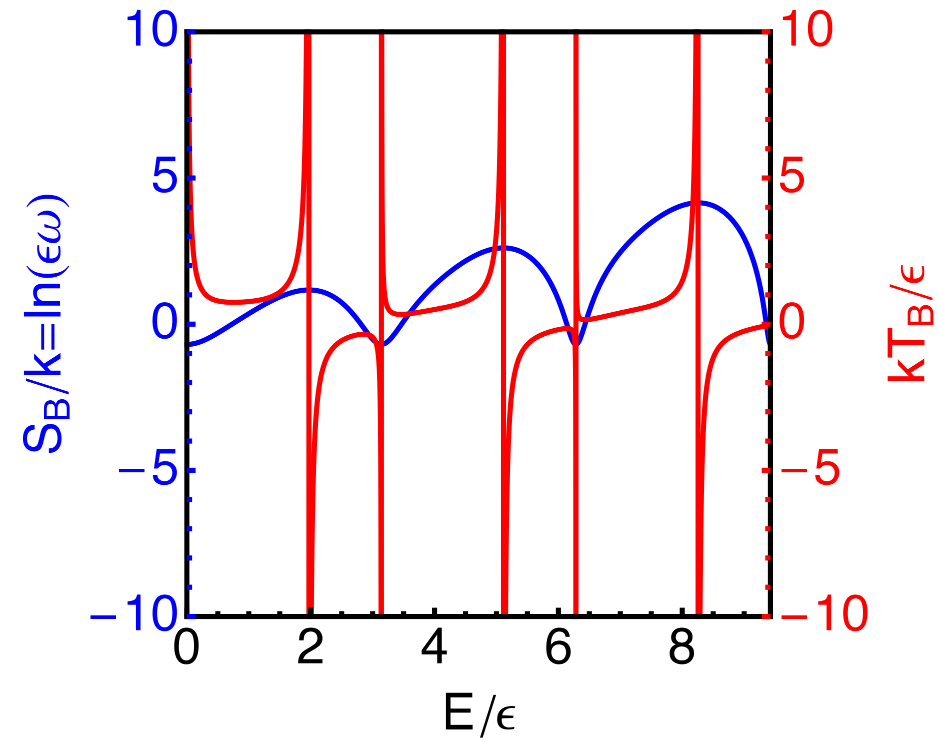
$$T_{\mathrm{B}}(E) = \frac{\omega}{\nu} \gtrless 0 \qquad\qquad T_{\mathrm{G}}(E) = \frac{\Omega}{\omega} \geq 0$$

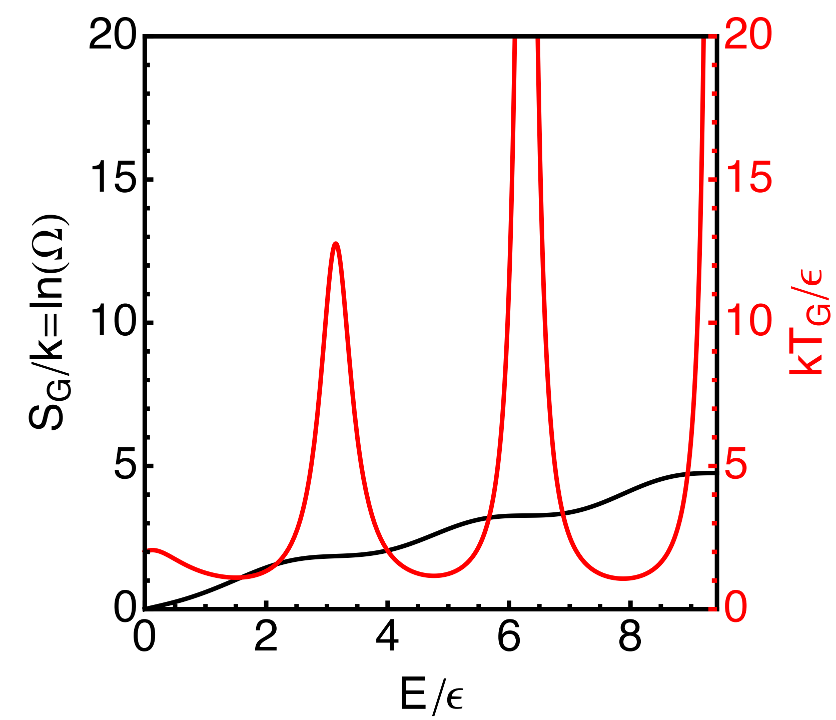
$$\nu(E,Z) = \partial\omega/\partial E,$$

‘Non-uniqueness’ of temperature

$$\Omega(E) = \exp\left[\frac{E}{2\epsilon} - \frac{1}{4}\sin\left(\frac{2E}{\epsilon}\right)\right] + \frac{E}{2\epsilon},$$







Temperature does NOT determine direction heat flow.

Energy is primary control parameter of MCE.

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

Proof:

$$k_\mathrm{B} T_\mathrm{G} = \frac{\Omega}{\Omega'} = \frac{\Omega}{\omega}, \qquad k_\mathrm{B} T_\mathrm{B} = \frac{\omega}{\omega'} = \frac{\Omega'}{\Omega''}$$

$$\frac{1}{C} \equiv \left(\frac{\partial T_\mathrm{G}}{\partial E}\right) = \frac{1}{k_\mathrm{B}} \left(\frac{\Omega}{\Omega'}\right)' = \frac{1}{k_\mathrm{B}} \frac{\Omega'\Omega' - \Omega\Omega''}{(\Omega')^2}$$

$$= \frac{1}{k_\mathrm{B}} \left[1 - \frac{\Omega\Omega''}{(\Omega')^2}\right] = \frac{1}{k_\mathrm{B}} \left(1 - \frac{T_\mathrm{G}}{T_\mathrm{B}}\right)$$

$\square$

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

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

e.g. for pressure ($\mu = 0$)

$$p = T\left(\frac{\partial S}{V}\right)_E = -\left(\frac{\partial E}{\partial V}\right)_S = -\left\langle \frac{\partial H}{\partial V} \right\rangle$$

First law

$$dE = \delta Q + \delta A = T\,dS - \sum_n p_n dZ_n$$

$$p_j = T\left(\frac{\partial S}{\partial Z_j}\right)_{E, Z_n \neq Z_j} \stackrel{!}{=} -\left\langle \frac{\partial H}{\partial Z_j} \right\rangle_E$$

Gibbs

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

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

see also Campisi, Physica A 2007

First law

$$dE = \delta Q + \delta A = T\,dS - \sum_n p_n dZ_n$$

$$p_j = T\left(\frac{\partial S}{\partial Z_j}\right)_{E,Z_n\neq Z_j} \overset{!}{=} -\left\langle \frac{\partial H}{\partial Z_j}\right\rangle_E$$

Gibbs ✓ $\Longrightarrow$ Boltzmann ✗

see also Campisi, Physica A 2007

Second law

Gibbs

$$S_{\mathrm{G}}(E) = \ln \Omega$$

$$\begin{aligned}
&\Omega(E_{\mathcal{A}} + E_{\mathcal{B}}) \\
&= \int_0^{E_{\mathcal{A}}+E_{\mathcal{B}}} \mathrm{d}E' \, \Omega_{\mathcal{A}}(E') \omega_{\mathcal{B}}(E_{\mathcal{A}} + E_{\mathcal{B}} - E') \\
&= \int_0^{E_{\mathcal{A}}+E_{\mathcal{B}}} \mathrm{d}E' \int_0^{E'} \mathrm{d}E'' \omega_{\mathcal{A}}(E'') \omega_{\mathcal{B}}(E_{\mathcal{A}} + E_{\mathcal{B}} - E') \\
&\geq \int_{E_{\mathcal{A}}}^{E_{\mathcal{A}}+E_{\mathcal{B}}} \mathrm{d}E' \int_0^{E_{\mathcal{A}}} \mathrm{d}E'' \omega_{\mathcal{A}}(E'') \omega_{\mathcal{B}}(E_{\mathcal{A}} + E_{\mathcal{B}} - E') \\
&= \int_0^{E_{\mathcal{A}}} \mathrm{d}E'' \omega_{\mathcal{A}}(E'') \int_0^{E_{\mathcal{B}}} \mathrm{d}E''' \omega_{\mathcal{B}}(E''') \\
&= \Omega_{\mathcal{A}}(E_{\mathcal{A}}) \, \Omega_{\mathcal{B}}(E_{\mathcal{B}}).
\end{aligned}$$

$$\Longrightarrow \quad S_{\mathrm{G}\mathcal{A}\mathcal{B}}(E_{\mathcal{A}} + E_{\mathcal{B}}) \geq S_{\mathrm{G}\mathcal{A}}(E_{\mathcal{A}}) + S_{\mathrm{G}\mathcal{B}}(E_{\mathcal{B}})$$ ✓

Second law

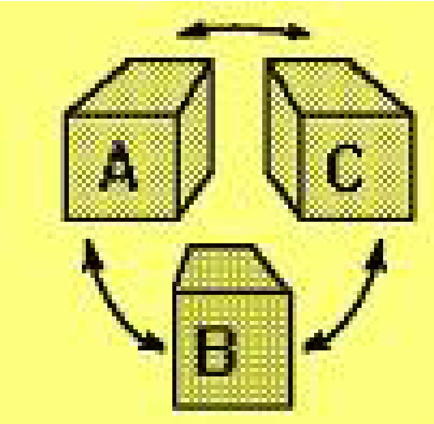
Boltzmann $$S_{\mathrm{B}}(E) = \ln(\epsilon\,\omega)$$

$$\epsilon\omega(E_{\mathcal{A}} + E_{\mathcal{B}}) = \epsilon \int_0^{E_{\mathcal{A}}+E_{\mathcal{B}}} \mathrm{d}E'\omega_{\mathcal{A}}(E')\omega_{\mathcal{B}}(E_{\mathcal{A}} + E_{\mathcal{B}} - E')$$

$$\not\geq \quad \epsilon^2\omega_{\mathcal{A}}(E_{\mathcal{A}})\omega_{\mathcal{B}}(E_{\mathcal{B}})$$

✗

Zeroth Law



Transitivity !

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

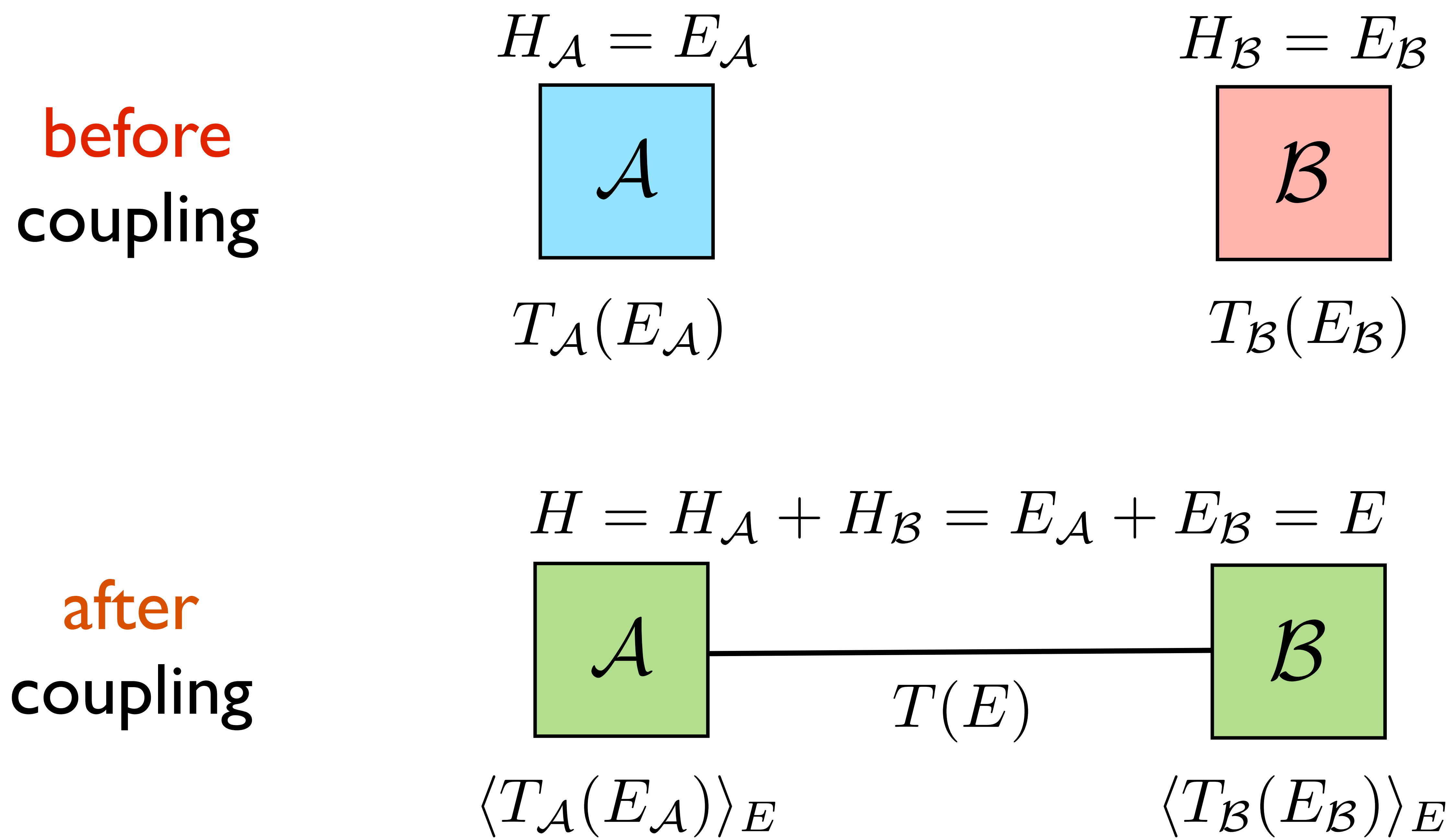
$$\text{B in equilibrium with C:} \quad f_{\mathrm{BC}}(p_{\mathrm{B}}, V_{\mathrm{B}}; p_{\mathrm{C}}, V_{\mathrm{C}}, \ldots) = 0$$

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

Allows the formal introduction of a temperature:

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

Thermal equilibrium

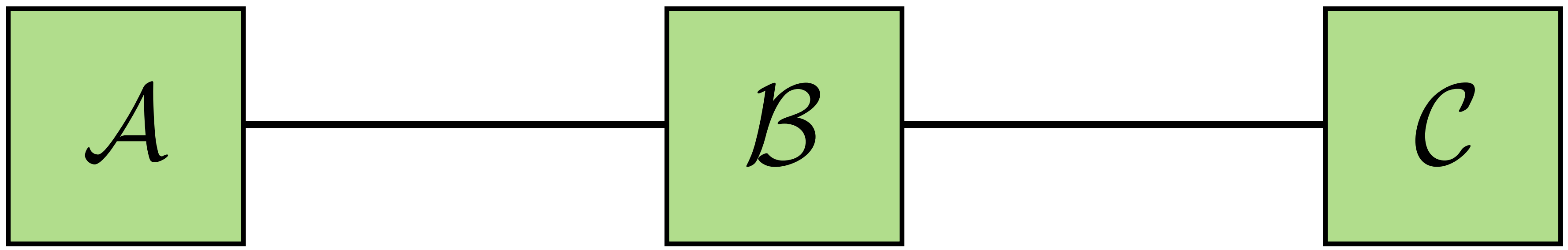


$$\langle T_i(E_i) \rangle_E = \int_0^\infty dE_i \; T_i(E_i)\, \pi_i(E_i|E)$$

$$\pi_{\mathcal{A}}(E_{\mathcal{A}}|E) = \frac{\omega_{\mathcal{A}}(E_{\mathcal{A}})\, \omega_{\mathcal{B}}(E - E_{\mathcal{A}})}{\omega(E)}.$$

Zeroth law

$$T(E)$$



$$\langle T_{\mathcal{A}}(E_{\mathcal{A}})\rangle_E \qquad \langle T_{\mathcal{B}}(E_{\mathcal{B}})\rangle_E \qquad \langle T_{\mathcal{C}}(E_{\mathcal{C}})\rangle_E$$

$$\langle T_i(E_i)\rangle_E \stackrel{!}{=} T(E)$$

Gibbs

$$\begin{aligned}
\langle T_{\mathrm{G}\mathcal{A}}(E_{\mathcal{A}})\rangle_E &= \int_0^\infty \mathrm{d}E_{\mathcal{A}}\, \frac{\Omega_{\mathcal{A}}(E_{\mathcal{A}})}{\omega_{\mathcal{A}}(E_{\mathcal{A}})}\, \frac{\omega_{\mathcal{A}}(E_{\mathcal{A}})\omega_{\mathcal{B}}(E-E_{\mathcal{A}})}{\omega(E)} \\
&= \frac{1}{\omega(E)} \int_0^E \mathrm{d}E_{\mathcal{A}}\, \Omega_{\mathcal{A}}(E_{\mathcal{A}})\omega_{\mathcal{B}}(E-E_{\mathcal{A}}) \\
&= T_{\mathrm{G}}(E).
\end{aligned}$$

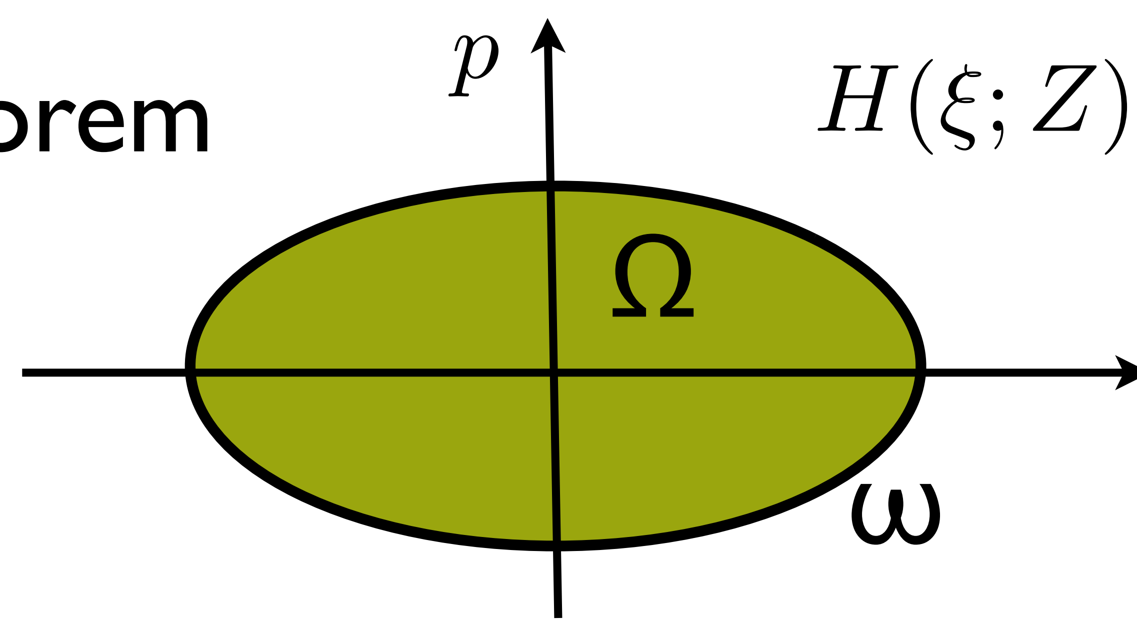
Entropy	$S(E)$	second law Eq. (38)	first law Eq. (37)	zeroth law Eq. (20)	equip artition equipartition
Gibbs	$\ln \Omega$	yes	yes	yes	yes
Penrose	$\ln \Omega + \ln\big(\Omega_\infty - \Omega\big) - \ln \Omega_\infty$	yes	yes	no	no
Complementary Gibbs	$\ln\big[\Omega_\infty - \Omega\big]$	yes	yes	no	no
Differential Boltzmann	$\ln\big[\Omega(E+\epsilon) - \Omega(E)\big]$	yes	no	no	no
Boltzmann	$\ln\big(\epsilon\omega\big)$	no	no	no	no

For Gibbs temperature & classical Hamiltonian systems even more ...

for all canonical coordinates $\xi = (\xi_1, \ldots)$ equipartition

$$\left\langle \xi_i \frac{\partial H}{\partial \xi_j} \right\rangle \equiv \mathrm{Tr}\left[\left(\xi_i \frac{\partial H}{\partial \xi_j} \right) \rho \right] = k_{\mathrm{B}} T_{\mathrm{G}} \delta_{ij}$$

... essentially Stokes theorem



$$H(\xi; Z) = E$$

A. I. Khinchin. *Mathematical Foundations of Statistical Mechanics*. Dover, New York, 1949.

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

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.

$$S_G(E, V, A) = k_B \ln[\Omega(E)]$$

$$k_B T_G = 2E, \qquad p_G \equiv T_G \left(\frac{\partial S_G}{\partial L}\right) = \frac{2E}{L}$$

$$p \equiv -\frac{\partial E}{\partial L} = \frac{2E}{L} = p_G$$

Inconsistent thermostatistics and negative absolute temperatures

Jörn Dunkel and Stefan Hilbert,

nature physics 10: 67-72 (2014)

& ! SUPPL. -MATERIAL !

? Negative Temperature ?

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

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

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

$$\omega = \frac{N!}{n_g! n_e!} \Rightarrow S_B = k_B \ln \omega$$

$$\Rightarrow \frac{1}{T_B} = \frac{\partial S_B}{\partial E}$$

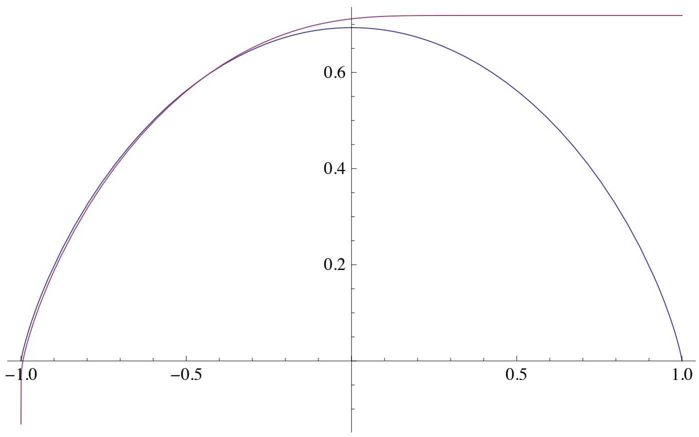
➡ $n_g = \frac{1}{2}\left(N - \frac{E}{\mu B}\right)$

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

```
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]=

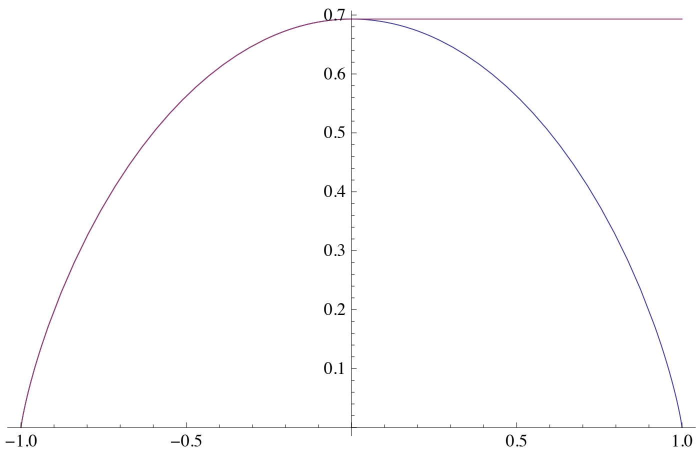


Purple: S_Phi /N
Blue: S_Omega/N

N=100

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

Out[25]=

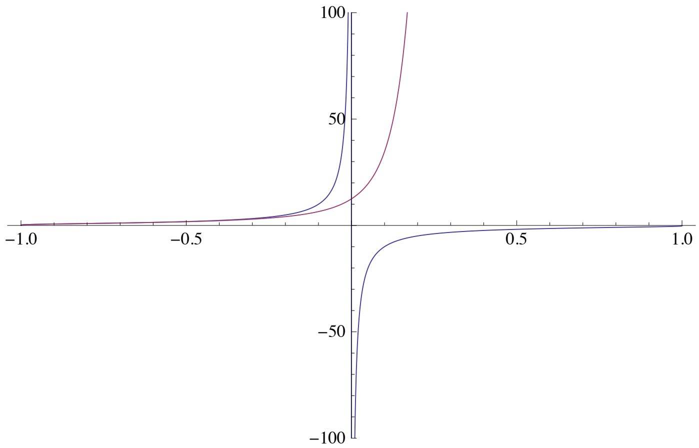


Purple: S_Phi /N
Blue: S_Omega/N

N=10^8

Limit Value = Log 2

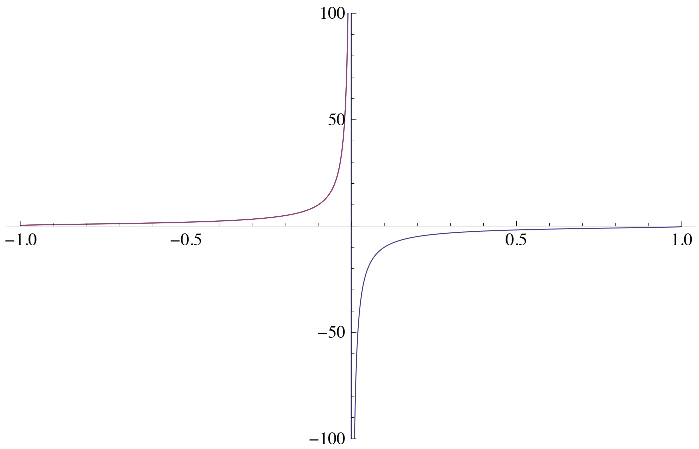
Out[26]=



Purple: T_Phi
Blue: T_Omega

N=100

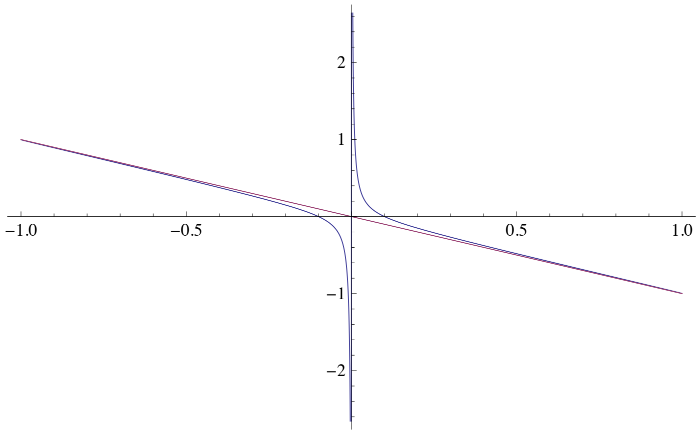
Out[27]=



Purple: T_Phi
Blue: T_Omega

N=10^8

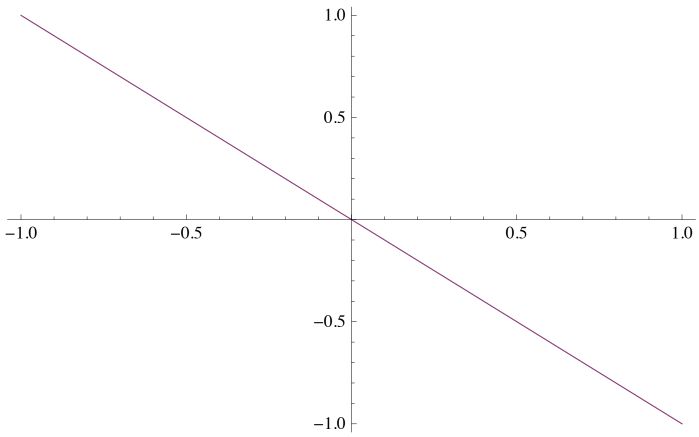
Out[28]=



Purple: M_Phi
Blue: M_Omega

N=100

Out[29]=



Purple: M_Phi
Blue: M_Omega

N=10^8

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*]

Ultra-cold boson gas in optical lattice 10^5 ^{39}K atoms

$$H = -J\sum_{\langle i,j\rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2}\sum_i \hat{n}_i(\hat{n}_i - 1) + V\sum_i \mathrm{r}_i^2 \hat{n}_i$$

via Feshbach resonance

- U>0: repulsive interactions
- U<0: attractive interactions

Claim: for U,V<0 spectrum bounded from above, population inversion in momentum space $\Rightarrow T < 0$

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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

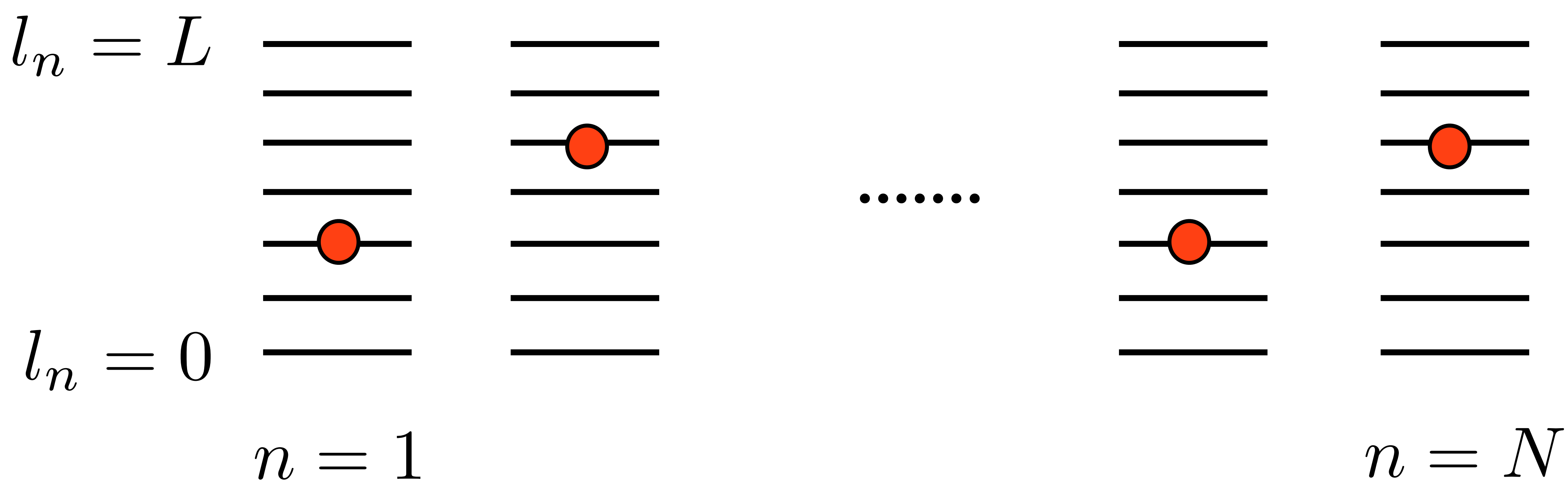
✓ Dark Energy

Generic spin or oscillator model

arxiv: 1304.2066

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

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



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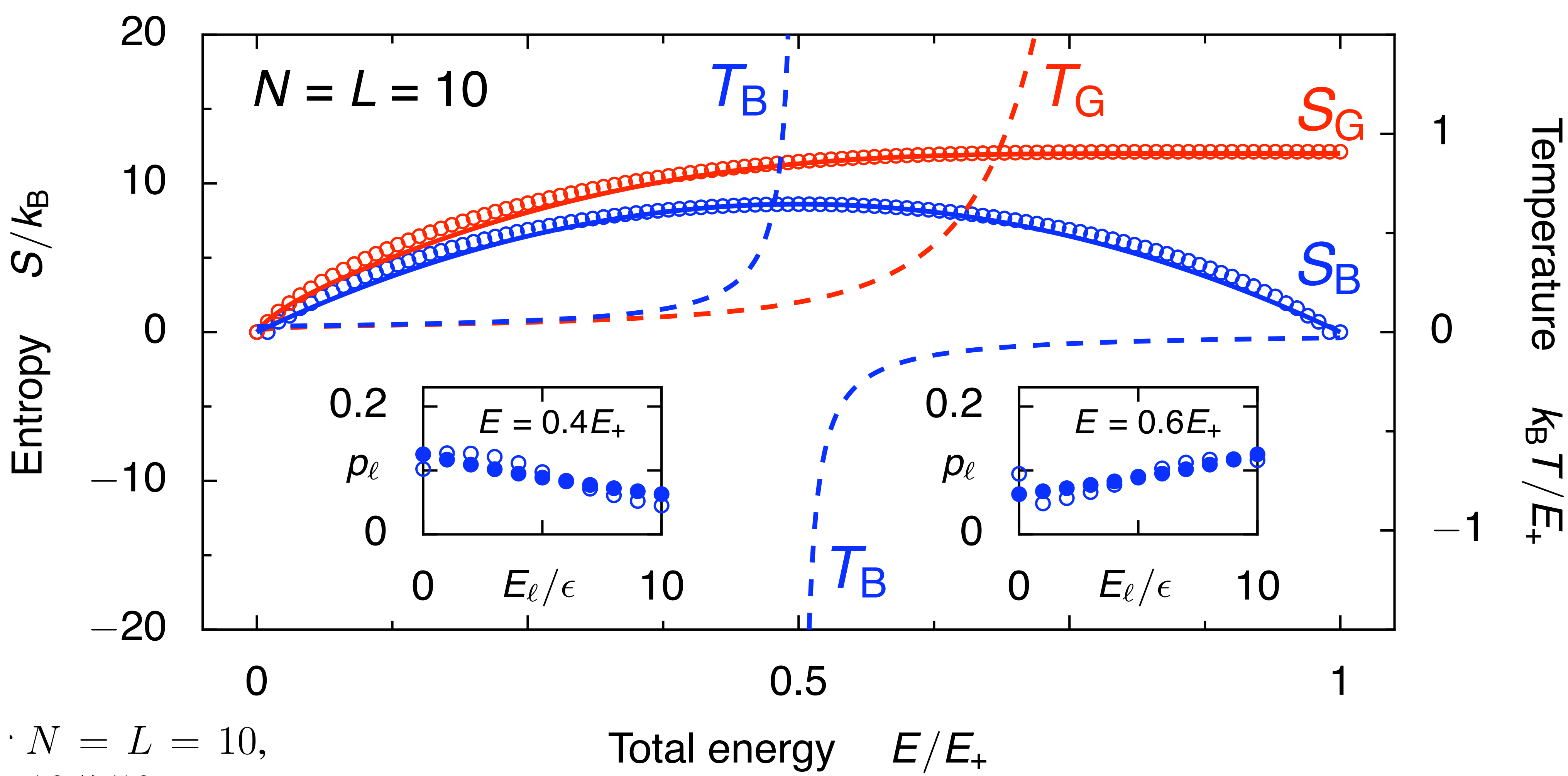
$$E_\Lambda = \epsilon(\ell_1 + \ldots + \ell_N) \qquad 0 \le E_\Lambda \le E_+ = \epsilon L N$$

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

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



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

but

$$T_G > 0$$

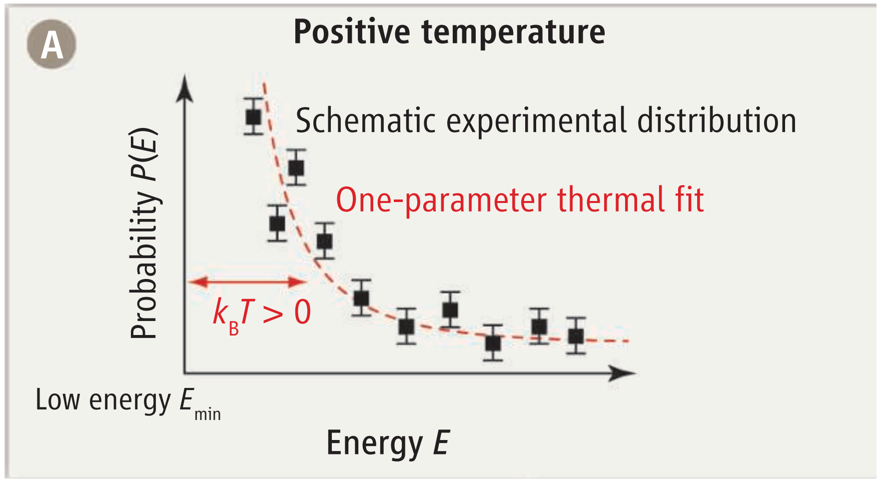
$N = L = 10$, 184756 states

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}

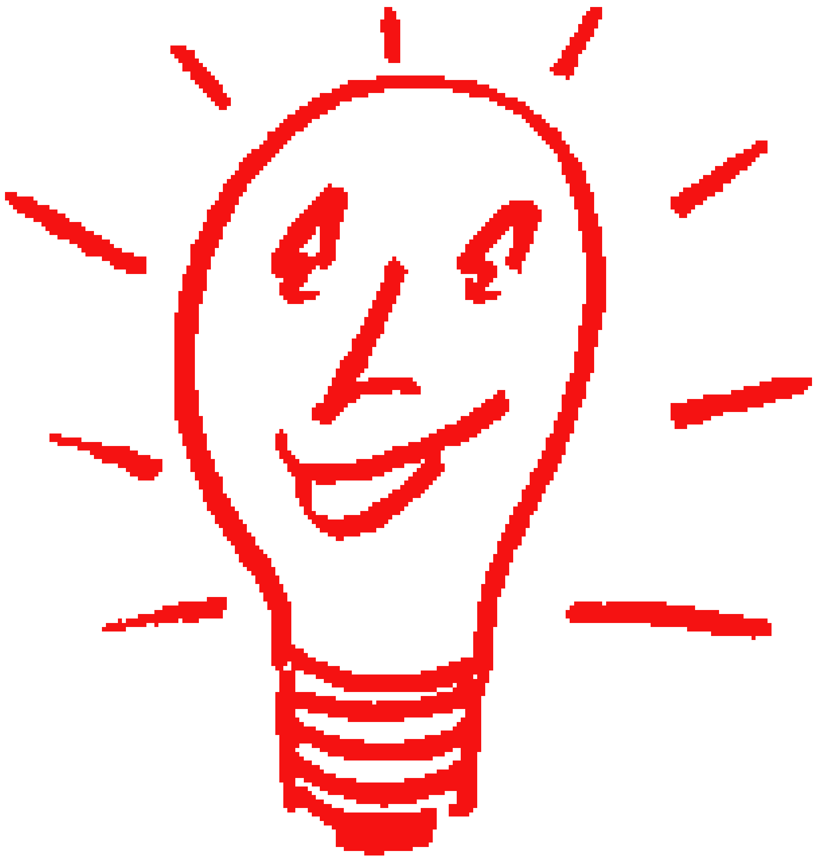
$\Rightarrow$ one-particle thermal fit does not give absolute $T = T_{\mathrm{G}}$

Generally

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

$$C = \left(\frac{\partial T_{\mathrm{G}}}{\partial E}\right)^{-1}$$

A QUESTION ?



Conclusions

- population inversion ⇨ microcanonical
- bounded spectrum ⇨ ensembles not equivalent
- consistent thermostatistics ⇨ Gibbs entropy
- temperature always positive
  (‘by construction’)
- no Carnot efficiencies > 1

Hilbert-Hänggi-Dunkel, Phys.Rev. E **90**: 062116 (2014)