Termodinámica estadística: Sistema de dos estados y temperaturas negativas

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Contexto

- Se trata de un problema actual controversial relacionado con la definición estadística de entropía.
- Ocurre cuando se impone una cota superior a los estados energéticos disponibles.
- Conduce a contribuciones negativas a la temperatura de un sistema por grados específicos de libertad.
- Este problema no ocurre si se usa la definición de Gibbs de entropía.

Nota: Este tema es opcional, complementario, y no se considerará para la evaluación.

Planteamiento

Sea un sistema con dos niveles posibles:

$$E_1 = -\varepsilon, \qquad E_2 = \varepsilon$$

tal que

$$\begin{aligned} N &= N_1 + N_2 \\ E &= N_1 E_1 + N_2 E_2 = (N_2 - N_1)\varepsilon \end{aligned}$$

Ejercicio: Expresa N_1 y N_2 en términos de E y N.

Resultado:

$$N_1 = \frac{1}{2}\left(N - \frac{E}{\varepsilon}\right) \qquad N_2 = \frac{1}{2}\left(N + \frac{E}{\varepsilon}\right)$$

El número de estados con energía $\boldsymbol{E}$ y $\boldsymbol{N}$ partículas es

$$\boldsymbol{\Omega(E,N) = \frac{N!}{N_1!N_2!} = \frac{N!}{\left[\frac{1}{2}\left(N-\frac{E}{\varepsilon}\right)\right]!\left[\frac{1}{2}\left(N+\frac{E}{\varepsilon}\right)\right]!}}$$

La entropía es $\boldsymbol{S(E,N) = k\ln\Omega(E,N)}$.

Ejercicio: Obtén la entropía del sistema mediante la aproximación de Stirling.

Resultado:

$$\boldsymbol{S(E,N) = k\left[N\ln N - \frac{1}{2}\left(N+\frac{E}{\varepsilon}\right)\ln\left(N+\frac{E}{\varepsilon}\right)\right.}$$
$$\boldsymbol{\left.-\frac{1}{2}\left(N-\frac{E}{\varepsilon}\right)\ln\left(N-\frac{E}{\varepsilon}\right)\right]}$$

Ejercicio:

Verifica que al dividir S entre Nk, se obtiene:

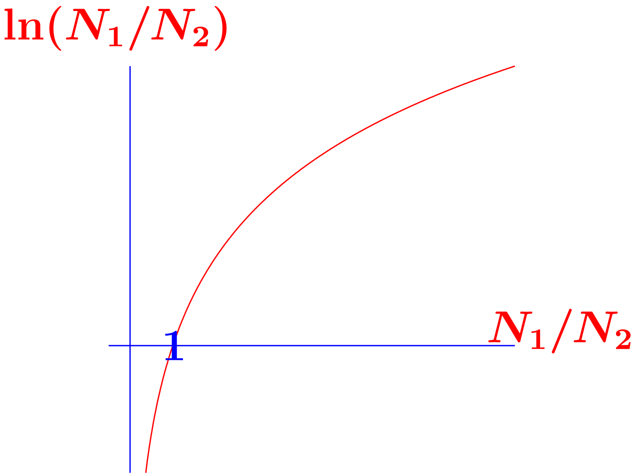
$$\begin{aligned} \frac{S}{Nk} &= \ln 2 \\ &\quad -\frac{1}{2}\left(1+\frac{E}{N\varepsilon}\right)\ln\left(1+\frac{E}{N\varepsilon}\right) \\ &\quad -\frac{1}{2}\left(1-\frac{E}{N\varepsilon}\right)\ln\left(1-\frac{E}{N\varepsilon}\right) \end{aligned}$$

Recordar que:

$$\ln \frac{N_1}{N_2} \approx \ln e^{\Delta E/kT} = \frac{\Delta E}{kT}, \qquad \Delta E = 2\varepsilon > 0$$

Por lo tanto:

$$\frac{1}{T} = \frac{k}{\Delta E} \ln \frac{N_1}{N_2}$$



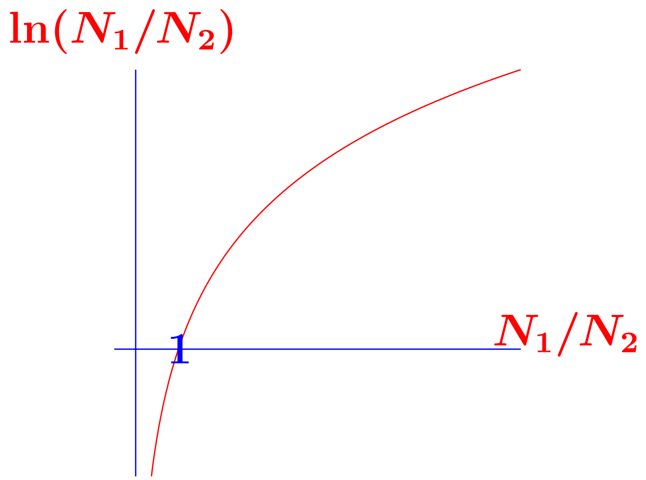
Casos:

(a) $N_1 > N_2, E < 0$:

$$\frac{N_1}{N_2} > 1, \qquad T > 0$$

(b) $N_1 = N_2, E = 0$:

$$\frac{N_1}{N_2} = 1, \qquad 1/T = 0$$



(c) $N_1 < N_2, E > 0$:

Suposición:

Un agente externo (ej: radiación láser) logra la inversión para $t < \tau$.

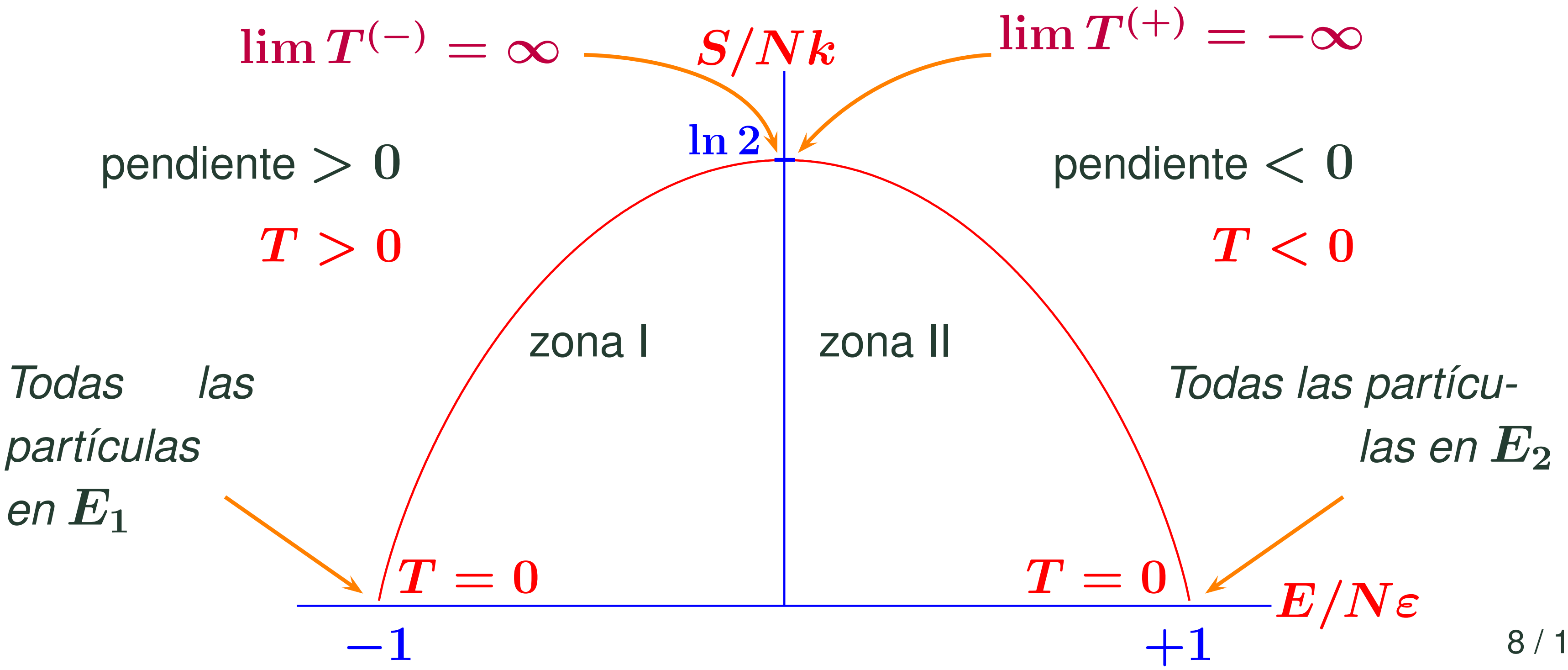
$$\frac{N_1}{N_2} < 1, \qquad T < 0$$

Recordar que: $$\left(\frac{\partial S}{\partial E}\right) = \frac{1}{T}$$

Por lo tanto:

$T > 0$, S aumenta con E
$T < 0$, S disminuye con E

Gráficamente:



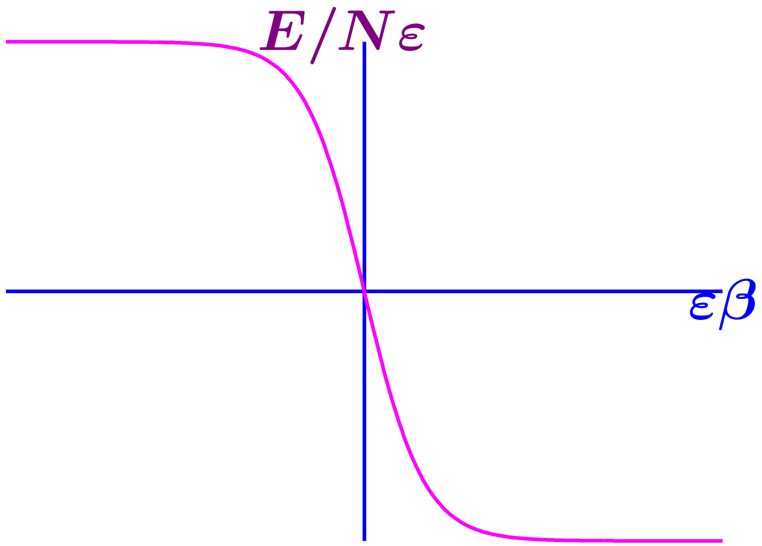
Además:

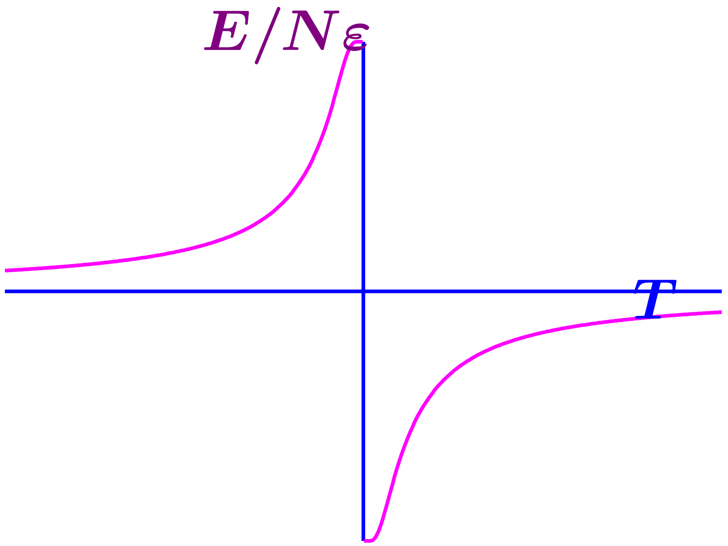
$$\left(\frac{\partial S}{\partial E}\right) = \frac{1}{T} = k\beta = \underset{\Uparrow}{\ldots} = \frac{k}{2\varepsilon}\ln\frac{N - E/\varepsilon}{N + E/\varepsilon}$$

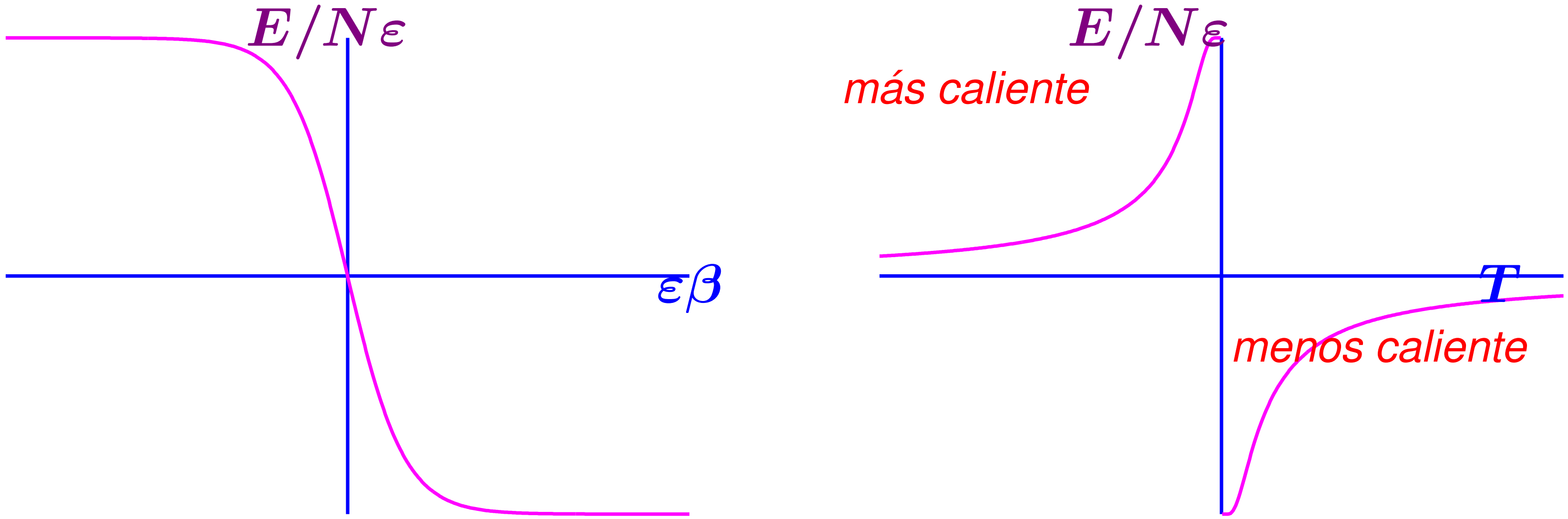
Tarea: realizar los pasos faltantes

Por lo tanto:

$$\frac{E}{N\varepsilon} = \frac{1 - e^{2\varepsilon\beta}}{1 + e^{2\varepsilon\beta}}$$

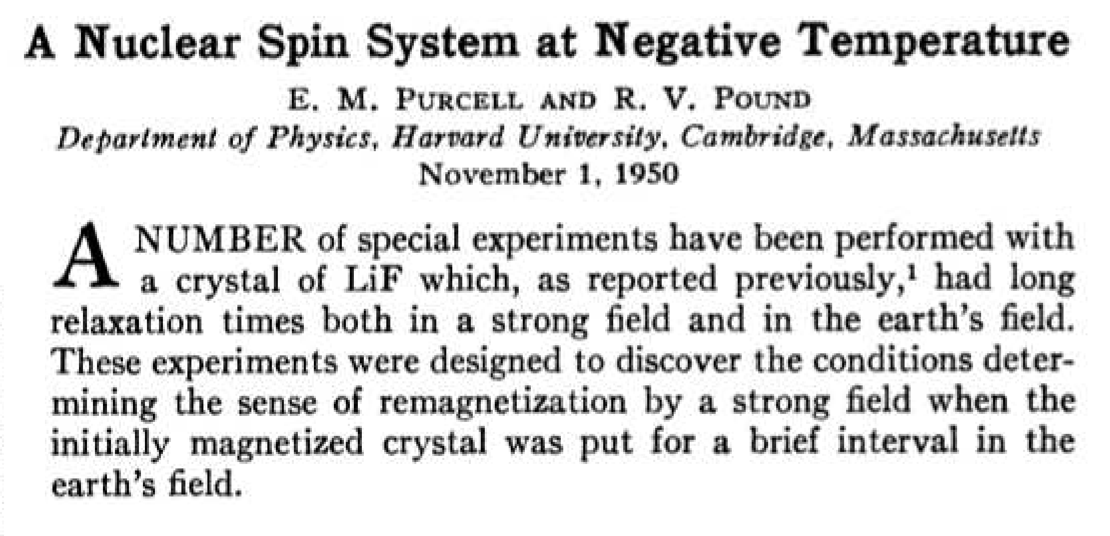






- Las temperaturas negativas corresponden a grados de libertad específicos.
- $T < 0$ corresponden a mayores E que $T > 0$.
- Se transfiere energía de un sistema con $T < 0$ a otro con $T > 0$.
- Escala de temperaturas:
  +0 K, +100 K, $\dots$, $+\infty$, $-\infty$, $\dots$, -100 K, -0 K

Evidencia experimental:



A Nuclear Spin System at Negative Temperature

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November 1, 1950

A NUMBER of special experiments have been performed with a crystal of LiF which, as reported previously,[1] had long relaxation times both in a strong field and in the earth's field. These experiments were designed to discover the conditions determining the sense of remagnetization by a strong field when the initially magnetized crystal was put for a brief interval in the earth's field.

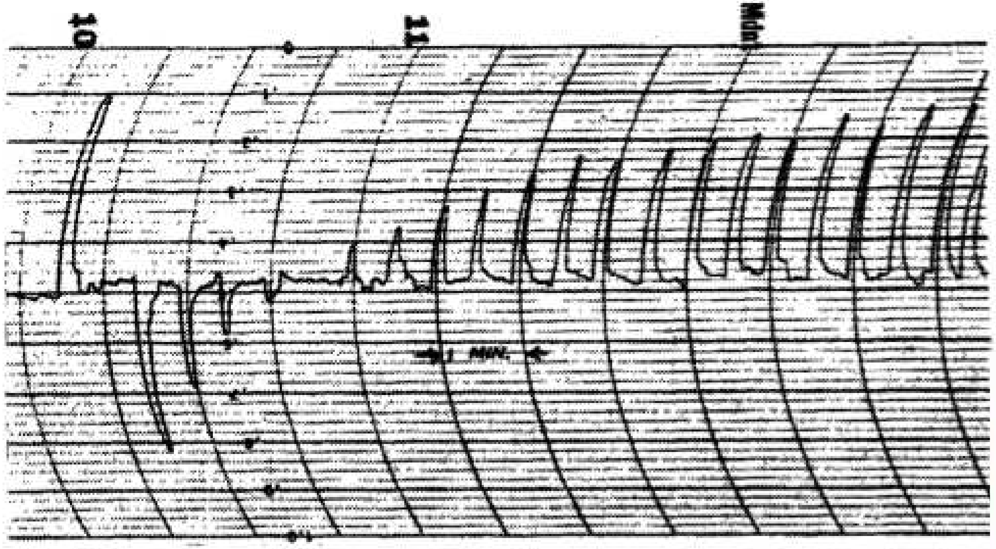
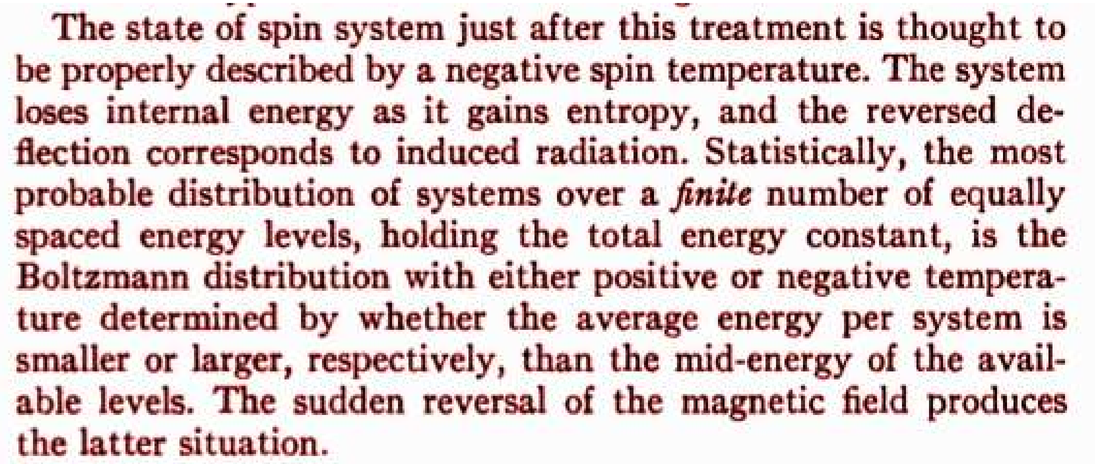
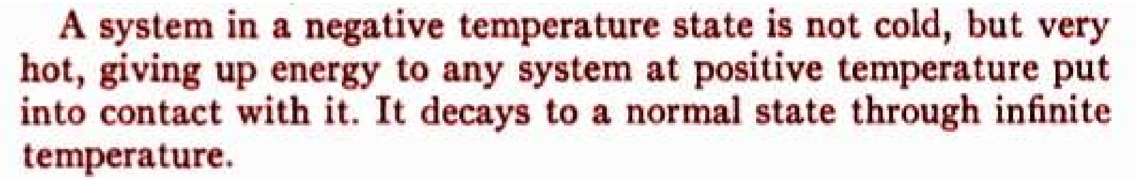


FIG. 1. A typical record of the reversed nuclear magnetization. On t left is a deflection characteristic of the normal state at equilibrium ma netization ($T\approx 300°$K), followed by the reversed deflection ($T\approx -350°$K decaying ($T\rightarrow -\infty$) through zero deflection ($T=\infty$) to the initial equ librium state.

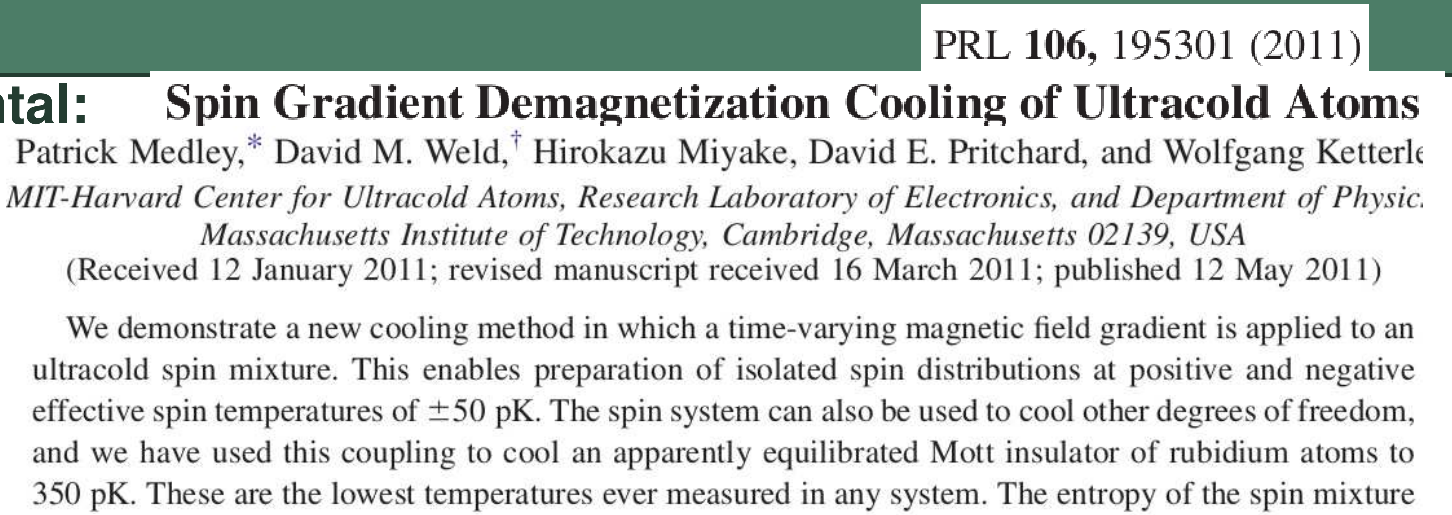


The state of spin system just after this treatment is thought to be properly described by a negative spin temperature. The system loses internal energy as it gains entropy, and the reversed deflection corresponds to induced radiation. Statistically, the most probable distribution of systems over a *finite* number of equally spaced energy levels, holding the total energy constant, is the Boltzmann distribution with either positive or negative temperature determined by whether the average energy per system is smaller or larger, respectively, than the mid-energy of the available levels. The sudden reversal of the magnetic field produces the latter situation.



A system in a negative temperature state is not cold, but very hot, giving up energy to any system at positive temperature put into contact with it. It decays to a normal state through infinite temperature.

Evidencia experimental:



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Spin Gradient Demagnetization Cooling of Ultracold Atoms

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We demonstrate a new cooling method in which a time-varying magnetic field gradient is applied to an ultracold spin mixture. This enables preparation of isolated spin distributions at positive and negative effective spin temperatures of ±50 pK. The spin system can also be used to cool other degrees of freedom, and we have used this coupling to cool an apparently equilibrated Mott insulator of rubidium atoms to 350 pK. These are the lowest temperatures ever measured in any system. The entropy of the spin mixture

magnetic ordering is expected.

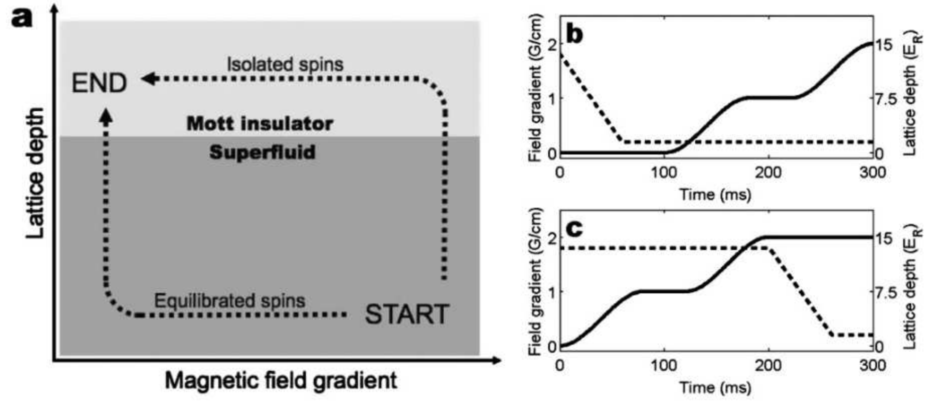


FIG. 1. Two different cooling protocols realizing the cases of isolated and equilibrated spin systems. (a) Experimental "phase diagram" of lattice depth vs applied gradient. Dashed lines show two different paths which connect the high-gradient superfluid state and the low-gradient Mott insulating state. (b) and (c) show the lattice depth (solid line) and gradient strength (dashed line) vs time for the two cases (equilibrated spins and isolated spins, respectively) in (a). The shape of the lattice ramp-up is designed to ensure maximum equilibration.

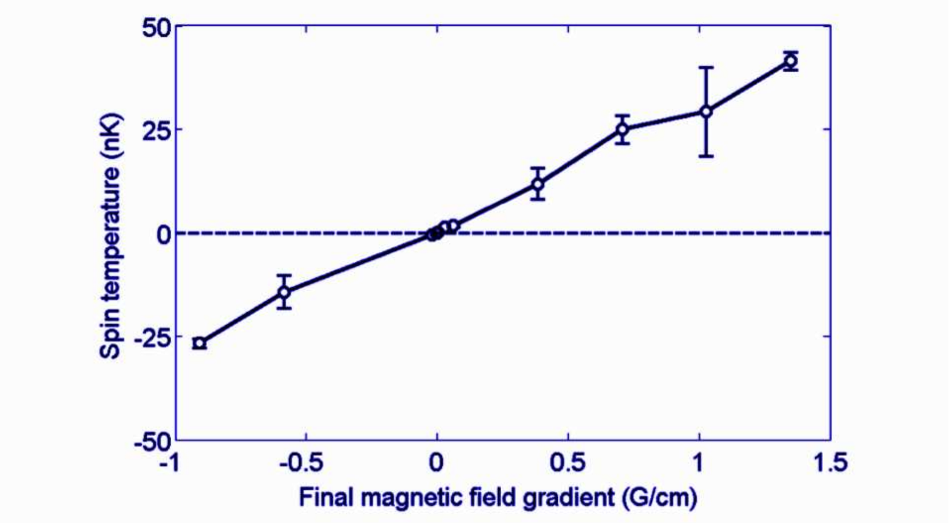
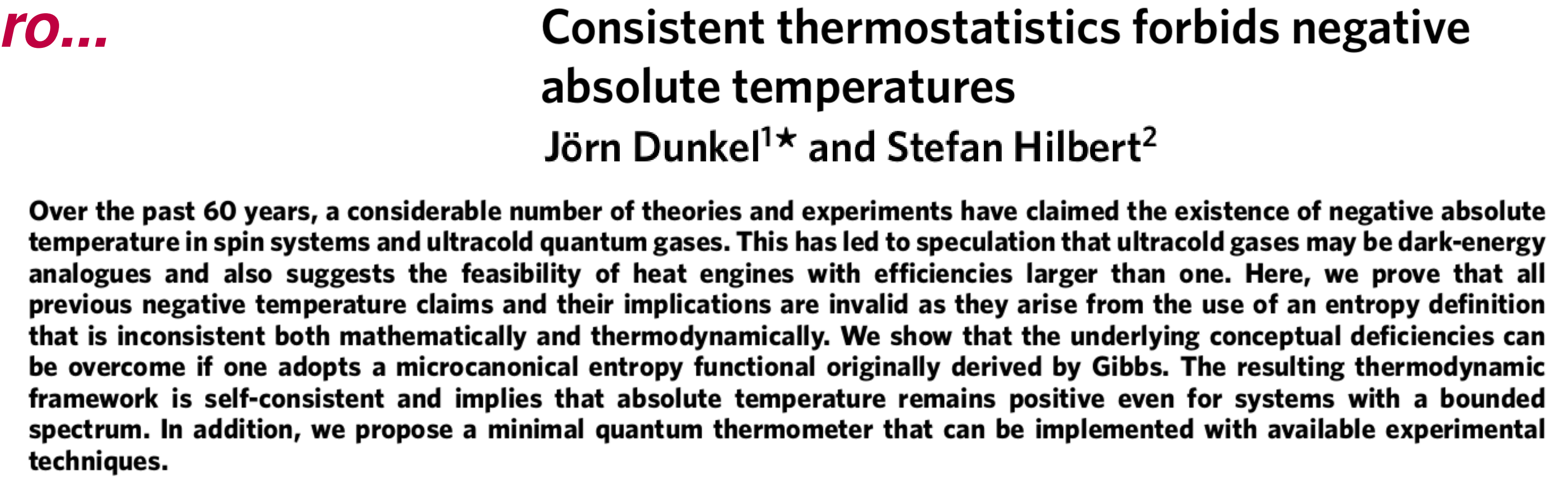


FIG. 2. Preparation of low positive and negative spin temperatures. Measured spin temperature vs final gradient, for the case of isolated spins. Error bars are statistical.

Pero...



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Consistent thermostatistics forbids negative absolute temperatures

Jörn Dunkel[1]* and Stefan Hilbert[2]

Over the past 60 years, a considerable number of theories and experiments have claimed the existence of negative absolute temperature in spin systems and ultracold quantum gases. This has led to speculation that ultracold gases may be dark-energy analogues and also suggests the feasibility of heat engines with efficiencies larger than one. Here, we prove that all previous negative temperature claims and their implications are invalid as they arise from the use of an entropy definition that is inconsistent both mathematically and thermodynamically. We show that the underlying conceptual deficiencies can be overcome if one adopts a microcanonical entropy functional originally derived by Gibbs. The resulting thermodynamic framework is self-consistent and implies that absolute temperature remains positive even for systems with a bounded spectrum. In addition, we propose a minimal quantum thermometer that can be implemented with available experimental techniques.

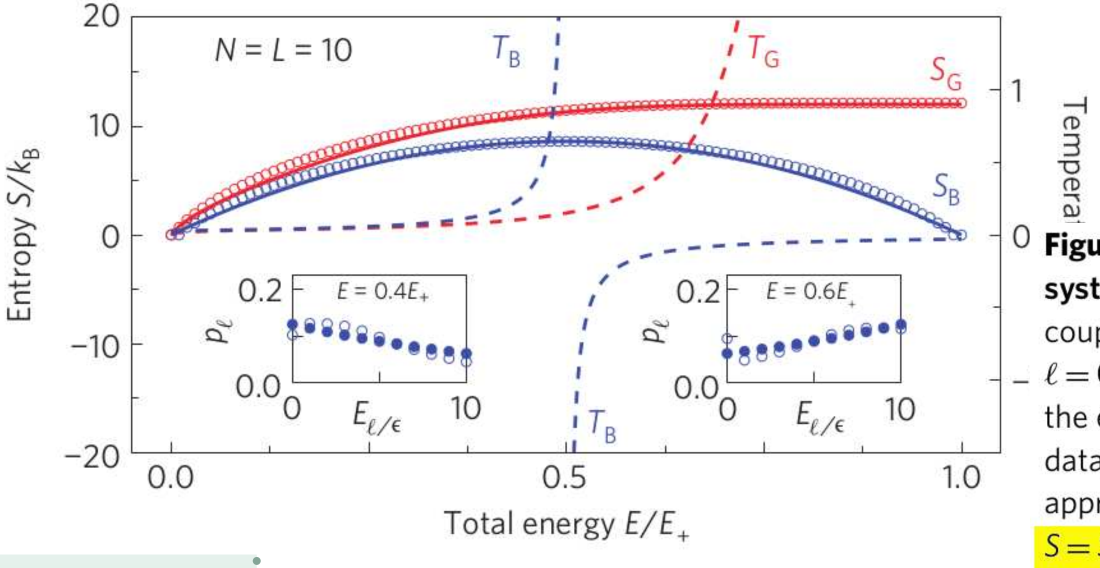

Figure 1 | Non-negativity of the absolute temperature in quantum systems with a bounded spectrum. Thermodynamic functions for N weakly coupled bosonic oscillators with $(L+1)$ single-particle levels $E_\ell = \ell\epsilon$, $\ell = 0, \ldots, L$, are shown for $N = L = 10$, corresponding to 184,756 states in the energy band $[E_-, E_+] = [0, LN\epsilon]$. Open circles show exact numerical data; lines represent analytical results based on the Gaussian approximation of the DOS ω. The thermodynamic Gibbs entropy $S = S_G = k_B \ln \Omega$ grows monotonically with the total energy E, whereas the Boltzmann (or surface) entropy $S_B = k_B \ln(\epsilon\omega)$ does not.

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