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# An Inequality for Partition Functions with Disturbed Hamiltonians

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We consider a thermodynamic system consisting of $n$ independent subsystems. Each subsystem is described by a Hamiltonian $H = H_0 + \alpha^i H_1$, $i = 1, 2,..., n$. We answer the question of how the entirety $\boldsymbol{\alpha} = (\alpha^1, \alpha^2,..., \alpha^n)$ must be varied in order to change the total partition function and the total free energy of the system monotonically.

**KEY WORDS:** Partition function; free energy; inequalities; majorization; Schur-convex functionals.

In this note the behavior of the partition function and the free energy of composite disturbed quantum mechanical systems subject to variations of their pertubation (or coupling) parameters is studied. Obviously, for such systems the statistical and thermodynamic quantities depend not only on the temperature, but also on these parameters. Hence there is a chance to control—in the simplest case to compensate—the temperature dependence of a certain quantity by its dependence on the perturbation parameters. A possible application could lie in constructing alternating processes taking their pattern from the adiabatic demagnetization in order to lower temperature. For such purposes it is essential to know what alterrations of the entire set of the pertubation parameters will cause a monotonic change of the quantity in question. It is precisely this in relation to the partition function and the free energy that will be developed. The mathematical background lies in enriching the usual considerations with some ideas of the majorization concept.

Let us start with the canonical partition function

$$Z = \operatorname{Tr} \exp(-\beta H) \tag{1}$$

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If we assume a Hamiltonian of the form $H = H_0 + \alpha H_1$, then we have not only

$$\frac{\partial^2}{\partial \beta^2} \ln Z(\beta, \alpha) \geqslant 0 \tag{2a}$$

but also

$$\frac{\partial^2}{\partial \alpha^2} \ln Z(\beta, \alpha) \geqslant 0 \tag{2b}$$

For proofs see, e.g., Bogoljubov[1] or Okubo and Isihara.[2]

Next we consider a thermodynamic system consisting of $n$ ($n$ finite) independent subsystems. Let these subsystems be in a common bath with inverse temperature $\beta$ and be described by Hamiltonians of the above-mentioned type differing only in the $\alpha^i$. Then for the partition function of the $i$th subsystem and the total partition function we clearly have, respectively,

$$Z^i(\alpha^i) = \mathrm{Tr}\, \exp[-\beta(H_0 + \alpha^i H_1)] \tag{3}$$

and

$$Z^{\mathrm{total}}(\boldsymbol{\alpha}) = \prod_{i=1}^{n} Z^i(\alpha^i) \tag{4}$$

where in $\boldsymbol{\alpha} = (\alpha^1, \alpha^2, ..., \alpha^n)$ the pertubation parameters (coupling strengths) are collected.

Now a rather natural question arises: Are there any handy conditions for changing the $n$-tuple $\boldsymbol{\alpha}$ into another one $\boldsymbol{\alpha}'$ so that the total partition function responds monotonically—say, decreases? For mathematical convenience we reformulate this somewhat: Characterize the class $\mathscr{K}_n$ of matrices $T$ defined by the following property:

$$\mathscr{K}_n := \{T\colon Z^{\mathrm{total}}(T\boldsymbol{\alpha}) \leqslant Z^{\mathrm{total}}(\boldsymbol{\alpha}), \forall \boldsymbol{\alpha}\} \tag{5a}$$

There is a surprisingly simple answer in terms of majorization techniques,[3-5] which we briefly recall:

(i) Let there be $\mathbf{x} = (x^1, x^2, ..., x^n)$ with $x^i \in \mathbb{R}$. Now one defines $\mathbf{x}' \prec \mathbf{x}$ (verbally: $\mathbf{x}$ majorizes $\mathbf{x}'$ or $\mathbf{x}'$ is more mixed than $\mathbf{x}$) iff there exists a doubly stochastic matrix T which fulfills $\mathbf{x}' = T\mathbf{x}$.

(ii) A doubly stochastic matrix has only nonnegative elements and the sum of an arbitrary row or column is equal to 1. The set of the $n$-dimensional, doubly stochastic matrices is usually denoted by $BST_n$.

(iii) A functional $\varphi(\mathbf{x})$ is called Schur-convex iff, whenever $\mathbf{x}' \prec \mathbf{x}$, an inequality $\varphi(\mathbf{x}') \leqslant \varphi(\mathbf{x})$ holds. (Unfortunately, the use of the direction of "$\prec$" differs in the literature.[6,7])

(iv) *Theorem:* Let $g$ be a continuous, nonnegative function on $J \subseteq \mathbb{R}$. Then the functional $\varphi(\mathbf{x}) = \prod_{i=1}^{n} g(x^i)$, with $\mathbf{x} \in J^n$, is Schur-convex iff $\log g(x)$ is convex.[3]

Now we may argue: Inequality (2b) ensures the convexity of $\ln Z^i(\alpha^i)$. Therefore, $Z^{\text{total}}(\boldsymbol{\alpha}) = \prod_{i=1}^{n} Z^i(\alpha^i)$ is a Schur-convex functional. Hence, whenever $\boldsymbol{\alpha}' \prec \boldsymbol{\alpha}$ holds, we know that $Z^{\text{total}}(\boldsymbol{\alpha}') \leqslant Z^{\text{total}}(\boldsymbol{\alpha})$ and we can identify a nontrivial subset of the sought matrices:

$$\mathscr{K}_n \supseteq BST_n \tag{5b}$$

(In the case of $\sum_{i=1}^{n} \lambda'^i = \sum_{i=1}^{n} \lambda^i$, $\mathscr{K}_n$ is even exhausted by $BST_n$.) In other words: The application of an arbitrary doubly stochastic matrix to an arbitrary $\boldsymbol{\alpha}$ will always diminish $Z^{\text{total}}(\boldsymbol{\alpha})$.

Let us also look at the total free energy of the above systems:

$$F^{\text{total}}(\boldsymbol{\alpha}) = \sum_{i=1}^{n} F^i(\alpha^i) \tag{6}$$

with

$$F^i(\alpha^i) = -\frac{1}{\beta} \ln Z^i(\alpha^i) \tag{7}$$

Analogous arguments lead to $F^{\text{total}}(\boldsymbol{\alpha}') \geqslant F^{\text{total}}(\boldsymbol{\alpha})$ whenever $\boldsymbol{\alpha}' = T\boldsymbol{\alpha}$ and $T \in BST_n$.

Restricting ourselves to a certain $J \subseteq \mathbb{R}$, say $0 \leqslant \alpha^i \leqslant 1$ with $\sum \alpha^i = 1$, we can give upper and lower limits for $F^{\text{total}}(\boldsymbol{\alpha})$. It is known[3] that $\hat{\boldsymbol{\alpha}} = (1, 0, 0,..., 0)$ (or a permutation of it) is the purest and $\hat{\hat{\boldsymbol{\alpha}}} = (1/n, 1/n,..., 1/n)$ is the most mixed $\boldsymbol{\alpha}$ distribution; more precisely: $\hat{\hat{\boldsymbol{\alpha}}} \prec \boldsymbol{\alpha} \prec \hat{\boldsymbol{\alpha}}$, $\forall \boldsymbol{\alpha}$. Hence we have, for reasons of continuity,

$$F^{\text{total}}(\hat{\hat{\boldsymbol{\alpha}}}) = F^{\text{total}}_{\max} \geqslant F^{\text{total}}(\boldsymbol{\alpha}) \geqslant F^{\text{total}}_{\min} = F^{\text{total}}(\hat{\boldsymbol{\alpha}}), \qquad \forall \boldsymbol{\alpha}$$

Straightforward calculation provides

$$F^{\text{total}}_{\min} = \left(-\frac{1}{\beta}\right) \{\ln \operatorname{Tr} \exp[-\beta(H_0 + H_1)] + (n-1) \ln \operatorname{Tr} \exp(-\beta H_0)\}$$

and

$$F^{\text{total}}_{\max} = \left(-\frac{n}{\beta}\right) \ln \operatorname{Tr} \exp\left[-\beta\left(H_0 + \frac{H_1}{n}\right)\right]$$

Finally, we point out the rather general nature of these results, since we did not need any additional requirements on the Hamiltonians $H_0$ and $H_1$ reflecting special physical properties of the subsystems.

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