On the Boundedness of Free Energy Functionals

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The boundedness of free energy functionals is examined. For several generic cases involving generalized energy and entropy measures, we show that free energy functionals defined on μ-space density functions are bounded from below.

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1 Introduction

The free energy principle is a fundamental concept of phenomenological thermodynamics and tells us that isothermal state changes do not increase the free energy of systems and that systems occupy stationary states of minimal free energy [1]. Recently, there is an increasing interest to exploit the free energy principle in order to describe many-body systems by means of free energy functionals of the form $F[P] = U[P] - \beta^{-1}S[P]$. Here, $U[P]$ denotes an internal energy functional or a measure of effort (e.g., in the case of neural network free energies). $\beta^{-1} > 0$ describes the strength of fluctuations and can often be identified with the temperature T of a system or the noise amplitude Q of a stochastic process. S describes a general entropy functional or an information measures. In both cases S measures the amount of disorder of a system and therefore will be called in what follows a disorder measure. The functionals F, U, and S are assumed to depend on a density function P that might correspond to a probability density or a particle number density. P depends on the M-dimensional state variable $\mathbf{x} \in \Omega$ of a many-body system, where Ω corresponds to the phase space of a single subsystem or particle of the system. That is, we deal with μ-space descriptions of many-body systems [1, 2, 3]. The free energy approach to many-body systems involving μ-space density functions has successfully been applied to real gases [4, 5], amorphous material [6, 7], mean field coupled many-body systems [8, 9, 10], and Fermi and Bose systems [11, 12, 13]. If free energy functionals are bounded from below then they describe systems that are globally stable. That is, they eventually converge to macroscopic stationary states with $\mathrm{d}F/\mathrm{d}t = 0$. The reason for this is that, on the one hand, state changes with $\beta^{-1} = \text{const}$ yield $\mathrm{d}F \leq 0$ but, on the other hand, we have $F \geq C > -\infty$ which implies $\lim_{t\to\infty} \mathrm{d}F/\mathrm{d}t = 0$. In particular, using nonlinear Fokker-Planck equations one can explicitly show that systems converge to stationary states if they are described by free energy measures that are bounded from below [8, 11, 12, 13]. Consequently, the boundedness of free energy functionals is a crucial property. Despite of the wide applicability of free energy functionals, a thorough discussion about this key property has not been carried out so far. In the following section we will address several generic cases for which the boundedness of free energy functionals can be proven.

2 Boundedness of free energies

Stationary states

Let us first characterize stationary states of systems described by μ-space free energy functionals $F[P]$. We assume that stationary states are given by distributions $P_{\rm st}$ that make F stationary under the normalization condition $\int_\Omega P \, {\rm d}^M x = 1$ which can equivalently be expressed as

$$\begin{aligned} Y[P_{\rm st}] &= F[P_{\rm st}] + \mu \left(1 - \int_\Omega P_{\rm st}(\mathbf{x}) \, {\rm d}^M x\right) \\ &= \text{stationary} \ . \end{aligned} \quad (1)$$

Here, μ is a Lagrange multiplier that can be interpreted as a chemical potential (see Eq. (3) below). The solutions $P_{\rm st}$ of Eq. (1) are given by

$$\begin{aligned} 0 = \delta Y[P_{\rm st}] &= \delta F - \mu \int_\Omega \delta P \, {\rm d}^M x \\ &= \delta U - \beta^{-1} \delta S - \mu \int_\Omega \delta P \, {\rm d}^M x \ . \end{aligned} \quad (2)$$

Since we require that $\delta Y[P_{\rm st}](\delta P)$ vanishes for all kind of small perturbations δP, the bracket in Eq. (2) must vanish and we get

$$\frac{\delta F}{\delta P_{\rm st}} = \mu \quad (3)$$

and

$$\frac{\delta S}{\delta P_{\rm st}} = \beta \left[\frac{\delta U}{\delta P_{\rm st}} - \mu\right] \ . \quad (4)$$

Next, we decompose $U[P]$ into its linear and nonlinear parts:

$$U[P] = U_{\rm L}[P] + U_{\rm NL}[P] \ , \quad (5)$$

where $U_{\rm L}[P]$ and $U_{\rm NL}[P]$ satisfy

$$U_{\rm L}[P] = \int_\Omega U_0(\mathbf{x}) P(\mathbf{x}) \, {\rm d}^M x \ , \quad (6)$$

$$U_{\rm NL}[P] = O(P^2) \ . \quad (7)$$

Note that a useful relation that will be use below is

$$\delta U_{\rm L}[P'](P) = U_{\rm L}[P] \ . \quad (8)$$

Furthermore, it is helpful to introduce the so-called distortion functional [9, 14, 15, 16]

$$G[u] = \exp\left\{-\frac{\delta S}{\delta u} - 1 + \beta \frac{\delta U_{\rm NL}}{\delta u}\right\} \ . \quad (9)$$

Then, Eq. (9) can equivalently be expressed as

$$\begin{aligned} G[P_{\rm st}] &= \exp\left\{-\frac{\delta S}{\delta P_{\rm st}} - 1 + \beta \frac{\delta U_{\rm NL}}{\delta P_{\rm st}}\right\} = \\ &= \exp\left\{-\beta \left[U_0(\mathbf{x}) - \mu\right] - 1\right\} \ . \end{aligned} \quad (10)$$

Using the Boltzmann distribution

$$W(\mathbf{x}) = \frac{\exp\{-\beta U_0(\mathbf{x})\}}{\int_\Omega \exp\{-\beta U_0(\mathbf{x})\} \, {\rm d}^M x} \ , \quad (11)$$

we obtain the mapping $P_{\rm st} \to W$ defined by

$$G[P_{\rm st}] = \frac{1}{Z} W(\mathbf{x}) \ . \quad (12)$$

Here, Z is a normalization constant depending on μ like $Z = [\int_\Omega \exp\{-\beta[U_0(\mathbf{x})] - \mu] - 1\} \, {\rm d}x]^{-1} > 0$. In order to interpret Z as a new normalization constant, we need to require that W indeed exists. That is, we assume that the integral $\int_\Omega \exp\{-\beta U_0(\mathbf{x})\} \, {\rm d}^M x$ is finite.

General Kullback measure

We consider a disorder measure $S[P]$ that satisfies the concavity inequality

$$S[P] \leq S[P_0] + \delta S[P_0](P - P_0) \quad (13)$$

for $P, P_0 > 0$. We assume that the equal sign holds only for $P = P_0$. Eq. (13) can be transformed into

$$S[P_0] - S[P] + \delta S[P_0](P - P_0) \geq 0 \ . \quad (14)$$

Using the inequality (14) we can introduce a semipositive definite measure [12, 13, 16]

$$K[P, P_0] = S[P_0] - S[P] + \delta S[P_0](P - P_0) \geq 0 \ . \quad (15)$$

The functional K takes two arguments: P and P_0. It can be regarded as a distance measure.

That is, it measures the difference between the probability densities P and P_0. If P equals P_0 we have $K = 0$. If P differs from P_0 we have $K > 0$:

$$K > 0 \Leftrightarrow P \neq P_0 \ , K = 0 \Leftrightarrow P = P_0 \ . \qquad (16)$$

We refer to K as a general Kullback measure because it recovers the Kullback-Leibner distance measure in the case of the BGS entropy (see below). Note that the general Kullback measures (15) can also be defined for two discrete probability distributions $\{p_i\}$ and $\{p_i^{(0)}\}$ and entropy measures of the form $S(p_i) = B[\sum_{i=1}^N s(p_i)]$:

$$K\Big(\{p_i\},\{p_i^{(0)}\}\Big) = S(\{p_i^{(0)}\}) - S(\{p_i\}) + \frac{\mathrm{d}B(z)}{\mathrm{d}z}\bigg|_{\sum_{i=1}^N s(p_i^{(0)})} \sum_{i=1}^N \frac{\mathrm{d}s(z)}{\mathrm{d}z}\bigg|_{p_i^{(0)}} \Big(p_i - p_i^{(0)}\Big) \ , \qquad (17)$$

see also [17] for the special case $B(z) = z$.

BGS-Kullback measure

For the BGS entropy $S[P] = -\int P \ln P \,\mathrm{d}^M x$, the general Kullback measure (15) reads

$$\begin{aligned} {}^{\mathrm{BGS}}K[P,P_0] &= -\int_\Omega P_0 \ln P_0 \,\mathrm{d}^M x + \int_\Omega P \ln P \,\mathrm{d}^M x \\ &\quad - \int_\Omega [1+\ln P_0](P-P_0)\,\mathrm{d}^M x \\ &= \int_\Omega P \ln\left[\frac{P}{P_0}\right] \mathrm{d}^M x \ . \end{aligned} \qquad (18)$$

This distance measure is known in the literature as Kullback-Leibner measure or Kullback measure [18, 19]. Since the BGS entropy satisfies the concavity inequality (13) the measure ${}^{\mathrm{BGS}}K$ is semi-positive definite. We would like to present here also an alternative prove of this property. We start off with the logarithm $\ln(x)$. The logarithm satisfies $\ln(1) = 0$ and it is also well-known that a straight line with slope one that intersect the x-axis at $x = 1$ is always larger than $\ln(x)$ except for $x = 1$ where both the line and logarithm equal zero. Therefore, we have the inequality

$$\ln(x) \leq x - 1 \ , \qquad (19)$$

which holds for $x > 0$. As mentioned already the equal sign holds for $x = 1$ only. Now, let us replace x by $P_0(\mathbf{x})/P(\mathbf{x})$ for $P, P_0 > 0$. Then, we conclude that

$$\begin{aligned} & \ln\left[\frac{P_0}{P}\right] \leq \frac{P_0}{P} - 1 \ , \\ \Rightarrow \quad & P \ln\left[\frac{P_0}{P}\right] \leq P_0 - P \ , \\ \Rightarrow \quad & \int_\Omega P \ln\left[\frac{P_0}{P}\right] \mathrm{d}^M x \leq 0 \ , \\ \Rightarrow \quad & {}^{\mathrm{BGS}}K[P,P_0] = \int_\Omega P \ln\left[\frac{P}{P_0}\right] \mathrm{d}^M x \geq 0 \ . \end{aligned} \qquad (20)$$

Note that in the derivation above we used the normalization condition in terms of $\int_\Omega [P_0 - P]\,\mathrm{d}^M x = 0$.

General Kullback measure for stationary probability densities

In particular, the general Kullback measure can be used to compare arbitrary probability densities P with stationary probability densities P_{st} obtained from the free energy principle. In this case, we put $P_0 = P_{\mathrm{st}}$ and Eq. (15) becomes

$$K[P,P_{\mathrm{st}}] = S[P_{\mathrm{st}}] - S[P] + \delta S[P_{\mathrm{st}}](P - P_{\mathrm{st}}) \ . \qquad (21)$$

From Eq. (2) it follows that P_{st} satisfies the relation

$$\delta S[P_{\mathrm{st}}](\delta P) = \beta \delta U[P_{\mathrm{st}}](\delta P) - \beta\mu \int_\Omega \delta P \,\mathrm{d}^M x \ . \qquad (22)$$

Consequently, Eq. (21) becomes

$$\begin{aligned} K[P,P_{\mathrm{st}}] &= S[P_{\mathrm{st}}] - S[P] + \beta\delta U[P_{\mathrm{st}}](P - P_{\mathrm{st}}) \\ &\quad - \beta\mu \underbrace{\int_\Omega (P - P_{\mathrm{st}})\,\mathrm{d}^M x}_{=0} \ . \end{aligned} \qquad (23)$$

That is, our final result reads

$$K[P,P_{\mathrm{st}}] = \beta\delta U[P_{\mathrm{st}}](P - P_{\mathrm{st}}) - S[P] + S[P_{\mathrm{st}}] \geq 0 \qquad (24)$$

If we split according to Eqs. (5,...,7) the energy measure U into a linear and nonlinear part and take into account that for arbitrary P' and P the equivalence $\delta U_{\rm L}[P'](P) = U_{\rm L}[P]$ holds, see Eq. (8), we can write Eq. (24) as

$$K[P, P_{\rm st}] = \beta\,(F[P] - F[P_{\rm st}]) + \beta\delta U_{\rm NL}[P_{\rm st}](P - P_{\rm st}) \ . \tag{25}$$

Linear energy functionals

The result (25) suggests to examine in more detail the case in which energy functionals can be written as $U = U_{\rm L} = \int_\Omega U_0(\mathbf{x})P(\mathbf{x})\,{\rm d}^M x$. Then, K reads [12]

$$K[P, P_{\rm st}] = -\,(S[P] - S[P_{\rm st}]) + \beta\,(U[P] - U[P_{\rm st}]) \ . \tag{26}$$

In the context of the BGS entropy and the so-called availability of systems this relation between the Kullback measure, on the one hand, and the energy and entropy terms, on the other hand, has been discussed, for example, in [20, 21]. Using the so-called Massieu potentials defined by

$$J[P] = S[P] - \beta U[P] \tag{27}$$

we can write K as the difference

$$K[P, P_{\rm st}] = -(J[P] - J[P_{\rm st}]) \ . \tag{28}$$

By means of the free energy, we can express Eq. (26) by

$$\beta^{-1}K[P, P_{\rm st}] = F[P] - F[P_{\rm st}] \ . \tag{29}$$

This relation can also be obtained from Eq. (25) by equating the $\delta U_{\rm NL}$-term to zero. From the semi-positivity of the general Kullback measure, we obtain the inequality

$$F[P] \geq F[P_{\rm st}] \ . \tag{30}$$

In order to exploit this inequality, we assume that the functional $F[P_{\rm st}]$ is finite: $|F[P_{\rm st}]| < C < \infty$. From $|F[P_{\rm st}]| < C$ it then follows that F is bounded from below:

$$|F[P_{\rm st}]| < C \Rightarrow F[P] = \text{bounded from below} \ . \tag{31}$$

Finally, we note that from (30) we conclude that for linear energy functionals the stationary states corresponds indeed to minima of free energy measure.

Negative concave energy functionals

We consider now a negative concave (or convex) energy functional U. In analogy with the inequality (13), U satisfies the convexity inequality

$$U[P] \geq U[P_0] + \delta U[P_0](P - P_0) \ . \tag{32}$$

In particular, for $P_0 = P_{\rm st}$ we have

$$\begin{aligned} & U[P] \geq U[P_{\rm st}] + \delta U[P_{\rm st}](P - P_{\rm st}) \\ \Rightarrow\quad & \delta U[P_{\rm st}](P - P_{\rm st}) \leq U[P] - U[P_{\rm st}] \ . \end{aligned} \tag{33}$$

Consequently, from Eq. (24) we obtain

$$\begin{aligned} 0 \ &\leq \ K[P, P_{\rm st}] \\ &= \ \beta\delta U[P_{\rm st}](P - P_{\rm st}) - S[P] + S[P_{\rm st}] \\ &\leq \ \beta\,(U[P] - U[P_{\rm st}]) - S[P] + S[P_{\rm st}] \ . \end{aligned} \tag{34}$$

Just as in the case of linear energy functional, we arrive at the result:

$$F[P] \geq F[P_{\rm st}] \ . \tag{35}$$

Nonlinear energy functionals in finite phase spaces

We consider systems with random variables defined on finite phase spaces Ω. We assume that the kernel of the functional U and the kernel of the functional $\delta U[P](P')$ are continuous functions. Then, these kernels are bounded from below and from above on the phase space Ω. Usually, we will then deal with functionals $U[P]$ and $\delta U[P](P')$ that are bounded like

$$\forall P : |U[P]| < C_1, \ \forall P, P' : |\delta U[P](P')| < C_2 \tag{36}$$

For example, for $U_0 \in C^0(\Omega)$ and $P \in C^0(\Omega)$ the integral $\int_\Omega U_0(\mathbf{x})P(\mathbf{x})\,{\rm d}^M x$ is larger than $\min_{\mathbf{x}\in\Omega}\{U_0(\mathbf{x})\}$ and smaller than $\max_{\mathbf{x}\in\Omega}\{U_0(\mathbf{x})\}$. From Eq. (24), we obtain

$$\begin{aligned} 0 &\leq K[P,P_{\rm st}] \\ &= S[P_{\rm st}]-S[P]+\beta\delta U[P_{\rm st}](P)-\delta U[P_{\rm st}](P_{\rm st}) \\ &\leq S[P_{\rm st}]-S[P]+2\beta C_2 \\ &\leq S[P_{\rm st}]-\beta U[P_{\rm st}]-S[P]+\beta U[P] \\ &\quad +2\beta C_2+\beta(U[P_{\rm st}]-U[P]) \\ &\leq \beta(F[P]-F[P_{\rm st}])+2\beta(C_1+C_2)\ . \end{aligned} \quad (37)$$

Consequently, if the integral $F[P_{\rm st}]$ exists (which is usually the case due to the finiteness of Ω), then $F[P]$ is bounded from below:

$$F[P]\geq F[P_{\rm st}]-2(C_1+C_2)\ . \quad (38)$$

The boundedness of free energy measures of systems with finite phase spaces can also be shown in an alternative fashion [22]. Let us consider a phase space Ω with $\int_\Omega {\rm d}^Mx=V<\infty$ (e.g., $\Omega=\prod_{i=1}^M[a_i,b_i]\Rightarrow V=\prod_{i=1}^M(b_i-a_i)$). Let $U[P]$ be bounded from below by $U[P]\geq U_{\rm min}$. Furthermore, we assume that S is maximal for the uniform distribution: $S_{\rm max}=S(P=1/\int_\Omega {\rm d}^Mx=1/V)$. Then, we obtain

$$F[P]=U[P]-\beta^{-1}S[P]\geq U_{\rm min}-\beta^{-1}S_{\rm max}\ . \quad (39)$$

Mean field energy functionals and BGS statistics

Of particular interest are systems that exhibit, on the one hand, BGS statistics and, on the other hand, mean field interactions between subsystems. The energy functional of this kind of systems reads

$$U=\int_\Omega U_0(\mathbf{x})P(\mathbf{x})\,{\rm d}^Mx+ +\frac{1}{2}\int_\Omega\int_\Omega U_{\rm MF}(\mathbf{x},\mathbf{y})P(\mathbf{x})P(\mathbf{y})\,{\rm d}^Mx\,{\rm d}^My \quad (40)$$

where the interaction potential $U_{\rm MF}$ satisfies the symmetry condition $U_{\rm MF}(\mathbf{x},\mathbf{y})=U_{\rm MF}(\mathbf{y},\mathbf{x})$. The entropy and information measure S is given by the BGS entropy. The inverse distortion functional (9) reads

$$G[u]=u\exp\left\{\beta\int_\Omega U_{\rm MF}(\mathbf{x},\mathbf{y})\,u(\mathbf{y})\,{\rm d}^My\right\}\ . \quad (41)$$

We define now the functional I given by

$$I[P,P_0]= -\frac{\beta}{2}\int_\Omega\int_\Omega U_{\rm MF}(\mathbf{x},\mathbf{y})P(\mathbf{x})P(\mathbf{y})\,{\rm d}^Mx\,{\rm d}^My +\int_\Omega P(\mathbf{x})\ln\left[\frac{G(P)}{G(P_0)}\right]\,{\rm d}^Mx \quad (42)$$

that involves two probability densities P and P_0 [9, 14]. For $U_{\rm MF}=0$ we have $G[u]=u$ and, consequently, $I[P,P_0]$ reduces to the BGS-Kullback measure (18). Eq. (42) can alternatively be expressed as

$$I[P,P_0]=\frac{\beta}{2}\int_\Omega\int_\Omega U_{\rm MF}(\mathbf{x},\mathbf{y})P(\mathbf{x})P(\mathbf{y})\,{\rm d}^Mx\,{\rm d}^My +\int_\Omega P(\mathbf{x})\ln\left[\frac{P}{G(P_0)}\right]\,{\rm d}^Mx\ . \quad (43)$$

The integral (43) can be used to compare stationary probability densities obtained from the free energy principle with arbitrary probability densities P. To this end, we put $P_0=P_{\rm st}$, where $P_{\rm st}$ satisfies Eq. (12). In doing so, we replace $G(P_0)$ by $G(P_{\rm st})=W/Z^*$ and obtain

$$\begin{aligned} I[P,P_{\rm st}] &= \ln Z^* \\ &+ \frac{\beta}{2}\int_\Omega\int_\Omega U_{\rm MF}(\mathbf{x},\mathbf{y})P(\mathbf{x})P(\mathbf{y})\,{\rm d}^Mx\,{\rm d}^My \\ &\quad \underbrace{+\int_\Omega P(\mathbf{x})\ln\left[\frac{P}{W}\right]\,{\rm d}^Mx}_{^{\rm BGS}K[P,W]\geq 0}\ . \end{aligned} \quad (44)$$

Note that Z^* is the normalization constant of $P_{\rm st}$. We assume that the mean field potential $U_{\rm MF}$ is bounded from below by $U_{\rm MF}(\mathbf{z})\geq U_{\rm MF-kernel,min}$ which implies that the ensemble average $f(\mathbf{x})=\int_\Omega U_{\rm MF}(\mathbf{x},\mathbf{y})P(\mathbf{y}){\rm d}^My$ is bounded from below by $U_{\rm MF,min}$: $\forall\mathbf{x}:f(\mathbf{x})\geq U_{\rm MF-kernel,min}$. This result, in turn, implies that the ensemble average $\int_\Omega f(\mathbf{x})P(\mathbf{x})\,{\rm d}^Mx$ is bounded from below by $U_{\rm MF-kernel,min}$. Consequently, the double integral occurring in Eq. (44) is bounded from below by $\beta U_{\rm MF-kernel,min}/2$ and from Eq. (44) we obtain

$$I[P,P_{\rm st}]\geq\ln Z^*+\frac{\beta}{2}U_{\rm MF-kernel,min}\ . \quad (45)$$

That is, $I[P, P_{\rm st}]$ is bounded from below. In addition, the functional $I[P, P_{\rm st}]$ is, up to a constant, equivalent to $\beta F[P]$. The reason for this is that the ${}^{\rm BGS}K[P, W]$ can be written as $-S[P] - \int_\Omega P(\mathbf{x}) \ln W(\mathbf{x})\, \mathrm{d}^M x$. Using Eq. (11) for $U(\mathbf{x}) = U_0(\mathbf{x})$ and the Boltzmann factor $Z_B = \int_\Omega \exp\{-\beta U_0(\mathbf{x})\}\, \mathrm{d}^M x$, we can write ${}^{\rm BGS}K[P, W]$ as $-S[P] + \beta \int_\Omega P(\mathbf{x}) U_0(\mathbf{x})\, \mathrm{d}^M x + \ln Z_B$. Substituting this result into Eq. (44) gives us

$$I[P, P_{\rm st}] = \ln(Z^* Z_B) - S[P] + \beta U[P] \qquad (46)$$

or, alternatively, the final result:

$$I[P, P_{\rm st}] = \beta F[P] + \ln[Z^* Z_B] \; . \qquad (47)$$

Comparing Eqs. (45) and (47) we obtain

$$F[P] \geq -\frac{\ln(Z_B)}{\beta} + \frac{1}{2} U_{\rm MF-kernel,min} \; . \qquad (48)$$

The inequality (48) states that in the context of the BGS statistics mean field systems with mean field interaction potentials that are bounded from below have free energy measures that are bounded from below as well. This result holds for mean field system defined on all kind of phase spaces. While for systems defined on finite phase spaces we have derived the same result under much weaker conditions in the previous section, the estimate (48) can in particular be used for systems defined on infinite phase spaces (e.g., $\Omega = \mathbb{R}^M$) and mixed phase spaces (e.g. $\Omega = \mathbb{R}^{M'} \times \prod_{i=1}^{M''} [a_i, b_i]$ with $M' + M'' = M$ such as phase oscillator systems with inertia terms).

Nonlinear energy functionals and BGS statistics

The functional (42) is a special case of the functional

$$I[P, P_0] = \int_\Omega \mathrm{d}^M x \int \mathrm{d}P \ln\left[\frac{G(P)}{G(P_0)}\right] \; . \qquad (49)$$

Here, we assume that we deal with the BGS statistics and a general nonlinear energy functional U composed of a linear part $U_{\rm L}$ and a nonlinear part $U_{\rm NL}$, see Eq. (5). Accordingly, G is given by

$$G[u] = u \exp\left\{\beta \frac{\delta U_{\rm NL}}{\delta u}\right\} \; , \qquad (50)$$

cf. Eq. (9). The expression $\int \mathrm{d}P \ldots$ denotes a functional integration, that is, an integration with respect to a function. Let $f(x)$ by a function defined on a one-dimensional domain Ω. Then, $\int_\Omega \mathrm{d}x [\int \mathrm{d}f\, g(f(x))]$ can be written as $\int_\Omega \int^{z=f(x)} g(z) \mathrm{d}z\, \mathrm{d}x$. That is, we integral with respect to z, replace in the result thus obtain z by $f(x)$, and finally integrate with respect to x. It is clear from the notion of a functional integration that the functional integration and the functional derivative can be regarded as inverse operations. For example, for the functional $Y[f] = \int_\Omega \mathrm{d}x [\int \mathrm{d}f\, g(f(x))]$ we get $\delta Y / \delta f = g(f)$ leading to $Y[f] = \int_\Omega \mathrm{d}x [\int \mathrm{d}f \delta Y / \delta f]$. For our purposes, however, we will not dwell into the formalism of functional integrations. We interpret the functional I as a functional that satisfies a particular ordinary first order differential equation. To this end, we introduce a real parameter κ and consider a probability density $\tilde{P}(\mathbf{x}, \kappa)$ depending on κ. Then, the integral (49) is defined as the integral $I[\tilde{P}, P_0]$ that satisfies

$$\frac{\mathrm{d}}{\mathrm{d}\kappa} I[\tilde{P}(\mathbf{x}; \kappa), P_0] = \int_\Omega \frac{\mathrm{d}\tilde{P}}{\mathrm{d}\kappa} \ln\left[\frac{G(\tilde{P})}{G(P_0)}\right] \; \mathrm{d}^M x \; . \qquad (51)$$

For $P_0 = P_{\rm st}$ the term $G(P_0)$ can be replaced by $G(P_{\rm st}) = W/Z^*$. Analogous to derivation of Eq. (47), we can then conclude that

$$\begin{aligned} &\frac{\mathrm{d}}{\mathrm{d}\kappa} I[\tilde{P}, P_{\rm st}] \\ &= \int_\Omega \frac{\mathrm{d}\tilde{P}}{\mathrm{d}\kappa} \ln[G(\tilde{P})] + \int_\Omega \frac{\mathrm{d}\tilde{P}}{\mathrm{d}\kappa} \ln\left(Z^* Z_B e^{\beta U_0}\right) \\ &= \frac{\mathrm{d}}{\mathrm{d}\kappa}\left[-S[\tilde{P}] + \beta U_{\rm NL}[\tilde{P}]\right] + \beta \frac{\mathrm{d}}{\mathrm{d}\kappa} \int_\Omega U_0 \tilde{P}\, \mathrm{d}^M x \end{aligned} \qquad (52)$$

Consequently, we can integrate both sides of Eq. (52) with respect to κ. Subsequently, we drop the parameter κ (that merely has been used to carry out the functional integration using standard techniques). The result reads:

$$I[P, P_{\rm st}] = \int_\Omega {\rm d}^M x \int {\rm d}P \ln\left[\frac{G(P)}{G(P_{\rm st})}\right] = \beta F[P] + I_0 \, . \quad (53)$$

I_0 denotes an integration constant. Since $F[P]$ can be decomposed into $F = U_{\rm NL} - \beta^{-1}\,{}^{\rm BGS}S + U_{\rm L}$ and $U_{\rm L} = \int_\Omega U_0(\mathbf{x})P(\mathbf{x})\,{\rm d}^M x$ can be written as $U_{\rm L} = -\beta^{-1}\int_\Omega P(\mathbf{x})\ln[Z_B W(\mathbf{x})]\,{\rm d}^M x$, we obtain $F = U_{\rm NL} - \beta^{-1}\ln Z_B + \beta^{-1}\int_\Omega P\ln[P/W]\,{\rm d}^M x$. Due to the semi-positivity of the BGS-Kullback measure (i.e., because of $\int_\Omega P\ln[P/W]\,{\rm d}^M x \geq 0$), we conclude that if the nonlinear energy functional is bounded from below by $U_{\rm NL,min}$, the free energy functional F and the functional I are bounded from below as well:

$$F[P] \geq -\frac{\ln Z_B}{\beta} + U_{\rm NL,min} \, , \quad (54)$$

$$\Rightarrow \quad I[P, P_{\rm st}] \geq \ln Z_B + \beta U_{\rm NL,min} + I_0 \, . \quad (55)$$

Finally, we would like to mention that from Eqs. (49) and (50) and the aforementioned inverse relation $\int_\Omega {\rm d}^M x[\int {\rm d}P \delta U_{\rm NL}/\delta P] = U_{\rm NL}[P]$, it follows that $I[P, P_0]$ can equivalently be expressed as

$$I[P, P_0] = \beta\, U_{\rm NL}[P] + \int_\Omega P(\mathbf{x})\ln\left[\frac{P}{G(P_0)}\right]\,{\rm d}^M x + I_0 \, . \quad (56)$$

That is, the functional (49) indeed generalizes the functional (43). Likewise, Eq. (49) generalizes Eq. (42). In order to see this, note that the mean field functional $Y[P] = 0.5\int_\Omega\int_\Omega U_{\rm MF}(\mathbf{x},\mathbf{y})P(\mathbf{x})P(\mathbf{y})\,{\rm d}^M x\,{\rm d}^M y$ with $U_{\rm MF}(\mathbf{x},\mathbf{y}) = U_{\rm MF}(\mathbf{y},\mathbf{x})$ satisfies $\int_\Omega\int_\Omega Y[\delta Y/\delta P]{\rm d}^M x\,{\rm d}^M y = \delta Y[P](P) = 2Y[P]$. Consequently, if $U_{\rm NL}$ corresponds solely to such a mean field functional we can add on the right hand side of Eq. (56) a zero in form of $-2\beta U_{\rm NL} + \beta\delta U_{\rm NL}[P](P)$ and write $\beta\delta U_{\rm NL}[P](P)$ as $\int_\Omega P\ln[\exp\{\beta\delta U_{\rm NL}/\delta P\}]\,{\rm d}^M x$ which yields Eq. (42).

Nonlinear free energy functionals with matching condition

We consider a system with a nonlinear energy functional U given by Eq. (5) and a general entropy and information measure S. We assume that the system has at least one stationary behavior for which the free energy $F = U - \beta^{-1}S$ and the nonlinear part $U_{\rm NL}$ of the energy measure are stationary: $\delta F[P_{\rm st}] = 0$ and $\delta U_{\rm NL}[P_{\rm st}] = 0$. We show now that this matching condition implies the boundedness of free energy measures. Our departure point is the free energy measure F given by $F = U_{\rm L} + U_{\rm NL} - \beta^{-1}S$. Since $P_{\rm st}$ solves the variational problem (1) and we have $\delta U_{\rm NL}[P_{\rm st}] = 0$, Eq. (2) becomes

$$\delta U[P_{\rm st}] - \beta^{-1}\delta S[P_{\rm st}] - \mu\int_\Omega \delta P{\rm d}^M x = 0 \quad (57)$$

which leads to

$$\delta U_{\rm L}[P_{\rm st}](\delta P) - \beta^{-1}\delta S[P_{\rm st}](\delta P) - \mu\int_\Omega \delta P{\rm d}^M x = 0 \, . \quad (58)$$

We proceed now as in previously discussed cases. From Eq. (58) it follows that $\delta S[P_{\rm st}](\epsilon) = \beta\delta U_{\rm L}[P_{\rm st}](\epsilon) - \beta\mu\int_\Omega \epsilon(\mathbf{x})\,{\rm d}^M x$. Substituting this result into Eq. (21), taking the normalization of P and $P_{\rm st}$ into account and the identity $\delta U_{\rm L}[P](P') = U[P']$ (see Eq. (8)), we obtain

$$S[P_{\rm st}] - S[P] + \beta U_{\rm L}[P] - \beta U_{\rm L}[P_{\rm st}])] \geq 0 \, . \quad (59)$$

Using the free energy measure $F = U_{\rm L} + U_{\rm NL} - \beta^{-1}S$, we can transform the inequality (59) into

$$F[P] \geq F[P_{\rm st}] - \beta U_{\rm NL}[P_{\rm st}] + \beta U_{\rm NL}[P] \, . \quad (60)$$

We finally assume that the nonlinear part $U_{\rm NL}$ of the system energy measure U is bounded from below: $\forall P : U_{\rm NL}[P] \geq U_{\rm NL,min}$. Then, from Eq. (60) we obtain

$$F[P] \geq F[P_{\rm st}] - \beta U_{\rm NL}[P_{\rm st}] + \beta U_{\rm NL,min} \, . \quad (61)$$

That is, provided that the integrals $F[P_{\rm st}]$ and $U_{\rm NL}[P_{\rm st}]$ exist (i.e, are finite), the free energy F is bounded from below.

generic type	$S =$	U	Ω	K, I	F[P]	$F[P_{\mathrm{st}}]$
A	general	U_{L}	finite/∞	K	bounded f.b.	minimal
B	general	negative concave	finite/∞	K	bounded f.b.	minimal
C	general	bounded f.b. & f.a.	finite	K	bounded f.b.	—
D	general	bounded f.b.	finite	—	bounded f.b.	—
E	${}^{\mathrm{BGS}}S$	bounded f.b. $U_{\mathrm{L}} + U_{\mathrm{MF}}$	finite/∞	I	bounded f.b.	—
F	${}^{\mathrm{BGS}}S$	bounded f.b. $U_{\mathrm{L}} + U_{\mathrm{NL}}$	finite/∞	I	bounded f.b.	—
G	general	matching condition, $U_{\mathrm{L}} + U_{\mathrm{NL}}$	finite/∞	K	bounded f.b.	—

Table 1. Boundedness of several generic free energy functionals of the form $F = U - \beta^{-1}S$ (f.b. = from below, f.a. = from above, ∞ = infinite phase space)

3 Conclusions

Let us summarize the results obtained in the previous section. We examined the boundedness of free energy measure for several generic cases. The conditions involved in these cases as well as the results are listed in Table 1.

From our preceding discussion it is clear that the boundedness of free energy functionals is due to a few fundamental ingredients. For systems described by finite phase spaces the boundedness results from follows assumptions: (i) energy measures are continuous and, therefore, bounded from below and above and (ii) stationary states exist with finite free energies. Alternatively, the boundedness is due to the assumptions: (i) energy measures are bounded from below and (ii) entropy and information measures exhibit a global maximum (which is usually given by the uniform distribution). The maximum corresponds to a finite real number. For systems defined on infinite phase spaces the boundedness of free energy measures is, roughly speaking, a consequence of the assumptions: (i) energy measures are bounded from below, (ii) entropy and information measures are concave measures, and (iii) there exists at least one stationary state with finite values for system energy, entropy or information, and free energy.

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