Temperature Relaxation between Systems with Negative Kelvin Temperatures

Ch. Zylka and G. Vojta
Sektion Physik, Karl-Marx-Universität Leipzig, DDR

Z. Naturforsch. **42 a**, 556–558 (1987); received October 4, 1986

We investigate the problem of distributing a given amount of heat among three systems under the following conditions: The systems are able to exhibit negative Kelvin temperatures, and heat equalization always fulfills a harmonic mixing rule $\bar{T} = 2\,T^{(1)} \cdot T^{(2)}/(T^{(1)} + T^{(2)})$. Just this happens for spin systems in the high temperature approximation.

1. Introduction

The starting point of this paper is the concept of an order structure (partial order) for (thermodynamic) states of classical or quantum systems in very general state spaces as introduced independently by Ruch and Schönhofer [1] and Uhlmann [2]; see also [3]. There are various indications that this concept should allow a more detailed understanding of irreversibility. One of the more fundamental questions to be asked is: What states are attainable at all, starting at a definite pure or mixed initial state? This question was to a large extent answered for heat exchange in ordinary systems with positive Kelvin temperatures [4]. Here we treat a more general case, viz. heat exchange in systems which are able to exhibit negative Kelvin temperatures.

The most prominent systems of this type are spin systems [5–7]. There exists a diversity of other systems with negative temperatures, e.g. two-dimensional plasmas in the guiding-center approximation [8] and two-dimensional turbulent fluids [9] showing a more or less complicated dependence of the internal energy on the (negative) temperature. Here we treat spin systems in a constant magnetic field of field strength H_0. One spin with the spin quantum number S has the energy

$$\varepsilon_m = -\gamma \hbar m H_0 , \quad m = S, S-1, \dots, -S . \tag{1}$$

The partition function for N independent spins yields the internal energy (in equilibrium)

$$U = -1/2\, N \gamma \hbar H_0 (g \coth g x - \coth x) \tag{2}$$

with $g = 2S + 1$, $x = \gamma \hbar H_0 / 2kT$. For the special case $S = 1/2$ one gets

$$U(T) = -(N \gamma \hbar H_0)/2 \cdot \tanh(\gamma \hbar H_0 / 2kT) \tag{3}$$

or in the so-called high-temperature approximation ($\gamma \hbar H_0 \ll kT$)

$$U(T) \approx -N(\gamma \hbar H_0/2)^2/kT . \tag{4}$$

For nuclear spins this approximation is usually valid down to very low temperatures [5–7, 10, 11]. The following treatment is applicable for all systems with $U(T) \propto 1/T$.

2. The Problem

The present note applies and extends the method and a previous result of one of the authors [4] on equalizing processes to systems with negative absolute temperatures. In [4] the question was answered which distributions of heat among n macroscopic bodies with equal heat capacities ($n \geqq 3$) – depending, of course, on the initial distribution – become attainable if heat is allowed to flow exclusively from the hotter to the cooler body.

The sets of accessible states turned out to be nonconvex polyhedra in a state space conveniently choosen. The mathematical idea lies in identifying the temperature distributions with a probability distribution p^i over n states ($i = 1, \dots, n$) and expressing heat transfer by means of double stochastic matrices. Doing this one soon meets with the rather well investigated theory of majorization, see e.g. [12, 13].

(For earlier applications of this concept to describe irreversibility we mainly refer to [3, 14, 15].) – Now we want to transfer the above mentioned

Reprint requests to Dr. Ch. Zylka, Sektion Physik, Karl-Marx-Universität, Karl-Marx-Platz 10, DDR-7010 Leipzig.

0932-0784 / 87 / 0600-0556 $ 01.30/0. – Please order a reprint rather than making your own copy.

result to more general states. Therefore we weaken the conditions for the probabilities p^i by replacing them by new quantities $\tilde{p}^i$ $(i = 1, \ldots, n)$ which are allowed to be negative and fulfill

$$\sum_{i=1}^{n} \tilde{p}^i = K, \tag{5}$$

where K be finite with positive or negative value (or value zero). Obviously the space of the sets $\tilde{p}^i$ is a convenient frame to handle systems with negative temperatures. As already mentioned, the high temperature approximation for spin systems provides $U \propto 1/T$. Assuming, for reasons of simplicity, equal heat capacities one immediately obtains a mixing rule of the type

$$\bar{T} = \frac{2\,T^{(1)}\,T^{(2)}}{T^{(1)} + T^{(2)}} \quad \text{with} \quad T^{(1)}, T^{(2)}, \bar{T} \gtreqless 0\,. \tag{6}$$

The reciprocal $1/\bar{T}$ of the mixing temperature $\bar{T}$ always lies between $1/T^{(1)}$ and $1/T^{(2)}$. This reflects nothing more than the concavity of $S(U)$: Since entropy should increase by any equalization $1/\bar{T}$ has to be "between" $1/T^{(1)}$ and $1/T^{(2)}$ (in the sense of Figure 1!).

Furthermore, we like to mention that (6) is experimentally checked, cf. [5, 10, 11].

Denoting the common heat capacity of the bodies by C, then via $C/T^{(i)} =: C \cdot \beta^{(i)} =: \tilde{p}^{(i)}$ one directly obtains elements of the state space $\tilde{\mathscr{S}}_n$. For its geometrical representation barycentric coordinates [16] are used. In order to illustrate them the case $n = 3$ with $K > 0$ is drawn in Figure 2.

One realizes that there is a one-to-one correspondence between $a\,\tilde{\boldsymbol{p}} \in \tilde{\mathscr{S}}_3$ and a point of the plane. Only the signs of the $\tilde{p}^{(i)}$ determine whether a point lies inside or otuside the strongly framed triangle.

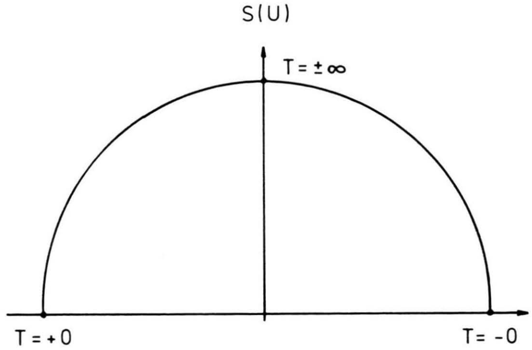

Fig. 1. Entropy versus internal energy for a system with both positive and negative temperatures.

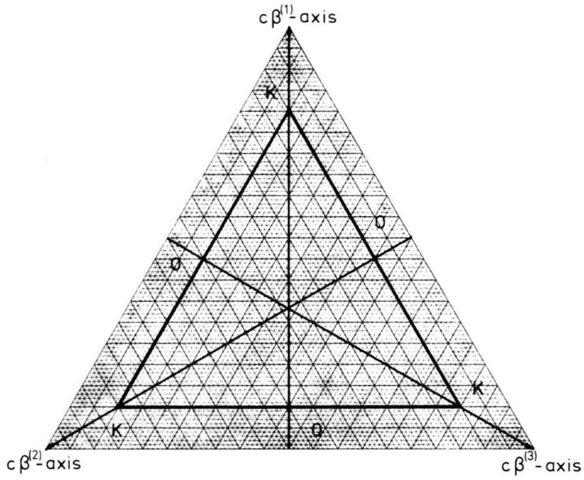

Fig. 2. The representation of $\tilde{\mathscr{S}}_3$ by means of barycentric coordinates.

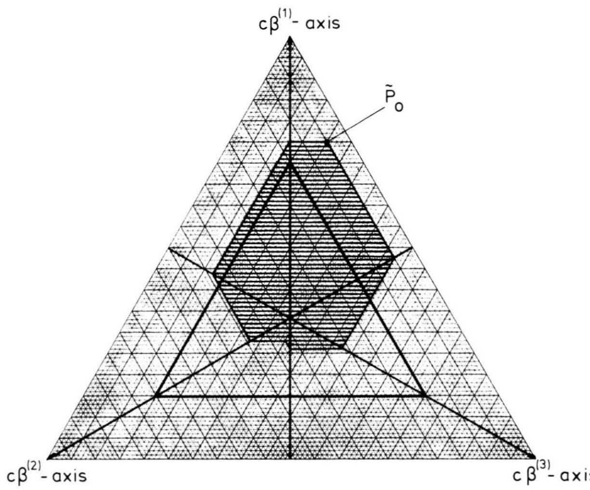

Fig. 3. The case $K > 0$ with $\beta^{(1)} > 0$, $\beta^{(2)} > 0$, and $\beta^{(3)} < 0$.

3. The Result

Let us consider the following cases separately: $K > 0$, $K = 0$, and $K < 0$.

The Case $K > 0$:

We use the homogeneity of the barycentric coordinates for the normalization $K \equiv 1$. With $C \equiv 1/3$ this leads to $\bar{\beta} = 1$, where $\bar{\beta}$ denotes the inverse tem-

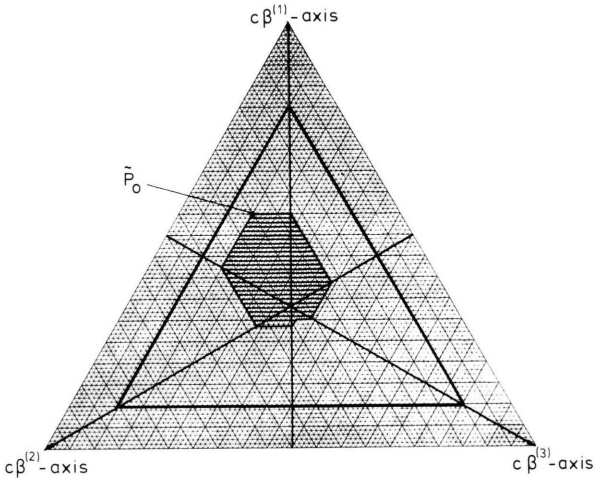

Fig. 4. The case $K > 0$ with $\beta^{(1)}, \beta^{(2)}, \beta^{(3)} > 0$.

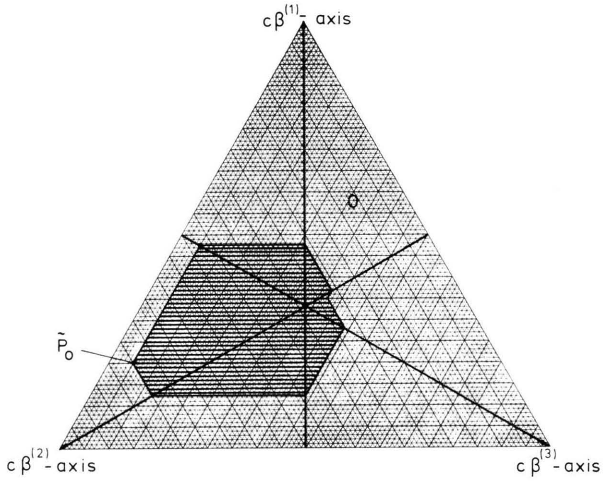

Fig. 5. The case $K = 0$ with $\beta^{(1)} < 0$, $\beta^{(2)} > 0$, and $\beta^{(3)} < 0$.

perature of the maximally equalized state. (The Boltzmann constant is now assumed to be 1.) The property (7) ensures that the construction procedure of [4] remains applicable and one obtains figures of the following type, where the hatched areas mark the set of the accessible states: Figures 3 and 4.

The Case $K = 0$:

Here we have $\bar{\beta} = 0$, and the triangle from Fig. 2 degenerates to a point. Therefore, not all the $\beta^{(i)}$ can have the same sign. The Fig. 5 shows one of the two possibilities.

The Case $K < 0$:

By formally substituting $C \to -C$ this case can obviously be traced back to the first one.

We want to stress that by a suitable choice of the initial state a non-trivial section of the set of attainable states and the set of states characterized by the same sign of temperature may appear. Due to the non-convexity of the former set this section should have an interesting shape in general.

Finally we remark that neither the consideration of more than three systems involved nor different heat capacities will lead to principal difficulties, see [17, 18].

The authors wish to thank Prof. A. Uhlmann and Dr. H. Schmiedel, Leipzig, for valuable discussions.

[1] E. Ruch and A. Schönhofer, Theor. Chim. Acta **19,** 225 (1970).
[2] A. Uhlmann, Wiss. Z. Karl-Marx-Universität Leipzig **21,** 421 (1972).
[3] F. Schlögl, Z. Phys. **B 25,** 411 (1976).
[4] Ch. Zylka, Theor. Chim. Acta **68,** 363 (1985).
[5] A. Abragam and W. G. Proctor, Phys. Rev. **109,** 1441 (1958).
[6] M. Goldmann, M. Chapellier, Vu Hoang Chau, and A. Abragam, Phys. Rev. **B 10,** 226 (1974).
[7] N. F. Ramsay, in: A Critical Review of Thermodynamics, Eds. B. Stuart, B. Gal-Or, A. J. Brainard, Mono Books, Baltimore 1970, p. 217.
[8] S. F. Edwards and J. B. Taylor, Proc. Roy. Soc. London A **336,** 257 (1974).
[9] R. H. Kraichnan and D. Montgomery, Rep. Progr. Phys. **43,** 54 (1980).
[10] A. Sawada, H. Yano, M. Kato, K. Iwahashi, and Y. Masuda, Phys. Rev. Lett. **56,** 1587 (1986).
[11] H. Suzuki, Y. Masuda, M. Miyamoto, T. Ohtsuka, and P. J. Walker, J. Low Temp. Phys. **62,** 497 (1986).
[12] G. H. Hardy, J. E. Littlewood, and G. Polya, Inequalities, University Press, Cambridge 1934.
[13] A. W. Marshall and J. Olkin, Inequalities. Theory of Majorisation and Its Application (in Russian), Isd. Mir, Moscow 1983.
[14] A. Uhlmann, Wiss. Z. Karl-Marx-Universität Leipzig **27,** 213 (1978).
[15] E. Ruch, R. Schranner, and T. H. Seligman, J. Chem. Phys. **69,** 389 (1978).
[16] A. F. Möbius, Der barycentrische Kalkül, Verlag J. A. Barth, Leipzig 1827.
[17] Ch. Zylka, Wiss. Z. Karl-Marx-Universität, Leipzig **34,** 598 (1985).
[18] Ch. Zylka, Publ. Joint Inst. Nucl. Res., E5-86-173, Dubna 1986.