

APPENDIX A

Mathematical supplement

A.1. Matrices and matrix norms

We consider $n \times n$ matrices with complex entries. Such a matrix a is *hermitian* if it equals its conjugate transpose, $a = a^*$; it is *non-negative* if $\langle \psi, a\psi \rangle \geq 0$ for all vectors ψ . A hermitian matrix a is diagonalizable: there is a unitary matrix U (meaning $U^* = U^{-1}$) such that U^*aU is diagonal. The eigenvalues of a hermitian matrix a are all real. A hermitian matrix is non-negative if and only if all its eigenvalues are non-negative.

If $D = \text{diag}(d_1, \dots, d_n)$ is a diagonal matrix, and f is a real-valued function whose domain contains all the entries d_i of D , then we define

$$f(D) = \text{diag}(f(d_1), \dots, f(d_n)). \quad (\text{A.1})$$

This definition extends to hermitian matrices via diagonalization: If a is a hermitian matrix and f is a real-valued function whose domain contains the spectrum of a , and a is diagonalized as $a = U \text{diag}(\lambda_1, \dots, \lambda_n) U^*$, then we define

$$f(a) = U \text{diag}(f(\lambda_1), \dots, f(\lambda_n)) U^*. \quad (\text{A.2})$$

For an arbitrary $n \times n$ matrix a , the matrix a^*a is hermitian. We define the *absolute value* by $|a| = (a^*a)^{\frac{1}{2}}$, where the square root of a^*a is defined as above. Then $|a|$ is hermitian. The p -norm of a matrix is then defined as

$$\|a\|_p = (\text{Tr } |a|^p)^{1/p}. \quad (\text{A.3})$$

We also define the *operator norm* of a by

$$\|a\| = \sup_{\psi \neq 0} \frac{\|a\psi\|}{\|\psi\|} \quad (\text{A.4})$$

where $\|\psi\| = (\sum_i |\psi_i|^2)^{1/2}$ is the usual vector norm. Note that $\|a\|_\infty = \lim_{p \rightarrow \infty} \|a\|_p = \|a\|$, the operator norm of a .

A.2. Hölder inequality for matrices

PROPOSITION A.1 (Hölder inequality for matrices). *If $1 \leq p, q, r \leq \infty$ with $\frac{1}{p} + \frac{1}{q} = \frac{1}{r}$, we have*

$$\|ab\|_r \leq \|a\|_p \|b\|_q.$$

It follows from a simple induction that

$$\left\| \prod_{j=1}^n a_j \right\|_r \leq \prod_{j=1}^n \|a_j\|_{p_j} \quad (\text{A.5})$$

whenever $1 \leq r, p_1, \dots, p_n$ with $\sum_{j=1}^n \frac{1}{p_j} = \frac{1}{r}$.

There are no short proofs in the case of matrices. The proof here is due to Fröhlich [1978] and it uses chessboard estimates. The proof of Proposition A.1 can be found after that of Lemma A.4.

LEMMA A.2 (Chessboard estimate). *For any $n \in \mathbb{N}$ and any matrices a_1, \dots, a_{2n} , we have*

$$|\text{Tr } a_1 \dots a_{2n}| \leq \prod_{i=1}^{2n} \left(\text{Tr } (a_i a_i^*)^n \right)^{1/2n}.$$

PROOF. Since $(a, b) \mapsto \text{Tr } a^* b$ is an inner product, we have the Cauchy–Schwarz inequality: $|\text{Tr } a b|^2 \leq \text{Tr } a^* a \text{Tr } b^* b$. The following inequality follows:

$$|\text{Tr } a_1 \dots a_{2n}|^2 \leq \text{Tr } (a_1 \dots a_n a_n^* \dots a_1^*) \text{Tr } (a_{2n}^* \dots a_{n+1}^* a_{n+1} \dots a_{2n}). \quad (\text{A.6})$$

This allows to use a reflection positivity argument. By replacing a_i with $a_i / \sqrt{\text{Tr } (a_i a_i^*)^n}$ it is enough to prove the inequality for matrices that satisfy $\text{Tr } (a_i a_i^*)^n = 1$; the general result follows from scaling. Note that the set of such matrices is compact.

Let a_1, \dots, a_{2n} be matrices that maximise $|\text{Tr } a_1 \dots a_{2n}|$, with maximum number of matching neighbours $a_{i+1} = a_i^*$. Suppose there exists an index j such that $a_{j+1} \neq a_j^*$. Using cyclicity, we can assume that $j = n$. By the inequality (A.6), $a_1, \dots, a_n, a_n^*, \dots, a_1^*$ and $a_{2n}^*, \dots, a_{n+1}^*, a_{n+1}, \dots, a_{2n}$ are also maximisers. At least one has strictly more matching neighbours, hence a contradiction. The maximum is then $\text{Tr } (a a^*)^n$ for some matrix $a \in \{a_1, \dots, a_n\}$, which is equal to 1. \square

Chessboard estimates allow to prove what is essentially the case $r = 1$ of Hölder’s inequality.

COROLLARY A.3. *We have*

$$|\text{Tr } a_1 \dots a_n| \leq \prod_{i=1}^n \|a_i\|_{p_i}$$

for all n and all $p_i \geq 1$ such that $\sum_{i=1}^n \frac{1}{p_i} = 1$.

PROOF. It suffices to consider rational p_i , by continuity. Let ℓ be a positive integer such that $2\ell/p_i$ is integer for all i . Let $a_i = U_i|a_i|$ be the polar decomposition of a_i , and let

$$b_i = |a_i|^{p_i/2\ell}, \quad \hat{b}_i = U_i|a_i|^{p_i/2\ell}. \quad (\text{A.7})$$

Then $a_i = \hat{b}_i b_i^{(2\ell/p_i)-1}$, and we have

$$\begin{aligned} |\text{Tr } a_1 \dots a_n| &= |\text{Tr } \hat{b}_1 \underbrace{b_1 \dots b_1}_{(2\ell/p_1)-1} \dots \hat{b}_n \underbrace{b_n \dots b_n}_{(2\ell/p_n)-1}| \\ &\leq \prod_{i=1}^n (\text{Tr } |a_i|^{p_i})^{1/p_i} \\ &= \prod_{i=1}^n \|a_i\|_{p_i}. \end{aligned} \quad (\text{A.8})$$

The inequality follows from Lemma A.2 and from the identities

$$\text{Tr } (b_i b_i^*)^\ell = \text{Tr } (\hat{b}_i \hat{b}_i^*)^\ell = \text{Tr } |a_i|^{p_i}. \quad (\text{A.9})$$

□

LEMMA A.4. *Let $r, r' \in [1, \infty]$ such that $\frac{1}{r} + \frac{1}{r'} = 1$. Then for any square matrix a , we have*

$$\|a\|_r = \max_{\|c\|_{r'}=1} \text{Tr } c^* a.$$

PROOF. The right side is smaller by Corollary A.3:

$$|\text{Tr } c^* a| \leq \|c\|_{r'} \|a\|_r = \|a\|_r. \quad (\text{A.10})$$

In order to check that this inequality is saturated, let $a = U|a|$ be the polar decomposition of a , and choose $c = \|a\|_r^{1-r} U|a|^{r-1}$. Then $\|c\|_{r'} = 1$ and $\text{Tr } c^* a = \|a\|_r$. □

PROOF OF PROPOSITION A.1. Starting with Lemma A.4 and then using Corollary A.3 with $a_1 = c^*$, $a_2 = a$, $a_3 = b$ and $p_1 = r$, $p_2 = p$, $p_3 = q$, we have

$$\begin{aligned} \|ab\|_r &= \sup_{\|c\|_{r'}=1} \text{Tr } c^* ab \\ &\leq \sup_{\|c\|_{r'}=1} \|c\|_{r'} \|a\|_p \|b\|_q. \end{aligned} \quad (\text{A.11})$$

□

A.3. Trotter and Duhamel

We now review a useful expansion for the exponential of a sum of two non-commuting operators, namely the Duhamel formula.

PROPOSITION A.5 (Lie–Trotter formula). *Let a, b be $n \times n$ matrices. Then*

$$e^{a+b} = \lim_{N \rightarrow \infty} \left(e^{\frac{1}{N}a} e^{\frac{1}{N}b} \right)^N = \lim_{N \rightarrow \infty} \left[e^{\frac{1}{N}a} \left(1 + \frac{1}{N}b \right) \right]^N.$$

PROOF. We prove the second formula — the mild changes for the other formula are straightforward. Let K_N be the matrix such that

$$e^{\frac{1}{N}a} \left(1 + \frac{1}{N}b \right) = 1 + \frac{1}{N}(a+b) + K_N. \quad (\text{A.12})$$

It is clear that $\|K_N\| = O(\frac{1}{N^2})$. We have

$$\left[e^{\frac{1}{N}a} \left(1 + \frac{1}{N}b \right) \right]^N = \left(1 + \frac{1}{N}(a+b) \right)^N + R_N, \quad (\text{A.13})$$

where R_N is a matrix whose norm satisfies

$$\|R_N\| \leq \sum_{k=0}^{N-1} \binom{N}{k} \|1 + \frac{1}{N}(a+b)\|^k \|K_N\|^{N-k} = O(\frac{1}{N}). \quad (\text{A.14})$$

The first term in the right side of (A.13) converges to e^{a+b} . \square

PROPOSITION A.6 (Duhamel formula). *Let a, b be $n \times n$ matrices. Then*

$$\begin{aligned} e^{a+b} &= e^a + \int_0^1 e^{ta} b e^{(1-t)(a+b)} dt \\ &= \sum_{k \geq 0} \int_{0 < t_1 < \dots < t_k < 1} dt_1 \dots dt_k e^{t_1 a} b e^{(t_2 - t_1)a} b \dots b e^{(1 - t_k)a}. \end{aligned}$$

PROOF. Let $F(s)$ be the matrix-valued function

$$F(s) = e^{sa} + \int_0^s e^{ta} b e^{(s-t)(a+b)} dt. \quad (\text{A.15})$$

We show that, for all s ,

$$e^{s(a+b)} = F(s). \quad (\text{A.16})$$

The derivative of $F(s)$ is

$$F'(s) = e^{sa} a + e^{sa} b + \int_0^s e^{ta} b e^{(s-t)(a+b)} (a+b) dt = F(s)(a+b). \quad (\text{A.17})$$

On the other hand, the derivative of $e^{s(a+b)}$ is $e^{s(a+b)}(a+b)$. The identity (A.16) clearly holds for $s = 0$ and, since both sides satisfy the same differential equation, they must be equal for all s .

We can iterate Duhamel's formula N times so as to get

$$\begin{aligned} e^{a+b} &= \sum_{k=0}^N \int_{0 < t_1 < \dots < t_k < 1} dt_1 \dots dt_k e^{t_1 a} b e^{(t_2 - t_1)a} b \dots b e^{(1 - t_k)a} \\ &+ \int_{0 < t_1 < \dots < t_N < 1} dt_1 \dots dt_N e^{t_1 a} b e^{(t_2 - t_1)a} b \dots b \left[e^{(1 - t_N)(a+b)} - e^{(1 - t_N)a} \right]. \end{aligned} \quad (\text{A.18})$$

Using $\|e^{ta}\| \leq e^{t\|a\|}$, the last line is less than $2e^{\|a\| + \|b\|} \frac{\|b\|^N}{N!}$ and so it vanishes in the limit $N \rightarrow \infty$. The summand is less than $e^{\|a\|} \frac{\|b\|^k}{k!}$, so that the sum is absolutely convergent. \square

A.4. Further matrix inequalities

PROPOSITION A.7 (Golden–Thompson inequality). *Let a, b be hermitian matrices. Then*

$$\text{Tr}(e^{a+b}) \leq \text{Tr}(e^a e^b).$$

PROOF. Hölder's inequality, in the form (A.5) with $r = 1$, $p_j = n$ and $a_j = ab$, implies that $|\text{Tr}(ab)^n| \leq \|ab\|_n^n$. The latter is equal to $\text{Tr}(a^2 b^2)^{n/2}$ since a, b are hermitian. Letting n be a power of 2, we can iterate and we get

$$\text{Tr}(ab)^n \leq \text{Tr} a^n b^n. \quad (\text{A.19})$$

We use this inequality with $a \mapsto e^{\frac{1}{n}a}$ and $b \mapsto e^{\frac{1}{n}b}$, which gives

$$\text{Tr}\left(e^{\frac{1}{n}a} e^{\frac{1}{n}b}\right)^n \leq \text{Tr} e^a e^b. \quad (\text{A.20})$$

The left side converges to $\text{Tr} e^{a+b}$ as $n \rightarrow \infty$ by the Trotter formula (Proposition A.5). \square

PROPOSITION A.8 (Klein inequality). *Let f be a convex differentiable function, and a, b be hermitian matrices with eigenvalues in the domain of f . Then*

$$\text{Tr}[f(a) - f(b) - (a - b)f'(b)] \geq 0.$$

With $f(s) = e^s$, exchanging a and b , we get

$$\text{Tr}(e^a - e^b) \leq \text{Tr}(a - b)e^a. \quad (\text{A.21})$$

PROOF. Let (ϕ_i) and (ψ_j) be orthonormal bases of eigenvectors of a and b , and let (α_i) and (β_j) the eigenvalues. Let $c_{ij} = \langle \phi_i, \psi_j \rangle$. Then

$$\begin{aligned}
 \langle \phi_i, [f(a) - f(b) - (a - b)f'(b)] \phi_i \rangle &= f(\alpha_i) - \sum_j |c_{ij}|^2 f(\beta_j) - \sum_j |c_{ij}|^2 (\alpha_i - \beta_j) f'(\beta_j) \\
 &= \sum_j |c_{ij}|^2 [f(\alpha_i) - f(\beta_j) - (\alpha_i - \beta_j) f'(\beta_j)] \\
 &\geq 0.
 \end{aligned} \tag{A.22}$$

□

PROPOSITION A.9 (Peierls–Bogolubov inequality). *Let f be convex on \mathbb{R} and a, h be hermitian matrices such that $\text{Tr } e^{-h} = 1$. Then*

$$f(\text{Tr } a e^{-h}) \leq \text{Tr } f(a) e^{-h}.$$

PROOF. Let (ϕ_i) and (η_i) be the eigenvectors and eigenvalues of h . Using Jensen's inequality twice,

$$\begin{aligned}
 f(\text{Tr } a e^{-h}) &= f\left(\sum_i \langle \phi_i, a \phi_i \rangle e^{-\eta_i}\right) \leq \sum_i f(\langle \phi_i, a \phi_i \rangle) e^{-\eta_i} \\
 &\leq \sum_i \langle \phi_i, f(a) \phi_i \rangle e^{-\eta_i} = \text{Tr } f(a) e^{-h}.
 \end{aligned} \tag{A.23}$$

□

PROPOSITION A.10 (Peierls inequality). *Let a be a hermitian matrix and (ϕ_i) an orthonormal set of vectors. Then*

$$\sum_i e^{\langle \phi_i, a \phi_i \rangle} \leq \text{Tr } e^a.$$

PROOF. Let α_j be the eigenvalues of a with corresponding orthonormal eigenvectors ψ_j . Then

$$e^{\langle \phi_i, a \phi_i \rangle} = \exp\left\{\sum_j \alpha_j |\langle \phi_i, \psi_j \rangle|^2\right\} \leq \sum_j |\langle \phi_i, \psi_j \rangle|^2 e^{\alpha_j}. \tag{A.24}$$

We used Jensen's inequality and

$$\sum_j |\langle \phi_i, \psi_j \rangle|^2 = \text{Tr } |\phi_i\rangle \langle \phi_i| = 1. \tag{A.25}$$

The claim follows by summing over i , using $\sum_i |\langle \phi_i, \psi_j \rangle|^2 = \text{Tr } |\psi_j\rangle \langle \psi_j| = 1$. □

A.5. About convex functions

Here is a simple result about convex functions on \mathbb{R} . Recall that the right and left derivatives of a convex function $f(s)$ at $s = 0$ are given respectively by $\partial_+ f(0) = \inf_{s>0} \frac{f(s)-f(0)}{s}$ and $\partial_- f(0) = \sup_{s<0} \frac{f(s)-f(0)}{s}$.

PROPOSITION A.11. *Let f_n be a sequence of continuously differentiable, convex functions on \mathbb{R} such that $f_n \rightarrow f$ pointwise. For each $m \in [\partial_- f(0), \partial_+ f(0)]$ there is a sequence $s_n \rightarrow 0$ such that $m = \lim_{n \rightarrow \infty} f'_n(s_n)$.*

PROOF. We claim the following: for any $\varepsilon, \delta > 0$ there is $N = N(\varepsilon, \delta)$ such that for any $n > N$ we have

$$f'_n(\delta) > \partial_+ f(0) - \varepsilon, \quad f'_n(-\delta) < \partial_- f(0) + \varepsilon. \quad (\text{A.26})$$

The result then follows using the mean value theorem for the continuous function $f'_n(s)$: if it is the case that $m \in [\partial_- f(0) + \varepsilon, \partial_+ f(0) - \varepsilon]$ then there is some $s_n \in [-\delta, \delta]$ satisfying $f'_n(s_n) = m$, otherwise we may take $s_n = \delta$ or $s_n = -\delta$.

We prove the claim for $\partial_+ f(0)$. We have

$$f'_n(\delta) \geq \frac{f_n(\delta) - f_n(\delta/2)}{\delta/2}, \quad \frac{f(\delta/2) - f(0)}{\delta/2} \geq \partial_+ f(0). \quad (\text{A.27})$$

Moreover,

$$\lim_{n \rightarrow \infty} \frac{f_n(\delta) - f_n(\delta/2)}{\delta/2} - \frac{f(\delta/2) - f(0)}{\delta/2} = \frac{f(\delta) - f(\delta/2)}{\delta/2} - \frac{f(\delta/2) - f(0)}{\delta/2} \geq 0. \quad (\text{A.28})$$

So for n large enough we have

$$f'_n(\delta) \geq \frac{f_n(\delta) - f_n(\delta/2)}{\delta/2} \geq \frac{f(\delta/2) - f(0)}{\delta/2} - \varepsilon \geq \partial_+ f(0) - \varepsilon, \quad (\text{A.29})$$

as claimed. \square