

## Energy and entropy: Path from game theory to statistical mechanics

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Statistical mechanics is based on the interplay between energy and entropy. Here we formalize this interplay via axiomatic bargaining theory (a branch of cooperative game theory), where entropy and negative energy are represented by utilities of two different players. Game-theoretic axioms provide a solution to the thermalization problem, which is complementary to existing physical approaches. We predict thermalization of a nonequilibrium statistical system employing the axiom of affine covariance, related to the freedom of changing initial points and dimensions for entropy and energy, together with the contraction invariance of the entropy-energy diagram. Thermalization to negative temperatures is allowed for active initial states. Demanding a symmetry between players determines the final state to be the Nash solution (well known in game theory), whose derivation is improved as a by-product of our analysis. The approach helps to retrodict nonequilibrium predecessors of a given equilibrium state.

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### I. INTRODUCTION

Entropy and energy are fundamental for statistical mechanics, because they define the concept of equilibrium [1–7]. The equilibrium (positive-temperature) Gibbs distribution can be obtained via maximizing entropy for a fixed average energy or via minimizing energy for a fixed entropy [1–7]. The first method refers to the postulate of the second law, which states that the entropy of an isolated system (hence fixed energy) tends to increase [1–7]. The second method reflects the postulate of maximal work [3,4]: The maximal work (energy difference) extracted from a given nonequilibrium state during a cyclic process is achieved for a fixed entropy and leaves the system in an equilibrium state. Both postulates have obvious limitations, e.g., the formulation of the second law assumes an idealization of isolated systems, while the maximal work postulate makes a strong assumption about the constant entropy.

Our aim here is to approach the problem of establishing an equilibrium state from the viewpoint of game theory. This includes solving the thermalization problem: when and how a statistical system that starts its evolution from a sufficiently macroscopic nonequilibrium state relaxes to thermal equilibrium [4,5]. We will argue that a branch of game theory, viz., bargaining, is capable of giving a versatile axiomatics for the thermalization problem of statistical mechanics that is complementary to physical approaches. More specifically, we propose that, within a sufficiently coarse-grained description

of a statistical system, its (average) negative energy  $U = -E$  and entropy  $S$  can play the role of payoffs (utilities) for two players that tend to maximize them “simultaneously”. The meaning of the latter term is given by several axioms that are inspired by the bargaining theory; see Table I for a dictionary of game theory and statistical physics and Appendix A for a brief introduction to bargaining.

The thermalization problem has been studied since the inception of statistical physics and it is still an active research field because dynamical (microscopic) mechanisms that lead to thermalizations are rather convoluted<sup>1</sup> (see [12,13] for reviews). In contrast to microscopic perspectives, our results allow one to deduce thermalization from a few axioms on entropy and energy. Though these axioms come from game theory, they do have a transparent physical meaning. In particular, our approach allows for retrodiction, i.e., investigation of nonequilibrium states that give rise to the given equilibrium state. We thus provide a different perspective on thermalization that starts from game-theoretic concepts.<sup>2</sup>

Game theory studies strategic interactions of rational agents (players) [8–11,27] given their utilities, possible strategies, the order of the move, and information that each of those agents has about the game and other players. The theory

<sup>1</sup>These difficulties are not related to incorporating probabilistic ideas into the theory, since they hold as well in quantum theory, which is inherently probabilistic.

<sup>2</sup>Applying physical ideas to economic behavior led to interesting research in econophysics [14–20] and in game theory [21–26]. This improved our understanding of cooperation mechanisms [21–25] and of stability [26]. Here we attempt the opposite move of applying game-theoretic ideas to statistical physics. In this context, note interesting analogies between the axiomatic features of entropy and utility [14].

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TABLE I. Dictionary of bargaining theory and statistical mechanics. Utilities (payoffs) are normally dimensionless and are defined subjectively, via preferences of a player [8–11] (see Appendix A). Entropy and energy are physical dimensional quantities [4–7]. The utility  $u(x_1, x_2)$  of the first player depends on its own actions  $x_1$ , but also on actions  $x_2$  of the second player, which has utility  $v(x_1, x_2)$  [8–10]. Entropy and energy depend on the probability of various states of the physical system [4–7]. Unlike actions, these probabilities do not naturally fragment into two different components. Hence it is unclear how to apply the noncooperative game theory to statistical mechanics. For cooperative game theory this problem is absent, since the actions need not be separated. All utility values from the feasible set are potential outcomes of bargaining. The feasible set is frequently (but not always) convex [8–10] (see Appendix A). In contrast, the entropy-energy diagram is not convex due to the minimal entropy curve (see Fig. 1). Its convexity is recovered after imposing Axioms 1 and 2 [see (8) and (9)]. Game theoretically, the defection point is a specific value of utilities which the players get if they fail to reach any cooperation [8–10] (see Appendix A). The defection point does not have any direct physical analogy, also because there is no natural separation of probabilities into two sets. Instead of it we need to employ the notion of the initial point that as such does not have game-theoretic analogies (at least within axiomatic bargaining). For a given set of utilities  $(u, v) \in \mathcal{D}$  from the feasible set  $\mathcal{D}$ , the Pareto set  $\mathcal{P}$  is defined as a subset of  $\mathcal{D}$  such that  $(\hat{u}, \hat{v}) \in \mathcal{P}$  if there does not exist any  $(w_1, w_2) \in \mathcal{D}$  with  $w_1 \geq \hat{u}$  and  $w_2 \geq \hat{v}$ , where at least one of the inequalities is strict [8–10]. Thus there are no utility values that are jointly better than any point from the Pareto set. Within statistical physics the Pareto line coincides with the branch of the maximum entropy curve with positive inverse temperatures  $\beta > 0$ , because this branch is also the minimum energy curve for a fixed entropy (cf. Fig. 1). If  $(x_1, x_2)$  vary over a convex set and if both  $u(x_1, x_2)$  and  $v(x_1, x_2)$  are concave functions of  $(x_1, x_2)$ , then every point from  $\mathcal{P}$  can be recovered from conditional maximization of  $u(x_1, x_2)$  with a fixed  $v(x_1, x_2)$  or vice versa [11] (Karlin’s lemma). Both entropy and energy are concave functions of probability and the probability itself is defined over a convex set (simplex). Hence Karlin’s lemma applies.

Bargaining theory	Statistical mechanics
Utilities of players	entropy and negative energy
Joint actions of players	probabilities of states for the physical system
Feasible set of utility values	entropy-energy diagram
Defection point	initial state
Pareto set	maximum entropy curve for positive inverse temperatures $\beta > 0$

started with zero-sum games, where the interests of players are strictly opposite to each other. Such agents have no reason to cooperate, i.e., meaningful actions are noncooperative [8–11]. Later on the restriction of opposite interests was dropped. For such nonzero sum games noncooperative solutions approaches are still meaningful.<sup>3</sup> Hence game theory divided into noncooperative and cooperative branches.

Cooperative game theory tries to predict the possible outcome of the game, where the formation of coalitions (a group of players who behave as an entity) and/or external enforcement mechanisms are accepted [8–10,21–25]. One of the points of cooperative games is that joint actions of players are allowed. The bargaining theory, where agents interact over sharing some good, is a branch of cooperative games. Strategic bargaining (cooperative) games tend to predict specific mechanisms according to which a certain compromise between the players is reached [10]. Axiomatic bargaining theory abstracts from specific scenarios of the bargaining process and finds possible compromises axiomatically [8,9,27]. The independence from specific details is the main advantage of axiomatic bargaining, an advantage it shares with (nonequilibrium) thermodynamics.

The rest of this paper is organized as follows. The next section studies the construction of the energy-entropy diagram. Some aspects of this diagram are known from textbooks [1–7], but here we present this key notion of statistical physics in its entirety. Section III poses our main problem and explains how axioms of bargaining theory apply to statistical physics. There we discuss the game-theoretic versus physical meaning

of those axioms, as well as account for their physical limitations. Table I presents a dictionary comparing the notions of axiomatic bargaining and statistical mechanics. Appendix A briefly reviews the bargaining theory. Section IV discusses thermalization, i.e., how and why (according to plausible axioms) a statistical system reaches equilibrium with positive or, depending on its initial conditions, negative temperatures. Predictions of thermalization are made more specific in Sec. V via the symmetry axiom. There we also deduce the famous Nash solution of axiomatic bargaining without the limitations of its previous derivations that prevent its application to physics. Section VI discusses the possibility of retrodicting from a given equilibrium state its predecessor nonequilibrium states. We summarize in Sec. VII. Several technical but pertinent problems are studied in Appendixes.

## II. ENTROPY-ENERGY DIAGRAM

We study a classical system with discrete states  $i = 1, \dots, n$  and respective energies  $\{\varepsilon_i\}_{i=1}^n$ . A statistical (generally nonequilibrium) state of the system is given by probabilities

$$\{p_i \geq 0\}_{i=1}^n, \quad \sum_{i=1}^n p_i = 1. \quad (1)$$

The entropy and negative average energy for such a state read, respectively [1–5],

$$S[p] = -k_B \sum_{i=1}^n p_i \ln p_i, \quad U[p] = - \sum_{i=1}^n \varepsilon_i p_i, \quad (2)$$

where  $k_B$  is Boltzmann’s constant. The Gibbsian equilibrium states are obtained by maximizing  $S[p]$  over (1) under a fixed

<sup>3</sup>Sometimes they are even preferable over cooperative ones, at least for one of the players; see, e.g., [8] for examples.

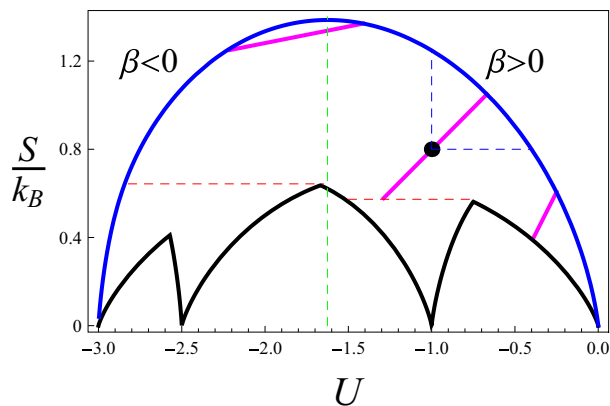


FIG. 1. Typical example of the entropy-energy diagram. The entropy is  $S$  and the negative energy  $U = -E$  for the four-level system with energies  $\varepsilon_1 = 0$ ,  $\varepsilon_2 = 1$ ,  $\varepsilon_3 = 2.5$ , and  $\varepsilon_4 = 3$  [cf. (1)–(3)]. The maximal and minimal entropy curves are blue and black, respectively. All physically acceptable values of entropy and energy are inside the domain bounded by blue and black curves. States below red dashed lines (both are lower than  $\ln 2$ ) are excluded by Axiom 2. The green dashed line shows  $U_{av} = -\frac{1}{4} \sum_{k=1}^4 \varepsilon_k$ ; it separates  $\beta > 0$  from  $\beta < 0$  [cf. (4)]. The black point denotes a possible initial state that holds Axiom 2. States inside dashed blue lines hold axiom 4. Magenta lines denote initial states that produce the same final state (14).

$$U = U[p] \text{ [1–5],}$$

$$p_i = e^{-\beta \varepsilon_i} / Z, \quad Z = \sum_{i=1}^n e^{-\beta \varepsilon_i}, \quad \beta = 1/k_B T, \quad (3)$$

where the inverse temperature  $\beta$  is uniquely determined from  $U[p] = U$ . The same result, but restricted to the positive-temperature branch  $\beta > 0$ , is obtained upon maximizing  $U[p]$  under fixed  $S$  [4,5]. This is why we frequently employ the negative energy together with entropy: Both are maximized in equilibrium.

Figure 1 shows a typical entropy-energy diagram on the  $(U, S)$  plane. Denoting the maximum entropy curve by  $S(U)$ , we see from (2) and (3) that  $S(U)$  achieves its maximum value  $\ln n$  for  $U = U_{av}$ :

$$S(U_{av}) = \ln n, \quad U_{av} \equiv -\frac{1}{n} \sum_{k=1}^n \varepsilon_k. \quad (4)$$

For  $U > U_{av}$  ( $U < U_{av}$ ),  $S(U)$  refers to  $\beta > 0$  ( $\beta < 0$ ).

The maximum entropy curve  $S(U)$  is smooth and bounds a convex domain due to concavity of  $S[p]$  ( $0 < \epsilon < 1$ ) [4,5]:  $S[\epsilon p + (1 - \epsilon)q] \geq \epsilon S[p] + (1 - \epsilon)S[q]$ . No probabilistic states are possible below the minimum entropy curve

$$S_{\min}(U) = \min_{p, U[p]=U} (S[p]). \quad (5)$$

Now  $S_{\min}(U)$  is an irregular curve, because minima of a concave function  $S[p]$  are reached for vertices of the allowed probability domain that combines (1) with the constraint  $U[p] = U$ . Hence only two probabilities are nonzero (see

Appendix B for details of deriving the minimum entropy curve). We have (cf. Fig. 1)

$$S_{\min}(U) \leq k_B \ln 2, \quad (6)$$

$$S_{\min}(-\varepsilon_i) = 0. \quad (7)$$

Due to (6) and (7), the minimal entropy curve is not a macroscopic concept, i.e., it is frequently overlooked in presentations of the energy-entropy diagram.

### III. STATEMENT OF THE PROBLEM AND AXIOMS 1–4

We emphasize that all the above features of the entropy-energy diagram hold for arbitrarily large but finite values of  $n$ . Let the statistical system be found initially at some point of the (nonequilibrium) entropy-energy diagram. We want to predict the long-time state of this system, knowing that its entropy and negative energy are going to be larger than their initial values. A basic example of this situation is when a thermally isolated statistical system<sup>4</sup> is subject to external fields that extract energy. Now in two extreme cases thermodynamics can determine the long-time state [1–3]. First, if there is a specific dynamic regime where the work-extraction process is neither slow nor fast, then the entropy is conserved and work extraction entails decreasing energy.<sup>5</sup> Consequently, through the extraction of as much work as possible, the system will finally reach equilibrium along the constant entropy [1–3]. Second, when no work exchange is present and the system is completely isolated, its entropy will increase until it finally reaches equilibrium along the constant energy path. This is the standard setup of the second law.

Realistically, both processes occur simultaneously, i.e., when both entropy and negative energy do not decrease. Can one still show that the system will reach a thermal equilibrium? If yes, can one bound its temperature?

The standard thermodynamics cannot answer these two questions due to insufficient information.<sup>6</sup> The questions can be answered within more detailed, nonequilibrium statistical mechanical theories [4,5]; however, such theories make a number of dynamical assumptions, e.g., they assume that internal constituents of the system move according to quantum Hamiltonian dynamics during the whole system's evolution

<sup>4</sup>“Thermally isolated” means that the system does not interact with external thermal baths, but may still interact with mechanical systems, i.e., sources of work. Formally, any process is thermally isolated if the system is enlarged by including there its environment (if this environment is known).

<sup>5</sup>The work-extraction process cannot be slow, since entropy will start to increase, as always with nonequilibrium, thermally isolated systems. It also cannot be fast, since such a process will induce its own entropy production. Hence the very existence of such a work extraction is an additional (and rather strong) postulate [2,3]. Thermally isolated processes that start from an equilibrium state need to be sufficiently slow to not produce entropy. The requirement of being sufficiently fast is absent here.

<sup>6</sup>For example, it can predict the final state (3) if we know that the system is attached to a much larger thermal bath at inverse temperature  $\beta$ , but we do not make such an assumption here.

[4,5] or they assume that the system is of hydrodynamic type with smooth density, velocity, and pressure fields [1]. The direct validity of such assumptions is difficult to address; hence specific axiomatic approaches can still be useful. Axiomatic approaches to equilibrium thermodynamics have a long history (see [2,28–30]). They revolve around axiomatic introduction of entropy, whereas we assume that the entropy holds its standard form.

We address the above questions via tools of axiomatic bargaining [8,9,27]; see Table I for a detailed comparison between bargaining theory and statistical physics and Appendix A for an introduction to bargaining. Given the initial, nonequilibrium state  $(U_i, S_i)$ , we look for the final state  $(U_f, S_f) = (U[p_f], S[p_f])$ . Axioms below will locate this final state on the entropy-energy diagram. For each axiom we comment separately on its physical vs game-theoretic meaning (frequently these are closely related). We also pay attention to the physical limitations of each axiom.

*Axiom 1: No decreasing.* We have

$$U_i \leq U_f, \quad S_i \leq S_f, \quad (8)$$

where at least one inequality is strict. This axiom excludes from consideration active nonequilibrium processes, where the energy is put in the system and/or its entropy is decreased. Nevertheless, (8) is a relatively weak axiom, e.g., there are infinitely many nonequilibrium states that are still compatible with it.

In bargaining problems the physical initial state is associated with the defection point, which is frequently the guaranteed outcome for both players (see Table I and Appendix A). Then (8) relates to the individual rationality of players, which plan to obtain anything better than the joint guaranteed payoff [8,9,27].

*Axiom 2: Choice of initial conditions.* We assume a nonequilibrium initial state, with entropy

$$S_i > k_B \ln 2. \quad (9)$$

This is a class of sufficiently macroscopic states for our purposes. In concrete cases this condition can be made weaker; e.g. for the case of Fig. 1 we can allow all initial states above dotted red lines. Now Axioms 1 and 2 ensure that the domain of allowed final states on the entropy-energy diagram is a convex set. Providing a relatively simple (convex) domain of allowed final states is the main physical aim of Axiom 2. The axiom is not especially restrictive, since  $k_B \ln 2$  is a small entropy for a macroscopic (even mesoscopic) system.

The axiom (9) is mostly absent from bargaining (game-theoretic) constructions, since there the convexity of the set of allowed states frequently comes from other sources, e.g., from the mean utility principle [8,9,27].

*Axiom 3: Affine covariance.* If the entropy-energy diagram  $(U, S)$  [including  $(U_i, S_i)$ ] is transformed as

$$(U, S) \rightarrow (a^{-1}U + d, b^{-1}S + c), \quad a > 0, b > 0, \quad (10)$$

where  $a > 0, b > 0$ , and  $c$  and  $d$  are arbitrary, then the final state  $(U_f, S_f)$  is transformed via the same rule (10) [8].

The physical meaning of this axiom is clarified in several steps. First of all, the factors  $c$  and  $d$  in (10) relate to the freedom of translating energy and entropy by an arbitrary amount, which is well known in physics. Naturally, we keep

this freedom here. Next we can change (different) dimensions of  $U$  and  $S$  without changing physics. Hence (10) should hold at least for those cases where  $a$  and  $b$  in (10) account for changes in dimensions. It remains to explain when (10) can be employed also for dimensionless  $a$  and  $b$ . If the final state  $(U_f, S_f)$  is assumed to be a functional of  $(U[p] - U_i, S[p] - S_i)$ ,

$$(U_f, S_f) = (\mathcal{G}_1[U - U_i, S - S_i], \mathcal{G}_2[U - U_i, S - S_i]), \quad (11)$$

then the validity of (10) for dimensionless  $a$  and  $b$  follows from the above freedom of changing dimensions. Thus (11) implies that  $U$  and  $S$  are autonomous variables that define the considered situation. If this is not the case, then Axiom 3 does not hold for dimensionless  $a$  and  $b$  (10).<sup>7</sup>

Recall that in an ordinary equilibrium situation entropy and (negative) energy can be taken as two independent variables which fully characterize the equilibrium state (on the same footing as, e.g., temperature and volume) [3]. Thus (11) generalizes the equilibrium situation and is intended to apply at least to certain nonequilibrium cases.

The game-theoretic meaning of Axiom 3 has two aspects. First, the utilities (being subjective quantities for defining preferences) are generally defined with the freedom of adding to the utility any number and multiplying it by a positive number [8,9,27]. Second, in bargaining it is frequently assumed that comparing different utilities directly with each other is not allowed [8,9,27]. This implies the freedom (10), where each utility is transformed independently.

*Axiom 4: Contraction invariance (independence of irrelevant alternatives)* [8]. Let  $\mathcal{D}'$  be a subset of the original entropy-energy diagram  $\mathcal{D}$ , with  $\mathcal{D}'$  containing both  $(S_i, U_i)$  and  $(S_f, U_f)$ . If now the set of allowed final states is restricted (contracted) from  $\mathcal{D}$  to  $\mathcal{D}'$ , then it still holds that  $(U_i, S_i) \rightarrow (U_f, S_f)$ .

Axiom 4 tells about any subset  $\mathcal{D}'$ , but below we will need it only for full-measure, well-behaved subsets that are similar to  $\mathcal{D}$ . The restriction to those subsets can be realized via suitable external fields.

Contraction invariance plays an important role in decision theory [8,9,27]. The intuition behind this axiom is *physical* and is akin to relaxation via comparing two states (which is realized, e.g., in Monte Carlo simulations): It assumes that the actual evolution  $(U_i, S_i) \rightarrow (U_f, S_f)$  amounts to selecting the “best” state via binary comparisons of diagram points. Hence restricting the set of alternatives, provided the best state is still allowed, cannot change the best. Physical limitations of Axiom 4 relate to situations where pairwise comparisons of states are not allowed (or are incomplete), as well as to those cases where the restriction  $\mathcal{D} \rightarrow \mathcal{D}'$  cannot be realized operationally.

<sup>7</sup>To give a concrete example, assume that the considered system is macroscopic and is attached to a thermal bath of a comparable size whose inverse temperature  $\beta_E$  is kept constant. Then we expect in (11) an additional dimensionless variable  $(U - U_i)\beta_E$  that does not change when changing dimensions but does change under (10) with dimensionless  $a$  and  $b$ . Hence we require that such dimensionless quantities are absent. This requirement need not always hold, thus limiting the applicability of Axiom 3.



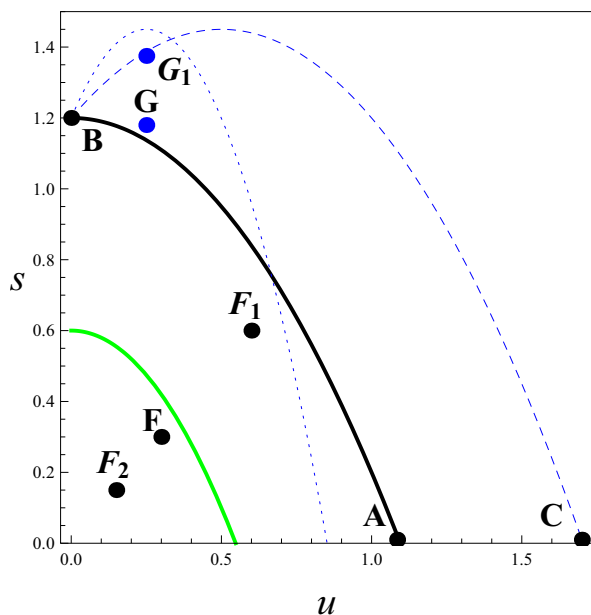


FIG. 2. Set of states in coordinates (12), i.e., the initial state is shifted to (0,0) via (10). The monotonic curve **BA** is a part of the maximum entropy curve for  $U_i \geq U_{av}$  (first scenario). The green curve is the image of **BA** under transformation (10) with  $a > 1$ ,  $b > 1$ , and  $c = d = 0$ . **BC** is a part of the maximum entropy curve for  $U_i < U_{av}$  (second scenario). The blue dotted curve is the image of **BC** after (10) with  $a > 1$ ,  $b = 1$ , and  $c = d = 0$ . Here **F**, **F**<sub>1</sub>, and **F**<sub>2</sub>, and **G** and **G**<sub>1</sub> are tentative final states for the first and second scenarios, respectively.

#### IV. THERMALIZATION

We have two possibilities for the initial state  $(U_i, S_i)$  [see (4) and Figs. 2 and 1]:  $U_i \geq U_{av}$  or  $U_i < U_{av}$ . Both scenarios are studied in coordinates

$$u = U - U_i, \quad s = S - S_i. \quad (12)$$

The transition to the new coordinates  $(u, s)$  is done via (10) with  $a = b = 1$  (see Fig. 2).

For  $U_i \geq U_{av}$ , all points on and below the maximum entropy curve **BA** [apart from (0,0)] are allowed as possible final states [see (8) and Fig. 2]. Assume that the final state **F**  $\equiv (\bar{u}, \bar{s}) \notin \mathbf{BA}$  [9] (cf. Fig. 2). Then there is a point **F**<sub>1</sub>  $\equiv (a_1\bar{u}, b_1\bar{s})$ , with  $a_1 \geq 1$  and  $b_1 \geq 1$  (at least one of these inequalities is strict).

We now apply (10) with  $a = a_1$ ,  $b = b_1$ , and  $c = d = 0$  to all points of the diagram. This transforms **F**<sub>1</sub>  $\rightarrow$  **F** and changes the original domain  $\mathcal{D} = \mathbf{OBA}$  [(0,0) = **O**] to the smaller domain  $\mathcal{D}' \subset \mathcal{D}$  (see Fig. 2, where  $\mathcal{D}'$  is below the green line). Now **F**  $\in \mathcal{D}'$ , due to **F**<sub>1</sub>  $\rightarrow$  **F**; however, we can regard  $\mathcal{D}'$  as just a subset of  $\in \mathcal{D}$  and apply to it Axiom 4. We now have two contradicting facts: Following Axiom 4, **F** should not change when going to a subset, but it should change **F**  $\rightarrow$  **F**<sub>2</sub> according to (10), i.e., Axiom 3. The contradiction is avoided only if **F** is on the maximum entropy curve **BA**, i.e., the final state has the form (3) with some temperature  $T$ .

For  $U_i < U_{av}$ , using (10) with  $a > 1$  is not useful, since the maximum entropy curve is not monotonic (see **BC** in Fig. 2). Then we get  $\mathcal{D}' \not\subset \mathcal{D}$  (see the domain below the blue

dotted line in Fig. 2) and then Axiom 4 does not apply. Note that the above nonmonotonic feature of **BC** is kept after any transformation (10).

Instead we employ (10) with  $a = 1$  and  $b > 1$  ( $c = d = 0$ ). Given a tentative final state **G**  $\equiv (\bar{u}, \bar{s})$ , we can reach the above contradiction only if there is a point **G**<sub>1</sub>  $\equiv (\bar{u}, b\bar{s})$  (see Fig. 2), i.e., the set of possible final states coincides with curve **BC** in Fig. 2.

Hence Axioms 1–4 imply thermalization: The final state is on the maximum entropy curve. Negative-temperature states are allowed by this derivation for  $U_i < U_{av}$ . Such initial states are active, i.e., they can provide work during a cyclic change of an external parameter [4]. The general definition [4] of an active state is given in terms of energies  $\{\varepsilon_i\}_{i=1}^n$  and probabilities  $\{p_i\}_{i=1}^n$  introduced in (1): The condition

$$(p_i - p_j)(\varepsilon_i - \varepsilon_j) > 0 \quad (13)$$

holds for at least for one pair  $(i, j)$ . For a negative-temperature state all pairs  $(i, j)$  hold (13). Negative temperatures are known for various systems whose energies are bounded from above (e.g., spin systems) [31–35].

Though we have shown that some equilibrium state will be achieved as a result of our axioms, we do not know precisely which temperature will be achieved by the above thermalization, since that depends on the details of the process, which are absent in our description. Below we show that the final temperature can be determined uniquely if we impose an additional axiom.

#### V. SYMMETRY AXIOM AND THE NASH SOLUTION

##### A. Axiom 5

The symmetry axiom below gives equal roles to both utilities provided all other conditions do not indicate an asymmetry between them. This axiom provides a natural middle situation between two extremes of conserving entropy or energy (cf. the discussion at the beginning of Sec. III).

*Axiom 5: Symmetry.* Make  $U$  and  $S$  dimensionless via (10). If the domain of allowed final states (8) is symmetric, i.e., it contains a point  $(U, S)$  if and only if it contains  $(S, U)$ , and so is the initial state ( $U_i = S_i$ ), then the final state is also symmetric  $(S_f, S_f)$ , if there are no reasons to regard the players asymmetrically.

Nash [27] and his numerous followers<sup>8</sup> [8–10] argued that the only final state satisfying Axioms 1–5 is

$$(U_N, S_N) = \operatorname{argmax}_{(U, S)} [(U - U_i)(S - S_i)], \quad (14)$$

where the maximum is reached on the maximum entropy curve restricted by (8). Since this curve is concave, the  $\operatorname{argmax}$  in (14) is unique (see Appendix C 1). Equation (14) shows that  $(U_N, S_N)$  refer to a  $\beta_N > 0$  [cf. (3)].

However, Refs. [9,27] derived (14) by making an additional assumption, viz., the domain restricted by (8) can be enlarged

<sup>8</sup>The solution (14) was found much earlier by Zeuthen [36], but it was based on a behavioristic, not an axiomatic approach. The solution by Zeuthen is discussed in Appendix A; see also [8].

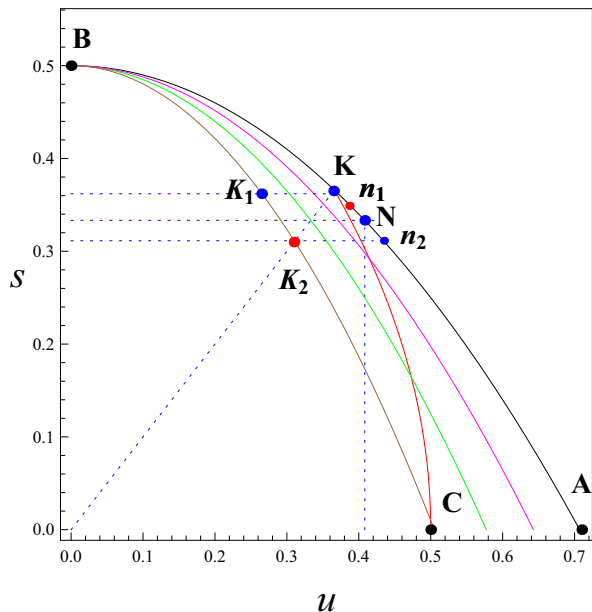


FIG. 3. Entropy-energy diagram in coordinates (12) with the initial state (0,0). The black curve **BA** is  $s(u)$ ; **N** is the corresponding solution (14). One of the blue dotted lines is  $s = u$ . **BKC** bounds a symmetric domain (with respect to  $s = u$ ), whose solution (14) is **K**. Curves are transformed via (16):  $s(a_0u)$  (green),  $s(a_1u)$  (magenta), and  $s(a_2u)$  (brown) [see after (17)].

into a larger domain (see Appendix C 2 for details). We cannot employ this assumption, since it is completely unphysical. Indeed, for a physical system with given energies  $\{\varepsilon_i\}_{i=1}^n$  there is simply no way we can enlarge the domain of allowed energies and entropies (see Fig. 1). The opposite operation of restricting the allowed domain can in principle be carried out via external fields and monitoring the system.

### B. Derivation of Nash’s solution

We will derive (14) using Axioms 1–5, but without the assumption. For clarity of our derivation, we will restrict ourselves to the case  $U > U_{av}$ , where the domain of allowed final states is bound by a *monotonic* curve according to Axioms 1 and 2 and the energy-entropy diagram; cf. the domain **BAO** in Fig. 2 [recall that **O** = (0, 0) there].

Figure 3 shows a typical example of the maximal entropy curve  $s(u)$  (denoted by **BA** in Fig. 3) in coordinates (12) with **O** ≡ (0, 0). The domain of states **BAO** allowed by Axiom 1 is not symmetric in the sense of Axiom 5, but it has the largest symmetric subset **OBKC** ⊂ **OBA**, where **K** is the solution of

$$s(\hat{u}) = \hat{u} \tag{15}$$

and **KC** is the inverse function  $s^{-1}(u)$  of  $s(u)$  (see Fig. 3). For **OBKC** Axiom 5 plus thermalization lead to **K** as the final state. Hence, for the original domain **BAO** the final state is located on the line **KA** (including **K**). Indeed, it has to be on **BA**, but locating it on **BK** contradicts Axiom 4, because if it were located on **BK**, it had to stay intact upon going from **OBA** to **OBKC** (but in reality it changes and becomes **K**).

In coordinates (12) the state (14) is given as  $(u_N, s(u_N))$  with  $u_N = \operatorname{argmax}_u [us(u)]$ . This is the point **N** in Fig. 3. Now

**N** should always be on the part of the maximum entropy curve that is allowed by the above argument, i.e.,  $\mathbf{N} \in \mathbf{KA}$  for Fig. 3 (see Appendix C 3 for the derivation).

The above restricting of the final state will be repeated after transformation (10) with  $b = 1$  and  $c = d = 0$ , where

$$s(u) \rightarrow s(au). \tag{16}$$

We choose  $a = a_0$  such that (cf. the green curve in Fig. 3)

$$\operatorname{argmax}_u [us(a_0u)] = \hat{u}_0, \quad \hat{u}_0 = s(a_0\hat{u}_0), \tag{17}$$

i.e., the transformed Nash solution (14) equals  $\hat{u}_0$  and lies on the  $s = u$  line (see Fig. 3). Now consider (16) under two other values of  $a$ :  $a_2 > a_0 > a_1$ .

After applying (16) with  $a = a_2$ , the transformed Nash solution lies on **BK<sub>2</sub>**, where **K<sub>2</sub>** is found from  $s(a_2u) = u$  (see Fig. 3). The transformed final state should be on **BK<sub>2</sub>**. This follows from the fact that the final state should be always on that part of the maximum entropy curve (for the present case this curve is **BC**) where the Nash solution is. Alternatively, the fact of being on **BK<sub>2</sub>** can be verified by carrying out the above construction of going from **OBC** to its maximal symmetric subset.

Moreover, the transformed final state should be between **K<sub>1</sub>** and **K<sub>2</sub>**, because before transformation it was on **KA**. Here **K** → **K<sub>1</sub>** under the transformation  $s(u) \rightarrow s(a_2u)$  (cf. Fig. 3). Going back to the original curve **KA**, we restrict the final state to lie between **K** and **n<sub>2</sub>** on **KA**, where **n<sub>2</sub>** goes to **K<sub>2</sub>** under applying (16) with  $a = a_2$  (see Fig. 3).

Applying (16) with  $a = a_1$ , we further restrict the final state to lie between **n<sub>1</sub>** and **n<sub>2</sub>** (see Fig. 3). Here **n<sub>1</sub>** is defined such that after applying (16) with  $a = a_1$ , it sits on the  $s = u$  line. For  $a_1 \rightarrow a_0 \leftarrow a_2$  we get **n<sub>1</sub>** → **N** ← **n<sub>2</sub>**, i.e., the final state coincides with (14).

Though (14) was established by making  $U$  and  $S$  dimensionless via (10), the form of (14) does not depend on this [i.e., within (14)  $U$  and  $S$  can be dimensional], precisely because (14) is invariant with respect to (10).

Above we focused on the case  $u_N > \hat{u}$ , i.e., when the Nash solution is located to the left of the  $s = u$  line. Likewise we can consider the case  $u_N < \hat{u}$  (cf. Fig. 4), where the above derivation applies with necessary modifications. To avoid carrying out this derivation again we can just interchange  $s$  and  $u$ .

## VI. RETRODICTING FROM AN EQUILIBRIUM STATE (WITHOUT CONSERVATION LAWS)

Given an equilibrium state  $(U(\beta), S(\beta))$  with  $\beta > 0$  we can identify it with the final state (14) and ask which initial states give rise to it. Such a question is possible to ask within standard thermodynamics only if the conservation law of entropy or energy is there. Note that  $(U_N, S_N)$  in (14) is determined from

$$\frac{d}{dU} \{(U - U_i)[S(U) - S_i]\} = 0, \tag{18}$$

where  $S(U)$  is the maximal entropy curve. Now employing (3) in (18) we get  $\frac{dS}{dU} = -\frac{1}{T}$ , where  $T = 1/\beta k_B$  is the

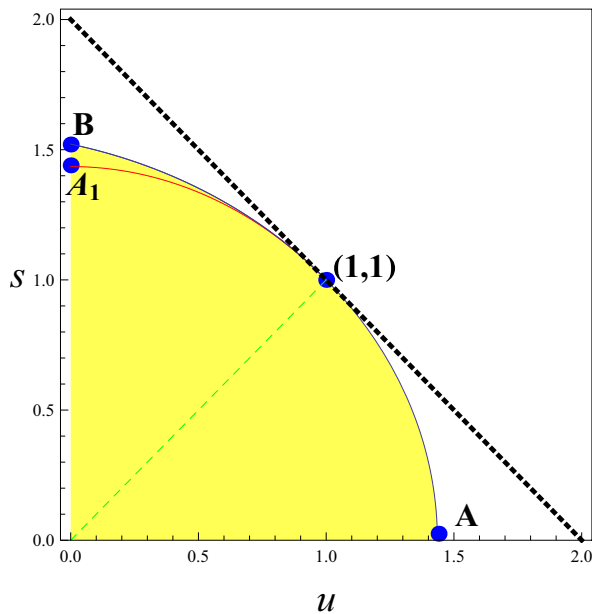


FIG. 4. Entropy-energy diagram in coordinates (12). The blue curve shows  $s(u)$ . The affine freedom is chosen such that the Nash solution (14) coincides with the point (1,1). The original domain of allowed states is filled in yellow. This domain is not symmetric with respect to  $s = u$ . This is seen by looking at the inverse function  $s^{-1}(u)$  (red line) of  $s(u)$ . The domain below  $AA_1$  is symmetric with respect to  $s = u$ .

temperature. Hence (18) leads to a line

$$\frac{S}{k_B} - \frac{S(\beta)}{k_B} = \beta[U - U(\beta)] \quad (19)$$

on the  $(U, S)$  entropy-energy diagram (see the magenta lines in Fig. 1). The line starts from  $(U(\beta), S(\beta))$  and represents possible initial states that lead to  $(U(\beta), S(\beta))$  according to (14). Figure 2 shows how these (magenta) lines end: They can end on the minimum entropy curve, at a point where the convexity of the domain is lost [e.g., at a point where (9) is violated], or at a boundary of the energy-entropy diagram. Thus, though neither energy nor entropy is conserved during thermalization, the assumption about their symmetry (i.e., Axiom 5) allows us to limit (within a finite line) the possible initial state that gives rise to the given thermalized (equilibrium) state.

### VII. SUMMARY AND OPEN PROBLEMS

The main message of this work is that results in nonequilibrium thermodynamics can be obtained via axioms of bargaining, a branch of game theory that describes consensus reaching. The latter is to be achieved between two players whose payoffs (utilities) are related, respectively, to entropy and negative energy. The formalization allows dealing with the problem of thermalization in a way that is complementary to existing physical approaches.

The description of thermalization is based on the energy-entropy diagram (see Sec. II) and Axioms 1–5. We will now briefly recall their physical meaning.

Axiom 1 excludes from consideration active processes, where, compared to the initial state, the energy of the system in the final state increases or its entropy decreases [see (8)].

Axiom 2 excludes very low initial entropies [see (9)], i.e., the initial entropy should be larger than the maximum (i.e., maximum of minimal) entropy. The necessity of this axiom is related to the complex structure of the energy-entropy diagram (see Fig. 1).

Axiom 3 is related to the freedom of adding an arbitrary constant to the energy and entropy, as well as to changing their dimensions without altering the physical content [see (10)].

Thus Axioms 1–3 insist on relatively obvious features, which are known in physics.

Axiom 4 (contraction invariance) introduces in a weak form a pairwise comparison between the states in terms of energy and entropy. This is the really nontrivial axiom, also because it demands the possibility to restrict the system to certain parts of the energy-entropy diagram. We opine that the physical content of this axiom, which is well known in decision theory, should be incorporated into statistical mechanics and lead to further pertinent conclusions.

Axioms 1–4 suffice for deriving thermalization, but they cannot determine which temperature will be reached. This temperature may even be negative depending on the initial state. Adding the last axiom, Axiom 5, which poses a symmetry between energy and entropy, allows us to deduce the Nash expression (14) for this (positive) temperature [cf. (14) and (3)].

Axioms 1 and 3–5 are mostly borrowed from bargaining theory and provided by physical meaning. However, our derivation of (14) is different and makes an important point, since it derives (14) without a hidden (and unphysical) assumption about the possibility to enlarge the domain of allowed payoffs (i.e., the energy-entropy diagram). While this hidden assumption is widely applied in axiomatic bargaining [8,9,27], its game-theoretic meaning is obscure, since it implies that payoffs are changed.

One open problem of this research is what happens when Axiom 5 is dropped, when one can argue that the final temperature will be determined from a generalization of (14),

$$(U_N(\alpha), S_N(\alpha)) = \operatorname{argmax}_{(U, S)} [(U - U_i)^{1-\alpha} (S - S_i)^\alpha], \quad (20)$$

where  $0 < \alpha < 1$  is a parameter. Equation (20) is known as the asymmetric Nash solution [9], but its status within our approach is yet unclear.

Another set of open problem concerns thermodynamic problems, where the known thermodynamic laws do not suffice for uniquely determining the final equilibrium state of a nonequilibrium system, e.g., the famous adiabatic piston problem [2] (see [37] for a review). We believe game-theoretic ideas may be useful for such problems.

### ACKNOWLEDGMENTS

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**APPENDIX A: SHORT INTRODUCTION TO BARGAINING**

The definition of axiomatic bargaining is presented in several places [8,9,27] and can be considered as standard in (cooperative) game theory. However, it also contains several subtle points that are interesting in view of its statistical physics applications explored in this work.

There are two players I and II with utilities  $u(x_1, x_2)$  and  $v(x_1, x_2)$ , respectively, and actions  $x_1$  and  $x_2$  that (for simplicity) are taken from a discrete set  $\mathcal{E}$ :  $x_1 \in \mathcal{E}$  and  $x_2 \in \mathcal{E}$  [8–11,27]. Hence the utility  $u(x_1, x_2)$  of I depends on its own actions  $x_1$ , but also on actions  $x_2$  of II. Utilities (or payoffs) are normally dimensionless and are defined subjectively, via preferences of the player [8–11,27]. The interests of I and II are defined by their utilities and are not opposite to each other; for example, it is generally not the case that  $u(x_1, x_2) + v(x_1, x_2) = 0$  for all pairs  $(x_1, x_2)$ . It is assumed that both utilities are known to I and II.

Now I and II enter into obligatorily negotiations (bargaining) with the aim to reach a consensus on a certain joint action that defines the solution of the bargaining game. Since joint actions can be realized via any joint probability  $p(x_1, x_2)$  for actions  $(x_1, x_2)$ , the set of all states  $\mathcal{D}$  (i.e., the feasible set) allowed for bargaining outcomes is defined via expected utilities:

$$u = \sum_{x_1, x_2} p(x_1, x_2) u(x_1, x_2), \tag{A1}$$

$$v = \sum_{x_1, x_2} p(x_1, x_2) v(x_1, x_2), \tag{A2}$$

for  $(u, v) \in \mathcal{D}$ . Hence  $\mathcal{D}$  is a convex set (cf. Fig. 2). The solution of the bargaining is a particular element of the feasible set  $\mathcal{D}$ . Alternatively,  $\mathcal{D}$  can be defined more abstractly, i.e., without an explicit reference to expected utilities (A1) and (A2); in that case, the convexity of  $\mathcal{D}$  is not guaranteed. For example, in the statistical physics application studied in the main text,  $\mathcal{D}$  is defined via the values of entropy and negative energy, and the convexity is generally not there without specific restrictions.

Sometimes  $\mathcal{D}$  is modified to be comprehensive [8–10], i.e., if  $(u, v) \in \mathcal{D}$ , then all points  $(w_1, w_2)$  with  $w_1 \leq u$  and  $w_2 \leq v$  are also included in  $\mathcal{D}$ . The feature of comprehensiveness is motivated by an observation that (arbitrary) worse utility values can be added to the existing feasible set [9,10]. The observation is not at all obvious (or innocent) even in the game-theoretic context [8]. It certainly does not apply to physics, as stressed in the caption of Table I.

If players I and II do not reach an agreement, then their payoffs are determined by a specific element

$$(u_d, v_d) \in \mathcal{D}, \tag{A3}$$

which is called a defection point [8–10]. Frequently,  $(u_d, v_d)$  is defined via guaranteed payoffs of the players. Recall that

the guaranteed payoffs for I and II read, respectively,

$$\max_{x_1} \min_{x_2} [u(x_1, x_2)], \tag{A4}$$

$$\max_{x_2} \min_{x_1} [v(x_1, x_2)]. \tag{A5}$$

The logic of (A4) for I is that for whatever action of I, the second player II will minimize the outcome of I. Hence I should choose the action that achieves the best among the worst. The same interpretation applies to (A5) for II.

One axiom that is frequently imposed on bargaining solutions is the Pareto optimality [8–11,27]. The definition of Pareto optimality is recalled in the caption of Table I. Using this concept, a restriction to solutions of the bargaining problem was proposed by von Neumann and Morgenstern [8]: It includes all  $(u, v) \in \mathcal{D}$  that are Pareto optimal and holds for  $u \geq u_d$  and  $v \geq v_d$  [cf. (A3)].

The Pareto optimality is motivated by the rationality of players, but we need to emphasize that this is not at all an obvious axiom; e.g., it is not clear (without further assumptions) how the players should reach a Pareto optimal point if they are not there. Hence we prefer an axiomatic structure proposed by Roth, where the Pareto optimality feature is derived from more intuitive axioms [9].

In this context we mention an elegant behavioristic scheme proposed by Zeuthen [36] that also avoids postulating the Pareto optimality and leads to the Nash solution (14) of the bargaining game [8]. Assume that I and II insist on outcomes  $(u_I, v_I)$  and  $(u_{II}, v_{II})$ , respectively. One of them should give up insisting, and Zeuthen assumed that in a fair situation this will be I, if its relative loss in giving up is smaller,

$$\frac{u_I - u_{II}}{u_I - u_d} < \frac{v_{II} - v_I}{v_{II} - v_d}, \tag{A6}$$

i.e.,

$$(u_{II} - u_d)(v_{II} - v_d) > (u_I - u_d)(v_I - v_d). \tag{A7}$$

After no more insisting on  $(u_I, v_I)$ , I should propose another solution  $(u'_I, v'_I)$ . With the same logic that leads to (A7), this solution should hold:  $(u'_I - u_d)(v'_I - v_d) > (u_{II} - u_d)(v_{II} - v_d)$ . Otherwise, II will keep on insisting at  $(u_{II}, v_{II})$ . This logic leads to the Nash solution

$$\max_{x_1, x_2} \{ [u(x_1, x_2) - u_d][v(x_1, x_2) - v_d] \}. \tag{A8}$$

**APPENDIX B: CALCULATION OF THE MINIMUM ENTROPY FOR A FIXED AVERAGE ENERGY**

Here we show how to minimize entropy

$$S_{\min}(E) = \min_p S[p], \quad S[p] = -k_B \sum_{i=1}^n p_i \ln p_i, \tag{B1}$$

over probabilities

$$\{p_i \geq 0\}_{i=1}^n, \quad \sum_{i=1}^n p_i = 1, \tag{B2}$$

for a fixed average energy

$$E = \sum_{i=1}^n \varepsilon_i p_i. \tag{B3}$$

Energy levels  $\{\varepsilon_i \geq 0\}_{i=1}^n$  are given.



Since  $S[p]$  is concave, its minimum is reached for vertices of the allowed probability domain. This domain is defined by the intersection of (B2) with probabilities that support the constraint (B3). Put differently, as many probabilities are nullified for the minimum of  $S[p]$  as allowed by (B3). Hence, at best, only two probabilities are nonzero.

We now order different energies as

$$\varepsilon_1 < \varepsilon_2 < \varepsilon_3 < \dots \tag{B4}$$

and define entropies  $s_{ij}(E)$ , where only states  $i$  and  $j$  with  $i < j$  have nonzero probabilities:

$$s_{ij}(E) = -\frac{E - \varepsilon_i}{\varepsilon_j - \varepsilon_i} \ln \frac{E - \varepsilon_i}{\varepsilon_j - \varepsilon_i} - \frac{\varepsilon_j - E}{\varepsilon_j - \varepsilon_i} \ln \frac{\varepsilon_j - E}{\varepsilon_j - \varepsilon_i}, \tag{B5}$$

$$\varepsilon_i \leq E \leq \varepsilon_j. \tag{B6}$$

The minimum entropy  $S_{\min}(E)$  under (B3) is found by looking, for a fixed  $E$ , at the minimum over all  $s_{ij}(E)$  whose argument supports that value of  $E$ . For example,  $S_{\min}(E)$  reads, from (B5) for  $n = 3$  (three different energies),

$$S_{\min}(E) = \min[s_{13}(E), \theta(\varepsilon_2 - E)s_{12}(E) + \theta(E - \varepsilon_2)s_{23}(E)], \tag{B7}$$

where  $\theta(x)$  is the step function [ $\theta(x > 0) = 1$  and  $\theta(x < 0) = 0$ ] and we assume  $\varepsilon_1 \leq E \leq \varepsilon_3$ . Likewise, for  $n = 4$ ,

$$\begin{aligned} S_{\min}(E) = & \min[s_{14}(E), \theta(\varepsilon_2 - E)s_{12}(E) \\ & + \theta(E - \varepsilon_2)\theta(\varepsilon_3 - E)s_{23}(E) \\ & + \theta(E - \varepsilon_3)s_{34}(E), \theta(\varepsilon_2 - E)s_{12}(E) \\ & + \theta(E - \varepsilon_2)s_{24}(E), \theta(\varepsilon_3 - E)s_{13}(E) \\ & + \theta(E - \varepsilon_3)s_{34}(E)], \end{aligned} \tag{B8}$$

where  $\varepsilon_1 \leq E \leq \varepsilon_4$ . Generalizations to  $n > 4$  are guessed from (B7) and (B8).

### APPENDIX C: FEATURES OF THE NASH SOLUTION (14)

#### 1. Concavity

Let us write (14) in coordinates (12),

$$u_N = \underset{u}{\operatorname{argmax}}[us(u)], \tag{C1}$$

where (for obvious reasons) the maximization was already restricted to the maximum entropy curve  $s(u)$ . Now recall that  $s(u)$  is a concave function. Local maxima of  $us(u)$  are found from [ $\frac{ds}{du} \equiv s'(u)$ ]

$$[us(u)]'|_{u=u_N} = u_N s'(u_N) + s(u_N) = 0. \tag{C2}$$

Calculating the second derivative and using (C2), we get

$$[us(u)]''|_{u=u_N} = -\frac{2s(u_N)}{u_N} + u_N s''(u_N) < 0. \tag{C3}$$

We see that solutions  $u_N$  of (C2) are indeed local maxima due to  $s''(u) < 0$  (concavity) and  $u \geq 0$  and  $s(u) \geq 0$ , as seen from (12).

We will now show that this local maximum is unique and hence coincides with the global maximum. For any concave function  $s(u)$  we have, for  $u_1 \neq u_2$ ,

$$s(u_1) - s(u_2) < s'(u_2)(u_1 - u_2). \tag{C4}$$

Employing (C4) for  $u_1 = u$  and  $u_2 = u_N$ , multiplying both sides of (C4) by  $u$ , and using (C2), we get

$$\begin{aligned} us(u) - u_N s(u_N) & < s'(u_N)(u - u_N)^2 \\ & = -\frac{s(u_N)}{u_N}(u - u_N)^2 < 0. \end{aligned} \tag{C5}$$

Hence  $u_N$  is the unique global maximum of  $us(u)$ .

#### 2. Comments on the textbook derivation of (14)

In the main text we emphasized that the derivation of the solution (14) for the axiomatic bargaining problem that was proposed by Nash [27] and is reproduced in textbooks [8–10] has a serious deficiency. Namely, (14) is derived under an additional assumption, viz., that one can enlarge the domain of the allowed state on which the solution is sought. This is a drawback already in the game-theoretic setup, because it means that the payoffs of the original game are (arbitrarily) modified. In contrast, restricting the domain of available states can be motivated by forbidding certain probabilistic states (i.e., joint actions of the original game), which can and should be viewed as a possible part of negotiations into which the players engage. For physical applications this assumption is especially unwarranted, since it means that the original (physical) entropy-energy phase diagram is arbitrarily modified.

We now demonstrate using the example of Fig. 4 how specifically this assumption is implemented. Figure 4 shows an entropy-energy diagram in relative coordinates (12) with  $s(u)$  being the maximum entropy curve. The affine transformation was chosen such that the Nash solution (14) coincides with the point (1,1). Now recall (C2). Once  $s(u_N) = u_N = 1$ , then  $\frac{ds(u_N)}{du} = -1$ , and since  $s(u)$  is a concave function, then all allowed states lie below the line  $2 - u$  (see Fig. 4). If now one considers a domain of *all* states ( $u \geq 0, s \geq 0$ ) [excluding the initial point (0,0)] lying below the line  $2 - u$  (this is *the* problematic move), then (1,1) is the unique solution in that larger domain. Moving back to the original domain and applying the contraction invariance axiom, we get that (1,1) is the solution of the original problem.

#### 3. Location of (14) on the maximum entropy curve

As mentioned in the main text, the application of Axioms 4 and 5 locates the Nash solution (14) on the maximum entropy curve such that it always lies on that part of the curve which is allowed according to Axiom 4. This result can be deduced from the fact that applying additional axioms (with respect to Axioms 1–5), one can deduce that (14) is the only solution [8,9,27]. Hence applying fewer axioms (i.e., applying only Axioms 1–5), one cannot conclude that (14) is not allowed. This argument is correct, but indirect; hence below we deduce the sought relation directly from equations.

Let us recall that  $\hat{u}$  is defined from  $s(\hat{u}) = \hat{u}$ ,  $s^{-1}(u)$  is the inverse function of  $s(u)$ , and  $u_N$  comes from (C1). We work out the concave function  $s(u)$  for  $u \simeq \hat{u}$ ,

$$us(u) - \hat{u}s(\hat{u}) = \hat{u}(u - \hat{u})[1 + s'(\hat{u})], \tag{C6}$$

$$s(u) - s^{-1}(u) = [s'(\hat{u})^2 - 1](u - \hat{u})/s'(\hat{u}), \tag{C7}$$

where  $s'(u) = ds/du$  and factors  $O(u - \hat{u})^2$  were neglected on the right-hand sides of (C6) and (C7).

For  $-1 < s'(u) < 0$  we have the situation shown in Fig. 3. Recalling that  $\hat{u} > 0$ , we see that (C6) predicts  $us(u) > \hat{u}s(\hat{u})$  for  $u > \hat{u}$ . Hence  $u_N > \hat{u}$ . Now (C7) confirms that  $s(u) > s^{-1}(u)$  for  $u > \hat{u}$ , as seen in Fig. 3. Thus  $u_N$  is in the allowed domain.

For  $-1 > s'(u)$  we have the analog of Fig. 3, which is reversed around the  $s = u$  line. Now (C6) shows that  $u_N < \hat{u}$ , while  $s(u) < s^{-1}(u)$  as implied by (C7). Again,  $u_N$  is in the allowed domain.

For  $1 > s'(\hat{u}) > 0$ , we always get  $u_N > \hat{u}$ .

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