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Negentropy in Many-Body Quantum Systems

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Academic Editors: Geert Verdoolaege and Kevin H. Knuth
Received: 25 June 2015; Accepted: 17 February 2016; Published: 22 February 2016

Abstract: Negentropy (negative entropy) is the negative contribution to the total entropy of correlated many-body environments. Negentropy can play a role in transferring its related stored mobilizable energy to colliding nuclei that participate in spontaneous or induced nuclear fusions in solid or liquid metals or in stellar plasmas. This energy transfer mechanism can explain the observed increase of nuclear fusion rates relative to the standard Salpeter screening. The importance of negentropy in these specific many-body quantum systems and its relation to many-body correlation entropy are discussed.

Keywords: negentropy; quantum systems; many-body correlation

1. Introduction

Negative entropy, or negentropy [1–3], can be defined as the specific entropy deficit of an ordered subsystem with respect to surrounding chaos. Negative entropy is used in information theory to measure the distance to normality, and it measures the difference in entropy between a given distribution and the Gaussian distribution, which is the distribution with the highest entropy [4,5].

It is well known that the "ultimate source of all our energy and negative entropy is the Sun" [6]. In addition to applications to the macroscopic world ranging from the biological [6] to the cosmological [7] context and quantum information [5], the concept of negentropy can also be useful in the quantum many-body world, e.g., in solid or liquid metals or in stellar plasmas where it can explain, at the microscopic level, how the reduced disorder or increase of information can result in increasing the spontaneous or induced fusion nuclear reactions. In this paper, we define as a many-body system the ensemble of sub-systems and the surroundings (or environment).

Our aim is to show how the physical concept of negentropy can be used in the above-mentioned selected physical processes that are observed in several laboratories. We discuss the interesting theoretical consequences of negentropy when applied to nuclear fusion rates in different many-body environments. We focus on fusion reactions in solid and liquid metals and in astrophysical stellar plasmas where strong enhancements of the fusion rates at low energy have been observed and cannot be completely explained by standard screening effects. We propose that negative entropy, in particular the negative contribution to entropy arising from two- and many-body correlations, has a great effect on the rates of nuclear fusions. The role of generalized statistics and energy-momentum quantum uncertainties was already explored elsewhere [8–10]; without the concept of negentropy, the role of correlations' negative entropy was described in our study on metal melting [11]. Other applications of negentropy are to be found in the study of black holes [12], in microbial life [13], in the field of the quantum mechanics information [14] and, finally, in the study of nanoparticles [15].

To the best of our knowledge, in the field of nuclear physics, this paper is the first attempt to apply the negentropy to observed nuclear fusion reactions. The advantages over other methods consist of the concise treatment of all of the effects due to the environment, at a microscopic level. These effects are contained in the negentropy expression. Negentropy is a reasonable scientific physical quantity because it is strictly related to all many-body effects and many-body quantum interactions and correlations beyond the ideal environment made of independent particles subject or not to short-range two-body interactions [16,17].

In thermodynamics and in statistical mechanics, the entropy enters with a central role into all of the laws concerning systems in equilibrium and in a non-equilibrium state, reversible and irreversible transformations and phase transitions in Boltzmann and Gibbs classical and quantum extensive and non-extensive distributions.

Entropy is usually given as a total, compact, positive expression always increasing during its time evolution. However, more generally, entropy is composed of a few terms, and at least one of them represents a negative contribution to its evaluation.

The negative entropy contribution is related to quantum exclusion and inclusion principles and to many-body correlations or interactions among the single elements or clusters of elements composing the system. Quantum exclusion and inclusion effects, correlations and/or interactions produce order in the system, decreasing the value of the total entropy.

From microscopic nuclear, atomic molecular, nano-physical theories, one can obtain the decrease of entropy in macroscopic thermodynamics. It is interesting to follow the function of the negative entropy contribution, different from the positive one, because negentropy is a stored mobilizable energy in an organized system. This quantity can be spontaneously transferred or exchanged among the elements or clusters of elements or from the environment to elements and subsystems. In our future research, we will consider negentropy to fully provide a quantitative explanation of experimental facts and results concerning nuclear fusion processes in solid and liquid metals, in standard and astrophysical plasmas, in Jovian planets and in general to make a step towards a dynamical electron screening theory, on the basis of a unifying character.

The plan of the paper is as follows. In Section 2, we describe how the negative part of the entropy contributes to transferring stored mobilizable energy. In Section 3, we briefly summarize those physical processes and the corresponding experiments where negentropy could be applied, while in Section 4, we comment on the validity of the ideal plasma model (a fully-disordered system) to describe the contribution of the environment to nuclear fusion reactions and the conditions when such an approximation becomes realistic: it appears that this ideal plasma approximation is not justifiable in solid or liquid metals, or in stellar plasmas. In Sections 5–7, we report the analytical expression of negentropy contributions in solid, liquid metal and stellar plasma, respectively. Our conclusions follow in Section 8.

2. Negative Entropy

Let us write the complete positive entropy S of a system as the sum of a positive contribution $S^+ > 0$ and a negative contribution $-S^-$ (negative entropy), with $S^- > 0$ and:

$$S = S^+ - S^- \,, \tag{1}$$

where $S > 0$ implies $S^+ > S^-$.

The quantity S^+ represents the extensive part, *i.e.*, comes from the kinetic component of the Hamiltonian of electrons, ions or nuclei that compose the system. The positive entropy S^+ coincides with total S when all kinds of interactions are negligible or weak and such that they can be included into the kinetic term S^+ of single particle motion and also when quantum effects are negligible.

At global thermodynamic equilibrium, $S = S^+$ and $S^- = 0$. The contribution S^- is given by correlations, due to two- or many-body interactions $(S_2 + S_x)$, or by quantum effects, such as Pauli blocking. The negative part of the entropy S^- reflects some order in the system relative to the disordered system as described by S^+ alone: $S^+ > S^-$ if the total entropy must be positive.

We now consider a generalized statistical mechanics, like, for instance, the Tsallis one, S_q [18], where q is the entropic parameter. S^+ can be identified by the extensive part of the whole entropy S, like, for instance, $S_{q=1}$, that is the maximum value (Boltzmann–Gibbs entropy). If we have to describe a system that is in a stationary metastable state with a long half-life, with particle interactions no longer negligible and many-body correlations, then the total entropy should be $S = S_q$ for a certain $q \neq 1$ value. Therefore, the system entropy is given by:

$$S_q = S_{q=1} - S^- \tag{2}$$

The negentropy of the system is the difference between the Boltzmann–Gibbs entropy ($q = 1$) and the Tsallis entropy with q different from one.

The negentropy can be written using several approximations and is a measure of the non-Gaussianity of the system [19,20]. Because negentropy, S^-, represents the particle correlations, these can be written also with the same approximations of negentropy, for instance the two-body correlation entropy:

$$S_2 = -\int g(r) \ln g(r)\, dr = S_{q=1} - S_q = S^- \tag{3}$$

From the curves calculated for $S_{q>1}$, we can obtain and clearly see that $S_{q=1} - S_{q>1} > 0$, then $S^- > 0$, as we expect for $q > 1$.

The states with $q \neq 1$ are metastable, and their entropy could be smaller than $S_{q=1}$. In any case, S_q is always positive, and we can set:

$$S \equiv S_q = S_{q=1} - \left(S_{q=1} - S_q\right) = S^+ - S^- \tag{4}$$

with S^- defined in Equation (3). A change in sign of S^- means that, with respect to the independent particle state, in one case ($S^- > 0$), the system has more order than in the other one ($S^- < 0$).

In generalized statistics based on the κ-entropy [21,22], this situation does not arise, since S^- is always positive for any value of κ.

The entropic parameter q was given from dynamical first principles, in implicit form, in [23], Equation (33), and was explicitly related to particle correlations and given for solar plasma in [24], Equations (15) and (16), in terms of plasma and ion-ion correlation parameters. A two-parameter entropy was reported the first time in [25], Equations (24) and (25), in terms of hypergeometric functions and later in [26], Equation (7.1). In the framework of κ-statistics, the κ entropic parameter is linked to special relativity calculus [21,22].

The negative entropy contribution is related to a stored mobilizable energy [4], *i.e.*, $NkTS^-$, where kT is the system mean energy per particle, N the number of particles that transfers energy and S^- the adimensional negentropy per particle. Let us consider, for instance, nuclear fusions in metals. This energy can be freely shared between the accelerated ions and the surrounding ions in the metal, without modifying the macroscopic parameters of the system. The energy coming from the negentropy of electrons in solid metals increases the effect of the standard electron screening. The nuclear fusion can be described by an incident particle with an effective kinetic energy equal to the beam energy plus the contributions from the standard electron screening and the energy from the negative entropy of the correlated surrounding ions.

At the classical level, if in a physical system the entropy decreases, this process is explained by saying that there is a contribution from negentropy (total entropy is always greater than zero). Negentropy is not only a conceptual, mathematical quantity. It represents a physical substance, the interactions and particle correlations beyond the ideality of the environment, excluding any change or violation of the three laws of thermodynamics. These laws could only be reformulated using the expression of $S = S^+ - S^-$, in order to control the behavior of S^+ and of S^-, separately. The entropy S should not be divided artificially; it must be expressed as the sum of the two contributions that take into account specific physical effects and considering how the presence of the negentropy contribution increases the order of the system. At the quantum level, in the case of fermions, the exclusion principle contributes to a certain negentropy. However, negentropy is not only a quantum effect, but can be simulated as a quantum effect. The quantum mechanics of fermions and bosons calculated for ideal systems should not be changed. If the systems are non-ideal, the distribution functions change, due to the presence of particle correlations beyond the ideality. This requires the introduction of q- or κ-Fermi–Dirac and q- or κ-Bose–Einstein, or Gentile, or Griffiths, or Swamy *et al.* [18,27,28] distribution functions, depending on the deviation from ideality considered.

To have an indication of the complexity of the system, we can define the quantity disorder D, the ratio of the entropy of the system, $S^+ - S^-$, and the maximum entropy of the system S^+ [29]. We have in our case $D = 1 - (S^-/S^+)$, if $S^- = 0$, then $D = 1$, and the disorder is maximum. The order is therefore given by $O = 1 - D = S^-/S^+$. When $S^- = S^+$, $O = 1$, and we have the maximum order.

3. Experiments

Let us list a few observations in several different environments where nuclear fusion reaction rates are larger than expected and comment on some proposed interpretations.

Laboratory experiments with deuterated metals: d-d nuclear fusion rates in metals are enhanced compared to rates between bare nuclei; fusion reactions of other light nuclei show similar enhancements. Such enhancements can be reproduced by models with a screening potential of 200–300 eV, which are however much higher than the few tenths of eV of the adiabatic limit [8].

At Gran Sasso Laboratory, fusion experiments measure the reactions of interest in stellar physics (fusion of light nuclei), therefore at an energy much lower than the Coulomb barrier, down to the Gamow peak for solar temperatures. The measured large enhancements cannot be explained with the non-dynamical standard Salpeter electron screening [30,31].

The Salpeter approach is strongly dependent on the assumption of an ideal plasma. However, we expect metal and stellar environments to be non-ideal plasmas with entropies that contain negative correlations and, therefore, very much different from the Boltzmann–Gibbs entropy.

Nuclear fusion reactions in the solar core: solar and neutrino physics is reasonably well understood, but some questions still need to be addressed. The solar interior plasma is not in a global thermodynamic equilibrium and should show small deviations from the Maxwell–Boltzmann (MB) distribution. Several authors [32–35] have been discussing these aspects for many years, almost since the birth of quantum mechanics. Recently, there have been some important applications of generalized statistical mechanics that helped to better describe ion and electron energy distributions in such environments.

These generalized thermostatistics allow modified high-energy tails, enhanced or depleted with respect to the MB distribution [9].

The effect of electron screening on nuclear fusions is still to be fully understood because of the lack of a dynamic screening theory, since the static Salpeter approach is unsatisfactory [36,37]. Deviations of a few percent from standard rates are expected and are within the experimental precision.

Fusions in liquid metals and entropic correlations: the Tohoku group has measured a different effective screening potential in solid and liquid lithium, and we have recently proposed that the two-body correlation gives a negative contribution to the entropy that could explain the different screening between solid and liquid metal [38] (additional details and results from the experiments of interest can be found in [39–43]).

The metal environment, where fusions are taking place, is often modeled as an ideal plasma, where the simple Salpeter screening formula can be used. In fact, Rolfs [44] called the metallic environment a "plasma of a poor man" and used a modified Debye electron screening to describe fusions in deuterated metals, this screening, however, violates one of the conditions for the validity of Debye screening: the number of particles with the Debye sphere should be larger.

Experiments of Gran Sasso, Bochum, Berlin and Tohoku pose the following question: what kind of plasma is found in the metal matrix? It would be important to compare the entropies and negentropies of the metals and plasmas and their analytical structures: are there any fundamental differences, or are they basically the same?

4. Validity of the Ideal Plasma Model: Comments and Requirements

In this section, we list the conditions under which the concept of the ideal plasma is valid. It is clear that the ideal plasma is an approximated model that describes the environment only in the limit that all of the conditions are verified. The real plasma entropy must contain negative contributions from many-body correlation entropy and quantum effects: these negative contributions constitute the negentropy. For instance, fusion rates in the Sun are often evaluated with a Maxwellian distribution for the relative velocities as expected in an ideal plasma, which however is only an approximation for the solar plasma [45].

Stellar plasmas are neutral plasmas. We call neutral plasma a system of particles that satisfies three conditions: (1) the Debye length is much smaller than the characteristic dimension of the system; (2) $N_{\mathrm{Debye}} \gg 1$, where N_{Debye} is the number of particles within the Debye sphere; (3) the mean time between neutral atom collisions, τ, is much larger than the inverse of the plasma frequency ω: $\omega\tau \gg 1$; otherwise, the system is a neutral gas and not a plasma.

The above-listed conditions imply that: (1) only binary collisions are important in an ideal plasma; (2) if t_{coll} is the typical duration of a collision, $\tau \ll t_{\mathrm{coll}}$, or that collisions are practically instantaneous (no memory effects); (3) correlations are absent in an ideal plasma, which can be described by Markovian dynamics; (4) the plasma parameter Γ, which measures the importance of the interaction energy relative to the kinetic energy, is much smaller than one; (5) the Boltzmann equation is valid and leads to an MB statistical distribution.

In the limit of the ideal plasma, bare thermonuclear fusion reactions are corrected by screening potential energy due to negative electrons and positive ions, energy that effectively can be added to the kinetic energy of the fusing ions and that, following Salpeter, can be calculated with the standard Debye–Hückel (DH) approach. Note that also the positive ions contribute to the DH screening.

Therefore, we need to answer the following questions: (1) Is the solar core plasma an ideal plasma? (2) Are solid or liquid metals with implanted deuterons where d-d fusions might take place ideal plasmas? (3) Is DH screening a good approximation to the environmental contribution to fusion rates in solar plasma, as well as in solid and liquid metals?

The following comments of Cox *et al.* [46], on thermonuclear fusion reactions in stars, are still relevant: "One usually assumes: (1) negligible radiative forces; (2) complete ionization; (3) Maxwellian velocity distributions and the same kinetic temperature for all ions and electrons; (4) diffusion velocities that are much smaller than mean thermal velocities; (5) no magnetic fields; (6) collisions dominated by classical interactions between two point particles; (7) plasma which can be considered dilute gas, *i.e.*, the ideal gas equation of state applies. When the number of particles in a Debye sphere around an ion is not greater than one, Assumption 6 and 7 above are incorrect. Ions are no longer effectively screened from their surrounding and multiple particle collisions and collective effects become important. The classical approach to calculating transport properties of ions using Boltzmann's equation becomes invalid. In the Sun, the number for particles per Debye sphere is only about 1.4 at the base of the convection zone, and 2.2 at the core, so the dilute gas approximation fails".

However, the use of the MB distribution and DH approach is often justified by saying that corrections should only be of a few percent. We pose another question: how well is a non-ideal plasma in (local) thermodynamic equilibrium? In this respect, a modified DH electron screening has been proposed [47].

The state of the art of the electron screening in nuclear fusions in stars has been summarized by Chabrier and Potekhin [48,49]. In addition, Dappen-Mussak [36,37] and Shaviv [50] have criticized the use of the stationary Salpeter screening. Bahacall *et al.* [51], on the other side, have strongly supported the Salpeter approach in stars, but their arguments have also been criticized [52,53].

In light of the above criticisms of the use of the ideal plasma approximation in stars and metals, to which we can add Wallace's [54–56] claim that solid and liquid metals are not plasmas, is the Salpeter approach, repeatedly used to interpret experimental data on nuclear fusion reactions, appropriate? Can some other limit (high density or low temperature) still justify the use of this approach? Can this approach be systematically improved?

5. Nuclear Fusions in Solid Metals

In nature, most fusion nuclear reactions do not take place in a vacuum. Therefore, it is important to examine the effects of the environment on fusion nuclear rates.

We are interested in environments where experimental results on fusion nuclear rates are available: solid and liquid simple metals, where accelerated charged particles of a beam interact with implanted deuterons, producing nuclear fusion and astrophysical stellar plasmas, like the solar core, where light nuclei produce thermonuclear reactions. In such cases, the observed nuclear rates are different from those derived just from screening. These rates can be described in terms of an incident energy larger than the one derived using electron screening. We show that this extra energy can be related to the negative entropy of the system.

Let us consider a solid simple metal, *i.e.*, a metal where electrons are nearly-free, that can be modeled by a collection of rigid ions and by weakly-interacting valence electrons that follow the Fermi statistics. Rigid ions have a closed-shell passive electron core plus active valence electrons that yield binding and excitations. Entropy, a measure of the number of occupied quantum states in the fluctuating equilibrium state, is the quantity of our interest. When interatomic forces are at a sufficiently short range, the cluster expansion for the entropy exists and converges at low density, and the entropy integration constant can be determined. This classical entropy contains the term ($3Nk\ln h$): the Planck constant h signals that states need to be discrete (quantized) in the classical formalism.

The entropy of a crystalline phase is:

$$S^c = S^c_{\mathrm{qh}} + S^c_{\mathrm{an}} + S^c_{\mathrm{el}} + S^c_{\mathrm{ei}} \tag{5}$$

where S^c_{qh} is the quasi-harmonic contribution, S^c_{an} the anharmonic, S^c_{el} the electronic contribution and S^c_{ei} the electron-ion interaction entropy, which often can be neglected.

Since the crystal structure, lattice parameters and average lattice properties can be described in terms of the phonon free energy, the phonon harmonic entropy, S^c_{ph}, can also describe quasi-harmonic entropy S^c_{qh} [56].

At sufficiently high temperatures, the nuclear motion approaches the classical limit and can be evaluated using harmonic lattice dynamics. For a monatomic crystal, the high-temperature expansion for S^c_{qh} (in k units) is:

$$S^c_{\mathrm{qh}} = 3\,N\left[1 - \ln\left(\frac{\theta_0}{T}\right) + \frac{1}{40}\left(\frac{\theta_2}{T}\right)^2 - \frac{1}{2240}\left(\frac{\theta_4}{T}\right)^2 + \ldots\right], \tag{6}$$

where θ_n are the phonon characteristic temperatures, and the leading high-temperature quantum term is:

$$S^c_Q = \frac{3\,N}{40}\left(\frac{\theta_2}{T}\right)^2 \tag{7}$$

In a metal, ion-ion interactions have a range shorter than Coulomb interactions, due to electronic screening. Metals are not high-temperature plasmas: the validity of the standard DH approach, often employed for calculating the effect of screening for nuclear fusions in metals, is questionable.

In a crystal, the quasi-harmonic entropy is positive. The exact non-harmonic contribution to entropy is not easily calculated, but this correction to the harmonic term is very small. The non-harmonic contribution can be extracted from experiment: the average value at the melting point is $S^c_{\mathrm{an}} = 0.06 \pm 0.10$ (in k units); however, values for Ag, Au, Zn and Pb have been reported to be negative, but negligibly small. Given the very small values, these kinds of negative entropy contributions can be safely neglected in our discussion.

Let us now consider the third contribution: the electronic component S^c_{el}. Note that also this contribution is much smaller than S^c_{qh}. The metals of interest are the nearly-free electron metals; therefore, this small positive contribution to the entropy can be evaluated to a good approximation using the expression for a free classical gas:

$$\frac{S^c_{\mathrm{el}}}{N} = \left[\ln\left(\frac{V}{\lambda^3_{\mathrm{th}}}\right) + \frac{3}{2} \right] - [\ln N - 1] = \ln\left(\frac{V}{N\lambda^3_{\mathrm{th}}}\right) + \frac{5}{2}\,, \tag{8}$$

with:

$$\lambda_{\mathrm{th}} = \hbar\sqrt{\frac{2\,\pi}{m\,k\,T}} \tag{9}$$

In the above formula, the first square bracket contains the result for distinguishable particles, while the second square bracket contains the correction that takes into account that electrons are undistinguishable. This correction reduces the classical entropy by $\ln N!$.

If we consider the quantum nature of electrons, which follows the Fermi–Dirac statistics, the entropy per particle becomes:

$$S^c_{\mathrm{el}} = -\int_0^\infty n(\epsilon)\;[f(\epsilon)\,\ln f(\epsilon) + (1 - f(\epsilon))\,\ln(1 - f(\epsilon))]\;d\epsilon\,, \tag{10}$$

with:

$$f(\epsilon) = e^{\beta(\mu-\epsilon)}, \tag{11}$$

and the one-electron energy levels (density of state) are:

$$n(\epsilon) = \frac{3}{2}\,\frac{Z\sqrt{\epsilon}}{\epsilon_{\mathrm{F}}^{3/2}}\,. \tag{12}$$

where Z is the number of electrons per atom.

We see that the entropy S^c_{el} is the sum of a positive and a negative part. The negative contribution is:

$$S^{c-}_{\mathrm{el}} = \int_0^\infty n(\epsilon)\,f(\epsilon)\;\ln(1 - f(\epsilon))\,d\epsilon < 0\,. \tag{13}$$

In a crystal metal, this negative contribution to the entropy of electrons is very small, and consequently, the stored mobilizable energy is small, as well.

6. Fusions in Liquid Metals

Liquid metals are strongly-coupled plasmas; for instance, liquid Li is described as Li^+ ions in a sea of negative electrons. The gas of degenerate conduction electrons forms a strongly-coupled quantum plasma, where the Fermi statistics plays an essential part, while the ions can be described as classical particles with long-range correlations. Ion and electron Debye screening is often derived by using the DH approach [38]. However, in these systems, the interaction energy per particle, U_I, is much larger than the kinetic energy K:

$$\langle U_I \rangle \gg \langle K \rangle \,. \tag{14}$$

Therefore, the question is whether the DH approximation is valid in liquid metals or in metals just below the melting temperature. Regarding this problem, Wallace writes in his book on liquid metals [56]: "Ion-ion interactions at moderate temperatures are of shorter range than Coulomb due to electron screening, so the metal is not a plasma and the DH limit is not the correct high temperature limit. In fact, cluster expansion provides a suitable high temperature limit for liquid metals."

Liquid metals are definitely not ideal plasmas. At room temperature, the electron number density, both in solids and liquids, is in the range $10^{22} \div 10^{23}$ cm^{-3}, much larger than the number densities in gases at standard conditions.

The entropy of a liquid metal is the sum of the small, but not completely negligible, electron and quantum contribution $S^\ell_{\rm el} + S^\ell_Q$, which can be well estimated in the free electron model, plus the ionic contribution that can be expanded in one-particle S^ℓ_1, two-particle S^ℓ_2 and many-particle S^ℓ_x entropies:

$$S^\ell = S^\ell_1 + S^\ell_2 + S^\ell_x + S^\ell_{\rm el} + S^\ell_{\rm Q} \,. \tag{15}$$

The contributions to the entropy of $S^\ell_{\rm el}$ and $S^\ell_{\rm Q}$ are very small, and we can neglect them. Otherwise, the main part of the entropy, the one due to ions, can be written as:

$$S^\ell_1 + S^\ell_2 + S^\ell_x = -\frac{N}{\rho} \int f(p)\, \ln\left(h^3 f(p)\right) dp - \sum_{n=2}^{N} \frac{\rho^n}{n!} \int \cdots \int g^{(n)}(\vec{r})\, \ln g^{(n)}(\vec{r})\, dr_1 \ldots dr_n \,, \tag{16}$$

where $\rho = V/N$ is the particle density, $g^{(n)}(\vec{r})$ is the normalized equilibrium n-particle (of mass M) correlation function and $f(p)$ is the equilibrium Boltzmann distribution:

$$f(p) = \rho \left(\frac{\beta}{2\,\pi\,M}\right)^{3/2} \exp\left(-\frac{\beta\,p^2}{2\,M}\right) . \tag{17}$$

The one-particle contribution to the entropy is the classical entropy of N distinguishable particles:

$$S^\ell_1 = N \left(\frac{3}{2} - \ln(\rho\,\lambda^3)\right) , \tag{18}$$

while the two-body contribution can be approximated as:

$$S^\ell_2 = -\frac{1}{2}\rho \int g(r)\, \ln g(r)\, dr \approx -\frac{1}{2}\rho\, \frac{V}{N} \,. \tag{19}$$

Note that the above equations show that entropies of both liquid and solid metals have negative contributions. The larger negative term is S^ℓ_2. While $S^\ell_x + S^\ell_{\rm Q}$ is also negative, it is much smaller and decrease as temperature increases.

The negative correlation entropy reflects correlations among the particles that induce some order in the liquid metal; in the solid, these correlations are almost absent, the ions being localized on the crystal lattice, and the negative part of the entropy is much smaller.

Any fluctuation near the stable equilibrium causes a negative entropy generation; near a stable stationary state is always expressed by a positive entropy generation.

Let us consider the entropy of a single atom of a liquid metal: its entropy is composed of a positive part, the one-body entropy, S_1^ℓ, and by a negative part $(S_2^\ell + S_x^\ell + S_Q^\ell)$, due to correlations. In addition, the electronic component has also positive and negative contributions, but it is numerically less important, and we shall neglect it for the moment.

A single atom can do work or give up energy to $k\,T\,S^{\ell-}$, where $S^{\ell-}$ is the total negative part of the entropy per atom, whose main contributions are S_2^ℓ and S_x^ℓ. The negative contribution of $S_2^\ell + S_x^\ell$ to the entropy can be interpreted as the correlation order in the system compared to the completely disordered one whose entropy is just the one-body part S_1^ℓ.

The mechanisms can involve a cluster of N atoms increasing the amount of mobilizable energy up to:

$$\mathcal{E} = N\,k\,T\,(S_2 + S_x + S_Q)\ . \tag{20}$$

Let us give some hints about the calculation of the number N of atoms or ions of the cluster or cage. Of course, average evaluations are reported just to show the order of magnitude; detailed results on a wide list of metals will be reported elsewhere. The correlation length L_c, following Wallace [54–56], is proportional to hard sphere diameter d: $L_c = x\,d$, with x of the order of $5 \div 10$ and $d = y\,a_o$, where a_o is the Bohr radius and y a parameter of the order $2 \div 3$. The parameter x depends on the metal and on the kinetic energy or temperature of the atom or ion. Assuming that the cage is a sphere, we take $N = (4/3)\,\pi\,x^3\,d^3\,n$, where n is the number density of the metal. In the case of deuterons in liquid lithium, we have $N \approx 1800$.

The measured cross-sections of the fusion of light nuclei, at very low energy (< 30 keV), in liquid lithium, are higher than the ones calculated in a vacuum. The total screening potential of 520 ± 190 eV that one should use to obtain the experimental rates of the reaction ^{6}Li(d, α)^{4}He is much greater than the prediction of about 70 eV. Furthermore, in gases and solid metals, the reported values of the screening potential are sensibly higher than the prediction. Standard atomic electron screening (DH approach) is not enough to explain the enhancement. The difference of the screening potential for the ^{6}Li(d, α)^{4}He reaction in liquid lithium can be compared to the screening potential of the same reaction in solid lithium (of about 310 eV). The difference of 210 eV can be explained with the help of the two-body correlation entropy (negative entropy), the same as can be used in evaluating the metal melting entropy.

The deuteron travels in the liquid lithium with a cage of N correlated ions that transfer the energy $\mathcal{E}$ of Equation (20) to the deuteron kinetic energy. The quantity $\mathcal{E}$ is about 210 eV if $N = 1800$, being $S_2 = -2.48$ eV as calculated in [57]. This is the required quantity that is in addition to energy effects due to electron screening and stopping power in order to quantitatively explain the experimental rates.

Other liquid metals of interest, due to large value of S_2, are In and Hg. We may argue that also for these metals, N is about the same order of magnitude as for lithium.

The two-body correlation energy is −3.39 eV for indium and −3.97 eV for mercury. Experiments of the fusion of deuterons inserted and traveling in the liquid and solid phase of these two metals should provide the validity of the proposed mechanism.

In conclusion, the mechanism proposed in this section explains the large liquid-solid difference of the effective screening potential that parameterizes the cross-section increment.

7. Fusion in Plasmas

In the previous section, we have shown that liquid metals have larger negative entropies, $[-(S_2^\ell + S_X^\ell + S_Q^\ell)]$, than solid metals because of the larger many-body correlations and that this larger negentropy can explain why in liquid metals the effective screening energy for the nuclear fusion reaction is about 300 eV higher than in solid metals.

In this section, we want to examine thoroughly the possibility that also stellar plasmas have negentropy contributions related to many-body correlations and that this negentropy could provide additional free energy to fusion reactions. This mechanism would increase the fusion rates above those expected by standard screening by a factor that could be large if this mobilizable energy is collected from many neighbor ions in the plasma.

The standard plasma enhancement of nuclear fusion rates is evaluated by means of the Salpeter static approach that modifies the two-body probability distribution at $r = 0$. This enhancement is equal to the difference of the excess free energy of the plasma before and after the reaction $[F_{\rm ex}(N_1, N_2, N_e) - F_{\rm ex}(N_1 - 2, N_2 + 1, N_e)]$, where $F_{\rm ex}$ is the excess free energy of a binary plasma composed by N_1 ions of Type 1, N_2 ions of Type 2 and N_e electrons, after fusion of two ions of Type 1 into an ion of Type 2 $N_1 \to N_1 - 2$ and $N_2 \to N_2 + 1$. Over the years, this excess free energy $F_{\rm ex}$ has been extensively studied and evaluated by many authors with different approaches [36,58–61].

Negentropy gives a positive contribution to the free energy [5]. From the relation $F = (U + p\,V) - k\,T\,(S^+ - S^-)$ and assuming that $F = F^+ - F^-$, we have that $(N_1 + N_2 + N_e)\,k\,T\,S^- = F^+ - (U + p\,V)$ and $F^- = (N_1 + N_2 + N_e)\,k\,T\,S^+$, where $k\,T\,S^-$ is the quantity of energy per ion that can be transferred at constant p and T. It is used to calculate the free energy F of a stellar plasma in deriving its equation of state: positive contributions (if any) to F have corresponding negentropy terms. The quantity $k\,T\,S^-$ is the average energy stored and mobilizable in the environment per single ion. This energy can be transferred to another ion: an ion can collect in principle this mobilizable energy from the N ions encountered during its collision mean free path $L_{ii} = 1/(\sigma_{ii} n_i)$ from one elastic Coulomb collision to another. The number $N = \pi\,d^2\,L_{ii}\,n_i$, where d is the range of ion-ion interaction, σ_{ii} the Coulomb cross-section and n_i the number density.

The total free energy of the system is often expressed as:

$$F = F^i_{\rm id} + F^e_{\rm id} + F_{\rm rad} + F_{\rm ex}\,, \tag{21}$$

where $F^i_{\rm id}$ is the ideal free energy of ions, $F^e_{\rm id}$ those of electrons, $F_{\rm rad}$ is the radiation free energy and $F_{\rm ex}$ is the excess free energy arising from non-ideal effects and:

$$F_{\rm ex} = F_C + F_{\rm neut}\,, \tag{22}$$

with:

$$F_C = N\,k\,T\,[N_e\,f_{ee} + N_i\,(f_{ii} + f_{ie})]\,, \tag{23}$$

and $N = N_i + N_e$. In Equation (23), f_{ii}, f_{ee}, f_{ie} are the reduced free energies, and $F_{\rm neut}$ is the free energy of neutral particles.

In almost all of the published papers, the analytical expression of F is derived from minimizing the partition function. The free energy is negative by definition, although we are interested in the positive contributions that come from correlations, and is related to negentropy. For instance, the expression for F given by Rogers *et al*. [60] has a positive contribution coming from DH screening:

$$F^{DH} = \frac{N\,k\,T}{12\,\pi\,n\,\lambda_D^3}\,, \tag{24}$$

where λ_D is the Debye screening length. Therefore, the negentropy for the core solar plasma described in [60], related to the free energy Equation (24), gives $k\,T\,S^- \approx 9.5$ eV per ion.

In a weakly-coupled plasma, positive contributions to the excess free energy F_{ex} can be found going beyond a random-phase approximation, as was done by Ichimaru and Kitamura [58]. These authors derive the expression:

$$\frac{F_{\rm ex}(N_1,\,N_2,\,N_e)}{(N_1+N_2)\,k\,T} = f_{\rm ex}(N_1,\,N_2,\,N_e) = -\frac{\Gamma^{3/2}}{\sqrt{3}} - \frac{\Gamma^3}{2}\left(\frac{3}{4}\ln(3\,\Gamma) + \gamma - \frac{11}{12}\right)\,, \tag{25}$$

where Γ is the effective plasma parameter and $\gamma = 0.57721$ is the Euler constant. The first and second terms of the above equation are the RPAand the non-RPA contributions, respectively.

The effective Coulomb coupling parameter for the solar interior is $\Gamma = 0.0737$, being $\rho = 148\ \mathrm{g/cm^3}$, $T = 1.36$ keV, hydrogen mass fraction $X_1 = 0.34$, helium mass fraction $X_2 = 1 - X_1 - X_3$, where $X_3 = 0.02$ is the mass fraction of heavy elements. Then, from Equation (25), we have $f_{\rm ex} = -0.011552\,(\mathrm{RPA}) + 0.000294\,(\mathrm{non-RPA})$.

The positive non-RPA term is about 2.5% of the RPA term. Therefore, for the solar core, the energy stored and mobilizable by a single ion is about:

$$k\,T_c\,S^- = n\,k\,T_c\,f_{\rm ex} = 0.4\,eV\,. \tag{26}$$

In the p-p reaction rates, for the case of pure hydrogen matter ($X_1 = 1$), we have $\Gamma = 0.0438$ and $f_{\rm ex} = -0.005292 + 0.001785$. This time, the non-RPA positive contribution is 33.7% of the RPA contribution. The stored and mobilizable energy per ion by negentropy S^- is:

$$k\,T_c\,S^- = n\,k\,T_c\,f_{\rm ex} = 2.5\,eV\,. \tag{27}$$

It is therefore necessary that a few tens (hundreds) of ions transfer stored energy to a colliding ion to increase the corresponding effective screening energy of some tenths (hundreds) of eV.

The evaluation of the number of effective ions in the cage N can follow the lines indicated above. Just to give the order of magnitude, we report that a hydrogen ion in the solar core plasma, considering an average number density, can receive, between two elastic Coulomb collisions, an added energy of a few hundred eV from a few hundred ions. Detailed evaluations and a comparison to existing data for the solar core are in progress and will be reported elsewhere.

In summary, negentropy contributions, related to the many-body correlation entropy, give a mechanism that can increase the standard screening energy of two nuclei reacting in a stellar plasma. This mechanism is equivalent to increasing the kinetic energy of the colliding nuclei, without affecting the total energy of the plasma and increasing nuclear fusion rates.

Moreover, let us summarize with some more details. If we suppose the total entropy S is given by the positive contribution only, $S = S^+$, then the fusion cross-sections are the standard well-known ones, at the fixed energy of the incident beam (in the metal matrix experiments), or at an average energy given by the temperature (in the stellar plasmas). The fusion rates can be evaluated by means of the MB energy-momentum distribution. All of the effects of the environment over the cross-sections are added through multiplicative factors, as the electron screening effect.

When, on the other hand, $S = S^+ - S^-$, then the fusion reactions take place at an energy usually greater than in the standard case (except for environments with retarding effects, if any). Let us consider the sub-system composed of ions or nuclei in a plasma environment. These particles, that react through a nuclear fusion, attempt to modify their environment (solid or liquid metal, stellar plasma) for their own needs by creating what for them is order (a new system, *i.e.*, heavier nucleus, composed of the previous two). The two nuclei keep energy from the environment through negentropy. The effective cross-section is the one that is measured (and must be evaluated) at a higher energy than in a vacuum. The entropy of the final nucleus is smaller than the sum of the two entropies of the fusing nuclei. The source of negative entropy is the sum of many-body correlations among particles of the environment. Greater is the negative contribution to entropy due to many-body particle correlations and higher is the energy of the fusing nuclei, and therefore, the cross-section depends on the negative entropy. The rates depend on the energy-momentum distribution function and, due to the presence of correlations, differ from the standard MB rates.

8. Conclusions

The entire entropy of a solid or liquid metal and of an astrophysical stellar plasma is an elaborated expression sum of many different positive and negative contributions from ions and electrons and their interactions. These entropies can be derived from direct calculations with expansion (usually to second order) in terms of a small parameter of the free energy of many-body classical and quantum systems, starting from the partition function. Different approaches include RPA and non-RPA calculations.

The entropy and free energy of an ensemble are related by well-known thermodynamics relations. In particular, the positivity of the total entropy of an ensemble corresponds to the negativity of the total free energy. Negative contributions to the total entropy, which is positive, come from correlations that reduce disorder in the system; examples can be found in the quantum correlations in the nearly free electron gas in solid metals, in the negative many-body correlations in liquid metals or in the non-RPA contribution to the entropy of an astrophysical stellar plasma. The free energy of an ideal non-relativistic classical plasma has only negative terms; therefore, negentropy is not to be considered under the assumption that the solar core is an ideal plasma. However, at very low temperatures, when the quantum effects of ion motion become important, the ideal plasma hypothesis could fail, and positive free energy contributions appear. In fact quantum effects, such as the Pauli principle for electrons, produce order in the system with the associated negative entropy. In the ideal plasma, the terms f_{ii}, f_{ee}, f_{ie} represent each a negative excess free energy. In non-ideal plasma, where correlations among plasma particles depending on all types of interactions are active, positive free energy contributions can be found, and negative entropy contributions should be considered.

This work draws attention to the role of these negative entropy contributions in several physical processes. The physical sources of these terms are the many-body interactions or correlations, or the non-linear or quantum effects.

Negentropy is related to the stored mobilizable energy per particle, $N\,k\,T\,S^{-}$, that can be transferred and occasionally reabsorbed. Many single components of the system (ions and electrons) can collectively transfer this energy to a single ion during its mean free path between elastic Coulomb collisions. If the two-particle distribution probability, at $r = 0$, is above a given threshold, the two ions (nuclei) can have a non-negligible probability to undergo a nuclear fusion reaction. Implanted deuterons and the incoming deuteron of an accelerated beam react in a liquid metal with an effective screening potential higher than in solid metal. In liquid metal, the about 300 eV energy difference in the screening potential between solid and liquid metal at temperatures just above melting can be explained by the energy $k\,T\,S_2^{-}$ coming from negentropy (negative two-body correlation entropy) of the liquid metal. In astrophysical plasmas, negentropy has a similar effect on the reacting nuclei.

The role of negentropy and its relation to many-body correlation entropy has been extensively explored and exploited in biophysics; this work starts to apply this concept to fields related to the microscopic quantum matter, but more needs to be done.

When considering fusion nuclear reactions not in a vacuum, as for instance in solid or liquid metals or stellar plasmas, the system must be considered as the sum of the relevant sub-systems, such as the reacting nuclei within their environment. The net effect of the environment on nuclear fusion rates is often easily estimated by the stationary Salpeter approach, which is valid in the appropriate contexts. However, the Salpeter approach is not sufficient in the many important physical applications, when two- and many-body correlations are not negligible and give important contributions to the entropy. These correlations, related to the negative contributions to the entropy (negentropy), determine the stored mobilizable energy, an energy that can be transferred to the nuclei participating to the nuclear reaction. In the case of fusing ions, an ion could gain the energy from at most the correlated ions in the path between two Coulomb elastic collisions.

Author Contributions: All authors performed the theoretical calculations, discussed the results, prepared the manuscript and commented on the manuscript at all stages. All authors have read and approved the final manuscript.

Conflicts of Interest: The authors declare no conflict of interest.

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