

Maximization of nuclear fusion reactivity via optimal energy distributions

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(Received 18 June 2026; accepted 2 October 2026; published 23 October 2026)

We investigate the optimization of nuclear fusion reactivity relative to the choice of energy probability distribution. A single Maxwell-Boltzmann (MB) distribution is found to be optimal in the region where reactivity is a concave function of the average available kinetic energy, specifically near the reactivity peak. Conversely, in regions where the reactivity curve is convex, optimization is achieved through a bimodal MB distribution. We then discuss our results in the context of three classes of generalized energy distributions (superstatistics), which are modeled as a continuum of MB distributions. As expected, in all cases examined, the reactivity gains provided by superstatistics are bounded by the proposed optimal distribution. Finally, we apply these findings to deuterium-deuterium and deuterium-tritium fusion processes using empirical parametrizations of their respective cross sections. For both reactions, employing optimal bimodal MB distributions at low average energies—of particular interest for magnetically confined plasmas—yields a reactivity enhancement of approximately a factor of 2.

DOI: [10.1103/xhzy-hxdw](https://doi.org/10.1103/xhzy-hxdw)

I. INTRODUCTION

The production of nonintermittent energy with low levels of air and water pollution is an important goal of science and technology in the first half of the 21st century. In this context, the most promising approach seems to be nuclear fusion, with the potential to significantly improve desirable features with respect to nuclear fission, the latter being a source of energy production since the 1950s. In addition, nuclear fusion studies play a crucial role in understanding complex nonlinear systems in general and plays a crucial role in a variety of processes in astrophysics, most notably stellar evolution and primordial nucleosynthesis. Efforts are ongoing to reach breakeven in the most promising case of deuterium-tritium (DT) fusion [1,2], in spite of the complications related to the need to produce and maintain enough levels of radioactive tritium. Next to this, deuterium-deuterium (DD) fusion processes have the advantages, with respect to DT, of widespread availability in water, a greater share of the energy self-igniting the reaction, and less damage induced by the emitted neutrons due to their lower energy, which also implies lower levels of environmental radioactivity. The biggest bottleneck for DD fusion is the fusion cross section, which peaks at a value

2 orders of magnitude lower than the corresponding peak for DT fusion, with its peak also occurring at much higher temperature.

While current efforts focused on DT fusion using magnetic confinement aim at increasing plasma volume or its density, it may also be worth discussing a possible path in which new physical effects are identified to catalyze DD fusion, hopefully recovering the 2 orders of magnitude gap in its cross section by boosting fusion reactivity [3]. With this goal in mind, some assumptions usually used in the evaluation of the dynamics of fusion processes have been scrutinized. For instance, the dependence of tunneling processes on the use of plane waves and Gaussian wave packets for the colliding ions in a thermonuclear reaction was analyzed [4]. There are no ideal plane waves in nature, and more specifically, this approximation is rather questionable in the case of confined gases because of both the size of the confinement of each individual ion and the presence of ion-ion and ion-electron scattering limiting the mean free path. In order to discriminate discrepancies due to the use of the Wentzel-Kramers-Brillouin approximation and its variants, the discussion has been framed within an exactly solvable potential [5]. Sensible differences in the tunneling coefficient and reactivities have been observed depending on the width of the Gaussian wave packet, as well as the temperature and the effective mass of the scatterers. This result for the parametrization of the fusion reaction via the Gamow factor typically used in astrophysics [6].

Furthermore, the assumption of an ideal thermal equilibrium related to Maxwell-Boltzmann (MB) distributions has been repeatedly challenged [3,7–18]. Indeed, maximizing fusion reactivity also implies the discussion of potential advantages in using energy distributions in which the high

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energy tail does not fall quickly at high energy like in the case of MB distributions due to their asymptotic exponential dependence on energy, in spite of the possible limitations due to the replenishing of the high energy tail if it is operated in a continuous mode [19]. In particular, attention has been focused on energy probability distributions representing generalizations of Lorentzian distributions, also named kappa (or κ) distributions [20]. These energy distributions were empirically discovered by fitting the data of electrons in space plasmas and then gained more foundational ground in the framework of nonextensive statistical mechanics [21,22]. Some examples of reactivity gain using κ distributions with respect to their MB counterparts were discussed in Ref. [15], including the case of Gaussian states. In the same contribution, the robustness of the results with respect to the choice of the potential barrier was also scrutinized.

Here, we extend the considerations reported in Ref. [15] to identify general conditions for the energy distribution required to optimize reactivity. Rather than assuming a specific non-Maxwellian distribution, we consider a general picture in which the system is described as a continuous mixture of MB distributions at different temperatures. This approach is well suited to systems that are locally in equilibrium but globally out of equilibrium. In such conditions, the system can be partitioned into small cells, each relaxing rapidly to a local MB distribution, while at larger scales the inverse temperature β fluctuates from cell to cell according to the distribution $f(\beta)$. This description has proven highly successful in capturing observed distributions across a wide range of physical [23–28] and nonphysical systems [29–31], which typically decay more slowly than the MB distribution, thereby opening the possibility of identifying temperature fluctuations that optimally enhance reactivities.

This paper is organized as follows. In Sec. II, we recall the formalism introduced in previous work [4,15] to incorporate generalized kinematic conditions for both the energy distribution of the particle ensemble and the momentum distribution of a single particle with a given energy. We also present the expression for the most general ensemble distribution as a continuous mixture of MB distributions with a normalized weight function $f(\beta)$. In Sec. II A, we establish the conditions under which $f(\beta)$ optimizes reactivity. This optimization is straightforward when the target reactivity is globally concave; applying Jensen’s inequality [32] demonstrates that the standard MB energy distribution is the optimal solution. However, physical constraints dictate that the reactivity cannot be concave everywhere, as it rapidly drops to zero at both low and high energies. Consequently, a more refined analysis is required, which is detailed in Sec. II B. Section III discusses the relationship between our optimization results and three classes of generalized energy distributions known as superstatistics. In Sec. IV, the results of Secs. II and III are applied to DT and DD fusion processes using the parametrization of the cross-section data described in Ref. [33], highlighting the advantages of employing the optimized distribution. Finally, concluding remarks on the applicability of our findings to optimizing fusion processes in magnetically confined plasmas are presented in Sec. V.

II. REACTIVITY FOR GENERALIZED KINEMATIC CONDITIONS

We start by summarizing results already discussed in Refs. [4,15] for reactivities evaluated using the scattering of ions and specifying the notation. The discussion is focused on, but not limited to, the simplest one-dimensional case for which we used analytical expressions for tunneling coefficients. The generalization to the three-dimensional case is, formally at least, straightforward.

The mutual scattering of ions at a characteristic momentum $\hbar K$ is well described by a stationary wave function $\psi_K(x)$, which is shaped by the mutual nuclear tunneling potential. While the standard approach involves plane waves, more general situations can arise and often offer clearer physical insight. For instance, $\psi_K(x)$ can be represented by a wave packet, such as the Gaussian wave packet considered in Ref. [4]. It is convenient to work in the reciprocal space k by writing the ionic wave function in terms of its Fourier transform $\varphi_K(k)$,

$$\psi_K(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \varphi_K(k) e^{ikx} dk, \quad (1)$$

which shows that $\psi_K(x)$ is a superposition of plane waves with wave vectors $k \in (-\infty, +\infty)$ distributed according to the probability density $P_K(k) = |\varphi_K(k)|^2$. With the choice $\psi_K(x) = [2/(\pi\xi^2)]^{1/4} e^{-(x-x_0)^2/\xi^2 + iKx}$, we have

$$P_K(k) = \frac{\xi}{\sqrt{2\pi}} e^{-\xi^2(k-K)^2/2}. \quad (2)$$

Note that these Gaussian wave packets have mean momentum $\langle \hbar k \rangle = \hbar K$ and mean kinetic energy $\langle \hbar^2 k^2 / (2m) \rangle = \hbar^2 (K^2 + \xi^{-2}) / (2m)$, the case of a pure plane wave with wave vector K being recovered for $\xi \rightarrow \infty$ when $P_K(k) \rightarrow \delta(k - K)$.

As stated, the above description applies to the case of monoenergetic ions with characteristic momentum $\hbar K$, which may occur in ion beams. In reality, especially for thermonuclear plasmas, the wave vector K should be considered a real parameter drawn from a statistical distribution $w(K)$ corresponding to some classical ionic setup. Thus, regarding $P_K(k)w(K)$ as the joint probability distribution of the wave vectors k and K allows us to consider fusion processes taking place in a statistical ensemble of nuclei represented by Gaussian wave packets with an arbitrary distribution of their mean momenta.

In the context of thermonuclear fusion, ions are usually assumed to follow a MB energy distribution. Accordingly, for $w(K)$ we take the following MB probability density, normalized to unity for $K \in (-\infty, +\infty)$:

$$w_{\text{MB}}(K; \beta) = \left(\frac{\beta}{\pi} \frac{\hbar^2}{2m} \right)^{1/2} e^{-\beta \hbar^2 K^2 / (2m)}. \quad (3)$$

As usual, $\beta = (k_B T)^{-1}$ is the inverse temperature characterizing the MB distribution, and m is the reduced mass of the two ions, a and b , involved in the fusion reaction, namely, $m = m_a m_b / (m_a + m_b)$.

An intensive measure of the reaction rates is provided by the reactivity $\langle \sigma(E) v(E) \rangle$, where $\langle \cdot \rangle$ denotes the average over the statistical distribution of the reactants, $\sigma(E)$ is the cross section of the process, and $v(E)$ is the velocity of the reduced

ion. In one dimension and for nuclei at energy $E = mv^2/2 = \hbar^2 k^2/(2m)$, the cross section is [34] $\sigma(E) = T(E)\pi/k^2$, and

$$\sigma(E)v(E) = \frac{\pi \hbar^2}{\sqrt{2m^3}} \frac{T(E)}{\sqrt{E}}. \quad (4)$$

For a statistical ensemble of nuclei as described above in terms of the wave vectors k and K , the reactivity must be averaged over the joint probability distribution $P_K(k)w(K)$:

$$\langle \sigma v \rangle = \frac{\pi \hbar^2}{\sqrt{2m^3}} \int_{-\infty}^{+\infty} dk \int_{-\infty}^{+\infty} dK \frac{T(E(k))}{\sqrt{E(k)}} P_K(k)w(K), \quad (5)$$

where $E(k) = \hbar^2 k^2/(2m)$.

In the case of Gaussian wave packets with mean momenta MB distributed at inverse temperature β , that is, for $P_K(k)w(K)$ given by (2) and (3), the integral over K in (5) can be performed by reducing the reactivity to the simpler expression

$$\langle \sigma v \rangle_{\text{MB}}(\beta) = \sqrt{\frac{\pi}{2}} \frac{\hbar \xi_{\text{eff}}}{m} \int_{-\infty}^{+\infty} dk \frac{T(E(k))}{k} e^{-\xi_{\text{eff}}^2 k^2/2}, \quad (6)$$

where $\xi_{\text{eff}}^{-2} = \xi^{-2} + m/(\beta \hbar^2)$. In the limit $\xi^2 \gg \beta \hbar^2/m$, i.e., for wave packets approximating a plane wave, the effective positional spreading becomes the De Broglie thermal wavelength $\xi_{\text{eff}} \simeq (\beta \hbar^2/m)^{1/2}$. In the opposite limit of spatially narrow wave packets, $\xi^2 \ll \beta \hbar^2/m$, we have $\xi_{\text{eff}} \simeq \xi$. Note that, even if we prepare the ions in states with positional variance of a quantum nature, at high enough temperatures, the relevant length scale below which quantum coherence is maintained no longer depends on the initial preparation, a result confirming earlier discussions [35,36].

A natural question is how the averaged reactivity (5) is affected by the distribution $w(K)$. For a MB distribution at a fixed inverse temperature β_0 , specifically, $w(K) = w_{\text{MB}}(K; \beta_0)$, we already obtained the result (6) with $\xi_{\text{eff}}^{-2} = \xi^{-2} + m/(\beta_0 \hbar^2)$. Here, we explore the most general case of a K distribution derived as a continuous mixture of MB distributions at any possible inverse temperature β :

$$w_f(K) = \int_0^\infty d\beta f(\beta; \beta_0) w_{\text{MB}}(K; \beta). \quad (7)$$

This distribution is fully characterized by a normalized weight function $f(\beta)$, with $\beta \geq 0$. More precisely, we specify that $f(\beta) = f(\beta; \beta_0)$ also includes a parametric dependence on $\beta_0 \geq 0$ to fairly compare it with the MB distribution at that inverse temperature. In fact, while for $f(\beta; \beta_0) = \delta(\beta - \beta_0)$ we have $w_f(K) = w_{\text{MB}}(K; \beta_0)$, for $f(\beta; \beta_0)$ to be a smooth function of β we require that the mean energy of $w_f(K)$ is equal to the mean energy of $w_{\text{MB}}(K; \beta_0)$. Recalling that the mean energy of a MB distribution at inverse temperature β amounts to $1/(2\beta)$, we conclude that $f(\beta; \beta_0)$ can be arbitrary as long as it is subject to the constraints

$$\begin{aligned} f(\beta; \beta_0) &\geq 0, \\ \int_0^\infty d\beta f(\beta; \beta_0) &= 1, \\ \int_0^\infty d\beta f(\beta; \beta_0) \frac{1}{2\beta} &= \frac{1}{2\beta_0}. \end{aligned} \quad (8)$$

A. Optimization for a concave reactivity

According to Eq. (5) and using the result (6), the average reactivity associated with the distribution (7) reduces to the following functional of $f(\beta; \beta_0)$:

$$\begin{aligned} \langle \sigma v \rangle_f(\beta_0) &= \frac{\pi \hbar^2}{\sqrt{2m^3}} \int_{-\infty}^{+\infty} dk \int_{-\infty}^{+\infty} dK \frac{T(E(k))}{\sqrt{E(k)}} P_K(k)w_f(K) \\ &= \int_0^\infty d\beta f(\beta; \beta_0) \langle \sigma v \rangle_{\text{MB}}(\beta). \end{aligned} \quad (9)$$

We seek to maximize the value of $\langle \sigma v \rangle_f(\beta_0)$ with the constraints (8) and compare the gain with respect to the MB average reactivity $\langle \sigma v \rangle_{\text{MB}}(\beta_0)$ at the same average energy $1/(2\beta_0)$. In the following, we will use $0 < \beta < \infty$ as the domain of $f(\beta; \beta_0)$ even if the support for this function is physically restricted to a finite interval $[\beta_{\text{min}}, \beta_{\text{max}}]$.

Based on the above statements, we are dealing with a constrained linear variational problem which is conveniently recast as a constrained probabilistic functional problem, namely, finding the probability density function (PDF) $f(\beta; \beta_0)$ such that

$$\begin{aligned} \mathbf{E}_f[\langle \sigma v \rangle_{\text{MB}}(\beta)] &\text{ is maximum,} \\ \mathbf{E}_f[\beta^{-1}] &= \beta_0^{-1}, \end{aligned} \quad (10)$$

where $\mathbf{E}_f(\cdot) = \int_0^\infty d\beta f(\beta; \beta_0)(\cdot)$ is the expectation induced by the PDF $f(\beta; \beta_0)$. It is easier if we rewrite the second equation of (10) as a condition involving a moment of first order. To this end, we change the variable $\beta = u^{-1}$ and define $p(u; u_0) = u^{-2} f(u^{-1}; u_0^{-1})$, where $u_0^{-1} = \beta_0$. Probability is conserved, $f(\beta; \beta_0) d\beta = -p(u; u_0) du$. In terms of the new PDF $p(u; u_0)$ and the assigned function $h(u) = \langle \sigma v \rangle_{\text{MB}}(u^{-1})$, the problem (10) becomes, for a given value of u_0 , the search for the PDF $p(u; u_0)$ such that

$$\begin{aligned} \mathbf{E}_p[h(u)] &\text{ is maximum,} \\ \mathbf{E}_p[u] &= u_0, \end{aligned} \quad (11)$$

where $\mathbf{E}_p(\cdot) = \int_0^\infty du p(u; u_0)(\cdot)$ is the expectation induced by $p(u; u_0)$. Note that $u(u_0)$ are twice the mean energy of a MB average reactivity at inverse temperature $\beta(\beta_0)$ and $h(u)$ is nothing but the MB average reactivity as a function of the thermal energy $u = k_B T = \beta^{-1}$.

Problem (11) falls within the class of the so-called generalized moment problems [37], more exactly, the sharp bounds on expectations [38,39], and its solution depends on the shape of $h(u)$ and, of course, the value of the parameter u_0 .

Let us assume that the domain of $h(u)$ is $(u_{\text{min}}, u_{\text{max}})$, possibly with $u_{\text{min}} = 0$ and $u_{\text{max}} = \infty$. If $h(u)$ is concave everywhere in its domain, the following Jensen inequality then applies for any $u \in (u_{\text{min}}, u_{\text{max}})$:

$$\mathbf{E}_p[h(u)] \leq h(\mathbf{E}_p[u]) = h(u_0). \quad (12)$$

The max of $\mathbf{E}_p[h(u)]$ is thus obtained by concentrating the PDF at point u_0 , namely,

$$p(u; u_0) = \delta(u - u_0). \quad (13)$$

Note that the constraint $\mathbf{E}_p[u] = u_0$ is satisfied and p is correctly normalized.

B. Reactivity with concave and convex regions

In general, $h(u)$ is not concave everywhere, and the solution of the problem (11) requires the introduction of its concave envelope $\hat{h}(u)$, namely, the tightest concave function lying above or on $h(u)$. It is easy to visualize $\hat{h}$ as a rubber band stretched over h (see Fig. 4 below). In fact, according to Carathéodory's theorem [40] applied to moment space, any valid expectation vector $(E[u], E[h(u)])$ lies on the concave envelope of the curve $\{(u, h(u)) : u \in (u_{\min}, u_{\max})\}$ and can be represented by a discrete probability measure with finite support. Specifically, since the constraint is given here by a moment of order 1 (the mean), the optimal PDF $p(u; u_0)$ is supported by at most two points.

Let $\hat{h}(u)$ be the smallest continuous concave function such that $\hat{h}(u) \geq h(u)$ for any $u \in (u_{\min}, u_{\max})$. This concave envelope is easily visualized in one dimension as the rubber band connecting the points $(u_{\min}, h(u_{\min}))$ and $(u_{\max}, h(u_{\max}))$ stretched over the h function's local maxima. Depending on the value of u_0 in $(u_{\min}, u_{\max})$, there are two different types of solutions $p(u; u_0)$ of (11).

If u_0 is in a range such that $\hat{h}(u_0) = h(u_0)$, namely, in the proximity of the maxima of $h(u)$ where this function is concave, then we have

$$p(u; u_0) = \delta(u - u_0), \quad (14)$$

the normalized distribution which, as we have already seen, maximizes the expectation of $h(u)$ satisfying, at the same time, the constraint on the average of u .

If u_0 is in a range, say, $u_1 \leq u_0 \leq u_2$ with $\hat{h}(u_1) = h(u_1)$, $\hat{h}(u_2) = h(u_2)$, and $\hat{h}(u) > h(u)$ for $u_1 < u < u_2$, it is more convenient to concentrate the probability at the end points u_1 and u_2 . To explain this behavior, we start observing that

$$E_p[h(u)] \leq E_p[\hat{h}(u)]. \quad (15)$$

Since $\hat{h}(u)$ is the function growing linearly from $(u_1, h(u_1))$ to $(u_2, h(u_2))$, namely,

$$\hat{h}(u) = h(u_1) + [h(u_2) - h(u_1)] \frac{u - u_1}{u_2 - u_1}, \quad u_1 \leq u \leq u_2, \quad (16)$$

for the linearity we have $E_p[\hat{h}(u)] = \hat{h}(E[u]) = \hat{h}(u_0)$, and we conclude that for any $u_0 \in [u_1, u_2]$

$$E_p[h(u)] \leq \hat{h}(u_0) = \frac{u_2 - u_0}{u_2 - u_1} h(u_1) + \frac{u_0 - u_1}{u_2 - u_1} h(u_2). \quad (17)$$

The max of $E_p[h(u)]$ is achieved when expression (17) holds with equality, i.e., when $p(u; u_0)$ concentrates the mass at u_1

and u_2 ,

$$p(u; u_0) = w_1 \delta(u - u_1) + w_2 \delta(u - u_2), \quad (18)$$

with weights

$$w_1 = \frac{u_2 - u_0}{u_2 - u_1}, \quad w_2 = \frac{u_0 - u_1}{u_2 - u_1}. \quad (19)$$

The PDF (18) is correctly normalized and satisfies the constraint $E_p[u] = u_0$. It only remains to discuss the nature of the end points u_1 and u_2 . Bearing in mind the rubber band analogy, there are four possible cases. We may have $u_1 = u_{\min}$ and $u_2 = u_{\max}$ or the two cases in which just one end point coincides with one end point of the domain,

$$u_1 = u_{\min}, \quad u_2 \text{ such that } h'(u_2) = \frac{h(u_2) - h(u_1)}{u_2 - u_1}, \quad (20)$$

$$u_1 \text{ such that } h'(u_1) = \frac{h(u_2) - h(u_1)}{u_2 - u_1}, \quad u_2 = u_{\max}, \quad (21)$$

or, last, $u_{\min} < u_1 < u_2 < u_{\max}$ determined by the bitangent condition

$$h'(u_1) = \frac{h(u_2) - h(u_1)}{u_2 - u_1} = h'(u_2). \quad (22)$$

Let us specialize the above general scheme to the case $h(u) = \langle \sigma v \rangle_{\text{MB}}(k_B T)$. For physical reasons, the MB reactivity is not concave everywhere [4]; it must vanish faster than linearly at small and large temperatures and reach a finite maximum value at an intermediate temperature. It follows that $h(u)$ is a bounded continuous function going from being convex to concave and then convex again in the domain $(u_{\min}, u_{\max})$. We thus divide this domain into three regions: the left region where $\hat{h}(u) > h(u)$ with end points

$$u_1^{(l)} = u_{\min}, \quad u_2^{(l)} \text{ such that } h'(u_2^{(l)}) = \frac{h(u_2^{(l)}) - h(u_1^{(l)})}{u_2^{(l)} - u_1^{(l)}}, \quad (23)$$

the right region where $\hat{h}(u) > h(u)$ with end points

$$u_1^{(r)} \text{ such that } h'(u_1^{(r)}) = \frac{h(u_2^{(r)}) - h(u_1^{(r)})}{u_2^{(r)} - u_1^{(r)}}, \quad u_2^{(r)} = u_{\max}, \quad (24)$$

and the remaining central region where $\hat{h}(u) = h(u)$. The concave envelope of $h(u)$ is the stepwise function

$$\hat{h}(u) = \begin{cases} \frac{u_2^{(l)} - u}{u_2^{(l)} - u_{\min}} h(u_{\min}) + \frac{u - u_{\min}}{u_2^{(l)} - u_{\min}} h(u_2^{(l)}) & u_{\min} < u < u_2^{(l)}, \\ h(u) & u_2^{(l)} \leq u \leq u_1^{(r)}, \\ \frac{u_{\max} - u}{u_{\max} - u_1^{(r)}} h(u_1^{(r)}) + \frac{u - u_1^{(r)}}{u_{\max} - u_1^{(r)}} h(u_{\max}) & u_1^{(r)} < u < u_{\max}. \end{cases} \quad (25)$$

Note that in Eq. (25) we are left with the simple task of determining the two points $u_2^{(l)}$ and $u_1^{(r)}$ from the values of $h(u)$ and its first derivative $h'(u)$, which we can consider known, at least numerically, at any point u .

In conclusion, according to (14) and (18), the optimal PDF $p_{\text{opt}}(u; u_0)$ solution of problem (11) is

$$p_{\text{opt}}(u; u_0) = \begin{cases} \frac{u_2^{(l)} - u_0}{u_2^{(l)} - u_{\min}} \delta(u - u_{\min}) + \frac{u_0 - u_{\min}}{u_2^{(l)} - u_{\min}} \delta(u - u_2^{(l)}) & u_{\min} < u_0 < u_2^{(l)}, \\ \delta(u - u_0) & u_2^{(l)} \leq u_0 \leq u_1^{(r)}, \\ \frac{u_{\max} - u_0}{u_{\max} - u_1^{(r)}} \delta(u - u_1^{(r)}) + \frac{u_0 - u_1^{(r)}}{u_{\max} - u_1^{(r)}} \delta(u - u_{\max}) & u_1^{(r)} < u_0 < u_{\max}. \end{cases} \quad (26)$$

Let $h_{\text{opt}}(u_0)$ be the optimal average reactivity corresponding to the above optimal PDF; we have

$$h_{\text{opt}}(u_0) = \int_0^\infty du p_{\text{opt}}(u; u_0) h(u) = \begin{cases} \frac{u_2^{(l)} - u_0}{u_2^{(l)} - u_{\min}} h(u_{\min}) + \frac{u_0 - u_{\min}}{u_2^{(l)} - u_{\min}} h(u_2^{(l)}) & u_{\min} < u_0 < u_2^{(l)}, \\ h(u_0) & u_2^{(l)} \leq u_0 \leq u_1^{(r)}, \\ \frac{u_{\max} - u_0}{u_{\max} - u_1^{(r)}} h(u_1^{(r)}) + \frac{u_0 - u_1^{(r)}}{u_{\max} - u_1^{(r)}} h(u_{\max}) & u_1^{(r)} < u_0 < u_{\max}. \end{cases} \quad (27)$$

By construction, the optimal average reactivity coincides with the concave envelope function, $h_{\text{opt}}(u_0) = \hat{h}(u_0)$. Viewed as a function of β_0 , the optimal average reactivity $\langle \sigma v \rangle_{\text{opt}}(\beta_0)$ is obtained from $h_{\text{opt}}(u_0)$ by applying the substitution $u_0 \rightarrow \beta_0^{-1}$.

We close this section with an important observation. The optimization procedure described above, despite being formulated for a one-dimensional setup with a MB distribution in momentum space, yields a completely general result. Indeed, the solution obtained for the constrained probabilistic functional problem stated in Eq. (10) remains valid for any arbitrary expression of $\langle \sigma v \rangle_{\text{MB}}(\beta)$, with the latter playing the role of the assigned function for which we must find the concave envelope.

III. OPTIMIZED ENERGY DISTRIBUTIONS AND SUPERSTATISTICS

Superstatistics are a way to generalize MB distributions, including the case of effective temperatures spread out in a continuum [23,27,41–43]. In this description, the system is viewed as a superposition of local equilibrium states, each characterized by a different value of β . The resulting energy distribution is therefore obtained by averaging the MB distribution over these inverse-temperature distributions $f(\beta)$ —nonnegative and normalized to unity once integrated in β —such that the energy distribution of the f superstatistics is written as

$$w_f(E) = \int_0^\infty d\beta f(\beta) w_{\text{MB}}(E; \beta), \quad (28)$$

where

$$w_{\text{MB}}(E; \beta) = \sqrt{\frac{\beta}{\pi E}} e^{-\beta E} \quad (29)$$

and

$$\int_0^\infty dE w_{\text{MB}}(E; \beta) = 1. \quad (30)$$

As usual, $\beta = 1/(k_B T)$ indicates the inverse temperature, with k_B being the Boltzmann constant.

Sometimes it is preferable to work in terms of wave vectors K instead of energies E . Assuming the dispersion relation of free particles, $E = \hbar^2 K^2 / (2m)$, the above relations for

the MB distribution become equivalent to Eq. (3). The f -superstatistics distribution expressed in terms of K is then as in Eq. (7),

$$w_f(K) = \int_0^\infty d\beta f(\beta) w_{\text{MB}}(K; \beta), \quad (31)$$

with $f(\beta) \geq 0$ and

$$\int_0^\infty d\beta f(\beta) = 1. \quad (32)$$

Note that, while the MB distribution is characterized by a given inverse temperature β connected to the average energy by

$$\begin{aligned} \int_0^\infty dE E w_{\text{MB}}(E; \beta) &= \int_{-\infty}^{+\infty} dK \frac{\hbar^2 K^2}{2m} w_{\text{MB}}(K; \beta) \\ &= \frac{1}{2\beta}, \end{aligned} \quad (33)$$

in the case of the f -superstatistics distributions we have only an effective inverse temperature defined via the average energy

$$\begin{aligned} \int_0^\infty dE E w_f(E) &= \int_{-\infty}^{+\infty} dK \frac{\hbar^2 K^2}{2m} w_f(K) \\ &= \int_0^\infty d\beta f(\beta) \frac{1}{2\beta}. \end{aligned} \quad (34)$$

We now focus on three representative examples of superstatistics: the χ^2 (type I), inverse χ^2 (type II), and log-normal (type III) classes. These constitute the main universality classes encountered across a wide range of physical systems and are supported by substantial observational evidence. They can be traced back to generic phenomenological mechanisms governing the stochastic fluctuations of β [44] and may also be derived from a maximum entropy framework under appropriate constraints [45].

In Fig. 1, we present examples of the distributions $f(\beta)$ for the three superstatistical classes, shown for different values of

$$q := \int_0^\infty d\beta f(\beta) \beta^2 \frac{1}{\beta_0^2} = \frac{\langle \beta^2 \rangle}{\beta_0^2}. \quad (35)$$

This parameter provides a common measure of inverse-temperature fluctuations since it is defined in the same way

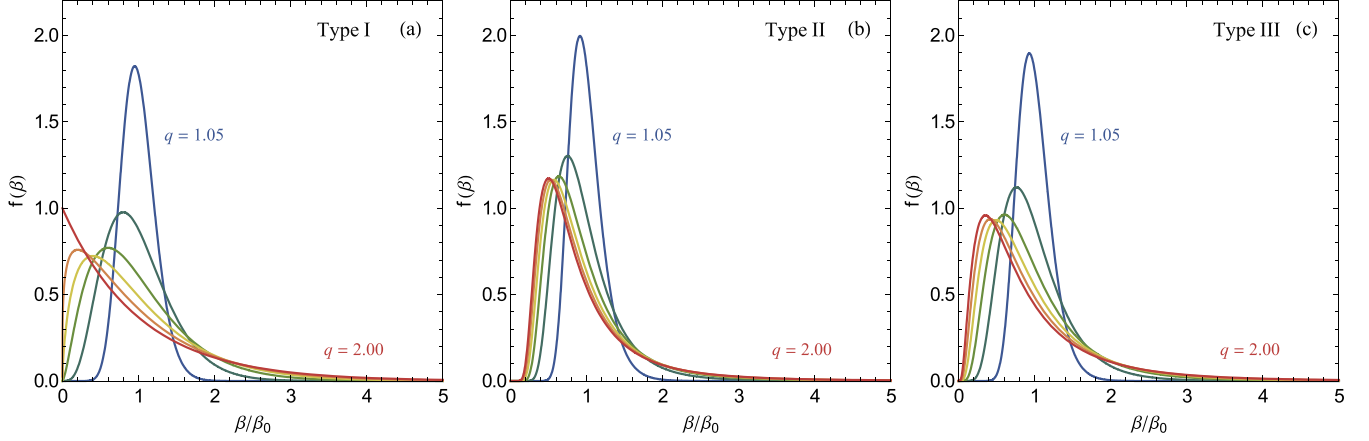


FIG. 1. Probability distributions $f(\beta)$ for the three representative superstatistics, parameterized by q , shown for different values, starting from the leftmost peak at $q = 2.0$ and going to the rightmost peak at $q = 1.05$, with intermediate values of $q = 1.20, 1.40, 1.60, 1.80$. In the limit $q \rightarrow 1$, $f(\beta)$ collapses to a Dirac δ distribution centered at β_0 , and the corresponding energy distribution reduces to the MB form.

for all three classes. Thus, comparing different distributions at the same value of q amounts to comparing them at the same degree of fluctuations. In the limit $q \rightarrow 1$, all three distributions collapse toward a Dirac δ centered at β_0 , recovering the MB limit. As q increases, the distributions broaden, and their weight is redistributed away from β_0 in a class-dependent way. It is noticeable that at least for the type-II and III superstatistics there is a leading contribution at the inverse temperature corresponding to an MB distribution, plus contributions with weight inversely proportional to the distance from the peak. In the case of type-I superstatistics, the peak of the distribution moves faster than the other two superstatistics toward $\beta = 0$, as shown more explicitly in Fig. 2 (a more detailed discussion is given below). In general, many statistical systems with a relatively small number of particles, either because they are of mesoscopic size or because they form small subsystems with partial, only local thermal equilibrium, are better described by a superstatistics taking into account temperature fluctuations absent in a more macroscopic system manifesting global equilibrium.

A useful way to quantify how the weight of each distribution shifts with increasing q is to locate its maximum.

Denoting by β_{peak} the value of β at which $f(\beta)$ is maximal, we obtain

$$\frac{\beta_{\text{peak}}}{\beta_0} = 2 - q \quad (36)$$

for type I,

$$\frac{\beta_{\text{peak}}}{\beta_0} = \frac{q}{3q - 2} \quad (37)$$

for type II, and

$$\frac{\beta_{\text{peak}}}{\beta_0} = q^{-3/2} \quad (38)$$

for type III. These three behaviors are shown in Fig. 2(a). In all cases, $\beta_{\text{peak}} \rightarrow \beta_0$ as $q \rightarrow 1$. As q increases, the peak moves toward smaller values of β , although with different rates depending on the class. In particular, type I reaches $\beta_{\text{peak}} = 0$ already at the limiting value $q = 2$, while type II tends to $\beta_0/3$ and type III tends to zero only asymptotically as $q \rightarrow \infty$.

In what follows, for each of these classes, we evaluate the reactivity under the condition of equal total energy and

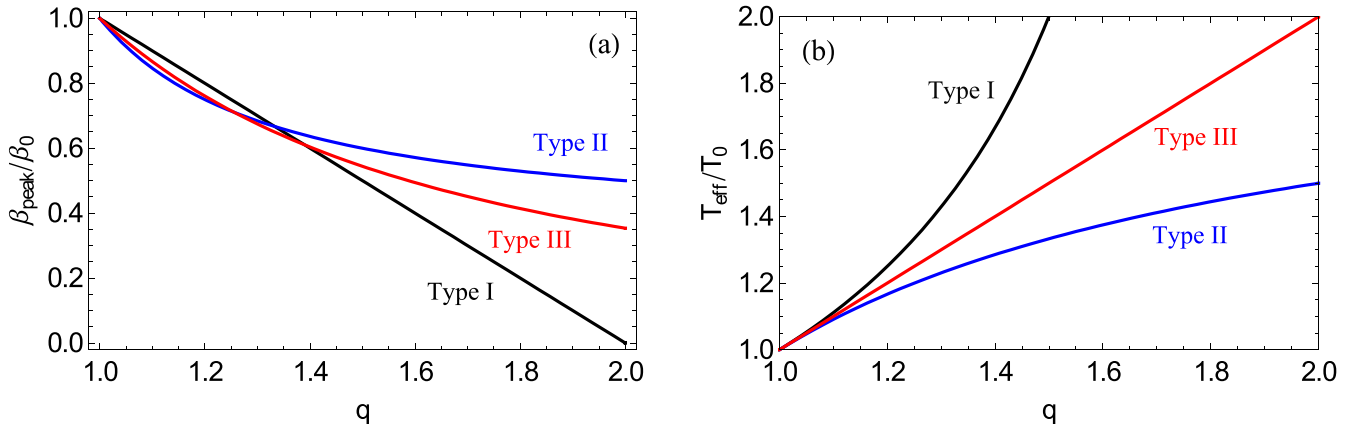


FIG. 2. (a) Position of the maximum of $f(\beta)$, β_{peak} , normalized to β_0 , as a function of the universal parameter q for the three superstatistics. (b) Effective temperature, normalized to the temperature T_0 of the MB energy distribution with the same average energy, versus q for the same three superstatistics.

compare it with the result obtained from the MB energy distribution with the same total energy. We also restrict ourselves to the plane-wave case, for which $P_K(k) = \delta(k - K)$ in Eq. (2). Since the parameter $q = \langle \beta^2 \rangle / \beta_0^2$ was already introduced as a common measure of the strength of inverse-temperature fluctuations, it will be used below to compare the three superstatistical classes at the same degree of departure from the MB limit.

For a more compact representation of the reactivity gains, we introduce the dimensionless energy variable $x := \beta_0 E(K) = \beta_0 \hbar^2 K^2 / 2m$ and the integral operator

$$\mathcal{G}_{\beta_0}[F] := \frac{\int_{-\infty}^{+\infty} dk \int_{-\infty}^{+\infty} dK \frac{T(E(k))}{\sqrt{E(k)}} P_K(k) F(x)}{\int_{-\infty}^{+\infty} dk \int_{-\infty}^{+\infty} dK \frac{T(E(k))}{\sqrt{E(k)}} P_K(k) e^{-x}}. \quad (39)$$

The dependence on the superstatistics class is then entirely contained in the function $F(x)$ and its associated prefactor.

A. Type I: χ^2 superstatistics

A relevant example of superstatistics consists of a choice of a two-parameter distribution $f = f_n(\beta; \beta_0)$ such that

$$f_n(\beta; \beta_0) = \frac{1}{\Gamma(n/2)} \left(\frac{n}{2\beta_0} \right)^{n/2} \beta^{n/2-1} e^{-n\beta/(2\beta_0)}, \quad (40)$$

which represents a χ^2 distribution of degree n with generic moment of order k ,

$$\langle \beta^k \rangle = \frac{\Gamma(n/2 + k)}{\Gamma(n/2)} \left(\frac{2\beta_0}{n} \right)^k, \quad (41)$$

from which we can identify the average value of the inverse temperature $\langle \beta \rangle = \beta_0$ and its variance

$$\Delta \beta^2 = \langle \beta^2 \rangle - \langle \beta \rangle^2 = \frac{2\beta_0^2}{n}. \quad (42)$$

It follows that for this superstatistics

$$q = \frac{\langle \beta^2 \rangle}{\beta_0^2} = 1 + \frac{2}{n}. \quad (43)$$

The resulting integral (31) is calculated analytically,

$$\begin{aligned} & \int_0^\infty d\beta f_n^{\chi^2}(\beta; \beta_0) w_{\text{MB}}(K, \beta) \\ &= \frac{1}{\Gamma(n/2)} \left(\frac{\hbar^2}{2\pi m} \right)^{1/2} \left(\frac{n}{2\beta_0} \right)^{n/2} \\ & \times \int_0^\infty d\beta \beta^{\frac{n-1}{2}} \exp \left[- \left(\frac{\hbar^2 K^2}{2m} + \frac{n}{2\beta_0} \right) \beta \right] \\ &= \frac{\Gamma(\frac{n+1}{2})}{\Gamma(n/2)} \left(\frac{\beta_0 \hbar^2}{\pi m n} \right)^{1/2} \left(1 + \frac{\beta_0 \hbar^2 K^2}{n m} \right)^{-\left(\frac{n+1}{2}\right)}. \end{aligned} \quad (44)$$

Note that the χ^2 distribution in Eq. (40) arises naturally when β results from the superposition of many independent random contributions, i.e., from an additive stochastic process [44]. In this case, β can be expressed as a sum of squared Gaussian variables, leading, by virtue of the central limit theorem, to a χ^2 distribution, where n represents the number of degrees

of freedom associated with the underlying fluctuations. The corresponding energy distributions, Eq. (44), exhibit power-law tails, making the χ^2 class particularly well suited to describe a wide range of nonequilibrium systems characterized by enhanced high-energy tails, as commonly observed in plasmas [46,47], gravitational systems [48–51], and various other physical contexts [52–56].

The reactivity gain obtained by comparing the χ^2 superstatistical distribution with the MB distribution at the same value of the inverse-temperature parameter β_0 , $G_n^{\chi^2}(\beta_0) = \langle \sigma v \rangle_f / \langle \sigma v \rangle_{\text{MB}}$, reads

$$G_n^{\chi^2}(\beta_0) = \frac{\Gamma(\frac{n+1}{2})}{\Gamma(\frac{n}{2})} \sqrt{\frac{2}{n}} \mathcal{G}_{\beta_0} \left[\left(1 + \frac{2x}{n} \right)^{-\frac{n+1}{2}} \right]. \quad (45)$$

B. Type II: Inverse χ^2 superstatistics

In the case of this second class of superstatistics, the temperature $T = \beta^{-1}$ is χ^2 distributed. That is,

$$f_n(T; T_0) = \frac{1}{\Gamma(n/2)} \left(\frac{n}{2T_0} \right)^{n/2} T^{n/2-1} e^{-nT/(2T_0)}, \quad (46)$$

where $T_0 = \langle T \rangle$. Changing variables to β (and using $|dT/d\beta| = \beta^{-2}$) yields

$$f_n(\beta) = \frac{1}{\Gamma(\frac{n}{2})} \left(\frac{n}{2T_0} \right)^{n/2} \beta^{-n/2-1} e^{-\frac{n}{2\beta T_0}}. \quad (47)$$

The mean of β is $\beta_0 \equiv \langle \beta \rangle = n/[(n-2)T_0]$, with $n > 2$. Using β_0 and redefining $n-2 \rightarrow n$, the inverse χ^2 distribution can be written as

$$f_n^{\text{inv}\chi^2}(\beta) = \frac{\beta_0}{\Gamma(\frac{n}{2})} \left(\frac{n\beta_0}{2} \right)^{n/2} \beta^{-n/2-2} e^{-\frac{n\beta_0}{2\beta}}, \quad (48)$$

with $n > 0$. The variance in this case is

$$\Delta \beta^2 = \langle \beta^2 \rangle - \langle \beta \rangle^2 = \frac{2}{n-2} \beta_0^2 \quad (49)$$

and

$$q = \frac{\langle \beta^2 \rangle}{\beta_0^2} = \frac{n}{n-2}. \quad (50)$$

The integral (31) now reads

$$\begin{aligned} & \int_0^\infty d\beta f_n^{\text{inv}\chi^2}(\beta; \beta_0) w_{\text{MB}}(K, \beta) \\ &= \frac{\beta_0}{\Gamma(n/2)} \left(\frac{n\beta_0}{2} \right)^{n/2} \left(\frac{\hbar^2}{2\pi m} \right)^{1/2} \\ & \times \int_0^\infty d\beta \beta^{-\left(\frac{n+3}{2}\right)} \exp \left[- \left(\frac{\beta \hbar^2 K^2}{2m} + \frac{n\beta_0}{2\beta} \right) \right] \\ &= \frac{2^{-(1+n/2)} n^{n/2}}{\Gamma(n/2)} \left(\frac{\beta_0 \hbar^2}{2\pi m} \right)^{1/2} \left(\frac{\beta_0 \hbar^2 K^2}{nm} \right)^{\frac{1+n}{4}} \\ & \times \mathcal{K}_{\frac{1+n}{2}} \left(\sqrt{n\beta_0 \hbar^2 K^2 / m} \right), \end{aligned} \quad (51)$$

where $\mathcal{K}_\alpha(x)$ is the modified Bessel function of the second kind. Note that the inverse χ^2 distribution (48) arises naturally when the inverse temperature β is governed by the inverse of an additive stochastic process, i.e., when $1/\beta$ results from

the superposition of many independent random contributions [44]. In this case, β can be interpreted as the inverse of a sum of squared Gaussian variables, leading to an inverse χ^2 distribution. The corresponding energy distributions in Eq. (51) then exhibits exponential decay in the tails. Such an exponential behavior has been documented in a variety of nonequilibrium systems, including vortex glasses and liquids [57], fusion plasmas [23], and harmonic oscillators coupled to solvent environments [58].

For the present superstatistics, the reactivity gain $G_n^{\text{inv}\chi^2}$ with respect to a MB distribution at the same inverse temperature β_0 is given by

$$G_n^{\text{inv}\chi^2} = \frac{2^{-(1+n/2)} n^{n/2}}{\Gamma(n/2)} \mathcal{G}_{\beta_0} \left[\left(\frac{2x}{n} \right)^{\frac{n+1}{4}} \mathcal{K}_{\frac{n+1}{2}}(\sqrt{2nx}) \right]. \quad (52)$$

C. Type III: Log-normal superstatistics

Finally, we consider the log-normal class, which naturally arises when the inverse temperature results from multiplicative random processes. In this case,

$$f_s(\beta) = \frac{1}{\sqrt{2\pi s\beta}} \exp\{-[\ln(\beta/\mu)]^2/(2s^2)\}, \quad (53)$$

where $\beta_0 = \mu e^{s^2/2}$. The variance is

$$\Delta\beta^2 = \langle\beta^2\rangle - \langle\beta\rangle^2 = (e^{s^2} - 1)\beta_0^2, \quad (54)$$

and therefore,

$$q = \frac{\langle\beta^2\rangle}{\beta_0^2} = e^{s^2}. \quad (55)$$

Equilibrium statistical mechanics is recovered in the limit $s \rightarrow 0$. The log-normal distribution arises naturally when the inverse temperature β is governed by a multiplicative stochastic process [44]. In this case, $\ln\beta$ results from the superposition of many independent random contributions and, by virtue of the central limit theorem, becomes Gaussian distributed. Consequently, β follows a log-normal distribution. The corresponding integral (31) cannot be evaluated in closed form and must therefore be computed numerically. Log-normal superstatistics is supported by empirical evidence from systems in which multiplicative and cascade processes, such as turbulence, play a central role [24,25]. It has also been successfully employed to describe distributions observed in space plasmas [27] and gravitational systems [28], as well as in a wide range of complex systems beyond physics [31,59].

For type III, with $y := \beta/\beta_0$, the reactivity gain G_s^{Ln} relative to the MB distribution at the same β_0 reads

$$G_s^{\text{Ln}} = \frac{1}{\sqrt{2\pi s}} \mathcal{G}_{\beta_0} \left[\int_0^\infty \frac{dy}{\sqrt{y}} e^{-xy - (\ln y + s^2/2)^2/(2s^2)} \right]. \quad (56)$$

Note that, in order to assess whether a given superstatistical distribution enhances the reactivity, the comparison should be performed at the same available kinetic energy $\langle E \rangle$, rather than at the same value of β_0 . For the three classes considered here, the average energy reads

$$\begin{aligned} \langle E \rangle &= \left(\frac{n}{n-2} \right) \frac{1}{2\beta_0} \quad (\text{type I}), \\ \langle E \rangle &= \left(\frac{n+2}{n} \right) \frac{1}{2\beta_0} \quad (\text{type II}), \\ \langle E \rangle &= \frac{e^{s^2}}{2\beta_0} \quad (\text{type III}). \end{aligned} \quad (57)$$

The resulting equal-energy reactivities can then be expressed as

$$\langle \sigma v \rangle_f = \left(\frac{\hbar^2}{2\pi m} \right)^{1/2} \int_{-\infty}^{+\infty} dk \int_{-\infty}^{+\infty} dK I_f(k, K). \quad (58)$$

The functions $I_f(k, K)$ corresponding to the different superstatistical classes, written in terms of the common parameter $q = \langle\beta^2\rangle/\beta_0^2$, are summarized in Table I.

From Eq. (57), it is useful to introduce an effective temperature T_{eff} , defined as the temperature a MB distribution would require to have the same average kinetic energy as the corresponding superstatistical distribution. This quantity is shown in Fig. 2(b) as a function of the common parameter q . Figure 2 shows that, for the three superstatistical classes, the effective temperature exceeds that of the corresponding MB distribution. Moreover, a clear hierarchy emerges: For the same value of q , type I exhibits the largest deviation from the Maxwellian reference, whereas type II remains the closest to it. This behavior is consistent with the trends observed in Fig. 1.

Finally, it should be noted that the power-law asymptotic behavior of the type-I distribution imposes restrictions on the parameter n , or, equivalently, on q . Requiring a finite average energy $\langle E \rangle$ (or a finite effective temperature T_{eff}) leads to $n > 2$, which is equivalent to $q < 2$. In addition, in the physically relevant three-dimensional case, quite general arguments suggest the stronger bound $q \lesssim 1.66$, which appears to be compatible with available real-world data [60].

TABLE I. Summary of the reactivities for the three classes of superstatistics. Shown are the relationships between the q parameter and the index usually denoting each superstatistics and the expressions for the integrand of the corresponding reactivities, expressed in terms of the average energy $\langle E \rangle$, as in Eq. (58).

Statistic	q parameter	$I_f(k, K)$ defined in Eq. (58)
χ^2	$1 + 2/n$	$\frac{\Gamma(\frac{q+1}{2(q-1)})}{\Gamma(\frac{1}{q-1})} \sqrt{\frac{q-1}{q-2}} \left(\frac{\hbar^2 k^2}{2m} \right)^{-1/2} T\left(\frac{\hbar^2 k^2}{2m} \right) P_K(k) \left(1 - \frac{(q-1)\hbar^2 K^2}{4(q-2)m\langle E \rangle} \right)^{-\frac{q+1}{2(q-1)}}$
Inverse χ^2	$n/(n-2)$	$\frac{2^{-5/2+\frac{1}{q-1}}}{\Gamma(2+\frac{1}{q-1})} \sqrt{\frac{2+\frac{1}{q-1}}{q-2}} \left(\frac{\hbar^2 k^2}{2m} \right)^{-1/2} T\left(\frac{\hbar^2 k^2}{2m} \right) P_K(k) \left(\frac{(2q-1)\hbar^2 K^2}{(q-1)m\langle E \rangle} \right)^{\frac{3q-1}{2(q-1)}} \mathcal{K}_{\frac{3q-1}{2(q-1)}} \left\{ \sqrt{(2q-1)\hbar^2 K^2 / [(q-1)m\langle E \rangle]} \right\}$
Log normal	$\exp(s^2)$	$\frac{1}{\sqrt{2\pi \ln(q)}} \left(\frac{\hbar^2 k^2}{2m} \right)^{-1/2} T\left(\frac{\hbar^2 k^2}{2m} \right) P_K(k) \int_0^\infty d\beta \sqrt{\frac{2(E)}{\beta}} \exp \left[-\frac{\beta \hbar^2 K^2}{2m} - \frac{[\ln(4\beta(E)/q)]^2}{2\ln(q)} \right]$

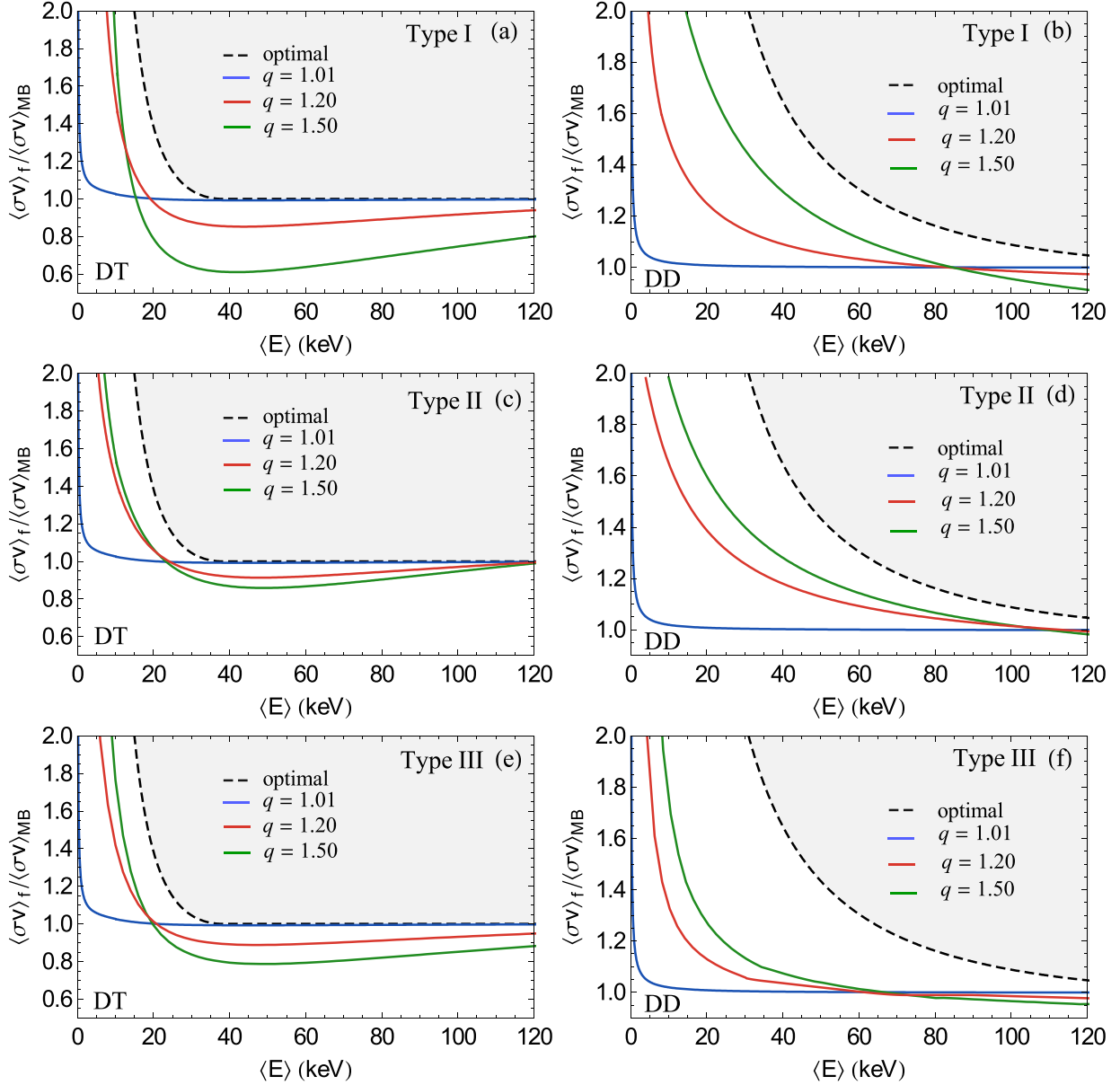


FIG. 3. Gain factor versus the average energy $\langle E \rangle$ for the three representative superstatistics, type I (top plots), type II (middle), and type III (bottom), each shown for three different values of q , and the exclusion region (in gray) for the optimal gain according to the concave envelope, delimited by the dashed line. The cases on the left are relative to DT fusion; the cases on the right are relative to DD fusion.

IV. REACTIVITY GAIN WITH EMPIRICAL FORMULAS FOR FUSION CROSS SECTIONS

As an application of the considerations described in the previous two sections, here, we consider the realistic case of DT and DD fusion reactivities. Following Ref. [33], the cross sections of these fusion processes are parametrized as

$$\sigma = S(E) \frac{e^{-B_G/\sqrt{E}}}{E}, \quad (59)$$

where $B_G = \pi\alpha Z_1 Z_2 \sqrt{2mc^2}$ is the Gamow constant, with α being the fine structure constant, m being the reduced mass, and Z_1 and Z_2 being the electric charges of the nuclei in elementary charge units, and $S(E)$ is the so-called astrophysical

S function, expressed in terms of a Padé polynomial as

$$S(E) = \frac{A_1 + E\{A_2 + E[A_3 + E(A_4 + EA_5)]\}}{1 + E\{B_1 + E[B_2 + E(B_3 + EB_4)]\}}, \quad (60)$$

with the values of B_G , A_i , and B_j , with $i = 1, \dots, 5$ and $j = 1, \dots, 4$, being reported in Table IV of Ref. [33] for various energy ranges depending on the specific fusion reaction. The above parameters are specified for both DT and DD fusion. For the DD case, the total reactivity includes the contributions from both reaction channels.

A first analysis consists of comparing the optimal reactivity discussed in Sec. II and the reactivities arising from the superstatistics in Sec. III, both using the empirical cross sections of Ref. [33]. Figure 3 shows the reactivity gain obtained using the three superstatistics described in Sec. III (top, middle,

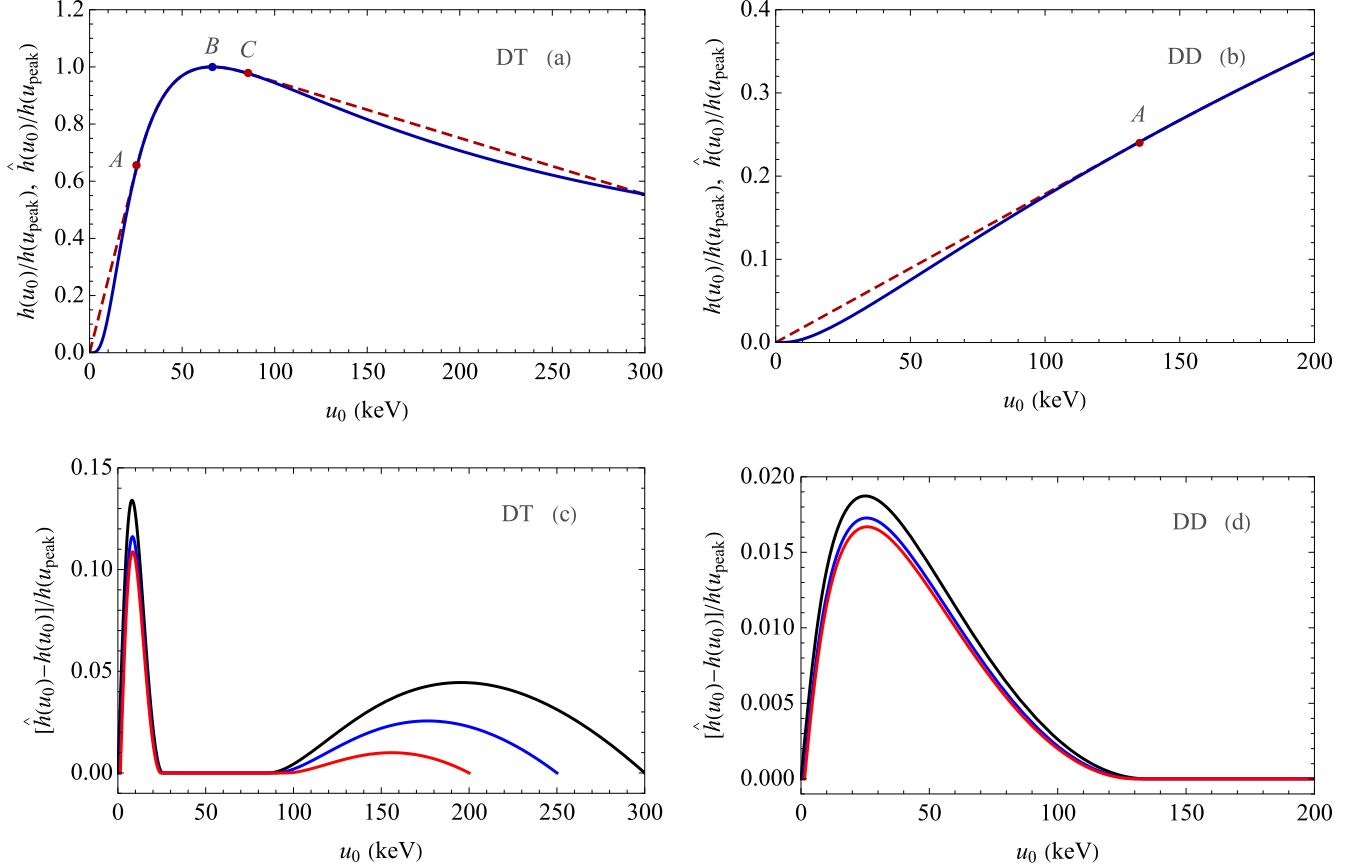


FIG. 4. Function $h(u_0)$ representing the empirical reactivity calculated from Ref. [33] (blue solid line) and its concave envelope $\hat{h}(u_0)$ (red dashed line) for (a) DT fusion and (b) DD fusion. In both cases, the functions are normalized to the peak value of $h(u)$ achieved at point B: $u_{\text{peak}} = 66.157$ keV for DT and $u_{\text{peak}} = 1.216$ MeV for DD (point not shown). In (a), the boundary points of the left and right regions where $\hat{h}(u_0) > h(u_0)$ are $u_1^{(l)} = u_{\text{min}} = 0$ keV, $u_2^{(l)} = 25.652$ keV (point A), $u_1^{(r)} = 85.386$ keV (point C), and $u_2^{(r)} = u_{\text{max}} = 300$ keV. Conversely, (b) shows only the left region with $u_1^{(l)} = u_{\text{min}} = 0$ keV and $u_2^{(l)} = 134.843$ keV (point A). Peak-normalized reactivity gain $[\hat{h}(u_0) - h(u_0)]/h(u_{\text{peak}})$ as a function of u_0 when using the optimized energy distribution for (c) DT and (d) DD. Three curves are shown in each panel, corresponding to different choices of u_{min} and u_{max} for DT (black: 0, 300; blue: 1, 250; red: 1.4, 200) and u_{min} for DD (black: 0; blue: 1; red: 1.4); all values are in keV.

and bottom rows) relative to the MB distribution at the same average energy for DT fusion (left column) and DD fusion (right column). All cases show an enhancement of reactivity at low average energies, confirming earlier results reported in Ref. [15]. In the case of DT fusion, such an enhancement at low average energy is followed by a suppression of reactivity at higher average energies, especially in the case of superstatistics of type I. In each panel of Fig. 3, the shaded region indicates the exclusion zone for the reactivity gain determined by the optimal reactivity in Sec. II, with its boundary represented by a dashed line. As expected, we find that the gain of each considered superstatistics is always upper bounded by the corresponding shaded contour. The distance of the superstatistics curves from the dashed line indicates that considerable gain can be further achieved by using the optimal reactivity.

The gain obtained from using optimized reactivities depends on the average energy; specifically, this gain occurs in the regions where the MB reactivity is exceeded by its concave envelope. As discussed in Sec. II, there are two such regions—one at low energy and the other at high energy [see Figs. 4(a) and 4(b) for the DT and DD fusion reactions]—and

their extensions depend on the choice of u_{min} and u_{max} , which define the boundaries of the supported MB distribution.

It is evident [see Figs. 4(c) and 4(d)] that the gain at low energies increases as u_{min} decreases, whereas at high energies, larger gains are achieved by increasing u_{max} . Indeed, decreasing u_{min} or increasing u_{max} shifts the matching points $u_2^{(l)}$ and $u_1^{(r)}$ closer to u_{peak} , causing the concave envelope to progressively exceed the MB reactivity. However, the actual gain in using the maximum span can be limited. First, the case of average energy close to 0 keV is not of physical or engineering interest because the absolute reactivity tends to zero in that limit anyway, and the measurements are limited to nonzero values of energy. Second, the maximum value of u_{max} is limited by the actual experimental data taken at the highest temperatures and can also be limited by the opening of new environmental conditions, for instance, the onset of an electron-positron plasma at temperatures of the order of 0.5–1 MeV.

The advantage of using an energy distribution based on the concave envelope with respect to a MB distribution with the same average energy can be evaluated for DT and DD reactions as follows. Regarding the DT fusion case, the peak

reactivity is found to be $h(u_{\text{peak}}) = 8.9 \times 10^{-16} \text{ cm}^3 \text{ s}^{-1}$, using the parametrization from Ref. [33]. At the reference energy of $u_0 = 10 \text{ keV}$, we find a maximum reactivity difference of $\hat{h}(u_0) - h(u_0) = 1.2 \times 10^{-16} \text{ cm}^3 \text{ s}^{-1}$, as shown in Fig. 4(c), where $[\hat{h}(u_0) - h(u_0)]/h(u_{\text{peak}}) \simeq 0.135$ in the most favorable case. Given $h(u_0) = 1.15 \times 10^{-16} \text{ cm}^3 \text{ s}^{-1}$, this corresponds to a reactivity gain of $\hat{h}(u_0)/h(u_0) = 2.04$ when we use the optimized energy distribution compared to a MB distribution with the same average energy u_0 . This optimized distribution is a bimodal MB energy distribution with $w_1 = 0.61$, as derived from Eq. (19). Repeating the calculation for DD fusion, we obtain a maximum reactivity gain of 1.7 at $u_0 = 23 \text{ keV}$, utilizing a bimodal MB energy distribution with $w_1 = 0.84$.

It is worth mentioning that this approximately twofold gain could take place in an energy region of immediate interest for magnetically confined plasmas. From a practical standpoint, the protocol will consist of using for the DT reaction, instead of a MB-distributed plasma at an average energy of $u_0 = 10 \text{ keV}$, a bimodal MB energy distribution made of a very cold plasma, at a percentage of $\simeq 60\%$, and a hot component at $u_0 \sim 25 \text{ keV}$. Bimodal MB distributions were already achieved at Joint European Torus (JET), as reported in Ref. [61] and more recently discussed in detail [62].

V. CONCLUSIONS

We discussed the optimization of fusion reactivity with respect to the energy distribution of the reacting ions, confirming the preliminary findings reported in Ref. [15] regarding the role of the concavity of the reactivity curve as a function of the average particle energy. This result is now established within the more rigorous framework of a constrained functional optimization problem, thereby increasing in clarity and generality. As long as the average energy remains within a range where the reactivity curve is concave, the MB energy distribution optimizes the reactivity. Outside this interval, the optimal solution is generally obtained by choosing a bimodal MB distribution with temperatures determined by the straight

lines that tangentially connect the boundary points of the two regions. While the three discussed classes of superstatistics can exceed the reactivity of their corresponding MB energy distributions, they all remain below the optimization boundary of the reactivity curve. Finally, we conjectured a relationship between optimized energy distributions and superstatistics. Most of these considerations on reactivity optimization can be extended to a more general setting, such as reactions of chemical and biological interest [63–65].

Regarding their applicability to confined plasmas, optimized energy distributions could play a significant role in an interesting regime centered around $u_0 \approx 10 \text{ keV}$ for DT fusion and $u_0 \approx 30 \text{ keV}$ for DD fusion. In these regions, one can expect peak-normalized reactivity gains $[\hat{h}(u_0) - h(u_0)]/h(u_{\text{peak}})$ of approximately 10% for DT and 1.5% for DD [see Figs. 4(c) and 4(d)], which translate into a boost in reactivity gain up to a factor of about 2 for both DD and DT mixtures. This requires envisaging demonstrations of engineered bimodal MB energy distributions. Within the context of a much simpler confinement geometry, such as a harmonic trap, numerical simulations have demonstrated that both bimodal MB [66] and κ energy distributions [67] are generated during a thermalization transient. In the former case, a mechanism was proposed where bimodal distributions arise from a local mismatch in heat capacities between the two species undergoing thermalization. A compelling future direction would be to extend these considerations to the more realistic confinement scenarios of tokamaks, leveraging existing codes designed to identify nonequilibrium plasma features [68,69].

ACKNOWLEDGMENT

We thank Lorenzo Bertini for a fruitful discussion on the solution of constrained linear variational problems.

DATA AVAILABILITY

There are no publicly available research data or software supporting this manuscript. Requests for further information or data should be sent to the authors.

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