Quantifying Knowledge Evolution with Thermodynamics: A Data-Driven Study of Scientific Concepts

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Abstract

In this work, we propose a thermodynamic framework to analyze the creative potential of scientific fields by examining over 11,000 scientific concepts across 500,000 publications from ArXiv (2002-2018). Our approach demonstrates that scientific concepts' term frequencies ($\boldsymbol{tf}$) follow a generalized Boltzmann distribution, enabling a rigorous thermodynamic description. We compute key thermodynamic properties of scientific concepts, treating them as closed thermodynamic systems. The observed most probable temperature, $\boldsymbol{T \simeq 3/2}$, corresponds to the maximum concept heat capacity, indicating a phase transition from non-equilibrium states with a linear energy spectrum to stable stationary states characterized by logarithmic energy spectra and power-law distributions of $\boldsymbol{tf}$. Concepts typically reach these stable states after being referenced in over 1,000 documents. The thermodynamic state space of scientific concepts is analyzed using data-driven diagrams, revealing correlations between energy, temperature, entropy, free energy, and residual entropy, which govern information transfer between concepts.

Keywords: Scientific Knowledge Dynamics, Knowledge Production, Statistical Mechanics of Knowledge, Thermodynamics of Information, Data-Driven Thermodynamic Models

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Nomenclature

tf Term frequency, the number of times $k \in \mathbb{Z}^+$ a specific concept appears in a document.
$N_c(t)$ Number of documents that contain a concept c up to time t.
$N_c(k,t)$ Number of documents that contain a concept c exactly k times up to time t.
$P_c(k,t)$ Probability of a concept being cited k times up to time t.
β Lagrangian multiplier associated with the inverse temperature ($\beta = \frac{1}{k_B T}$).
λ Lagrangian multiplier associated with the linear contribution to the system's energy.
$P_c(\{k\},t)$ Probability mass function of a mesostate at time t.
$\Pi_c(k,t;\beta,\lambda)$ Probability mass function of a macrostate at time t.
S_{micro} Microstate entropy per document, representing maximum uncertainty in the system and equals $\ln N_c(t)$.
S_{meso} Mesostate entropy per document, based on the $P_c(k,t)$ probabilities of concept frequencies.
S_{macro} Macrostate entropy per document, related to the thermodynamic entropy of the system.
S_{therm} Thermodynamic entropy, defined as $S_{\text{therm}} = k_B S_{\text{macro}}$.
R Residual entropy, the difference between macrostate and mesostate entropies ($S_{\text{macro}} - S_{\text{meso}}$).
A Helmholtz free energy per document of a concept, the usable energy in a closed thermodynamic system.
T Temperature of the concept.
k_B Boltzmann constant, we use $k_B = 1$ for numerical calculations.
Z Partition function, used in defining the probability mass function of a concept's macrostate.
$\langle k \rangle$ Expected value the first moment of $P_c(\{k\},t)$.
$\langle \ln k \rangle$ Expected value of the log-moment of $P_c(\{k\},t)$.
E Concept internal energy per document, defined as $\langle \ln k \rangle + \lambda \langle k \rangle / \beta$.
Q Entropy efficiency, the ratio of macrostate entropy to internal energy ($Q = S_{\text{macro}}/E$).
ΔR Change in residual entropy over time interval Δt.
C Heat capacity, the rate of change of internal energy with respect to temperature ($C = \partial E/\partial T$).
TR Residual energy, representing the energy tied up in the system's entropy.
η_{inf} Information flow efficiency, defined as ($\Delta R/\Delta S_{\text{meso}}$).

1 Introduction

The concept of discovery and scientific progress is closely tied to the exchange of ideas through collaboration and the application of models across disciplines. Numerous studies have explored these connections, emphasizing that while future discoveries are unpredictable, analyzing the historical trajectory of scientific fields provides essential insights [1–3]. These insights form the basis of a structured approach to understanding the process of discovery.

Central to this process is bridging logical gaps between scientific concepts and facilitating the diffusion of information [4–8]. However, investigating the emergence of scientific innovation remains a complex challenge. Previous studies have examined this from diverse perspectives, including philosophy, sociology, history of science, and quantitative methods such as citation analysis and network science [9–11]. The availability of vast metadata from electronically published scientific literature enables large-scale, data-driven analyses of the structure and dynamics of scientific innovation.

A promising direction for advancing our understanding of knowledge production lies in the study of concept-based knowledge networks encoded in scientific communication [12–14]. These networks are defined by scientific concepts, represented as key phrases that capture the ontology of a field. As scientific progress continues, the meanings of these concepts evolve, and new concepts emerge, reflecting the current state of knowledge.

While many existing studies have focused on detecting keyword communities within scholarly publications—using techniques from keyword co-occurrence to advanced word embedding models—these approaches often fail to capture the dynamic evolution of knowledge [15–17]. Additionally, the study of static complex networks usually involves computationally intensive calculations, especially for large networks. One approach, proposed by Martini et al. [13], uses Shannon residual entropy to select concepts with specific properties, reducing computational complexity and revealing hidden topics.

Building on this work, we propose a novel approach to analyze scientific concepts as interacting thermodynamic systems. By applying methods from statistical physics and thermodynamics, we study the transfer of information and the production of knowledge. This approach not only uncovers static relationships between concepts but also provides insights into their temporal evolution, offering a deeper perspective on how scientific knowledge develops over time.

The key connection between thermodynamics and information science lies in the recognition that entropy is not an intrinsic property but depends on the variables used to describe a system. Under certain conditions, the entropy of a scientific concept follows a generalized Boltzmann distribution, allowing for a thermodynamic description [18, 19]. The distribution of concept term frequencies extracted from scientific documents conforms to a power-law-modified exponential distribution [13]. This enables us to interpret the generalized energy of a system, which corresponds to the effort required to organize a set of microstates describing a scientific concept. Martini initially derived the model for the probability mass function using Jaynes' 'MaxEnt' method [13], and we extend this to explore the relationship between entropy maximization and concept energy [20].

In this research, we extend these thermodynamic principles to examine scientific concepts as evolving systems. The size of a concept as an information system can be understood through the number of active information connections with other concepts in a network. This behavior mirrors the complexity of neural networks, where the system's behavior changes as the number of connections increases [21–24].

The connection between information and energy provides a framework for understanding the dynamics of knowledge production and dissemination in scientific communities. This perspective, grounded in thermodynamic reasoning, allows us to investigate phase transitions where concepts shift in significance and to uncover emergent properties that reflect the evolution of scientific ideas over time [25, 26].

The aims of this research are: (i) to calculate the internal energy, Helmholtz free energy, temperature, and heat capacity of scientific concepts as closed thermodynamic systems [13]; (ii) to use a data-driven approach based on term frequencies of over 12,000 concepts across 500,000 scientific papers from ArXiv (2002-2018) to map the state space of the concept knowledge network; and (iii) to examine the dynamics of this state space, focusing on densely populated regions representing the most probable values of thermodynamic parameters.

The paper is organized as follows. Section 2 elaborates on the states that describe concepts as information systems, introducing definitions of information and thermodynamic entropy. Section 3 discusses the connection between Helmholtz free energy, thermodynamic work, residual entropy, and knowledge production. Section 4 presents thermodynamic diagrams of the knowledge network state maps. Finally, Section 5 concludes with insights and future directions.

2 Information and thermodynamic entropy

The correspondence between thermodynamic entropy and its information analog, introduced by Shannon, has sparked numerous debates and misconceptions within the scientific community [18, 27, 28]. Thermodynamic entropy, a concept deeply rooted in classical physics, describes the measure of disorder or randomness within a physical system. In contrast, Shannon entropy, originating from information theory, quantifies the uncertainty or unpredictability inherent in a set of data or information [29]. The potential solution to understanding how these concepts are related lies in recognizing that entropy should not be viewed as an inherent property of the system itself but rather as a characteristic of how we describe it [30, 31]. As Caticha stated it [32], "*entropy is fundamentally tied to our method of observation and description rather than being an intrinsic property of the system under study.*" More explicitly, entropy is a function of the macroscopic variables chosen to define the macrostate. For instance, different macrostates, based on varying choices of variables, will correspond to different entropy values for the same system. However, entropy is not solely dependent on the macrostate. As demonstrated below, entropy reflects an information difference between various descriptions of the same system. Besides the macrostate, we can also consider the set of microstates and mesostates. The differences in entropy among these states indicate the amount of additional information required to identify the other states.

Having a concept c, we will define the set of its microstates associated with probability $1/N_c(t)$ for a concept to be found in the document published until date t, where $N_c(t)$ is the number of documents that contain concept c. Uniform probability distribution of the concept microstates and corresponding maximal value of the entropy per document $S_{\text{micro}} = \ln N_c(t)$ corresponds to the absolute minimum information we have about the system in this representation [33, 34].

The more detailed text analysis of the documents enables the collection of additional information about concept occurrences, or concept frequencies denoted as tf. Grouping documents based on extracted frequency values $tf = k, k \in \mathbb{Z}^+$ associates the probabilities for a concept to be cited precisely k times with a set of *mesostates*. The probability of a particular frequency is given by the ratio $P_c(k,t) = N_c(k,t)/N_c(t)$, where $N_c(k,t)$ is the number of documents that mention a concept k times up to time t. The corresponding Shannon entropy per document is then given by [1].

$$S_{\mathrm{meso}}(t) = -\sum_{k=1}^{\max(tf_c)} P_c(k,t) \ln P_c(k,t). \quad (1)$$

The lower value of the mesostate entropy $S_{\mathrm{meso}} < S_{\mathrm{micro}}$ reflects the presence of additional information about the concept in this state, thereby reducing its uncertainty. The natural question arises: what is the minimum value of k that should be used to define the corresponding entropy? Martini addressed this question in [13] and concluded that entropy defined with $k > 0$ provides greater descriptive power for topic classification in the concepts network. The choice $k_{\min} = 1$ in our case is motivated by the proposed thermodynamic framework, where it sets the minimum energy level $\ln 1 = 0$ for the logarithmic bath of a concept as a thermodynamic system.

The Jaynes MaxEnt principle [31] allows us to define a normalized macrostate probability mass function $\Pi_c(\{k\},t)$ of a concept as the one that maximizes the S_{meso} entropy. Applied constraints in the form the first moment $\langle k \rangle$ and log-moment $\langle \ln k \rangle$ of $P_c(\{k\},t)$ gives [35]:

$$\Pi_c(k,t;\beta,\lambda) = \frac{1}{Z}\frac{e^{-\lambda k}}{k^{\beta}}, \quad Z = \sum_{k=1}^{\infty} \frac{e^{-\lambda k}}{k^{\beta}} = Li_{\beta}(e^{-\lambda}) \quad (2)$$

where Z is polylogarithm Li of order β and argument $e^{-\lambda}$ for the Lagrangian multipliers $\lambda > 0$ and β [13]. Corresponding macrostate entropy is then given by

$$S_{\mathrm{macro}} = \ln Z + \beta \left(\langle \ln k \rangle + \frac{\lambda}{\beta} \langle k \rangle\right) \quad (3)$$

with

$$\langle k \rangle = \frac{Li_{\beta-1}(e^{-\lambda})}{Li_{\beta}(e^{-\lambda})}, \quad \langle \ln k \rangle = -\frac{\partial_{\beta} Li_{\beta}(e^{-\lambda})}{Li_{\beta}(e^{-\lambda})}. \quad (4)$$

Similar results were obtained in [36] where it was shown that power-law and exponential distributions independently maximize the ratio $Q = S_{\mathrm{macro}}/E$ with the exponents β or λ approximated to it [37, 38].

Following the formalism developed in [18], the Eq.(2) can be understood as a generalized Boltzmann distribution of a concept as a system of logical particles, each

[1] The units of entropy in this study are denoted as *nats*, corresponding to base 'e' (Euler's number) logarithms, which are used throughout. While it is more common in the literature to use the base-2 logarithm, in that case, the units of entropy are expressed in *bits*, aligning with the binary digit terminology commonly associated with information theory.

representing a scientific document. The entropy of the macrostate S_{macro} is then related to thermodynamic entropy S_{therm} as:

$$S_{\text{therm}} = k_B S_{\text{macro}} = k_B(\beta E + \ln Z), \tag{5}$$

where k_B is a Boltzmann constant and is set to be one to simplify matters, so β corresponds to inverse temperature $1/T$ and E is the average internal energy per document:

$$E = \langle \ln k \rangle + \frac{\lambda}{\beta} \langle k \rangle. \tag{6}$$

In physics, the concept of internal energy (E) defines heat, and when a hypothetical reference frame is attached to a concept, there is no distinction between the total energy and the internal energy of the system. Consequently, the second term $\beta^{-1} \ln Z$ in Eq.(5), which is typically associated with the motion of a system's boundaries (such as changes in volume), is exclusively linked to work. However, since concepts, as informational entities, lack traditional spatial boundaries, calculating work based on changes in volume becomes nontrivial.

To circumvent this complexity, we estimate the average work from changes in the system's free energy. This approach allows us to effectively account for all informational interactions between concepts. In the following section, we will employ Helmholtz free energy and Jarzynski's equality [39, 40] to quantify thermodynamic work and relate it to the system's entropy and information production.

3 Residual entropy and free energy

As evident from the previous section, a scientific concept at moment t can be represented as a closed thermodynamic system, with its energy defined by Eq.(6). In our framework, a scientific concept reaches a state of equilibrium when the Shannon entropy S_{meso} equals the thermodynamic entropy S_{therm}, as defined by Eq.5. In this equilibrium state, the concept's informational structure has stabilized, meaning that its interactions within the broader knowledge network no longer produce significant changes in entropy or new informational contributions. Such concepts, termed 'basic' or 'generic' in [13], are often considered irrelevant for fine-grained topic detection within concept networks. These concepts typically appear in almost every document in a given collection, representing broad, overarching topics that, in some cases, can be identified with entire scientific fields.

For concepts that do not reach this equilibrium state, we observe the inequality $S_{\text{macro}} > S_{\text{meso}}$, indicating that these concepts are still in non-equilibrium. In this non-equilibrium state, these concepts are actively undergoing changes, suggesting that they are still contributing to the dynamic evolution of scientific knowledge. Such concepts may represent emerging or highly specialized topics that have not yet stabilized into a steady state, making them more relevant for fine-grained topic detection and deeper analysis of knowledge production.

The amount of additional information required to specify the mesostate concerning a macrostate can be quantified via residual entropy $R = S_{\text{macro}} - S_{\text{meso}}$ that can be expressed as the Kullback-Leibler divergence (see proof in [13]) between mesostate and macrostate as a state of instantaneous thermodynamic equilibrium:

$$R(t) = D_{KL}(P_c||\Pi_c) = \sum_k P_c(k,t) \ln \frac{P_c(k,t)}{\Pi(k,t)} \geq 0. \tag{7}$$

The net change in residual entropy, $\Delta R = R_f - R_i$, when the system transitions from an initial state i to a final state f, quantifies the entropy production within the system [41, 42]. This residual entropy is given by the difference $\Delta R = \Delta S_{\text{macro}} - \Delta S_{\text{meso}}$. While ΔR is typically negative and decreases as the system approaches its Gibbs state representation, both S_{macro} and S_{meso} may either decrease or increase simultaneously during this process, depending on the relative magnitudes of ΔS_{macro} and ΔS_{meso}. Specifically, when $\Delta S_{\text{macro}} > \Delta S_{\text{meso}}$, both entropies tend to decrease, and when $\Delta S_{\text{macro}} < \Delta S_{\text{meso}}$, both entropies tend to increase. Alternatively, the system may display asynchronous dynamics, where $\Delta S_{\text{macro}} < 0$ and $\Delta S_{\text{meso}} > 0$. According to the second law of thermodynamics, the residual entropy must continue to decrease, ensuring that any process within the system drives it toward equilibrium, thereby guaranteeing the irreversibility of natural non-equilibrium processes.

We know from physics that the entropy of a system may decrease when work is performed on it. In our case, this can result in R increasing during specific periods of time. However, the total entropy of the combined isolated system (the system plus its surroundings) must remain constant or increase, as required by the second law of thermodynamics. Drawing an analogy to a thermodynamic system in equilibrium, an increase in residual entropy R becomes particularly intriguing, as it reflects the "useful work" required to move the system away from equilibrium. In the context of an information system, this "work" corresponds to the additional *useful information* R transmitted into the system, which alters its mesostate. Thus, under certain conditions, we can expect R to increase, particularly when external influences introduce new information that shifts the system out of its current equilibrium.

In thermodynamics, the amount of energy that can be converted to work and is not tied up in the entropy of the system is given by Helmholtz free energy:

$$A = E - k_B T S_{\text{macro}} = -k_B T \ln Z. \tag{8}$$

The change in Helmholtz free energy ΔA tells us about the maximum obtainable work from a process when the system passes from some initial i to the final f state. Helmholtz's free energy change ΔA reaches its minimum value at equilibrium, and no work is made by the system if $\Delta A \to 0$ and $\Delta R \to 0$. Non-equilibrium systems can do work, and the change in Helmholtz free energy (ΔA) reflects the maximum theoretical work obtainable under constant temperature and systems volume V. This ΔA value can be positive or negative depending on whether the system does work on the surroundings ($\Delta A > 0$) or the surroundings do work on the system ($\Delta A < 0$).

The relation of useful information R to Helmholtz free energy is then followed from Eq.(8):

$$R = \frac{E - A}{k_B T} - S_{\text{meso}} \quad (T, V = const). \tag{9}$$

The useful expression to quantify work that is valid for the systems in- and far-from-equilibrium regime is given by the recently discovered Jarzynski equality [39] representing the relationship between the difference in free energy ΔA of two equilibrium ensembles and the amount of work W needed to switch between them in a finite amount of time:

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta A}. \tag{10}$$

Here, $\langle ... \rangle$ indicates an average over multiple process repetitions when experiments are conducted on physical systems.

Noting that Helmholtz free energy is a function of state from Eq.(10), we can measure the work needed to drive the system between i and f states separated by the time interval Δt as proportional to ΔA. In the case of the isothermal process, the analytical expression for the free energy change is simple and given by:

$$\Delta A = A_f - A_i = \Delta E - T(\Delta R + \Delta S_{\text{meso}}) = \Delta E - T \Delta S_{\text{macro}}. \tag{11}$$

In this case, we can also write a simple analytical expression for the efficiency of information flow η_{inf} represented by the dimensionless ratio of information transfer ΔR over total irreversible entropy production ΔS_{meso} [43]. Using Eq.(11) we get:

$$\eta_{inf} = \frac{\Delta R}{\Delta S_{\text{meso}}} = \frac{1}{k_B T} \frac{\Delta E - \Delta A}{\Delta S_{\text{meso}}} - 1 = \frac{\Delta S_{\text{macro}}}{\Delta S_{\text{meso}}} - 1. \tag{12}$$

We can see that for the reversible near equilibrium processes $\Delta S_{\text{macro}} \approx \Delta S_{\text{meso}}$, $\Delta S_{\text{macro}} / \Delta E = 1/T$ and $\Delta A = 0$ the efficiency of information flow is minimal $\eta_{\text{inf}} = 0$ unlike thermodynamic efficiency which is maximized in equilibrium [43].

As we will show below, concepts that are used in a sufficiently large number of documents all reach equilibrium at specific temperatures and, consequently, all have low values of η_{inf}. In contrast, new concepts have larger values of information flow efficiency as their residual and S_{meso} entropy vary significantly during their state evolution.

This thermodynamic analogy reveals a deep connection between the effective use of information by an information system and its thermodynamic efficiency. As the system evolves, it performs computations by changing its state in response to external inputs—in our case, the changing term frequencies (tf) of concepts across new documents. The system retains information about past fluctuations in its environment, and some of this information helps predict future changes [44]. However, as a concept approaches thermodynamic (or "infodynamic") equilibrium, the efficiency of information flow, η_{inf}, decreases, indicating that the concept no longer generates significant new information. Instead, equilibrium concepts tend to act as recipients of the work performed by other, more dynamic concepts within the network. Concepts with higher information flow efficiency, typically those further from equilibrium, are responsible for reshaping the concept network by performing informational "work" that drives changes and influences the relationships between concepts. In contrast, equilibrium concepts stabilize the network and integrate these changes, preserving the knowledge they accumulate over time. In the following section, we will illustrate these dynamics using thermodynamic diagrams, providing examples that demonstrate how concepts with varying levels of information flow efficiency influence the overall structure of the concept network.

4 Thermodynamic diagrams

In this section, we will calculate the macrostate parameters β and λ from Eq.(2) based on historical data about concepts tf and analyze the concept's state space using thermodynamic diagrams. For each of 13945 concepts recorded in our database, we estimate these parameters by numerically fitting the empirical mesostate distribution formed for specific time intervals using *maximum likelihood* estimation method. We cross-check the results by requiring that for obtained β and λ, the Eq.(4) must hold with a tolerance of $< 10^{-5}$ when $\langle \ln k \rangle$ and $\langle k \rangle$ are obtained directly from empirical data.

Figure 1 presents a heat map illustrating the distribution of concepts across different values of the state parameters β and λ. We can see that the largest number of concepts have λ in the interval from 0 to 0.15 and β from 1 to 2. The maximum concept density in macrostate parameters space shifts from $\beta = 2$ when $\lambda = 0$ to $\beta = 1.6$ when $\lambda = 0.15$. Similar results were previously obtained in [13] where the mean value for the inverse temperature distribution was reported to be $\overline{\beta} \sim 3/2$. This value remains almost constant for the studied period with $\overline{\beta} = 1.51$ until the end of 2010 to $\overline{\beta} = 1.61$ in 2018.

The difference between states with different β and λ is better understood in terms of probabilities of *information channels* $K = \{k\}$ that form the mesostate distribution. The number of microstates (documents) that contribute to a particular channel k quantifies the history of a system along the specific microscopic phase-space path. The probability for the system to follow this path is then given by $P_c(k, t)$, which changes over time as the system receives new information about new relevant microstates. For the concepts with a large number of microstates, we have an almost sequential filling of information channels starting from $k = 1$, which has the largest probability $P_c(k = 1, t)$ and which is decreasing for $k > 1$ mostly in a power law manner with non-zero probabilities for $k >> 1$.

Our analysis shows that the larger the values of β, the narrower will be the channel band with small k indexes and consequently lower entropy S_{meso}, S_{macro}, energy E, and temperature. For most concepts, λ, in this case, is small, and consequently, the linear contribution to E in Eq.(6) compared to the logarithmic term. From Fig.1, we can see that the number of concepts with the pure logarithmic spectrum, i.e., when $\lambda \to 0$ is increasing towards $\beta = 2$ and then decreasing when $\beta > 2$. The role of a linear term in E becomes more important as the temperature of a system increases. Our results show that the number of concepts with combined spectrum rises towards $\lambda = 0.1$ until $\beta \to 1$. For higher temperatures, the linear spectrum becomes dominant.

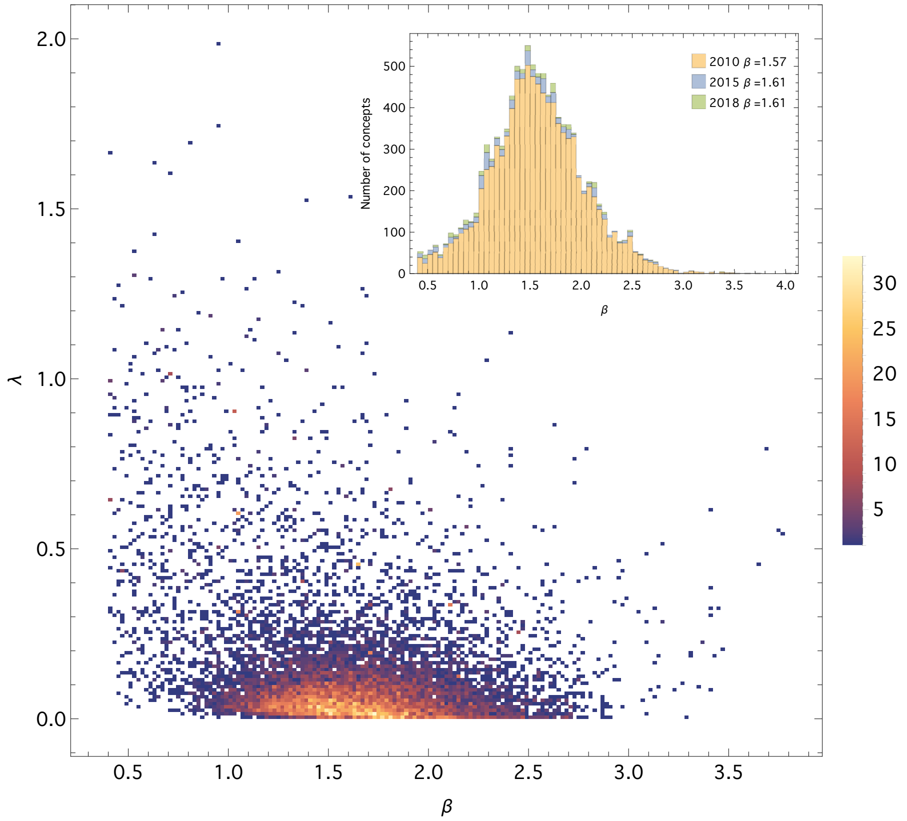

Fig. 1 A heat map illustrating the distribution of macrostate parameters for 11737 scientific concepts. The sub-figure demonstrates the distribution of inverse temperature β (where $\beta > 0.001$) and the evolution of the distribution over three time periods, beginning in 2002 and concluding in 2010, 2015, and 2018. The mean value of β, which is specified, is calculated at the end of each period.

Our results complement and extend previous research in social collaborations [36] where it was shown that for the pure power-law distributions if $\beta > 2$, the main contribution in E is made by the low energy (low k) information channels. If $\beta < 2$, more contribution is obtained from high energy (high k) channels, and when $\beta = 2$, all channels contribute evenly. Those conclusions were made assuming an infinite number of information channels k, but their number in real-world datasets is not infinite. Exponential cut-off in the macrostate probability mass function $\Pi_c(k,t)$ accounts for this fact by setting it to zero for some $k > k_{max}$. The smaller β, the larger λ is required to keep $\langle k \rangle$ from becoming infinite. When λ is large and β is small, the entropy of the concept is influenced by both the logarithmic and linear contributions, leading to a complex interplay of information channels with varying probabilities.

In each studied period, there exists a group of new concepts whose states are so far from equilibrium that their macrostate parameters cannot be accurately estimated based on the available term frequency (tf) distribution. These concepts represent novelties within the document collection that may later gain broader frequencies and either evolve into distinct topics or integrate into existing ones. However, during the study period, these concepts appear in only a small number of documents. As a result, their microstates are characterized primarily by a single occurrence ($k = 1$), leading to a mesostate entropy of $S_{\text{meso}} = 0$. Such concepts are excluded from the macrostate parameter estimation process but are reintroduced in later periods when their distributions become sufficient to allow accurate model fitting.

While different time periods can be analyzed by shifting the initial and final dates, we opt to fix the initial date and extend the final date, gradually incorporating more data. Concepts excluded in shorter periods due to insufficient data may reappear in longer periods when enough data is available, enabling the estimation of their thermodynamic parameters. However, our current dataset extends only to 2018, limiting our ability to shift the final date further. Consequently, 2,208 concepts with insufficient data are not analyzed in this study but could be included in future analyses if data from later years become available. An example of this issue is demonstrated by the concept 'Anomalous Hall effect,' which, as shown in Fig. 2, required four years of data collection (from 2000 to 2004) to obtain the thermodynamic parameters with the necessary level of accuracy.

Figure 2 indicates values of the concept's state parameters in 2018 concerning the time of their origin in the texts of the studied collection of documents. We can conclude that states with minimal residual entropy $R \to 0$, associated with the state of thermodynamic (infodynamic) equilibrium, are more common to concepts first introduced in the oldest documents, although instantaneous equilibrium can be reached by the relatively new concepts also. From Fig. 2(c), we can see that not all 'old' concepts have maximal entropy (minimal R), but many have power-law tf distribution (i.e. $\lambda \to 0$). Concepts that appeared in a state of stationary thermodynamic equilibrium, when R is constant and small for an extended period (marked green in Fig. 2), appeared to have both of these properties – near power-law distribution ($\lambda \sim 0.02$) and maximal possible entropy at $R \to 0$. We can assume that this limit is a future of all old concepts with well-established context meaning, which is what we can expect in the case of physical systems according to the second law of thermodynamics.

Figures 2(a),(d) show that the free energy A and temperature of concepts in a state of stationary equilibrium tend to specific non-zero values, indicating a stable balance between the entropic forces and the energy landscape governing the frequency distribution of these concepts. Other concepts that appeared in the state of instantaneous equilibrium have similar values of the (inverse) temperature, close to the most probable $\beta = 3/2$ evident from Fig. 1, but for many of them, free energy A has smaller values than for the stationary state concepts.

As we can see from Figs. 2 and 3, the state of a concept is a function of the number of documents where it can be found. The 'age' of a concept and the number of such papers are correlated quantities such that older concepts tend to appear in a larger number of documents. We can conclude that if the number of such papers exceeds 1000, the state of a concept is mostly in equilibrium (having maximum entropy for the particular term frequency distribution, meaning that Shannon-Gibbs and Boltzmann state descriptions yield the same entropy). Concepts' term frequency distributions tend to become more power-law-like as the number of relevant documents increases. The

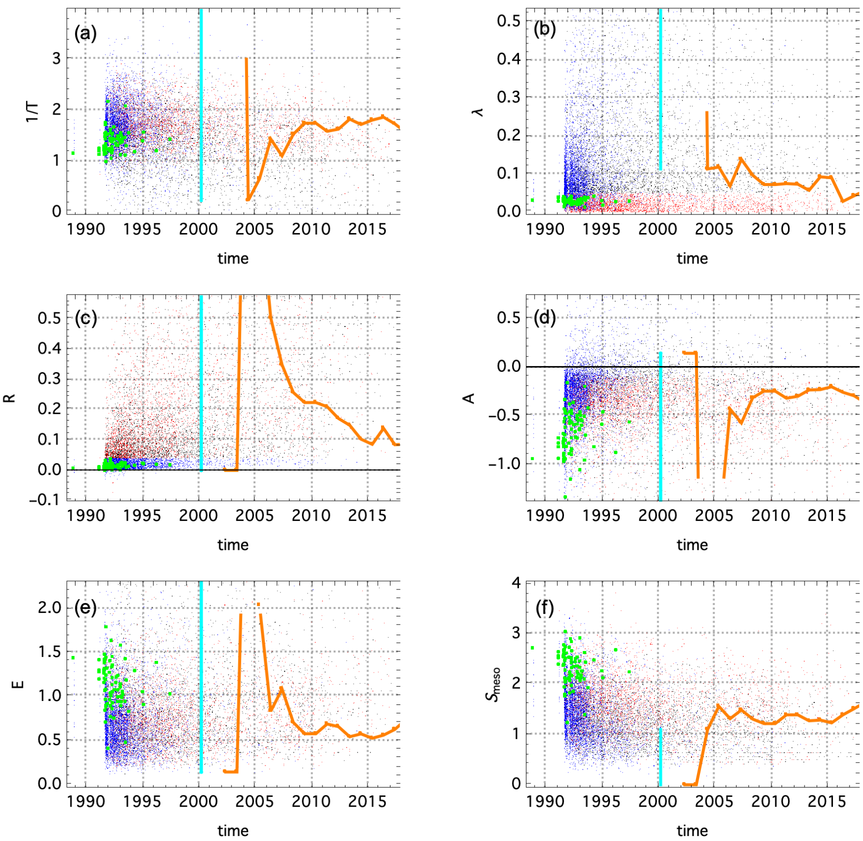

Fig. 2 Thermodynamic state parameters β, λ, residual entropy R, free energy A, internal energy E, and mesostate entropy $S_{\rm meso}$ for 11,737 physical concepts, estimated from term frequency (tf) data spanning from 1991 to 2018. Concepts are ordered by the time of their first mention in the studied collection (ArXiv, which began accepting documents on August 14, 1991). Blue dots represent concepts with $R < 0.04$. Green dots indicate concepts that remained with $R < 0.04$ between 2010 and 2018. Red dots highlight concepts exhibiting a near power-law term frequency distribution ($\lambda < 0.04$), while black dots represent all other concepts. The orange line traces the state evolution of the 'Anomalous Hall effect' concept.

most frequent concepts are in a stationary state, tend to be the oldest, and have, on average, larger values for entropy and internal energy compared to other equilibrium state concepts. The amount of free energy is generally lower for such concepts than for any others, indicating that they have done more work on their surroundings. Their current free energy change has to be the lowest among other equilibrium concepts.

4.1 Energy-entropy diagram.

To explore concepts' state space, we map their states in a series of diagrams. One of the common diagrams is an energy-entropy (E-E) diagram shown in Fig. 4 and Fig. 5. Dashed blue lines on these diagrams represent the largest $S_{\rm macro}$ entropy for different constant cut-off parameter values $\lambda > 0$ calculated from Eqs. (3),(4) and (6). The solid

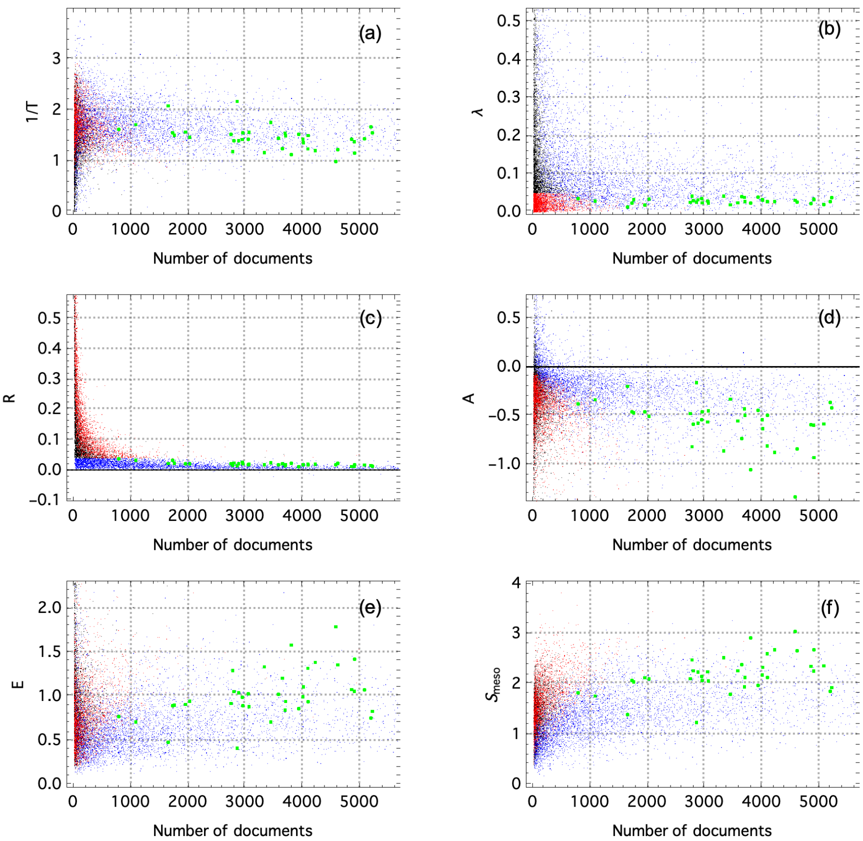

Fig. 3 The concept state parameters and thermodynamic quantities as a function of the number of documents. Non-equilibrium concepts are shown in red and black; stationary state concepts are in green, and concepts with small residual entropy R are in blue.

blue line shows the maximal entropy of a macrostate obtained if the distribution is very close to the power-law (i.e., $\lambda = 0.001$). From Fig. 4 diagram, we can conclude that the state of instantaneous thermodynamic equilibrium is possible for almost any value of λ parameter. Still, most concepts reach stable equilibrium when $\lambda < 0.05$. In Fig.5, we see examples of stable equilibrium concepts such as "Diquark" and "Mass," which maintain nearly constant energy and entropy over a 15-year period. The "Diquark" concept shows a gradual decrease in both residual and mesostate entropy, with slight oscillations around a specific temperature. Averaging its dynamics over the observed period (2002–2018), we can infer from Eq.(11) that its free energy $\Delta A > 0$, indicating that the concept performs a certain amount of work on surrounding concepts.

The "Mass" concept provides another example of state evolution, with its residual entropy remaining small and nearly constant ($\Delta R \sim 0$) throughout the entire period. By averaging its state dynamics from 2004 to 2017, we observe that the internal energy change is negligible ($\Delta E = 0$), while $\Delta S_{\mathrm{macro}} > 0$. According to Eq. (11), this results in negative free energy change ($\Delta A < 0$), suggesting that the surrounding concepts are performing work on the "Mass" concept, driving its evolution.

A third example of concept state dynamics is the "Anomalous Hall effect." In Fig.5, we observe the combined mesostate (orange line) and macrostate (red line) dynamics of this concept in energy-entropy coordinates. Over time, it exhibits a continuous decrease in residual entropy R and internal energy E as the concept evolves. By 2018, it reached equilibrium at a temperature of $\beta = 1.5$. Early in the studied period, particularly in 2004, the state parameters of this concept showed much larger fluctuations, which diminished as it approached equilibrium closer to 2018, as shown similarly in Fig.2.

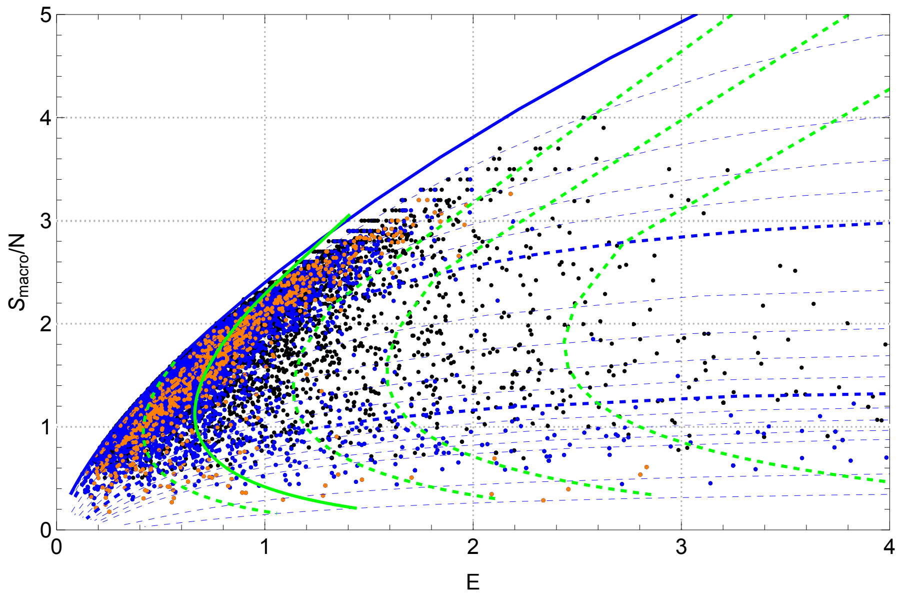

Fig. 4 Entropy-energy diagram for 11737 physical concepts as of the end of 2018. The blue lines (solid and dashed) correspond to the $S_{\text{macro}}(E(\lambda = c, \beta))$ function for specific values of $c = \{0.001, 0.01, 0.03, 0.05, 0.07, 0.09, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1, 1.5, 2\}$ from top to bottom. The green lines represent isotherms for $\beta = \{0.5, 1, 1.5, 2\}$ from right to left, with the solid green line for $\beta = 1.5$. Concepts for which $R > 0.04$ are depicted with black color dots and the ones with $R < 0.04$ and $R < 0.005$ are depicted as blue and orange color, respectively.

The example of the 'Anomalous Hall effect' concept is representative of most new concepts until they reach instantaneous equilibrium at maximum possible entropy S and minimal energy E. This behavior aligns with what we expect from physical closed thermodynamic systems. As suggested by Peng et al. [36], the ratio termed *entropy efficiency*, $Q = S_{\text{macro}}/E$, which is maximized for equilibrium states, represents another interpretation of the second law: "a system would use the minimum energy to produce the same amount of entropy." In Fig. 6, we show the diagram of states for entropy efficiency Q plotted against inverse temperature.

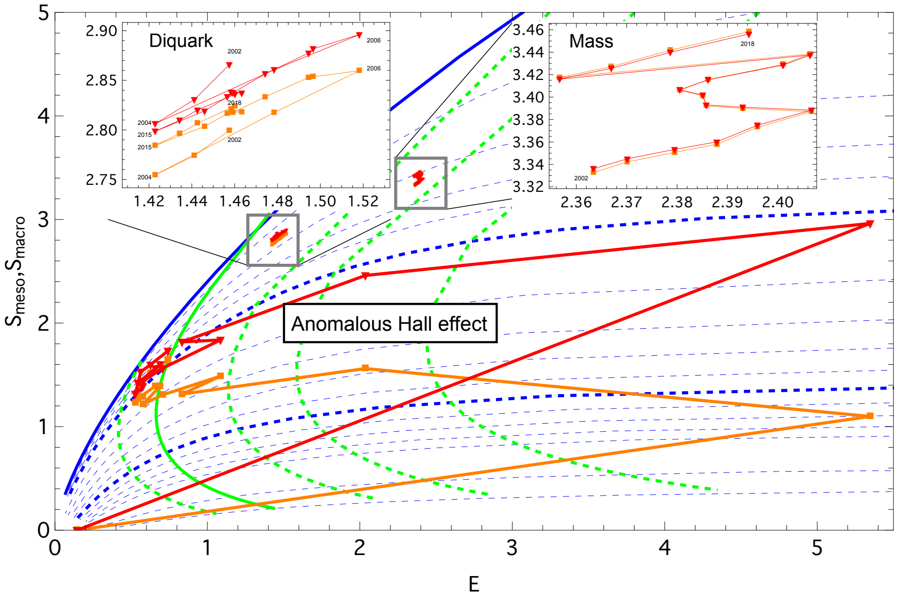

Fig. 5 State dynamics of the "Mass," "Diquark," and "Anomalous Hall effect" concepts for the period 2002–2018. Orange and red lines represent the evolution of the mesostate and macrostate, respectively. The blue lines (solid and dashed) correspond to the function $S_{\mathrm{macro}}(E(\lambda, \beta))$, with varying β and specific values of $\lambda = 0.001, 0.01, 0.03, 0.05, 0.07, 0.09, 0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1, 1.5, 2,$ arranged from top to bottom. Green lines represent isotherms for varying λ at constant $\beta = 0.5, 0.75, 1, 1.5, 2$, progressing from right to left, with the solid green line corresponding to $\beta = 1.5$

As we can see from Fig. 6, there is an almost linear correlation between the largest possible entropy efficiency Q for a concept and its inverse temperature. Concepts with the smallest R and λ appear to have the highest entropy efficiency, and the concept of "Anomalous Hall effect" state dynamics shows how general concepts reach this limit.

We can see that entropy efficiency is increasing towards lower temperatures, which explains the observed in Fig. 6 state dynamics of non-equilibrium and equilibrium concepts. The evolution of equilibrium concepts towards higher efficiency is much slower than for non-equilibrium systems, suggesting the exiting of different information (energy) exchange mechanisms for these systems.

4.2 Free energy diagrams.

In this section, we analyze diagrams showing the relationship between Helmholtz free energy and other thermodynamic functions and state parameters. In Fig. 7, we observe that non-equilibrium concepts with near power-law tf distributions ($\lambda \to 0$) correspond to macrostates with the largest values of $E - A = TS_{\mathrm{macro}} > 0$ and $A < 0$, which represent energy tied up in entropy at a given temperature. As temperature increases ($\beta \to 0$), this energy grows and becomes divergent below $\beta = 1$. In contrast, equilibrium concepts generally exhibit smaller values of $E - A$, especially when A is positive.

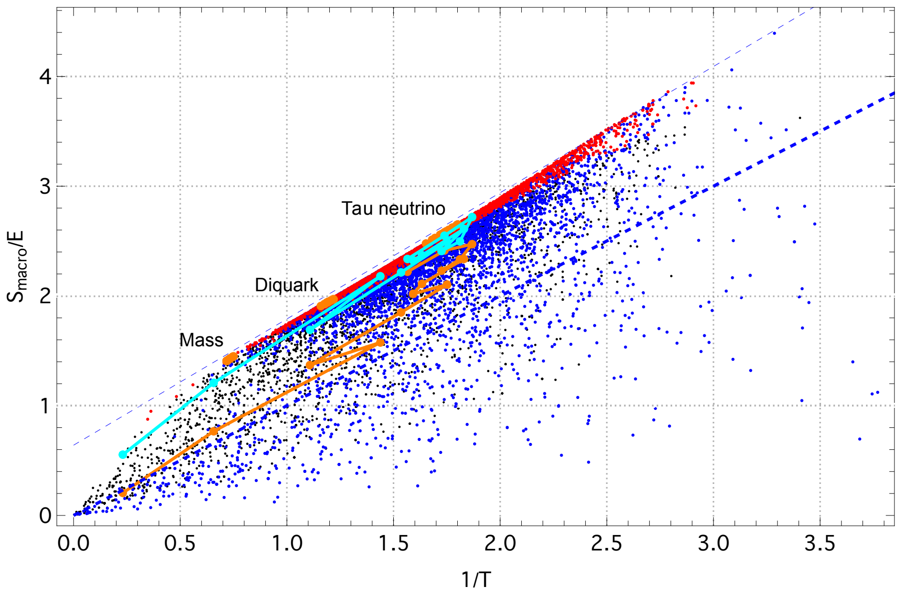

Fig. 6 Temperature diagram for entropy efficiency $Q = S/E$. Concepts with small residual entropy are marked in blue, and concepts with a near power-law term frequency (tf) distribution are marked in red. Historical values for the equilibrium concepts "Mass," "Diquark," and "Tau neutrino" are shown in orange. The dynamics of the non-equilibrium concept "Anomalous Hall effect" are represented in cyan for the macrostate and orange for the mesostate. The dashed lines represent the linear functions $Q = \beta$ (bottom dashed line) and $Q = 0.66 + 1.15\beta$ (top dashed line).

Among equilibrium concepts, those with the smallest average λ have the highest values of TS_{macro}. The difference in TS_{macro} between equilibrium and non-equilibrium concepts becomes less pronounced at lower temperatures, and after $\beta = 2.8$, almost all concepts appear in equilibrium.

Both E and A reach minimum values at specific temperatures and λ values. The minimum internal energy E increases with temperature and λ, primarily represented by equilibrium concepts. Across a broad range of temperatures, the energy minimum corresponds to λ values between 0.2 and 0.4 (see Fig.8), indicating that both terms in Eq.(6) contribute to the system's internal energy. In contrast, the minimum free energy A is mostly associated with non-equilibrium concepts close to power-law tf distributions.

The residual energy $TR = TS_{\text{macro}} - TS_{\text{meso}}$ distinguishes non-equilibrium concepts with near power-law distributions from equilibrium concepts at the same temperature. This residual energy can be seen as a form of potential energy that complements free energy A and is necessary to adjust the probabilities of information channels k in the mesostate to maximize entropy. As previously mentioned, the residual entropy R represents the information required to define the mesostate based on the macrostate description. When a concept reaches equilibrium, $R \to 0$, and any net change in residual entropy $\Delta R < 0$ indicates information transferred from the system to its surroundings.

The system utilizes the residual energy TR for information transfer, functioning as a creative potential realized through increasing mutual information with other concepts. This residual energy is used to perform work by creating or strengthening mutual information, thus enhancing the dynamic complexity of the knowledge network as it assimilates new information. If mutual information cannot be decreased, the process becomes irreversible. However, studies have shown that mutual information can decrease, albeit less frequently [45]. In such cases, a concept absorbs additional information from its surroundings, increasing both its free energy and residual entropy.

As shown in Fig. 8, the energy-temperature dynamics of the "Anomalous Hall effect" concept illustrate a thermodynamic process that starts in a non-equilibrium state. As temperature fluctuations subside, the concept gradually approaches equilibrium.

In Fig.7, concepts with the smallest $\lambda < 0.05$ (shown in red) are predominantly non-equilibrium concepts in the early stages of their evolution, whose mesostates are characterized mainly by a logarithmic energy spectrum. Fig.9 highlights an interesting property of these concepts: the dimensionless ratio A/E, derived from Eq. (9), remains nearly constant over a wide range of a quantity that can be described as the *mesostate free energy efficiency*, $1 - TS_{\mathrm{meso}}/E$. This quantity can be interpreted as a measure of the system's efficiency in utilizing energy for work rather than for sustaining entropy.

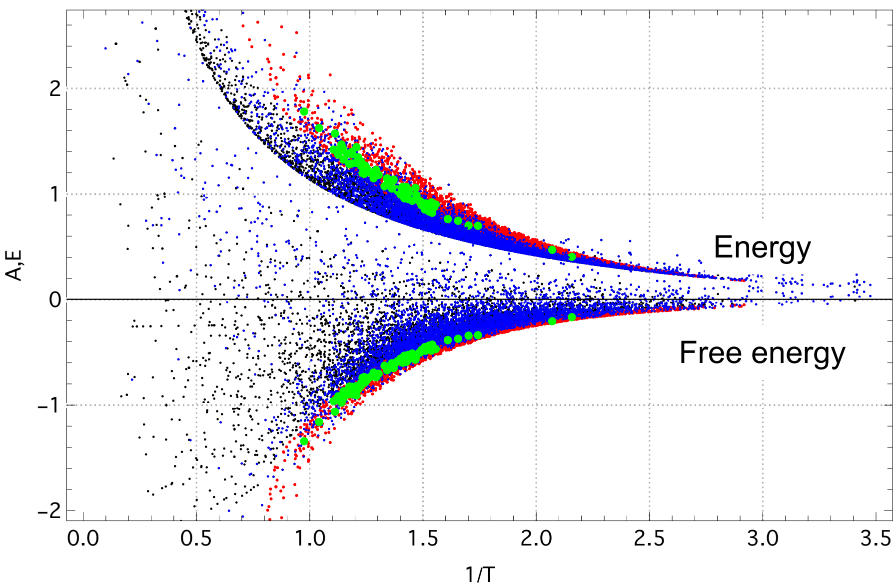

Fig. 7 Free energy A and average internal energy per document E temperature diagram for concepts with $\lambda < 0.05$ (red dots), with $R < 0.04$ (blue dots), and all other concepts (black dots). The green color identifies concepts in a stationary state with residual entropy remained $R < 0.04$ from 2010 to 2018.

Fig.9 provides a clear depiction of concept states with varying values of normalized creative energy potential, TR/E, represented by the vertical distance from the state's

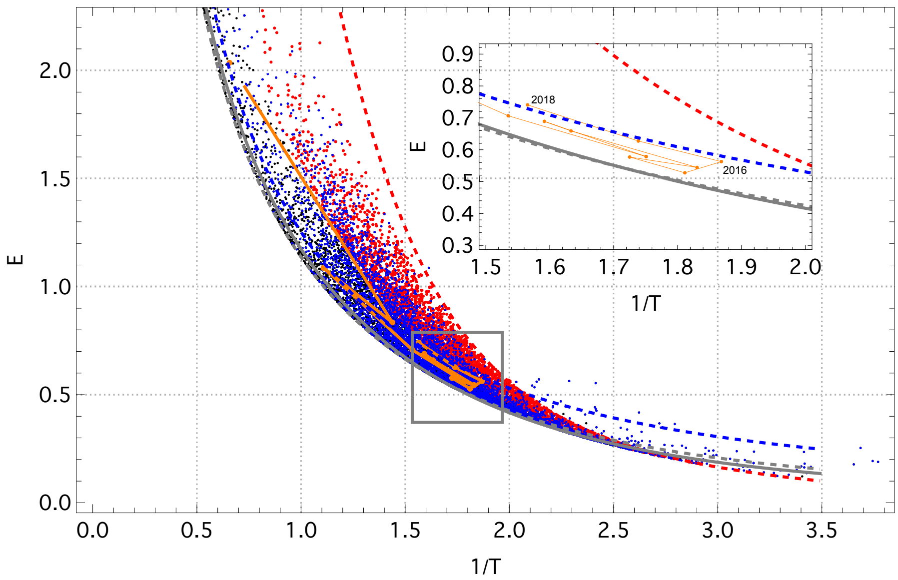

Fig. 8 Energy-temperature diagram. The red and blue dashed lines represent the $E(\beta)$ dependence for fixed $\lambda = 0.001$ and $\lambda = 0.8$, respectively. Gray lines correspond to $\lambda = 0.2$ and $\lambda = 0.3$ (dashed) and highlight the minimum $E(\beta)$ function over a wide range of temperatures. The orange line shows the state dynamics of the "Anomalous Hall effect" concept.

position on the diagram to the diagonal line. This diagonal line corresponds to states of instantaneous thermodynamic equilibrium with $R \to 0$ (marked by blue color). The line marks the position of all possible macrostates, while the mesostates appear below this line. Over time, all states below this diagonal gradually drift toward stable stationary states, marked in green. Examples of possible state dynamics, such as those of the "Anomalous Hall effect," "Electron-positron collider," and "Gravitational disruption" concepts, demonstrate two types of behavior, as previously observed in Fig.5. These systems either evolve to a stationary equilibrium state while their residual entropy R changes (non- equilibrium dynamics) or remain constant (equilibrium dynamics). The diagram in Fig. 9 also shows that the most probable state evolution trajectory has A/E value tightly distributed around -0.5, which corresponds to states power-law tf distribution.

The limited range of A/E values for near power-law non-equilibrium states suggests that the proportion of internal energy E in the free energy A for these states remains relatively stable, despite potential variations in entropy and temperature. The negative value of the most probable $A/E \sim -0.5$ indicates that most of the energy is tied up in entropy, suggesting a most probable value for $TS_{\text{meso}}/E \sim 3/2$ across the entire temperature range. In cases of small temperature oscillations and logarithmic energy spectra, the concept state dynamics align with the indicated parameters during information transfer. This might imply a robust mechanism of energy allocation and utilization within the network of concepts that follow a power-law distribution of term frequencies. Furthermore, this group of concepts exhibits the largest heat capacity (see Fig. 10), $C = \partial E/\partial T$, compared to others, indicating a higher capacity to absorb and retain heat energy.

The heat capacity C of the concepts is maximized around the most probable temperature and eventually becomes zero at very high ($\beta \to 0$) or very low ($\beta \to 3.5$) temperatures. The equilibrium concepts show various values of C across the available range of temperatures. Concepts in a stable equilibrium state (green color on Fig. 10) have a larger heat capacity and temperature, among other equilibrium concepts with small residual entropy R.

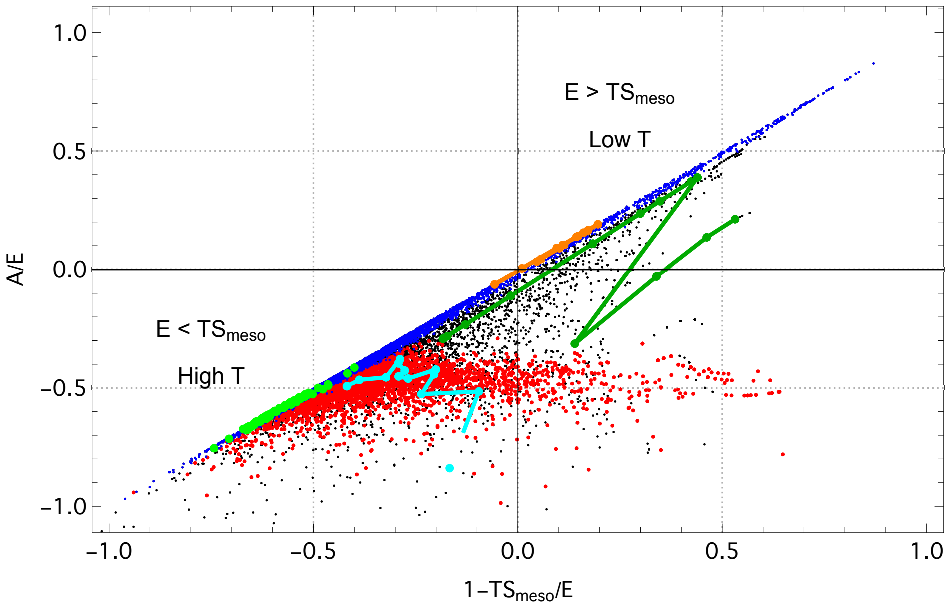

Fig. 9 State diagram showing the correlation between A/E and $1-TS_{\mathrm{meso}}/E$ for concepts. Concepts with macrostates where $\lambda < 0.05$ are depicted as red dots, and those with $R < 0.04$ are shown as blue dots. Concepts in stable stationary states are represented by green dots, while all other concepts are indicated by black dots. The state dynamics for the concepts "Anomalous Hall effect," "Electron-positron collider," and "Gravitational disruption" are shown by cyan, orange, and dark green lines, respectively.

The value of a concept's free energy changes along its state trajectory, reflecting its role in interacting with its surroundings. A concept can either transfer energy (information) to or receive it from the thermostat with which it interacts. In this way, a concept performs work on other concepts, or a group of concepts performs work on this particular concept, altering the direction of information transfer.

Concepts in a state of stationary equilibrium exhibit minimal variations in free energy and residual entropy relative to other concepts. In contrast, concepts with a term frequency (tf) distribution close to a power law but not yet in equilibrium tend to experience the largest average decrease in their residual entropy. This decrease corresponds to increased knowledge production as they progress toward equilibrium.

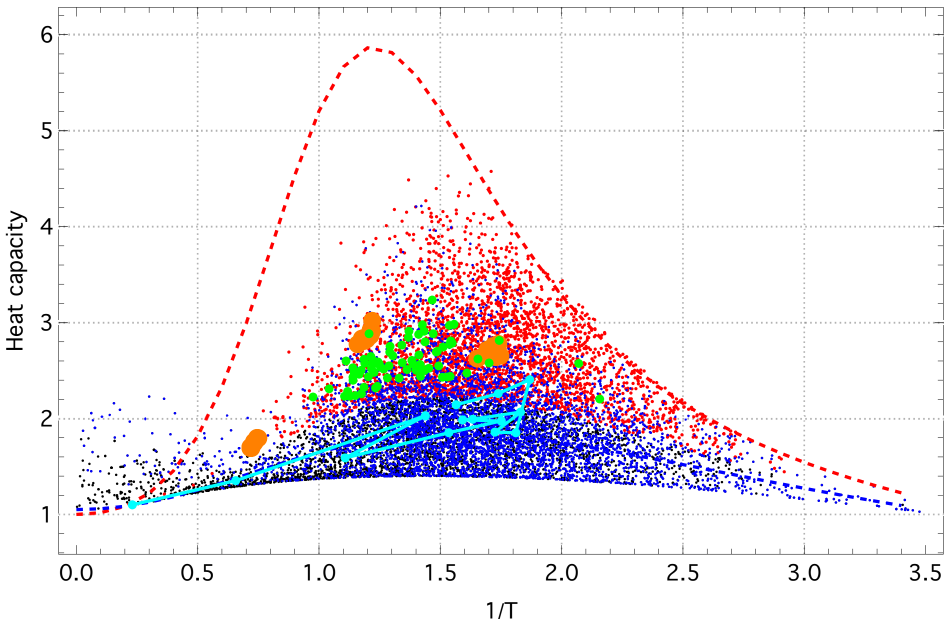

Fig. 10 Heat capacity of concepts from temperature is shown for the several types of concepts: concepts with $\lambda < 0.05$ (red dots), with $R < 0.04$ (blue dots), concepts in stable equilibrium (green dots), and all other concepts (black dots). The heat capacity dynamics are calculated for three equilibrium concepts "Mass", "Diquark" and "Tau neutrino" (orange color) and non-equilibrium concept "Anomalous hall effect" (cyan color). The derivative $\partial E/\partial T$ calculated using Eqs.(6 and (4)) for the constant $\lambda = 0.001$ (red dashed line) and $\lambda = 0.0042$ (blue dashed line)

5 Conclusions

In this study, we applied a thermodynamic framework to the analysis of scientific concepts, providing new quantitative insights into how knowledge evolves and stabilizes over time. By treating scientific concepts as closed thermodynamic systems, we modeled their behavior using thermodynamic quantities such as entropy, free energy, temperature, and heat capacity. This approach introduced an additional dimension to the analysis of concepts as information units, capturing the dynamic processes of knowledge creation and evolution. Our method offers a novel perspective on how scientific ideas grow, interact, and influence underlying knowledge networks.

One key finding was the observation that the term frequency (tf) distribution of scientific concepts follows a generalized Boltzmann distribution, a hallmark of systems in thermodynamic equilibrium. By analyzing over 11,000 concepts across more than 500,000 documents from ArXiv (2002–2018), we confirmed Martini's previous result [13] that the most probable tf distribution power-law exponent is $\beta \approx 3/2$. This corresponds to the most probable temperature across a collection of concepts, analogous to the fixed point in physical systems where equilibrium is achieved through long-term stochastic interactions.

A novel aspect of this study is the identification of a phase transition in the evolution of scientific concepts. Initially, concepts exhibit a linear energy spectrum with an exponential term frequency distribution—characteristic of early adoption with limited engagement. As these concepts gain traction, they undergo a phase transition into a state characterized by a logarithmic energy spectrum and a power-law frequency distribution. This shift represents the transition to mainstream acceptance, where the concept becomes deeply integrated into the knowledge network. Such phase transitions are akin to those observed in physical systems, highlighting the applicability of thermodynamic models to understanding nonlinear knowledge dynamics.

Our analysis of heat capacity further revealed that non-equilibrium concepts still gaining recognition exhibit near power-law frequency distributions and reach maximal heat capacity around the most probable temperature. At this stage, these concepts are highly responsive to external stimuli, suggesting intense information exchange and potential for further development before reaching equilibrium. The maximal heat capacity indicates their capacity to absorb new information and innovate.

An important finding concerns the relationship between free energy and residual entropy within the system, which governs the dynamics of concept space. The evolution of concepts follows a trajectory that minimizes both free energy and residual entropy. Minimizing free energy corresponds to a concept reaching a more stable and integrated state within the knowledge network, reducing the energy required to maintain its position. At the same time, minimizing residual entropy reflects the reduction of hidden complexity, as the concept's relationships within the network become clearer and more defined. Concepts with lower free energy are more likely to dominate and stabilize within the network, while concepts with higher residual entropy remain flexible, capable of integrating diverse perspectives and ideas. This balance between free energy and entropy plays a crucial role in shaping the structure and evolution of knowledge networks.

The minimization of free energy and residual entropy represents the stabilization of concepts as they move from non-equilibrium states to equilibrium. Early-stage concepts, with high free energy and residual entropy, are in a state of flux, absorbing new information and fluctuating in response to external influences. As they evolve, they undergo phase transitions, decreasing both their free energy and residual entropy, indicating a move toward stability and greater influence within the network. This dynamic reflects how scientific knowledge grows and solidifies over time.

The thermodynamic model developed in this study provides a robust, interdisciplinary framework for analyzing the dynamics of knowledge production. By applying classical thermodynamic principles to scientific concepts, we quantified the stages of concept development and mapped their trajectories within knowledge networks. This framework offers predictive insights into the future trajectory of emerging concepts, helping researchers identify those most likely to become influential or dominant based on their thermodynamic properties.

Moreover, identifying phase transitions and the role of heat capacity in concept evolution underscores the nonlinear nature of knowledge growth. Periods of intense innovation are often followed by stabilization as concepts reach equilibrium. These findings may help inform strategies for fostering innovation, particularly by targeting concepts in their early stages when they are most responsive to new information and external influences.

In conclusion, this study demonstrates the power of thermodynamic models in analyzing the evolution of scientific knowledge. By quantifying key parameters such as temperature, free energy, and heat capacity, we gained a deeper understanding of how scientific concepts grow, evolve, and stabilize within knowledge networks. The phase transitions observed further underscore the dynamic and nonlinear nature of knowledge creation, providing valuable insights into the processes that drive scientific innovation. The minimization of free energy and residual entropy within the concept space illustrates how concepts move toward stability and influence. This framework opens new avenues for future research, particularly in exploring the universality of these findings across different disciplines and tracking the evolution of emerging fields. As scientific knowledge continues to expand, applying thermodynamic principles to information systems will serve as a powerful tool for understanding and predicting the trajectory of innovation in science.

Supplementary information. This document provides additional materials to support the findings discussed in the main text. All supplementary figures are made available via Zenodo. These supplementary materials are intended to enhance understanding by allowing users to interactively explore the thermodynamic properties of scientific concepts through the use of active tooltips embedded within the figures.

1. Supplementary Figures in `.cdf` Format

The supplementary figures are provided in `.cdf` (Computable Document Format), which allows for dynamic interactivity. Each figure contains active tooltips that provide detailed information on data points when hovered over.

The `.cdf` format is supported by free software such as Wolfram Player, which can be downloaded from here. Once installed, users can open and interact with the figures provided.

- **Figure S1**: *Entropy efficiency diagram*
  Temperature diagram for entropy efficiency $Q = S/E$. Concepts with small residual entropy are marked in blue, and concepts with a near power-law term frequency (tf) distribution are marked in red. Historical values for the equilibrium concepts "Mass", "Diquark", and "Tau neutrino" are shown in orange. The dynamics of the non-equilibrium concept "Anomalous Hall effect" are represented in cyan for the macrostate and orange for the mesostate. Active tooltips provide name of concepts on the diagram for each data point.
- **Figure S2**: *Temperature dependence of internal and Helmholts free energy.*
  Free energy A and average internal energy per document E temperature diagram for concepts with $\lambda < 0.05$ (red dots), with $R < 0.04$ (blue dots), and all other concepts (black dots). The green color identifies concepts in a stationary state with residual entropy remained $R < 0.04$ from 2010 to 2018. Active tooltips provide name of concepts on the diagram for each data point.
- **Figure S3**: *Free energy conversion efficiency*
  State diagram showing the correlation between A/E and $1-TS_{\text{meso}}/E$ for concepts. Red dots represent those with macrostates characterized by $\lambda < 0.05$, while blue dots indicate those with $R < 0.04$. Concepts in a stable stationary state are depicted as green dots, and all others as black dots. The state dynamics for the "Anomalous

Hall effect," "Electron-positron collider," and "Gravitational disruption" concepts are represented by cyan, orange, and dark green lines, respectively.

- **Figure S4**: *Entropy reduction ratio – temperature diagram.*
State diagram showing the correlation between entropy reduction ratio TS_{macro}/E and temperature $1/T$ for concepts. Concepts with macrostates where $\lambda < 0.05$ are depicted as red dots, and those with $R < 0.04$ are shown as blue dots but have $\lambda > 0.05$. The state dynamics for the equilibrium concepts "Mass," "Diquark" and "Tau-neutrino" are shown by orange color and for "Anomalous Hall effect" by cyan color".

2. How to Access the Supplementary Materials

All supplementary materials, including the `.cdf` figures, datasets, and code, can be accessed via Zenodo at the following link:

`10.5281/zenodo.13889772`

Please ensure that you have the necessary software (e.g., Wolfram Player for `.cdf` files) installed before accessing the interactive figures. For questions or support regarding the supplementary materials, please contact the corresponding author.

3. Citation

When using or referencing these supplementary materials, please cite both the main publication and the Zenodo repository using the following format:

- **Main Paper**: [Full citation of the paper]
- **Zenodo Supplementary Materials**: 10.5281/zenodo.13889772

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- **Materials availability**: All materials related to the research (such as supplementary files) are available and can be accessed via Zenodo: `10.5281/zenodo.13889772`.
- **Code availability**: Not applicable.
- **Author contributions**:
  - Artem Chumachenko: Conceptualization, Methodology, Formal analysis, Investigation, Writing – original draft.
  - Brett Buttlierie: Writing – review & editing.

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