A multiobjective optimization approach to statistical mechanics

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Optimization problems have been the subject of statistical physics approximations, given the natural connection between fitness optimina in rugged landscapes, disordered systems, and their underlying Hamiltonians. As models of evolutionary complexity, they help building appropriate frameworks to define the space of the possible and the nature of transitions among different optimal solutions. Simple models are especially relevant when considering tradeoffs between cost and efficiency, where optimal solutions involve a compromise between both. The theory of Pareto Optimality (or Multi-Objective Optimization, MOO) is a general method that encompasses all optimal solutions as long as no bias toward any of the objectives exists. In such framework, families of optimal solutions lie on a well defined subset of the underlying function space: the so called Pareto front. The diverse formulations of the theory, as proposed within evolutionary theory, economics, or engineering hide a number of universal traits, which we study here under the light of statistical thermodynamics. We show that thermodynamics can be treated as an MOO problem, using the associated potentials as constraints. More importantly, we show that there is an equivalence between the structure of the Pareto front and the Gibbs surface as defined in thermodynamics. These equivalences are illustrated with standard examples of statistical physics and the general consequences of our results are discussed.

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I. INTRODUCTION

Most complex systems result from both evolutionary or design processes where multiple traits need to be simultaneously considered while searching for optimal solutions [1]. This includes living as well as technological and economic systems and, not surprisingly, there is a dedicated literature that develops the problem of how to define the paths and boundaries of the optimal trajectories [2–6]. Theoretical developments started with the formal search of economic efficiency, which – by definition – is a multidimensional task that incorporates different traits (and scales). But the basic concept turned much more general as a way of approaching any class of problem involving the simultaneous optimization of several competing objectives. This situation is common both to engineers and in biological evolution. In both cases, there is usually a conflict between cost and efficiency. The parallelisms between fields are further highlighted by the fact that many engineering endeavors can actually be addressed by means of computer-based selection Darwinian processes.

In all these fields, it is found that every problem has a space of possible solutions (consistent with the economic, biological, or technological reality) limited by some boundary that defines the frontier with the domain of the unreachably. Typically, starting from a population of initial conditions, the evolutionary dynamics under Pareto optimality (see Methods) generates a “final” population of best-fit solutions that appear scattered over that boundary, known as the Pareto front. This subset can have different geometric and statistical features. Are there universal properties common to all of these case studies? Can the constraints that operate in Multi Objective Optimization (MOO) problems be mapped into some fundamental set of concepts beyond the specific nature of each case study?

Statistical physics has addressed different aspects of optimization problems [7–12] and their associated phase transitions [13–17]. In these studies, a single-component fitness function (i.e. a single objective optimization, SOO) is considered. However, little attention has been payed to the physics of Pareto Optimality despite its great impact in many areas [18–27]. In MOO we deal with the simultaneous optimization of $K$ target functions ($T_f \equiv \{t_k, k = 1, ..., K\}$). The sought solution is the most optimal tradeoff between the $t_k$. An abundant literature exists with methods to locate these tradeoffs [2–6], but it is not so widespread outside economics or very specific scopes in engineering. Some researchers have taken an alternate and intuitive path by treating intrinsically multiobjective problems as single objective ones using global fitness functions such as:

$$\Omega = \sum_k \lambda_k t_k.$$  

This approach presents some inconveniences: i) Different $t_k$ might not be commensurable as they usually have distinct dimensionality. ii) The $\lambda_k$ (metaparameters external to the problem) introduce arbitrary (and potentially subjective) biases towards the different $t_k$. And, iii) minimizing for different values of $\lambda_k$ might fail to reproduce optimal tradeoffs...
optimization tasks are assumed to be minimizations unless indicated otherwise. Thermodynamics and illustration with two relevant examples follows in section II B. Without loss of generality all thermodynamics and Pareto optimality. The theoretical framework is explained in section II A. Its application to our theory is built (figure 1). The main findings in this article are of a theoretical nature and bridge between definitions in the Methods section. Importantly, we define Pareto optimality and the Pareto front, upon which weighting linearly the different targets with a set of external parameters \( \Lambda \) depending on the problem under research – as will become clear later. However, collapsing MOO into SOO (as in equation 1) happened to be a very fruitful line of research. When varying the \( \lambda_k \) under which optimization took place, authors found phase transition-like behaviors. Such phenomena were reported in very diverse systems from complex networks [28–32] to models of human language [33–36].

We wanted to understand these results from a pure MOO perspective and see how they would reflect on ongoing MOO research. Therefore we developed a theoretical framework that relates a general MOO to its collapsed SOO version and we investigated under what circumstances should phase transitions and other phenomena arise. In doing so we discovered a close correspondence of our framework with old ideas in classic thermodynamics [37–39] that are not being fully exploited until recently. The kind of problems studied in this paper include thermodynamics, but are more general. We indicate the equivalence between relevant thermodynamic objects and the corresponding elements of this more general framework.

From a purely thermodynamical point of view our results are not completely novel. We draw inspiration from the findings of Gibbs [37–39] who identified the thermodynamic state of a system as the point tangent to an abstract surface whose normal vector indicated the temperature and pressure of the system. Phase transitions are associated to concavities and non-analyticities of this surface. In this paper we show the equivalence of this surface and the Pareto front of a corresponding multiobjective optimization problem in thermodynamics. We show that any MOO system with an associated Pareto front presents the same kind of behaviors regarding concavities and non-analyticities when they are collapsed into SOO problems, thus the Pareto front becomes a conceptual cornerstone in generalizing phase transitions to any system outside thermodynamics or statistical mechanics. Accordingly, the existing efforts to classify phase transitions exhaustively under the light of the Gibbs surface [40–42] become of immediate interest to the research of Pareto optimality.

II. RESULTS

In the literature we can find different approaches to MOO. For consistency, we revise standard notation and definitions in the Methods section. Importantly, we define Pareto optimality and the Pareto front, upon which our theory is built (figure 1). The main findings in this article are of a theoretical nature and bridge between thermodynamics and Pareto optimality. The theoretical framework is explained in section II A. Its application to thermodynamics and illustration with two relevant examples follows in section II B. Without loss of generality all optimization tasks are assumed to be minimizations unless indicated otherwise.

A. Theoretical framework

Given an MOO with K target functions \( T_f \equiv \{t_k, k = 1,...,K\} \) we define the most simple SOO problem by weighting linearly the different targets with a set of external parameters \( \Lambda \equiv \{\lambda_k; k = 1,...,K\} \). This produces a global fitness function:

\[
\Omega\{T_f(x); \Lambda\} = \sum_k \lambda_k t_k(x). \tag{2}
\]

A set \( \Lambda \) with fixed values \( \lambda_k \) yields one SOO, thus equation 2 defines a parameterized family of SOOs. We will study such SOOs, the constraints that the Pareto front imposes to their solutions, and the relationships between different SOOs of the same family. The validity of the results holds for any positive, real set \( \Lambda \); but for convenience: i) We take \( K = 2 \), which simplifies the graphic representations and contains the most relevant situations possible. Some remarks are given about \( K > 2 \). ii) We require \( \sum_k \lambda_k = 1 \) without loss of generality. For \( K = 2 \) then \( \lambda_1 = \lambda \), \( \lambda_2 = 1 - \lambda \), and \( \Omega = \lambda t_1 + (1 - \lambda) t_2 \); greatly simplifying the analysis. iii) We impose \( \lambda_k \neq 0 \) \( \forall k \). The case \( \lambda_k = 0 \) is briefly commented bellow.

For given \( \lambda_k \) one definite SOO problem is posed. Then, equation 2 with fixed \( \Omega \) defines equifitness surfaces noted \( \tau_\Lambda(\Omega) \). Each \( \tau_\Lambda(\Omega) \) constitutes a \( K - 1 \) dimensional hyperplane in the \( K \)-dimensional space of target functions (or target space, see Methods). For \( K = 2 \) (figure 1) these surfaces are defined as:

\[
\tau_\Lambda(\Omega) \equiv \left\{ \left(t_1, t_2\right) \mid \frac{\Omega}{1 - \lambda} - \frac{\lambda}{1 - \lambda} t_1 \right\}. \tag{3}
\]

The slope of \( \tau_\Lambda(\Omega) \) along each possible direction \( \hat{t}_k \) in the target space only depends on \( \Lambda \); different \( \tau_\Lambda(\Omega) \) for a given SOO problem are parallel to each other. The crossing of \( \tau_\Lambda(\Omega) \) with each axis \( \hat{t}_k \) is proportional to \( \Omega \). (From equation 3 for \( K = 2 \) the crossing with the vertical axis is \( \Omega/(1 - \lambda) \) and with the horizontal axis is \( \Omega/\lambda \).) These
FIG. 1: An MOO-SOO system, step by step. a Upon a set $X$ of arbitrary objects we define an optimization task that consists on the minimization of $t_1, t_2 \in T_f$. These functions map each object $x \in X$ in the target space – in this case, the real plane. b In this space, dominance and Pareto optimality introduce a partial ordering of the elements $x \in X$. The Pareto front (thick brown line) consists of all Pareto optimal solutions and offers the most optimal tradeoff possible between the conflicting targets $t_1$ and $t_2$. This is the solution of the MOO. c Collapsing the targets with equation 2 defines SOOs parameterized by the parameters $\lambda_k$. In this two-dimensional case one parameter $\lambda$ suffices to parameterize all possible SOOs. For fixed $\lambda$ one SOO is posed whose solution usually lies where lines of equal fitness $\tau_\lambda(\Omega)$ (straight black lines) match the tangent of the Pareto front where it has slope $d = -\lambda/(1 - \lambda)$. Graphically, any optimization that proceeds gradually towards the best $\Omega$ can be seen as pushing these straight lines as much as possible against the front. d Changing the parameter $\lambda$ we visit an SOOs of the same family. The solutions to related SOOs are bound to belong to the same Pareto front, thus its differential geometry in the target space (see methods) plays a paramount role. If the Pareto front is convex, it is smoothly visited for different values of $\lambda$. Any order parameter is then a smooth function of $\lambda$. 
crossings are a function of $\Omega$ and $\lambda_k$ alone. With $\lambda_k$ given and constant, minimizing $\Omega$ means finding $\tau(\tilde{\Omega})$ with $\tilde{\Omega}$ the lowest value possible such that $\tau(\tilde{\Omega})$ still intersects the Pareto front. Graphically, this is equivalent to pushing the equifitness surfaces against the Pareto front as much as possible (figure 1b). Hyperplanes with lower $\Omega$ exist, but the Pareto front sets the limit of feasibility: any solution with $\Omega < \tilde{\Omega}$ cannot be physically realized. The SOO optimum lays on the Pareto front, as can be proved. (From Methods, take $y \notin \Pi$, then $\exists x \in \Pi$, $x < y$; thus at least for one $k' \in \{1, \ldots, K\}$ we have $t_{k'}(x) < t_{k'}(y)$, implying $\{T_f(x); \lambda\} < \{T_f(y); \lambda\}$ and $y$ cannot be SOO optimal.)

The SOO optimum usually lays at the point $x \in \Pi$ where $\tau(\lambda)$ is tangent to the Pareto front (figure 1d). The exceptions to this rule constitute the most interesting cases. The solution to different SOOs (defined by different values of $\lambda$) are found in different points along the front. The relationships within a family of SOO problems is thus partly encoded in the differential geometry of this surface. To explore the many possibilities we use the concavity/convexity convention explained in Methods. We also adopt a dynamic point of view in which $\lambda$ is varied infinitesimally slow, thus transitioning between different SOOs of a same family.

The most simple case happens for convex Pareto fronts whose tangent in the $t_1 - t_2$ plane is well defined in its interior and its slope spans the interval $(-\infty, 0)$ (figure 1c). Then, the solution to the SOO posed by a given $\lambda$ is always found where the Pareto front has slope $d = -\lambda/(1 - \lambda)$ and $\tau(\lambda)$ matches the tangent of the front. A differential increase $\lambda \to \lambda + D\lambda$ causes a differential modification $d 	o d + (\lambda - 1) D\lambda$. For $\lambda \in (0, 1)$, $d \in (0, -\infty)$ and there is a well posed SOO problem for each $\lambda$, each with a different solution. As we vary $\lambda$, successive SOO solutions roll smoothly over the front. The plot of any order parameter $\theta$ (see Methods) renders a continuous, differential function of $\lambda$ that lacks any relevant features.

**FIG. 2: Convex Pareto front with a tangent whose slope does not span the whole range $(-\infty, 0)$.** a The slope of the tangent of the Pareto front spans $d \in (-\infty, d^*)$, thus the lower-right end of the Pareto front is the SOO optimum for several $\lambda < \lambda^*$ (open circle). For $\lambda > \lambda^*$ the SOO optima are reached in a differentiable fashion as for fully convex fronts (filled circle). When measuring an order parameter $\theta$ (inset) we find that for $\lambda < \lambda^*, \theta$ does not change because the SOO optimum is one and the same; but its derivative is not zero for $\lambda > \lambda^*$. This causes an abrupt shift in $\frac{d\theta}{d\lambda}$ at $\lambda^*$ while $\theta(\lambda)$ remains continuous always. b The exact same situation happens if the pathology is found at the upper-left end of the Pareto front. c Following the same reasoning, an ill defined derivative is associated with two consecutive second order phase transitions. In the insets of each panel they are shown possible plots of $\theta$ vs. $\lambda$. Note that the inset plots are only an illustration: the actual shape can vary and the curved stretches would depend on the differential geometry of the Pareto front, among other factors specific to each order parameter.

In figure 2a, b, and c we represent convex Pareto fronts whose slopes span $d \in (-\infty, d^*)$, $d \in (d^*, 0)$, and $d \in (-\infty, d^-) \cup (d^+, 0)$ respectively; with $-\infty < d^* < d^-, d^+ < 0$. In all three cases we find convex stretches of the front with well defined values of their slopes $d$. With $\lambda = -d/(1 - d)$ we reveal the intervals $\lambda \in [\lambda^*, 1]$, $\lambda \in [0, \lambda^*]$, and $\lambda \in [0, \lambda^*] \cup (\lambda^-, 1]$ respectively; with $\lambda^*, \lambda^- \equiv -d^*/(1 - d^*, \pm)$. For these intervals they are defined a series of SOO problems whose solutions are always found where the $\tau(\lambda)$ match the tangent of the Pareto front. These can be smoothly visited as $\lambda$ changes infinitesimally slow, just as in the trivial case above.

Consider now figure 2a as $\lambda \to (\lambda^*)^+$ and for $0 < \lambda < \lambda^*$. We can define SOO problems in this range (gray fan in figure 2a), but the abrupt end of the Pareto front implies that the solution to all these SOOs is the same. This happens again as $\lambda \to (\lambda^*)^-$ in figure 2b and as we approach $\lambda^+$ from below and $\lambda^-$ from above in figure 2c. For SOOs defined by $\lambda \in (0, \lambda^*)$, $\lambda \in (\lambda^-, 1]$, and $\lambda \in (\lambda^+, \lambda^-)$ respectively, the solution is one and the same. Thus, as we vary $\lambda$ within these intervals any order parameter measured upon this same SOO solution remains unchanged: $\frac{d\theta}{d\lambda} = 0$. But the same order parameters change at non-zero rates as we approach $\lambda^*, \pm$. Because every point of the
front can be reached continuously while varying $\lambda$, plotting $\theta$ (figure 2 insets) produces a continuous graph with a discontinuity in the derivatives. This is the fingerprint of **second order phase transitions** and is coherent with an interpretation based on the thermodynamic Gibbs surface [38, 39] (although these transitions were not described by Gibbs using this tool).

In thermodynamics, **first order phase transitions** and metastability are associated to concavities in the Gibbs surface [38, 39]. The same is true about the MOO studied here, for which the Pareto front is the equivalent to the Gibbs surface – indeed, we propose that the Pareto front is more general than the Gibbs surface since thermodynamics can be written as the kind of problems under research here, as discussed later.

[FIG. 3: Concave Pareto front, or fronts with concavities. a] The easiest case to illustrate first order phase transitions is a fully concave Pareto front. Only two solutions are ever SOO global optima: one of them is reached for every $\lambda > \lambda^*$ and the other one for every $\lambda < \lambda^*$. For $\lambda = \lambda^*$ both solutions coexist. When plotting an order parameter against $\lambda$ (inset) we observe a sharp discontinuity at $\lambda = \lambda^*$, as in documented first order phase transitions. In b and c similar but more general cases are illustrated. In c, the $\theta$ vs. $\lambda$ inset plot is interesting in that while $\theta(\lambda)$ is not continuous, its derivative (dashed lines) is perfectly continuous. In all three cases, the concavities of the Pareto front contain some solutions that could be reached as metastable states.

Take the fully concave front from figure 3a. A critical value of $\lambda$ is defined by the slope $d^*$ of the straight line joining the two ends of the Pareto front: $\lambda^* \equiv \frac{-d^*}{1-d^*}$. The solution to any SOO defined by $\lambda < \lambda^*$ is located at the lower right end of the Pareto front, while for SOOs defined by $\lambda > \lambda^*$ the solution is found at the upper left end. Both extremes coexist for $\lambda = \lambda^*$, as is characteristic of first order phase transitions. There is not smoothly rolling over the front when varying $\lambda$ now, only one sudden shift between radically different optima as we transit through $\lambda^*$. Because below and above this value the optima are the same for the many different SOOs posed by different $\lambda \gtrless \lambda^*$, any order parameter remains constant below and above $\lambda^*$; but there is a gap between both constant values (figure 3b, inset). Once again, this is characteristic of first order phase transitions.

Pareto optimal solutions inside the concavity are never global optima for the posed SOOs. Some of these solutions might be metastable – i.e. locally optimal – as in thermodynamics. In real systems they remain stable as long as the system is spared from huge perturbations – e.g. as it happens with supercooled water.

These situations (first order phase transitions, phase coexistence, and metastability) happen in Pareto fronts with concavities, even if combined with convex parts (figures 3b and c). In both cases we observe a finite gap as we plot any order parameter $\theta$ as a function of $\lambda$. Interestingly, $\frac{d\theta}{d\lambda}$ remains always continuous in figure 3b even when $\theta$ itself is not. A consequence of these considerations is that SOO solutions are restricted to the convex hull of the Pareto front.

Phase transitions are among the most interesting phenomena accounted for by the Pareto front, which generalizes the Gibbs surface for the studied MOO-SOO systems. Because of the equivalence between both objects, we remit the reader to more specialized literature that builds upon the Gibbs surface to discuss features such as the critical or spinoidal points [40–42], which are interesting specially to thermodynamic systems. Other accidents might show up in the Pareto front that have not been discussed in the thermodynamic literature to the best of our knowledge:

- If the Pareto front is a straight segment in the $t_1 - t_2$ plane we define a critical value $\lambda^* \equiv \frac{-d^*}{1-d^*}$ with $d^*$ the slope of the segment. In figure 4a a situation similar to first order phase transitions is found with either extreme of the Pareto front solving the SOOs defined by $\lambda \gtrless \lambda^*$ respectively. Besides, any solution of the Pareto front is optimal at this critical value. Optima at $\lambda = \lambda^*$ contain both $\lambda < \lambda^*$ and $\lambda > \lambda^*$ phases (as in first order phase transition coexistence) but for this singular value of $\lambda$ it is also present a repertoire of solutions not visited
under any other circumstance, making this situation strictly different from thermodynamic phase coexistence. This repertoire of solutions not only solves the MOO and the $\lambda^*-\text{SOO}$. It also presents a great diversity and is perhaps ready to adapt to further external requirements that we might impose, portraying a very interesting situation. Straight stretches of the front might also happen along second order phase transitions, (figure 4b). Then, an infinite divergence of the derivative of any order parameter takes place as $\lambda \to \lambda^*$ (figure 4b inset), which is characteristic of critical systems.

- Allowing $\lambda = 0$ is the only situation in which solutions not in the Pareto front solve an SOO (figure 4c). At least one of these solutions must be Pareto optimal, though. This case is straightaway incorporated in the general framework: if such an extension of the Pareto front exists, it is equivalent to a straight stretch as described above. Allowing $\lambda_k = 0$ does not alter our theory.

- We assumed that the $\lambda_k$ are the only relevant control parameters, but it is easy to conceive other external variables modifying the shape of the Pareto front or its constituents. Such cases could prompt phase transitions to existence or erase them. (This can also be due to the varying of some $\lambda_k$ if $K > 2$, as noted for the Gibbs surface [42].) Parameters changing the constituents of the front could trigger drastic changes not studied here.

### B. Thermodynamics as a multiobjective optimization problem

Considering thermodynamics as a MOO deserves a lengthy discussion undertaken in appendix A. This section follows the next plot: i) it is proposed a legitimate MOO involving entropy and energy optimization for an arbitrary physical system, ii) this problem is solved through the Pareto formalism, iii) the MOO is collapsed into a relevant family of SOOs parameterized through a parameter akin to $\lambda$ above, iv) it is shown that the SOO solutions correspond precisely to configurations of the chosen physical system in thermodynamic equilibrium. The theory is illustrated through the Ising and Potts models for which phase transitions are uncovered by the Pareto front. We focus on the results here, the detailed calculations made for these models are shifted to appendix B.

Take an arbitrary physical system that can occupy any state $\sigma_j$ of its phase space $\sigma_j \in \Sigma$. Each $\sigma_j$ is a physical configuration with an energy $E_j$. Consider an arbitrary ensemble for this system $P_i$, in which $\sigma_j$ shows up with probability $P_i(\sigma_j)$. Consider, indeed, all possible ensembles $P$ ($P_i \in P$), each of them an arbitrary, mathematically
plausible probability distribution over the phase space. Upon each $P_i$ we define the functionals:

$$U\{P_i, \Sigma\} = \sum_j P_i(\sigma_j)E_j,$$

$$S\{P_i, \Sigma\} = -\sum_j P_i(\sigma_j)\log(P_i(\sigma_j)); \quad (4)$$

i.e. the internal energy and entropy of the ensemble $P_i$. These functionals are rigorously defined irrespective of whether they bear any physical meaning. Furthermore, $P_i$ is an arbitrary probability distribution, thus there is not any guarantee (neither necessity, so far) that $U\{P_i, \Sigma\}$ or $S\{P_i, \Sigma\}$ obey any relevant relationship.

These functions map each and every $P_i \in P$ into the $U = S$ plane, where dominancy and Pareto optimality are well defined. Within $P$, let us find the subset $P_{\Pi} \subset P$ of probability distributions $P_{\nu} \in P_{\Pi}$ that minimize $U\{P_{\nu}, S\}$ and maximize $S\{P_{\nu}, S\}$ simultaneously. This is a legitimate MOO problem, again irrespective of whether it has got any physical relevance. We can solve this problem just for the sake of it. Its solution consists precisely of all $P_{\nu} \in P_{\Pi}$; this is the Pareto front of the MOO and it constitutes the optimal tradeoff between the functionals from equation \[(4)\]. This reduces the number of relevant ensembles for us: among all $P_i \in P$ we focus now on $P_{\nu} \in P_{\Pi}$, but still there is no guarantee nor any need that these ensembles present notable physical properties. They are just probability distributions laying on the Pareto front of an ad-hoc MOO.

Consider now the family of SOOs defined by:

$$\min \{\Omega(U, S; \lambda_U, \lambda_S) \equiv \lambda_U U + \lambda_S S\} \Rightarrow \min \left\{\Omega \equiv \frac{U}{\lambda_U} + \frac{S}{\lambda_S}\right\}. \quad (5)$$

This collapses the original MOO into a series of SOOs interrelated because their solutions lay upon the convex hull of $P_{\Pi}$ in the $U = S$ plane. These SOOs are subjected to the observations demonstrated above. Phase transitions might arise for singular values $(\lambda_U/\lambda_S)^{\pm}$ due to concavities and non-analyticities of the Pareto front.

Again, these are phase transitions of a fabricated problem. Let us find a link with the known physical reality of equilibrium thermodynamic systems. Following the second law of thermodynamics, we find the ensembles that maximize $S$ for fixed values of $U$. These correspond to the microcanonical ensemble that are mapped into the $U = S$ plane through equation \[(4)\] describing a curve. For each fixed $U$ we attain the maximum possible $S$, reconstructing the Pareto front of the MOO above (see appendix \[A\] for details). Irrespective of whether thermodynamics consists in a MOO, microcanonical ensembles are linked to the Pareto front of a legitimate MOO.

The laws of thermodynamics also imply that

$$F = U - TS = U - S/\beta \quad \text{(6)}$$

is minimized in equilibrium at a fixed temperature \[39\]. Thermodynamic canonical ensembles embody this minimization. Identifying $\Omega \equiv F$ and $\lambda_S/\lambda_U \equiv -T = -1/\beta$ in equation \[(5)\] the relevant $(\lambda_U/\lambda_S)^{\pm}$ correspond to temperature values at which phase transitions occur. Irrespective of whether thermodynamics consists of an MOO-SOO setup, canonical ensembles are constrained by the rules that reveal phase transitions in such systems. These rules assign first order phase transitions to concavities of the Pareto front. Due to these concavities, the front and its convex hull – i.e. the mapping of microcanonical and canonical ensembles into the $U = S$ plane – differ, yielding valid all results from the study of ensemble inequivalence \[43\] \[44\]. Consistently, second order phase transitions correspond to sharp edges of the Pareto front.

As a final remark (further discussion in appendix \[A\]), thermodynamic systems described by internal energy, entropy, and volume find their microcanonical ensembles laying on the Gibbs surface $G = U - TS - pV$ \[35\] \[70\]. This corresponds to the Pareto front of an adequate MOO problem. Phase transitions are identified for singular values of temperature and pressure.

The Ising and Potts models illustrate first and second order phase transitions respectively. General versions of these models have been solved using ensemble inequivalence \[43\] \[44\], but they are discussed here because they allow an almost complete analytic resolution (see appendix \[B\] for detailed calculations).

The Ising model presents a convex Pareto front (figure \[5\]a). This front results a function $S = S(U)$ well defined for $U \in [-Jz/2, 0]$ ($J$ being the coupling constant of the model and $z$ the number of nearest-neighboring spins). Entropy is maximized, as opposed to the minimization of target functions throughout the text. The only modification is that the Pareto front has positive slope. Otherwise, exactly as solutions for SOO with fixed $\lambda$ where found where the slope...
**FIG. 5: Pareto fronts for the Ising and Potts models.**

*a* The Pareto front of the mean-field Ising model (black, equation B2) is convex but its slope does not span all possible values that the parameter $\beta$ explores. Therefore, different SOOs have the same solution: the most entropic upper right end of the front. At $\beta = 1/J_z$ (SOO indicated by the red straight line) a second order phase transition takes place.

*b* A sample of some arbitrary ensembles distributions $P = \{p_1, p_2, p_3\}$ for the $q = 3$ Potts model (blue crosses) is dominated by the Pareto front (red, equation B8). Barely noticeable, the right upper corner portrays a concavity, indicating a first order phase transition. 

*c* The concavity becomes obvious when analyzing the slope of the front, which is not monotonously decreasing.

The front matched $d \equiv -\lambda/(1 - \lambda)$, solutions for fixed $\beta$ are associated to some slope $d(\beta)$. From equation 6 we get curves of constant free energy $\tau_{\beta}(F)$ just as we got equifitness surfaces $\tau_{\lambda}(\Omega)$ before:

$$\tau_{\beta}(F) = \{(U, S) | S = \beta U - \beta F\},$$

revealing that SOO solutions are found now precisely where $\partial S/\partial U = d = \beta$. The derivative $\partial S/\partial U$ tends to $+\infty$ for $U \to (-J_z/2)^+$, meaning that this end of the front is only reached for $\beta \to +\infty$ (zero temperature). Nothing remarkable happens here. At the other end of the Pareto front $\partial S/\partial U$ tends to $1/J_z$ for $U \to 0^-$. Thus, the range $\beta \in (1/J_z, 0]$ defines SOOs whose solutions are always the most entropic configuration of the Ising model. At $\beta \geq 1/J_z$ the SOO solution leaves the disordered phase towards the ordered, magnetic one.

The Potts model (figure 5b and c) presents a concavity in the upper right end of its Pareto front. This implies a first order phase transition from the most entropic configuration to the ordered state, as it is known [45]. Calculations based on the convex hull of this front (appendix B2) match those obtained elsewhere [46]. Again, nothing remarkable happens at the lower left end of the front, which is reached for $\beta \to +\infty$ ($T \to 0$).

**III. DISCUSSION**

In this paper we presented a theoretical framework to discuss MOOs collapsed into families of SOOs. This offered in turn an approach to statistical mechanics from an MOO perspective. In doing so, we have uncovered the equivalence of key objects in MOO (the Pareto front) and building blocks of thermodynamics (the Gibbs surface). Consequently, we have found that phase transitions are not exclusive of this physical theory, but a universal phenomenon natural to any MOO-SOO system. We provide a robust generalization of the concept of phase transition outside its traditional field where they are defined in terms of ensembles and non-analyticities of order parameters. With the proposed framework, we can straightforwardly investigate phase transitions in any system as soon as we can define the relevant MOO problem.

Our framework reveals that old, elegant ideas from thermodynamics [37,39] apply to more general situations than originally envisioned for. The framework also proposes a valid mechanism (MOO collapse into SOOs) of why such a scheme works in its original scope. With the equivalence that we show between our framework and profound concepts in thermodynamics [37,42], we bridge MOO with statistical mechanics and call for a transfer of tools across fields. In the MOO literature we did not find any interpretation of the results in the terms discussed here; not even in recent breakthroughs that bring together MOO and ecology or molecular biology [25–27]. A revision of these works from the proposed point of view becomes compelling. Meanwhile, contributions that somehow overlook the MOO nature of the investigated problems [28–36] persistently reported phase transitions and related phenomenology that can now be understood within a more integrative framework.

In thermodynamics a mechanism naturally collapses MOO into SOO: entropy is available heat and a variation of volume requires work – both eventually linked to energy. In Pareto optimality studies, some authors integrate MOO into SOO for simplicity. Then the $\lambda_k$ can be subjective and are justified because the solutions obtained help
us understand our research problems. In recent approaches to multiobjective aspects of biology \cite{25, 27}, the MOO-SOO nature of such systems is taken for granted because a global fitness function must emerge from Darwinian natural selection. In \cite{25, 27}, several tasks $P_1, ..., P_K$ contribute to the fitness of a species through $F = F(P_1, ..., P_K)$. Improvements in any $P_k$ might raise the overall fitness justifying an MOO study. But the consequences of the MOO-SOO combination are not explored. Our framework relies on the existence of this integration that in the case of thermodynamics and other problems happens through a linear combination of the targets. The scenario found in \cite{25, 27} becomes interesting because the MOO-SOO collapse imposed by $F = F(P_1, ..., P_K)$ is not necessarily linear. In a linear integration SOO optima are always mutually non-dominating, thus SOO and MOO problems can be simultaneously solved. This might not be the case for non-linear fitness functions, opening interesting possibilities associated to biological fitness.

IV. METHODS

A. Elements and solutions of multiobjective optimization

This section provides a common ground on MOO that can be found in the literature \cite{2–6}. As in the main text, we assume minimization without loss of generality (the same results could be obtained for maximization or mixed optimization of target and fitness functions).

Consider a set $X$ of objects upon which we enforce a minimization. We refer to all objects $x \in X$ as feasible or candidate solutions. Objects outside $X$ are not feasible for our problem either because they are physically impossible to realize or because they violate some requested mathematical constraint. The imposed optimization implies that among all objects $x \in X$ we wish to find the subset $\Pi \subset X$ that minimizes a series of given mathematical functions. The set $T_f \equiv \{ t_k(x); k = 1, ..., K \}$ is composed by the $K$ target functions that we wish to minimize. The $t_k(x)$ may be any physical, geometrical, topological, or any other numerical aspect that we might measure upon objects $x \in X$. The set $T_f$ establishes a mapping between $X$ and $\mathbb{R}^K$ (assuming $t_k \in T_f$ as real valued). We refer to $\mathbb{R}^K$ as the target space. Normal vectors $\hat{t}_k$ along the direction of maximal increase of each target constitute an orthonormal base and indicate the axis of $\mathbb{R}^K$. For $K = 2$ the target space reduces to the $t_1 - t_2$ plane.

As a naive illustration of these mathematical elements consider networks of $N$ nodes with one connected component and the simultaneous minimization of i) the average path length between nodes and ii) the number of links implementing the network. The set $X$ consists of all possible networks of $N$ nodes with just one components – any network not complying with these conditions is not feasible for our problem. $T_f$ is comprised by i) the average path length and ii) the number of edges, which are two geometrical features that we can measure in any connected network. These functions map each network of $X$ into one point of $\mathbb{R}^2$ – i.e. in the $t_1 - t_2$ plane (figure 1a). This problem is explored in a forthcoming paper \cite{47}.

For $K = 1$, one single functions $t_1$ is minimized. We face a Single Objective Optimization (SOO). All optimal solutions $x \in \Pi \subset X$ are mapped onto just one point of the real line. $\Pi$ might consist of many elements, but choosing between them is trivial regarding this optimization task because every $x \in \Pi$ presents the same value of $t_1(x)$. This function encloses all the relevant information and it induces an almost perfect ordering of $X$ in $\mathbb{R}$.

The picture changes for $K \geq 2$, a genuine Multi Objective Optimization (MOO). Then, it is usually impossible to induce a perfect ordering of $X$ in $\mathbb{R}^K$. At best we can find tradeoffs between the different targets involved. Solutions $x \in \Pi$ lay along the optimal tradeoff. Picking up between them implies biasing the optimization towards some of the targets, which is something that we ideally wish to avoid. In SOO it is almost always possible to say ‘a solution $x \in X$ is objectively better than another solution $y \in X’$. In MOO it is usual to find $t_1(x) < t_1(y)$ while $t_2(x) > t_2(y)$, thus we cannot say ‘$x$ is objectively better/worst than $y’$ unless we emphasize one target over the other – which, again, is something that we do not want.

We introduce some standard concepts to solve these situations. Recall the set of candidate solutions $X$ and that it is mapped onto $\mathbb{R}^K$ by $T_f(X)$ (figure 1b). In $\mathbb{R}^K$ we can define:

**Definition 1 (Dominance)** A candidate solution $x$ dominates another $y$ (and we denote it $x \prec y$) if:

$$t_k(x) \leq t_k(y) \quad \forall \quad k = 1, ..., K;$$

$$\exists k' \in \{1, ..., K\} | t_{k'}(x) < t_{k'}(y).$$

If a solution dominates another it is objectively better – i.e. more optimal – regarding all MOO targets (figure 1b). But we cannot say anything about two mutually non-dominated solutions. Considering not a couple of solutions ($x$ and $y$), but the whole mapping of $X$ in $\mathbb{R}^K$, we introduce:
Definition 2 (Pareto optimal) A feasible solution $x \in X$ is Pareto optimal if it does not exist any other feasible solution $y \in X$ such that $y < x$.

This definition automatically accounts for the result of SOO, in which all Pareto optimal solutions map into the same point of the real line. In $\mathbb{R}^K$ with $K > 1$ the set of Pareto optimal solutions does not usually map into one point. We define:

Definition 3 (Pareto front) We name Pareto front (and denote it $\Pi$ with $\Pi \subset X$) to the set of Pareto optimal solutions of an MOO. This object is mapped into $\mathbb{R}^K$ by $T_f$ yielding a hypersurface $T_f(\Pi)$ of dimension $K - 1$ or lower. We shall refer to $T_f(\Pi)$ or $\Pi$ as Pareto front indistinctly.

The Pareto front (sketched in figure 1) has got some properties:

1. There are not any $y \in X$ that dominate any $x \in \Pi$, thus solutions from the Pareto front are mutually non-dominating.

2. All $z \in (X - \Pi)$ are dominated by some $x \in \Pi$ (otherwise $z$ is Pareto optimal itself).

3. It is impossible to enhance the performance of a solution of the Pareto front with respect to some $t_k$ without worsening its performance with respect to other(s) $t_{k'}$. Otherwise, the enhanced solution would dominate the original one, which could not belong to the Pareto front.

We can give an alternative definition of the Pareto front based on properties 1 and 2:

Definition 4 (Pareto front) We identify the Pareto front as the subset $\Pi \subset X$ such that:

$$
\forall \quad x, y \in \Pi, \ x \not\preceq y \land y \not\preceq x;
\forall \quad z \in (X - \Pi), \ \exists x \in \Pi \mid x < z.
$$

The mapping $T_f(\Pi)$ of the Pareto front in $\mathbb{R}^K$ may be discrete, finite, or continuous, and concave or convex (see the concavity definition bellow). The essence of the theory introduced here is already captured by MOOs whose Pareto front is a continuous, almost everywhere derivable $K - 1$ dimensional surface in $\mathbb{R}^K$.

The Pareto front constitutes a frontier between what is feasible and unfeasible given the constraints posed by $X$ and $T_f$. When comparing two solutions from the front it is impossible to claim one more optimal than another without introducing a bias towards some target function(s). However, there is a sense of optimality that this scheme grasps: it yields the most optimal tradeoff between different targets. Important challenges remain: “How do we interpret this tradeoff?” “How do we choose a solution if we need to implement one, say in an engineering problem?” The theory developed in this work sheds some light upon these questions.

### B. Concavity/convexity and order parameters

The theoretical framework that we introduce requires a definition of concavity and convexity. Therefore we need a notion of up and down, which we take as given by the equifitness surfaces $\tau(\Omega)$ introduced in section II A. These objects arise from the collapse of MOO into SOOs. SOOs define a perfect ordering of their domains. Consequently, a gradient of optimization emerges (figures 4 and 5). Now it is possible to talk about concavities in a robust way.

As for order parameters, we admit any physical, geometrical, topological, or any other features that we can measure on the elements of $X$. We just require i) that they make different phases distinguishable (they would be poor order parameters otherwise) and ii) that non-trivial behaviors arise out of the optimization dynamics exclusively – if not, we might encounter order parameters that become singular for some mathematical reason not relevant to our study. Importantly, if the chosen indicators obey these conditions, singularities arise for all order parameters simultaneously.

For an arbitrary order parameter $\theta$ the first condition implies that if $x, y \in X$ are mapped into the same point ($T_f(x) = T_f(y)$), then $\theta(x) = \theta(y)$. The opposite ($\theta(x) = \theta(y) \Rightarrow T_f(x) = T_f(y)$) is only required whenever $x \not\preceq y$ and $y \not\preceq x$. This last condition guarantees that two points with different values of the order parameter are never mapped into the same point of the Pareto front in $\mathbb{R}^K$. Accordingly, different phases have different $\theta$. The second condition is satisfied for $\theta$ such that $x, y \in X$ with $T_f(x) = T_f(y) + D\mathbb{R}^K$ implies $\theta(x) = \theta(y) + D\theta$, $D\mathbb{R}^K$ and $D\theta$ standing for arbitrary differential modifications. Then $\theta$ will not present non-analitics other than those revealed by the theory above. Following these conditions, the $t_k(x)$ themselves are valid order parameters.
FIG. 6: A working definition of concave and convex. For an open curve we can safely define concave and convex stretches as soon as we introduce an absolute up-down directionality. The $\tau(\Omega)$ and the optimization gradient that they force upon $\mathbb{R}^2$ are the right objects for us to define up and down. We see how a concavity is revealed in the Pareto front (dashed line).

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VI. AUTHORS CONTRIBUTIONS

LS and RS designed research and wrote the paper. LS developed the models and simulations under the supervision of RS.

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Appendix A: A discussion of thermodynamics as an MOO problem.

In section II B we proved how the solutions to an adequate MOO-SOO problem based on a physical system must correspond precisely to the canonical ensembles of that system in thermodynamic equilibrium. The most delicate part of that process is showing that the microcanonical ensemble reconstructs the Pareto front of the relevant MOO problem. We devote some space here to better clarify this point. Also, SOOs were defined based on equation 6, appropriate for systems described in terms of internal energy and entropy. Other physical systems involve volume in their descriptions. In them, the relevant thermodynamic potential (and the corresponding MOO-SOO problem) is given by the Gibbs potential. A brief discussion about such a potential and its connection to MOO follows at the end of this section.

![Diagram](image)

**FIG. 7: Laws of thermodynamics and the Pareto front.** a According to the second law of thermodynamics, at constant internal energy the microcanonical ensemble is the one that maximizes the entropy (dashed rectangle). Implementing this maximization for varying energy yields a function on the $U - S$ space that for thermodynamic systems is usually monotonously increasing with $U$. This guarantees that any two points on this curve are mutually non-dominated. There cannot be any point above this curve (that point would be reached for the corresponding energy, otherwise), thus the obtained curve must match the Pareto front of the corresponding MOO problem. b This curve would not match the front only if the microcanonic entropy were not monotonously increasing with $U$. This is an odd situation in thermodynamics. These non-increasing stretches would necessarily lay inside a cavity (marked by the blue straight line) and would never show up in thermodynamic equilibrium. c Such situation can also happen beyond a global maximum of the entropy, which is only reached for $T = 0$ (blue). Points of the microcanonical entropy beyond this maximum would require $\partial S/\partial U = 1/T < 0$ (red). In both b and c the entropy of microcanonic ensembles still contains the whole Pareto front (brown) and, of course, its convex hull.

The reconstruction of the Pareto front through microcanonical ensembles derives from the second law of thermodynamics. This states that microcanonical ensembles are those that maximize the entropy for a fixed value of internal energy. This maximization for fixed energy is illustrated in figure 7a. Each microcanonical ensemble is mapped into the $U - S$ plane through equations describing a curve. This curve must be a function $S = \bar{S}(U)$. Otherwise, for a value of $U$ two or more values of $S$ would be assigned, and only one of them could me maximum. The lower values would not correspond to any microcanonical ensemble, accordingly.

Consider the situation in which the curve $S = \bar{S}(U)$ is monotonically increasing. This means that a greater internal energy has always associated a greater degeneracy, which makes sense in a physical context. However, there are mathematical descriptions of physical systems in which this is not the case. These exceptions usually arise in mathematical idealizations compatible with a given model that often lead to exotic parameterizations such as negative temperatures. But these situations bear not relevance for the description of thermodynamic equilibrium systems. This will be clarified below.

Once again, let us assume that $S = \bar{S}(U)$ is monotonically increasing. This guarantees that $S = \bar{S}(U)$ matches the Pareto front of the given problem. For each $U_j > U_i$ necessarily $\bar{S}(U_j) > \bar{S}(U_i)$, thus in this curve there are not any two $U_i < U_j$ such that $\bar{S}(U_i) > \bar{S}(U_j)$, which would imply $U_i \succ U_j$. Furthermore, any ensemble mapped into a point $(U_i, S_i)$ outside this curve is necessarily dominated by some microcanonical ensemble mapped into $(U_j, \bar{S}(U_j))$, because by definition of microcanonical ensembles through the second law of thermodynamics, $\bar{S}(U_i) > S_i$ for that given value $U_i$. This is true for any energy value. Summing up: i) points along the curve $S = \bar{S}(U)$ are mutually non-dominated and ii) for any physically plausible point $(U, S)$ outside this curve there is at least one point that
belongs to the curve and dominates \((U, S)\). This two premises satisfy the second definition of the Pareto front given in Methods. Once microcanonical ensembles reconstruct the front of the proposed MOO, the collapse into SOOs and phase transitions related to accidents in the Pareto front follow naturally.

Let us analyze hypothetical situations like those depicted in figures 7a and c, where the function \(S = S(U)\) is not monotonically increasing. We do not worry ourselves with the physical reality of such descriptions. Our concern is to show that equilibrium thermodynamics are still well represented by the convex hull of the Pareto front and that all the points made in this paper remain true. Given the definition of dominance form the Methods section and applying the reasoning in the paragraph above, we note that the Pareto front of the relevant MOO problem is still fully reconstructed by the curve \(S = S(U)\) (the front is contained in this curve). Non-increasing stretches of \(S = S(U)\) then lay inside a cavity (figure 7b) or after the global maximum of the function (figure 7c). If they are inside a cavity, such situations can never arise in thermodynamic equilibrium, whose canonical ensembles are strictly mapped into the convex hull of the Pareto front. These points are bypassed by a first order phase transitions. In the other situation, note that the slope of the Pareto front at the global maximum (whose limit from below is perfectly reconstructed by the microcanonical ensemble) is necessarily 0, meaning that such situation is only reached at \(\beta = 0 \Rightarrow T \rightarrow +\infty\). Reaching solutions beyond the global maximum implies considering \(\beta = 1/T < 0\), which is not a realistic situation. Thus non monotonously increasing functions \(S = S(U)\) do not affect the general framework because they are situations that we are not concerned with in thermodynamic equilibrium. For MOO-SOO systems others than thermodynamics we do not rely on microcanonical ensembles, but on the Pareto front straightaway, in which non-dominated regions (i.e. non monotonic surfaces with respect to some of the target functions) never show up.

Our work follows closely the ideas of Gibbs [37, 38] that were immediately featured by Maxwell [39], but that otherwise did not become mainstream in the study of statistical mechanics. Gibbs’ graphic method relied on the existence of a surface upon which dwell all possible states of a thermodynamic species in equilibrium. This surface is defined by the Gibbs potential:

\[
G(p, T) = U + pV - TS,
\]

which plays now the role of equation 6 both in thermodynamics and in our theoretical framework. We identify the target functions \(U, S, \) and \(V\); and the control parameters \(T\) and \(p\). We discuss \(p\) and \(V\) below.

In the original account this surface is associated to a given thermodynamic species and it is shown that its convex hull is reached at thermodynamic equilibrium through the optimization of equation (A1) which is a free energy minimization. Then, the tangent plane to this surface at a given state – i.e. at a given point of the surface – is defined by a normal vector whose components are precisely related to the pressure and temperature of that equilibrium state [39].

This ingenious picture received renewed attention recently as it is investigated along the concept of ensemble inequivalence and used to explain more thermodynamic features [40, 41]. The Gibbs surface is fabricated thanks to the microcanonical ensemble and it can be convex or concave, while a thermodynamic canonical ensemble can only be convex. Whenever \(G\) becomes concave both ensembles must diverge geometrically in the \(U - V - S\) space. This makes the canonical ensemble non-analytic at the inequivalence points which is reflected as a first order phase transition in the corresponding physical system. Another source of non-analyticity happens whenever the microcanonical ensemble renders a convex, non-derivable Gibbs surface as seen in the body of the paper.

Collapsing of MOO into SOOs (as in equation 2) is a remarkable step. One of the initial motivations of MOO is that the target functions might be incommensurable: they might have different dimensions and represent such disparate features that an objective pondering of both quantities together does not make sense. That is why solving MOO through equation 2 might connote highly subjective decisions. Weighting targets with different dimensionality into a same fitness function means translating all targets into similar units such that their preponderance in the optimization can be directly assessed. The processes by which this is done might be different for each MOO-SOO problem, but they are of undeniable value.

In the case of thermodynamic systems, we know how \(TS \equiv S/\beta\) is related to a quantity of heat: i.e. entropy is potentially energy once a temperature is given. This allows the internal energy and the entropy to be mutually commensurable by means of the temperature. The minimization of the free energy in equation (A1) thus, follows by the understanding that any existing free energy must be utilized – thus its amount in a system reduced. This energy can be used to reach through unstable thermodynamic states up to the optima of a system [39]. This deems the MOO-SOO collapse a feature of the canonical ensemble alone. It also explains why some non-analyticities of the microcanonical ensemble are not visible [42].

We have already interpreted \(U, S\) and \(T\) from an MOO perspective. We also commented that \(p\) plays the role of one of the \(\lambda_k\) in the MOO-SOO framework and in Gibbs’ graphical method. Accordingly, the volume plays the role of a target for optimization. In equation (A1) \(V\) appears with the same sign as \(U\) so it must be minimized. The linking
of volume to the free energy by the pressure tells us exactly how a volume is turned into available or required energy (work) at that given pressure – i.e. how it is made commensurable with the energy and the heat.

An intuitive way to see that volume is being minimized is that as we increase pressure – i.e. as we augment the preponderance of volume in the single objective optimization of the Gibbs potential – states with each time lower volumes are achieved: we proceed to further minimums in volume. This is so if we make a rigorous interpretation from the mathematical perspective of the MOO-SOO problem. But pressure and volume are so intuitively associated to our physical experience of the world that it may become cumbersome to conceive pressure as weighting the importance of volume within an optimization framework. We can also look at expression \( A_1 \) from an alternative perspective if the volume (instead of the pressure) is manipulated externally and considered as a control parameter akin to some \( \lambda_k \): then the pressure becomes a target function for the MOO, and once again we seek its minimum. This is a more intuitive interpretation: as we increase the volume – i.e. the importance of pressure towards the SOO – a thermodynamic system gets redistributed as to decrease its averaged internal forces. When we reduce the volume of a system, its parts again fall into place as to minimize the mutual forces they exert on each other – i.e. as to minimize pressure. The MOO-SOO system, once again, accounts for relevant features of the physical system under research.

**Appendix B: Careful resolution of the Ising and the Potts model from a MOO perspective**

As noted in the main text, the Ising and the Potts models and more general versions of them have been solved using the concept of ensemble inequivalence \([43, 44]\), which is comprehensively explained by the Pareto optimality approach introduced here. We illustrate thermodynamic phase transitions with the Pareto front through these models because of their historical importance and because they allow a complete analytical treatment. The details of the calculations follow.

### 1. The mean-field Ising model – a second order phase transition

We use a standard mean-field Hamiltonian for the Ising model

\[ H = - \frac{J}{2} \sum_{(j,k)} s_j s_k \]

with \( J \) the coupling constant and the sum running over \( z \) neighboring spins. We parameterize the system with the probability \( p \) that we find the mean-field spin in the up state. It becomes easy to write down the entropy and the internal energy of the system in terms of \( p \):

\[
S = -p \cdot \log(p) - (1 - p) \cdot \log(1 - p),
\]

\[
U = -\frac{Jz}{2} (2p - 1)^2.
\]

(S1)

Solving this last expression for \( p \), we can also write the entropy as a function of the internal energy alone:

\[
\bar{S}(U) = -\frac{1}{2} \{1 + f(U)\} \log \left(\frac{1 + f(U)}{1 - f(U)}\right) - \log \left(\frac{1 - f(U)}{2}\right),
\]

(B2)

with:

\[
f(U) \equiv +\sqrt{-\frac{2U}{Jz}}.
\]

(B3)

Equation \( B_2 \) (represented in figure 5a) gives us \( S \) as a function of \( U \) \((S = \bar{S}(U))\) for all possible states that the model can be found into, disregard of whether or not these states correspond to thermodynamic equilibrium situations or to microcanonical ensembles. Because for this model equation \( B_2 \) is a function, for each \( U \) \( \bar{S}(U) \) is also maximal – i.e. every state of the system corresponds to a microcanonical ensemble itself. This is valid for this lucky model, but not necessarily true in a general case.

This curve also constitutes the Pareto front of the corresponding MOO problem (minimizing \( U \) and maximizing \( S \) from equations [3]), as is expected given the correspondence between the microcanonical ensembles and Pareto optimal solutions. Let us analyze the Pareto optimality of equation \( B_2 \). First we note that \( \bar{S}(U) \) is only real and well defined for \( U \in [-Jz/2, 0] \), the range of available energies for the model. In this range:

\[
\frac{d\bar{S}}{dU} = -\frac{1}{2} f'(U) \log \left\{ \frac{1 + f(U)}{1 - f(U)} \right\} > 0,
\]

(B4)
\[ \beta \text{Ising model undergoes at precisely illustrated in figure 2, and is associated to second order phase transitions as the one that we know that the mean-field } (J \text{ with } \beta) \text{Pareto front continuously. The transition between a persistent solution for } \beta \text{ where their tangent matches the slope of the corresponding } \tau \text{ thus } \bar{S}(U) \text{transitions for any } \beta \text{Going back to the well behaved range of } \beta \text{ decrease at the upper right end of the front which corresponds to the state with more entropy and energy. If we further assume that any other state is equally likely } p \text{we have too many degrees of freedom. In figure 5 we represent a sample of valid points for } \beta \text{S}(U) \text{is monotonously increasing, which guarantees that its points in the } U - S \text{ plane do not dominate each other regarding energy minimization and entropy maximization. Because this curve comprises everything that is possible in the system under research and because its constituting points are mutually non-dominated, it must be the Pareto front itself. Besides, } \frac{d \bar{S}}{dU} \text{ is positive and monotonously decreasing for } U \in (-Jz/2, 0); \text{ thus there are not concavities in the Pareto front: we rule out first order phase transitions. We can also rule out second order phase transitions in the interior of } U \in (-Jz/2, 0) \text{ because the derivative is well defined everywhere. Second order phase transitions are thus restricted to } U = -Jz/2 \text{ or } U = 0. \text{ We inspect } \frac{d \bar{S}}{dU} \text{ as } U \text{ tends to these points. After some algebra we arrive to:}
\]

\[ \lim_{U \to 0} \frac{d \bar{S}}{dU} = \frac{1}{Jz}, \quad (B5) \]

and:

\[ \lim_{U \to (-Jz/2)^+} \frac{d \bar{S}}{dU} = +\infty. \quad (B6) \]

As we saw in section II.B for the SOO posed at temperature \( T = 1/\beta \) we typically reach points of the Pareto front where their tangent matches the slope of the corresponding \( \tau_\beta(F) \) (equation 3). The derivative \( \frac{d \bar{S}}{dU} \) as we approach \( U = -Jz/2 \) is infinite, meaning that we will reach this end of the Pareto front only at \( \beta \to \infty \) (zero temperature). There is not any remarkable behavior here. At the other end of the Pareto front the derivative is not 0, but a finite positive number. This means that already for \( \beta = \frac{1}{Jz} \) the free energy optimum – i.e. the SOO solution – is located at the upper right end of the front which corresponds to the state with more entropy and energy. If we further decrease \( \beta \) we will not be reaching any novel solutions: the SOO optima remain the most entropic state of the system. Going back to the well behaved range of \( \beta \), as we increase it above \( \frac{1}{Jz} \) the SOO solutions begin to roll over the Pareto front continuously. The transition between a persistent solution for \( \beta \in [0, 1/Jz] \) and a varying solution in the regime \( \beta \in [1/Jz, \infty) \) implies a discontinuity in the derivative of any order parameter. This is analogous to the cases illustrated in figure 2 and is associated to second order phase transitions as the one that we know that the mean-field Ising model undergoes at precisely \( \beta = \beta^* \equiv \frac{1}{Jz} \).

2. The mean-field Potts model – a first order phase transition.

We repeat the same operations with the Bragg-Williams approximation to the Potts model. This has been solved somewhere else [45] using other methods. This choice of implementing the mean-field presents first order phase transitions for any \( q \geq 3 \), where \( q \) is the number of available states for each spin. For a discussion of the Bragg-Williams against other mean-field approaches to the Potts model see [46].

Following [45], we write down the entropy and energy of the system:

\[ S = - \sum_{j=1}^{q} p_j \log(p_j), \]

\[ U = -\frac{J}{2} \sum_{j=1}^{q} p_j^2; \quad (B7) \]

with \( J \) and \( z \) still the coupling and the number of neighbors. Now \( U \) and \( S \) are parameterized by the probabilities \( p_j \) \((j = 1,\ldots,q)\) of finding a spin in each of the \( q \geq 3 \) states. The normalization \( \sum_j p_j = 1 \) means that there are \( q - 1 \) parameters and we cannot write \( S = \bar{S}(U) \) as before unless we make some assumption. Let us prefer one arbitrary state (say \( j = 1 \)) over the others. Let us call \( p \) to the probability of finding a spin in that preferred state, and let us further assume that any other state is equally likely \( p_{j'} = (1 - p)/(q - 1) \), now with \( j' = 2,\ldots,q \). This is analytically justified in the literature [45] and later by our arguments about Pareto dominance. We note that, unlike for the Ising model, states compatible with the premises of the system will not usually be constrained to a curve because we have too many degrees of freedom. In figure 3b we represent a sample of valid points for \( q = 3 \): all of them can happen ideally, but a few of them Pareto dominate some others thus not all of these configurations will be reached in thermodynamic equilibrium.
Thanks to the previous symmetry breaking to favor one state over the others we can write down the following curve:

\[
\bar{S}(U) = -\frac{1 + f_q(U)}{q} \log \left( \frac{(q-1)(1 + f_q(U))}{q - 1 - f_q(U)} \right) \\
-\log \left( \frac{q - 1 - f_q(U)}{q(q - 1)} \right).
\] (B8)

This is the counterpart of equation [B2] only now:

\[
f_q(U) \equiv \sqrt{(1 - q) \left[ 1 + 2qUzJ \right]},
\] (B9)

represented in figure 5b for \( q = 3 \). We can appreciate that it is monotonously growing as a function of \( U \): its point are mutually non-dominated and constitute the Pareto front. The fact that there is not any point in the previous sample that Pareto dominates any point in this curve indicates that our symmetry breaking hypothesis – favoring one spin state over the others – is correct. It can be analytically proved, indeed [45]. We can hardly appreciate that a concavity exists in the upper right part of the Pareto front. This becomes more obvious when analyzing \( \frac{d\bar{S}}{dU} \) (figure 5c), which is not monotonously decreasing.

Most of the Pareto front is continually visited: as we vary \( \beta \), the SOO solutions roll over its convex lower-left part. It can be shown once more that the less energetic end is reached only for \( \beta \to +\infty \) and \( T = 0 \), so that there is not any remarkable feature in that temperature range. Once again, it exists a value \( \beta_c \) below which the solution is persistently the most entropic one. At exactly \( \beta = \beta_c \) that solution coexists with another one in the convex part of \( \bar{S}(U) \).

To locate \( \beta_c \) we plot \( \frac{d\bar{S}}{dU} \) and we compare it to the slope \( \frac{\Delta S}{\Delta U} \) of the straight line that connects the upper-right with other points of the Pareto front (figure 5c, inset). Where both functions intersect we have identified the line of phase coexistence. Its slope is precisely \( \beta_c \). We collect \( \beta \) for Potts models with different parameter values \( q \) in figure 8b. These results match those known from the literature [45].

![Figure 8](image)

**FIG. 8:** Pareto front for the mean-field Potts with different \( q \). a For \( q = 3 \) (red), \( q = 5 \) (green), \( q = 8 \) (black), and \( q = 10 \) (blue); although hardly noticeable, all these fronts have got concave stretches towards their upper-right ends. This indicates that all of them undergo first order phase transitions from the most disordered state to a more ordered phase where symmetry has been broken to favor just one of the states. A Pareto front for \( q \) dominates the Pareto front for every \( q' < q \) indicating that this system will never leave empty one of its available states spontaneously, except in the most ordered state. b Inverse temperature at which the mean-field Potts model presents its first order phase transition for \( q = 3, \ldots, 10 \). The results match perfectly those from the literature [45].

Because the two coexisting solutions are far away in the Pareto front, at \( \beta = \beta_c \) the systems undergoes a drastic change – as opposed to the continuous transition from the Ising model. This is coherent with the first order phase transition situation illustrated in figure 3. This is the kind of phase transition that we know that our model presents.
In figure 8 we represent the Pareto front for many values of $q$. We observe that solutions for $q$ dominate solutions for any $q' < q$, leading to the interesting and trivial observation that an instance with higher $q$ does not spontaneously decay towards one with less available states by setting some $p_{j'} = 0$. This is well known for the Potts model, but such an interesting scenario should not be discarded in general for a different problem, and the Pareto front could provide a formalism to detect such a possibility.