

## MATRIX INEQUALITIES IN STATISTICAL MECHANICS

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ABSTRACT: Some matrix inequalities used in statistical mechanics are presented. A straightforward proof of the *Thermodynamic Inequality* is given and its equivalence to the Peierls–Bogoliubov inequality is shown.

### 1. Golden–Thompson Inequality

One of the earlier inequalities involving traces of matrices applied to statistical mechanics is the Golden–Thompson inequality. In 1965, Golden [8], Symanzik [17], and C. Thompson [18], independently proved that

$$\mathrm{tr}(e^{A+B}) \leq \mathrm{tr}(e^A e^B) \quad (1.1)$$

holds when  $A$  and  $B$  are Hermitian matrices. From (1.1) Thompson derived a convexity property that was used to obtain an upper bound for the *partition function* of an antiferromagnetic chain  $\mathrm{tr}(e^{-H/\Theta})$ , where  $H$ , a Hermitian operator, is the Hamiltonian of the physical system, and  $\Theta = kT$  where  $k$  is the Boltzmann constant and  $T$  is the absolute temperature. Golden [8] obtained lower bounds for the *Helmholtz free-energy function* for a system in statistical or thermodynamic equilibrium. The Helmholtz free-energy function is given by

$$F = -\Theta \log \mathrm{tr}(e^{-H/\Theta}).$$

Indeed, for any partition of the Hamiltonian  $H = H_1 + H_2$ , the exponential can be represented by the well-known Lie–Trotter formula (for a proof see, for example, [5] or [20])

$$e^{-H/\Theta} = \lim_{n \rightarrow \infty} (e^{-H_1/n\Theta} e^{-H_2/n\Theta})^n. \quad (1.2)$$

Since the exponential of a Hermitian matrix is a positive definite matrix, and recalling the following inequality for positive definite matrices  $A$  and  $B$  (see, e.g., [8])

$$\mathrm{tr}(AB)^{2p+1} \leq \mathrm{tr}(A^2 B^2)^{2p}, \quad p \text{ a non-negative integer,} \quad (1.3)$$

we have

$$\begin{aligned}
\mathrm{tr} (e^{-H_1/\Theta} e^{-H_2/\Theta}) &\geq \mathrm{tr} (e^{-H_1/2\Theta} e^{-H_2/2\Theta})^2 \\
&\geq \mathrm{tr} (e^{-H_1/2^p\Theta} e^{-H_2/2^p\Theta})^{2^p} \\
&\geq \mathrm{tr} (e^{-H_1/2^q\Theta} e^{-H_2/2^q\Theta})^{2^q} \\
&\geq \mathrm{tr} e^{-H/\Theta}, \quad p \leq q.
\end{aligned} \tag{1.4}$$

Regardless of the mode of partition of the Hamiltonian, these inequalities provide a set of nested lower bounds for the Helmholtz free energy. Let  $H = H_1 + H_2$  (in particular,  $H_1$  may be thought of as the kinetic energy and  $H_2$  as the potential energy of the system). In a classical model,  $H_1$  and  $H_2$  commute and so the partition function coincides with  $\mathrm{tr} (e^{-H_1/\Theta} e^{-H_2/\Theta})$ . This commutativity of  $H_1$  and  $H_2$  does not occur in quantal models. For a non-negative integer  $q$ , consider

$$F_q = -\Theta \log \mathrm{tr} (e^{-H_1/2^q\Theta} e^{-H_2/2^q\Theta})^{2^q}.$$

As a consequence of (1.4) and of the increasing monotonicity of the log function, we have

$$F_p \leq F_q \leq F, \quad p \leq q.$$

If  $q = 0$ , then the Helmholtz function  $F_0 = -\Theta \log \mathrm{tr} (e^{-H_1/\Theta} e^{-H_2/\Theta})$  corresponds to what may be termed the *pseudoclassical* case. Since  $F \geq F_0$ , the classical Helmholtz function provides a lower bound approximation to the correct quantum mechanical Helmholtz function [12]. The Golden–Thompson trace inequality has been generalized in several ways (e.g. [1, 4, 6, 9, 14, 19]). For instance, Cohen, Friedland, Kato and Kelly [6] proved inequalities of the form

$$\phi(e^{A+B}) \leq \phi(e^A e^B),$$

where  $A$  and  $B$  belong to  $M_n$ , the algebra of  $n \times n$  complex matrices, and  $\phi$  is a real-valued continuous function of the eigenvalues of its matrix argument. For example,  $\phi(A)$  might be the *spectral radius* of  $A$ , which is the maximum of the magnitudes of the eigenvalues of  $A$ .

## 2. Log Majorization and Golden–Thompson Type Inequalities

For a Hermitian matrix  $A$  in  $M_n$ , we assume that the eigenvalues  $\lambda_i(A)$ ,  $i = 1, \dots, n$ , are arranged in a nonincreasing order  $\lambda_1(A) \geq \dots \geq \lambda_n(A)$ . For

Hermitian matrices  $A$  and  $B$ , we write  $A \succ B$  to denote the *majorization*  $[\lambda_i(A)] \succ [\lambda_i(B)]$ , that is,

$$\sum_{i=1}^k \lambda_i(A) \geq \sum_{i=1}^k \lambda_i(B), \quad k = 1, \dots, n, \quad (2.1)$$

$$\sum_{i=1}^n \lambda_i(A) = \sum_{i=1}^n \lambda_i(B). \quad (2.2)$$

If (2.1) holds but not necessarily (2.2), we say that  $A$  *weakly majorizes*  $B$ , and write  $A \succ_w B$ . When  $A$  and  $B$  are positive definite matrices, we write  $A \prec_{\log} B$  to denote the majorization  $\log A \prec \log B$ , that is,

$$\prod_{i=1}^k \lambda_i(A) \leq \prod_{i=1}^k \lambda_i(B), \quad k = 1, \dots, n-1,$$

$$\prod_{i=1}^n \lambda_i(A) = \prod_{i=1}^n \lambda_i(B).$$

Lenard [14] and Thompson [19] extended the Golden–Thompson inequality to

$$e^{A+B} \prec_w e^{B/2} e^A e^{B/2},$$

or equivalently, to  $\|e^{A+B}\| \leq \|e^{B/2} e^A e^{B/2}\|$ , for any unitarily invariant norm  $\|\cdot\|$  and  $A$  and  $B$  Hermitian matrices. Araki [2] proved that

$$\mathrm{tr}(A^{1/2} B A^{1/2})^{rs} \leq \mathrm{tr}(A^{r/2} B^r A^{r/2})^s, \quad (2.3)$$

for  $A$  and  $B$  positive semidefinite matrices,  $r \geq 1$  and  $s > 0$ . Lieb and Thirring [15] proved the case  $s = 1$  and applied the result to get inequalities for the moments of the eigenvalues of the Schrödinger Hamiltonian. The Araki–Lieb–Thirring inequality (2.3) is also closely related to the Golden–Thompson inequality. Its special case  $r = 2$  and  $s = 2^p$ , with  $p \in \mathbb{N}_0$ , is just (1.3). Kosaki [11] showed that the above inequality remains valid in the setup of general von Neumann algebras. Araki [2] obtained a more general log majorization which is equivalent to

$$(A^{q/2} B^q A^{q/2})^{1/q} \prec_{\log} (A^{p/2} B^p A^{p/2})^{1/p}, \quad 0 < q \leq p. \quad (2.4)$$

Using this result and the Lie–Trotter formula (1.2), Hiai and Petz [9] strengthened the Golden–Thompson trace inequality for Hermitian matrices  $A$  and  $B$ :

$$\mathrm{tr}(e^{A+B}) \leq \mathrm{tr}(e^{pA/2} e^{pB} e^{pA/2})^{1/p}, \quad p > 0. \quad (2.5)$$

In [7], Cohen obtained some spectral inequalities for matrix exponentials, some of which extend Bernstein inequality [4],

$$\mathrm{tr}(e^T e^{T^*}) \leq \mathrm{tr}(e^{T+T^*}),$$

(which is valid for any operator  $T$ ), to partial traces defined by

$$\mathrm{tr}_j^{(k)}(X) = \sum_{i=1}^j \lambda_i(X^{(k)}), \quad k = 1, \dots, n, \quad j = 1, \dots, C_k^n,$$

where  $X^{(k)}$  denotes the  $k$ th compound of  $X \in M_n$ , and where its eigenvalues are labeled in nonincreasing magnitude  $|\lambda_1(X^{(k)})| \geq \dots \geq |\lambda_{C_k^n}(X^{(k)})|$ . For example,  $\mathrm{tr}_n^{(1)}(X) = \mathrm{tr}(X)$  and, when  $X$  is a positive semi-definite matrix,  $\mathrm{tr}_1^{(k)}(X) = \prod_{i=1}^k \lambda_i(X)$ .

The following log majorization for the exponential of an arbitrary matrix  $T$  is just a restatement of one of the inequalities in [7],

$$|e^T| \prec_{\log} e^{\mathrm{Re}T},$$

where  $\mathrm{Re}T := (T + T^*)/2$  and  $|e^T|^2 := e^T e^{T^*}$ . Since for any matrix  $X$ ,

$$|X^s| \prec_{\log} |X|^s, \quad s \in \mathbb{N}, \quad (2.6)$$

the following refinement of the above log majorization holds:

$$|e^{sT}|^{1/s} \prec_{\log} |e^T| \prec_{\log} |e^{T/p}|^p \prec_{\log} e^{\mathrm{Re}T}, \quad s, p \in \mathbb{N}. \quad (2.7)$$

The first and second log majorizations follow from (2.6) with  $X = e^T$  and with  $X = e^{T/p}$ ,  $s = p$ , respectively. The last log majorization follows from (2.6) and (2.7), with  $p \in \mathbb{N}$ ,  $q$  a multiple of  $p$ ,  $X = e^{T/q}$  and  $s = q/p$ , that is

$$|e^{T/p}|^p \prec_{\log} |e^{T/q}|^q;$$

and by using once more the Lie–Trotter formula. In particular, replacing  $X$  by  $X^{(k)}$  in (2.6), having in mind the Binet–Cauchy formula  $(XY)^{(k)} = X^{(k)}Y^{(k)}$  for  $X, Y$  belonging to  $M_n$ , and noting that  $(X^*)^{(k)} = (X^{(k)})^*$ , we

prove the validity of (2.6) and (2.7) for the  $k$ th compounds. Since log majorization implies weak majorization, we have the strengthened version of Bernstein inequality:

$$\mathrm{tr}_j^{(k)}(e^{T/p} e^{T^*/p})^p \leq \mathrm{tr}_j^{(k)}(e^{T+T^*}), \quad p \in \mathbb{N}, \quad k = 1, \dots, n, \quad j = 1, \dots, C_k^n.$$

Replacing  $A$  and  $B$  in (2.4) by  $A^{(k)}$  and  $B^{(k)}$ , respectively, and using the elementary properties of the  $k$ th compounds, we easily obtain the strengthened version of Golden–Thompson inequality (2.5) for partial traces.

### 3. Thermodynamic Inequality

In statistical mechanics, the statistical properties of complex physical systems are described by *density matrices*. A density matrix  $D$  is a positive semidefinite matrix such that  $\mathrm{tr}(D) = 1$ . The eigenvalues of a density matrix are the *probabilities* of the physical states described by the corresponding eigenvectors. The *entropy* of a statistical state described by the density matrix  $D$  is defined by

$$S(D) = -\mathrm{tr}(D \log D)$$

(convention:  $x \log x = 0$  if  $x = 0$ ). For the energy operator  $H$  ( $H$  is Hermitian), the statistical average of the energy is

$$E = \mathrm{tr}(HD).$$

It is an important problem to determine the maximum of the function

$$\psi(D) = \mathrm{tr}(HD) + \Theta \mathrm{tr}(D \log D),$$

which is an approximation to the Helmholtz free energy. For convenience we take  $\Theta = -1$ , which is meaningful in finite dimensional vector spaces. Denoting a positive definite matrix  $D$  by  $D > 0$ , we shall now prove:

#### Theorem 1

(a) Let  $H$  be a Hermitian matrix. Then

$$\log \mathrm{tr}(e^H) = \max\{\mathrm{tr}(HD) + S(D) : D > 0, \mathrm{tr}(D) = 1\}.$$

(b) Let  $D > 0$ , such that  $\mathrm{tr}(D) = 1$ . Then

$$-S(D) = \max\{\mathrm{tr}(HD) - \log \mathrm{tr}(e^H) : H \text{ Hermitian}\}.$$

*Proof.* (a) For every Hermitian  $S$ , and for each  $t \in \mathbb{R}$  in a neighborhood of 0, consider the differentiable function

$$f(t) = \psi(e^{-itS} D e^{itS}). \quad (3.1)$$

Observing that  $e^{itS} = I + itS + \dots$  is a unitary matrix and recalling that the trace is invariant under unitary similarity, we see that  $f(t)$  can take the form

$$f(t) = \operatorname{tr}(H e^{-itS} D e^{itS}) - \operatorname{tr}(D \log D).$$

By the extremum condition, it follows that

$$f'(0) = i \operatorname{tr}(S[H, D]) = 0,$$

where as usual,  $[H, D] = HD - DH$  is the commutator of the matrices  $H$  and  $D$ . Since  $S$  is arbitrary, we conclude that  $[H, D] = 0$  and so  $e^H$  and  $D$  also commute. Having in mind that  $\operatorname{tr}(D) = 1$ , we get

$$\operatorname{tr}(HD) + S(D) = \operatorname{tr}[D(\log e^H - \log D)] = \log \operatorname{tr}(e^H) - \operatorname{tr}[D(\log \operatorname{tr}(e^H) + \log D - \log e^H)].$$

Recalling that  $e^H$  and  $D$  commute, it can be easily seen that this last expression is equal to

$$\log \operatorname{tr}(e^H) - \operatorname{tr}[e^H D e^{-H} \log(\operatorname{tr}(e^H) D e^{-H})].$$

Taking  $C = \operatorname{tr}(e^H) D e^{-H}$ , we obtain

$$\begin{aligned} \log \operatorname{tr}(e^H) - \operatorname{tr}[e^H D e^{-H} \log(\operatorname{tr}(e^H) D e^{-H})] &= \log \operatorname{tr}(e^H) - [\operatorname{tr}(e^H)]^{-1} \operatorname{tr}[e^H C \log C] \\ &= \log \operatorname{tr}(e^H) - [\operatorname{tr}(e^H)]^{-1} \operatorname{tr}[e^H(C \log C - C + I)]. \end{aligned} \quad (3.2)$$

Observing that  $x \log x - x + 1 \geq 0$  for  $x \geq 0$ , we conclude that (3.2) is less or equal to  $\log \operatorname{tr}(e^H)$  and equality occurs only if  $C = I$ , that is,  $D = e^H / \operatorname{tr}(e^H)$ . On the other hand, if  $D = e^H / \operatorname{tr}(e^H)$ , easy calculations show that  $\psi(e^H / \operatorname{tr}(e^H)) = \log \operatorname{tr}(e^H)$  and part (a) of the Theorem is proved.

Next, since

$$\operatorname{tr}((H + Ik)D) - \log \operatorname{tr}(e^{H+Ik}) = \operatorname{tr}(HD) - \log \operatorname{tr}(e^H), \quad k \in \mathbb{R},$$

we may assume that  $\operatorname{tr}(e^H) = 1$ .

Following an analogous argument to the one in the first step of the proof of (a), we can show that the maximum of  $\operatorname{tr}(HD) - \log \operatorname{tr}(e^H)$  for Hermitian  $H$ , occurs when  $[H, D] = 0$ . Thus  $[D, e^H] = 0$ . Since under our assumptions,  $\operatorname{tr}(D) - \operatorname{tr}(e^H) = 0$ , we have:

$$-\operatorname{tr}(HD) + \operatorname{tr}(D \log D) = \operatorname{tr}[e^H D e^{-H} \log(D e^{-H})] - \operatorname{tr}(e^H D e^{-H}) + \operatorname{tr}(e^H) =$$

$$\operatorname{tr}[e^H(Z \log Z - Z + I)] \geq 0, \quad Z = De^{-H}.$$

Hence, the maximum occurs when  $H = \log D$ , and (b) follows.  $\square$

Theorem 1 implies the important *Thermodynamic Inequality* [10]:

$$\log \operatorname{tr}(e^H) \geq \operatorname{tr}(HD) + S(D).$$

The maximum  $\log \operatorname{tr}(e^H)$  is the free energy of equilibrium. For other proofs see [3, 10]. From the proof of Theorem 1, it follows that the occurrence of equality in the Thermodynamic Inequality is characterized by  $D = e^H / \operatorname{tr}(e^H)$ .

For  $A > 0$  and  $B > 0$ , the *relative entropy of Umegaki* is defined by

$$S(A, B) = \operatorname{tr}[A(\log A - \log B)].$$

Clearly,  $S(A, I) = -S(A)$ .

Approximations of the relative entropy were discussed, for instance, by Ruskai and Stillinger [16]. Considering  $u(p) = \frac{1}{p} \operatorname{tr}(A^{1+p}B^{-p} - A)$ ,  $0 < p \leq 1$ , they proved that

$$u(-p) \leq S(A, B) \leq u(p) \tag{3.3}$$

and showed that the bounds  $u(-p)$  and  $u(p)$  tend to  $S(A, B)$  as  $p \rightarrow 0$ . Exploiting Richardson extrapolation, Ruskai and Stillinger also noticed that the average of these bounds can be used to improve estimates of thermodynamic variables such as the free energy. Note that the left-hand-side of (3.3) with  $p = 1$  yields the Klein inequality.

Hiai and Petz [9] obtained the following bounds for the relative entropy:

$$\frac{1}{p} \operatorname{tr}(A \log(B^{-p/2} A^p B^{-p/2})) \leq S(A, B) \leq \frac{1}{p} \operatorname{tr}(A \log(A^{p/2} B^{-p} A^{p/2})), \quad p > 0$$

where, again, both bounds converge to  $S(A, B)$  as  $p \rightarrow 0$ . Since  $\log x - x + 1 \leq 0$  for  $x \geq 0$ , the upper bound is a better estimate than  $u(p)$  in (3.3). However, the lower bound does not improve the one we shall present in part (c) of Theorem 2.

Let  $H_n$  denote the real vector space of  $n \times n$  Hermitian matrices, endowed with the inner product  $\langle X, Y \rangle = \operatorname{tr}(XY)$ . Given a function  $f : H_n \rightarrow (-\infty, +\infty)$ , the conjugate function, or the *Legendre transform* of  $f$  is the function  $f^* : H_n \rightarrow (-\infty, +\infty)$  defined by

$$f^*(Y) = \sup\{\operatorname{tr}(XY) - f(X) : X \text{ Hermitian}\}.$$

The following corollary, which trivially follows from Theorem 1, shows that the relative entropy  $S(A, B)$ , viewed as a function of a positive definite matrix  $A$  of trace 1, is the Legendre transform of  $\log \operatorname{tr}(e^{H+\log B})$ , where  $B$  is positive definite, and vice-versa.

**Corollary (Hiai and Petz, [9])**

(a) *Let  $H$  be a Hermitian matrix and  $B > 0$ . Then*

$$\log \operatorname{tr}(e^{H+\log B}) = \max\{\operatorname{tr}(AH) - S(A, B) : A > 0, \operatorname{tr}(A) = 1\}.$$

(b) *Let  $A > 0$  such that  $\operatorname{tr}(A) = 1$ , and let  $K$  be a Hermitian matrix. Then*

$$S(A, e^K) = \max\{\operatorname{tr}(AH) - \log \operatorname{tr}(e^{H+K}) : H \text{ Hermitian}\}.$$

#### 4. Peierls–Bogoliubov Inequality

It is often difficult to calculate the value of the partition function  $\operatorname{tr}(e^H)$ . It is simpler to compute the related quantity  $\operatorname{tr}(e^{H_0})$ , where  $H_0$  is a convenient approximation to  $H$ . Indeed, let  $H = H_0 + V$ . The Peierls–Bogoliubov inequality [10] provides useful information on  $\operatorname{tr}(e^{H_0+V})$  from  $\operatorname{tr}(e^{H_0})$ . This inequality states that, for two Hermitian operators  $A$  and  $B$ ,

$$\operatorname{tr}(e^{A+B}) \geq \operatorname{tr}(e^A) e^{\operatorname{tr}(Be^A)/\operatorname{tr}(e^A)}.$$

This inequality can be easily derived from the Thermodynamic Inequality by considering  $H = A+B$  and  $D = e^A/\operatorname{tr}(e^A)$ . Having in mind the condition for equality in the Thermodynamic Inequality, it can be easily seen that equality occurs if and only if  $B$  is a scalar matrix.

For  $0 \leq \alpha \leq 1$ , the  $\alpha$ -power mean of matrices  $A > 0$  and  $B \geq 0$  is defined by

$$A\#_{\alpha}B = A^{1/2}(A^{-1/2}BA^{-1/2})^{\alpha}A^{1/2}.$$

In particular,  $A\#_{1/2}B = A\#B$  is the geometric mean of  $A$  and  $B$ .

Given Hermitian matrices  $A$  and  $B$ , it would be interesting to compare the lower bound for  $\operatorname{tr}(e^{(1-\alpha)A+\alpha B})$  provided by the Peierls–Bogoliubov inequality and by Hiai and Petz [9], in terms of the  $\alpha$ -power mean:

$$\operatorname{tr}(e^{pA}\#_{\alpha}e^{pB})^{1/p}, \quad p > 0.$$

We finally prove: **Theorem 2.** *The following conditions are equivalent:*

(a) *If  $H$  and  $K$  are Hermitian matrices, then*

$$\operatorname{tr}(e^{H+K}) \geq \operatorname{tr}(e^H) e^{\operatorname{tr}(e^H K)/\operatorname{tr}(e^H)}.$$



(b) If  $A > 0$  such that  $\text{tr}(A) = 1$ , and  $D$  is Hermitian, then

$$\log \text{tr}(e^D) \geq \text{tr}(AD) + S(A).$$

(c) If  $A > 0$  and  $B > 0$ , then

$$\text{tr}[A(\log \text{tr}(A) - \log \text{tr}(B))] \leq S(A, B).$$

*Proof.* (a)  $\Rightarrow$  (b): Let  $A > 0$  with  $\text{tr}(A) = 1$ . Then there exists a Hermitian

matrix  $H$  such that  $A = e^H$ . If  $D$  is Hermitian, then  $K = D - \log A$  is also Hermitian. Hence, by (a),

$$\text{tr}(e^D) \geq \text{tr}(A) e^{\text{tr}(AD - A \log A)/\text{tr}(A)} = e^{\text{tr}(AD) + S(A)},$$

and by the monotonicity of the logarithm function, (b) follows. (b)  $\Rightarrow$  (c):

Let  $A > 0$  and  $B > 0$ . Replacing in (b) the matrix  $A$  by  $A/\text{tr}(A)$  and taking  $D = \log B$ , we have

$$\log \text{tr}(B) \geq \frac{1}{\text{tr}(A)} \text{tr}\left[A\left(\log B - \log \frac{A}{\text{tr}(A)}\right)\right].$$

By multiplying both sides of this inequality by  $-\text{tr}(A)$ , we have

$$-\text{tr}(A \log \text{tr}(B)) \leq S(A, B) - \text{tr}(A \log \text{tr}(A)),$$

and so (c) holds. (c)  $\Rightarrow$  (a): Let  $H$  and  $K$  be Hermitian matrices. Taking in

(c)  $A = e^H$  and  $B = e^{H+K}$ , we obtain

$$\text{tr}(e^H)(\log \text{tr}(e^H) - \log \text{tr}(e^{H+K})) \leq S(e^H, e^{H+K}) = -\text{tr}(e^H K). \quad (4.1)$$

Dividing both sides of (4.1) by  $-\text{tr}(e^H)$  and taking the exponential, (a) follows.  $\square$

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