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ON AN INEQUALITY INVOLVING POWER AND CONTRACTION OF MATRICES WITH AND WITHOUT TRACE

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ABSTRACT. Let A and B be positive semidefinite matrices. Assuming that the eigenvalues of B are less than one, we prove the following trace inequalities

$$\operatorname{Tr}\left\{(BA^{\alpha}B)^{1/\alpha}\right\} \leq \operatorname{Tr}\left\{(BA^{\beta}B)^{1/\beta}\right\}$$

and

$$\operatorname{Tr}\left\{ \left(BA^{\alpha}B\right)^{1/\alpha}\right\} \leq \operatorname{Tr}\left\{ \left(B^{\alpha/\beta}A^{\alpha}B^{\alpha/\beta}\right)^{1/\alpha}\right\} ,$$

for all $0 < \alpha \leq \beta$. Moreover we prove that

$$\operatorname{Tr}\left\{\left(B^{\alpha/\beta}A^{\alpha}B^{\alpha/\beta}\right)^{1/\alpha}\right\} \leq \operatorname{Tr}\left\{\left(BA^{\beta}B\right)^{1/\beta}\right\} \,,$$

for all $0<\alpha\leq\beta$ and $0<\alpha\leq1.$ Furthermore we prove that

$$(BA^{\alpha}B)^{1/\alpha} \leq (BA^{\beta}B)^{1/\beta}$$

in the cases (a) $1 \le \alpha \le \beta$ or (b) $\frac{1}{2} \le \alpha \le \beta$ and $\beta \ge 1$. Further we present counterexamples involving 2×2 matrices showing that the last inequality is, in general, violated in case that neither (a) nor (b) is fulfilled.

Key words and phrases: Trace inequalities, Operator inequalities, Positive semidefinite matrix, Operator monotony, Operator concavity.

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1. INTRODUCTION

Let M_n be the space of $n \times n$ complex matrices. We say that $A \in M_n$ is positive if A is Hermitian, that is $A^* = A$, and its eigenvalues $\lambda_i(A)$ (i = 1, ..., n) are nonnegative. A positive matrix A is denoted by $0 \le A$ and we say that $A \le B$ if $0 \le B - A$. The identity matrix is denoted by I.

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Our main result is the proof of the following inequalities involving the matrix $(BA^{\alpha}B)^{1/\alpha}$ with $\alpha > 0$:

Theorem 1.1. Let be $A, B \in M_n$ with $0 \le A$ and $0 \le B \le I$. Defining

$$H(\alpha) := (BA^{\alpha}B)^{1/\alpha} \quad and \quad h(\alpha) := \operatorname{Tr} \{H(\alpha)\}$$

we prove the following operator and trace inequalities.

a) For all $1 \leq \alpha \leq \beta$ we have

(1.1)
$$H(\alpha) \le H(\beta) .$$

b') For all $1/2 \le \alpha \le 1$ and $\beta = 1$ we have

(1.2)
$$H(\alpha) \le H(\beta = 1)$$

b") For all $0 < \alpha < 1/2$ and $\beta = 1$ we can find matrices $A \ge 0$ and $0 \le B \le I$ such that

(1.3)
$$H(\alpha) \nleq H(\beta = 1)$$

b) *Combining a*) with b')

$$(1.4) H(\alpha) \le H(\beta)$$

holds for all $1/2 \le \alpha \le \beta$ and $\beta \ge 1$. c) For all $0 < \alpha < \beta$ we prove that

(1.5)
$$h(\alpha) \le h(\beta), \quad \text{that is,} \quad \operatorname{Tr}\left\{ (BA^{\alpha}B)^{1/\alpha} \right\} \le \operatorname{Tr}\left\{ (BA^{\beta}B)^{1/\beta} \right\} .$$

d) For all $0 < \alpha \leq \beta$ we have

(1.6)
$$\operatorname{Tr}\left\{ (BA^{\alpha}B)^{1/\alpha} \right\} \leq \operatorname{Tr}\left\{ \left(B^{\alpha/\beta}A^{\alpha}B^{\alpha/\beta} \right)^{1/\alpha} \right\}$$

e) For all $0 < \alpha \leq \beta$ and $0 < \alpha \leq 1$ we prove that

(1.7)
$$\operatorname{Tr}\left\{\left(B^{\alpha/\beta}A^{\alpha}B^{\alpha/\beta}\right)^{1/\alpha}\right\} \leq \operatorname{Tr}\left\{\left(BA^{\beta}B\right)^{1/\beta}\right\}$$

Remark 1.2. The item a) is the main inequality of Theorem 1.1. As we will see, it is a direct consequence of the following result of F. Hansen [8]:

"If f is an operator monotone function defined on the interval $[0,\infty)$, then $Kf(X)K^* \leq f(KXK^*)$ holds for every $X \geq 0$ and contraction K." See also Lemma 2.1.

A proof of c) can be obtained combining a) with d) and e). More precisely, c) follows from a) in the case $\alpha \ge 1$ and from d) and e) in the case $0 < \alpha \le 1$. The author would like to thank F. Hansen for indicating a simpler proof of c) which does not make use of d) and e). This simpler proof is presented below.

We would like to state our discussion, motivation and background of Theorem 1.1 as follows. A motivation to prove the inequality (1.5) is the application of the well-known trace inequality $|\text{Tr}\{X\}| \leq \text{Tr}\{|X|\}, X \in M_n$ for the particular case where X = AB with $0 \leq A$ and $0 \leq B \leq I$. Here we use the definition $|X| := (X^*X)^{1/2}$. Applying this trace inequality we obtain $h(1) \leq h(2)$, because:

(1.8)
$$h(1) := \operatorname{Tr}\{BAB\} = \operatorname{Tr}\{AB^2\} = \operatorname{Tr}\{A^{1/2}B^2A^{1/2}\}$$
$$\leq \operatorname{Tr}\{A^{1/2}BA^{1/2}\} = \operatorname{Tr}\{AB\}$$
$$\leq \operatorname{Tr}\{|AB|\} = \operatorname{Tr}\{(BA^2B)^{1/2}\} =: h(2) ,$$

where in the first inequality of (1.8) we used that $0 \le B^2 \le B$ since $0 \le B \le I$. We also used that $|\text{Tr}\{AB\}| = \text{Tr}\{AB\}$ because $\text{Tr}\{AB\} = \text{Tr}\{A^{1/2}BA^{1/2}\} \ge 0$ since both A and B are positive matrices. Similar to (1.8), we can also show that $h\left(\frac{1}{2^{k+1}}\right) \le h\left(\frac{1}{2^k}\right)$ for k = 0, 1, 2, ...

Considering the special case $\alpha = 1/2$ and $\beta = 1$ of (1.2) we can easily prove that $H(1/2) \le H(1)$, namely:

$$BAB - (BA^{1/2}B)^2 = BA^{1/2}A^{1/2}B - BA^{1/2}B^2A^{1/2}B = BA^{1/2}(I - B^2)A^{1/2}B \ge 0$$

because $0 \le B \le I$ and so $I - B^2 \ge 0$.

Now we put the inequalities presented in Theorem 1.1 in the context of known results. More precisely, we will derive two particular cases of (1.5) and (1.1) from [1], [3], [11], [10] and [6]. However, we need to impose some restrictions on A and B in the hypothesis of theorem 1.1. These restrictions are 1) B is a projection and 2) $0 \le B \le A \le I$.

- 1) Considering the restriction that B = P is a projection we can show the following two particular cases of (1.5):
 - The first particular case of (1.5) is

(1.9)
$$h(1/k) \le h(1)$$
 for all $k = 1, 2, 3, ...$

We can derive this trace inequality using the following result by Ando, Hiai and Okubo [1]:

"For semidefinite matrices A, B the inequaltity

$$\operatorname{Tr}\{A^{p_1}B^{q_1}\cdots A^{p_N}B^{q_N}\} < \operatorname{Tr}\{AB\}$$

holds with p_i , $q_i \ge 0$ and $\sum_{i=1}^{N} p_i = \sum_{i=1}^{N} q_i = 1$." Applying this result to B = P and $p_i = q_i = 1/k$ we have

$$h(1) = \operatorname{Tr}\{PAP\} = \operatorname{Tr}\{AP\} \ge \operatorname{Tr}\left\{A^{\frac{1}{k}}P \cdots A^{\frac{1}{k}}P\right\}$$
$$= \operatorname{Tr}\left\{\left(PA^{\frac{1}{k}}P\right) \cdots \left(PA^{\frac{1}{k}}P\right)\right\}$$
$$= \operatorname{Tr}\left\{(PA^{1/k}P)^{k}\right\} = h(1/k) ,$$

which proves (1.9).

• The second particular case of (1.5) is

$$h(\alpha) \le h(1)$$
 for all $0 < \alpha \le 1$.

This trace inequality can be derived from the Berezin-Lieb inequality ([3], [11]). To understand this, recall that the Berezin-Lieb inequality states that $\text{Tr}\{f(PXP)\} \leq \text{Tr}\{Pf(X)P\}$ holds if P is a projection and f is a convex function on an interval containing the spectrum of X. Now taking $X = A^{\alpha}$ and $f(\lambda) = \lambda^{1/\alpha}$ ($0 < \alpha \leq 1$) we obtain (1.10), because

$$h(\alpha) = \operatorname{Tr}\left\{ (PA^{\alpha}P)^{1/\alpha} \right\} \le \operatorname{Tr}\left\{ P(A^{\alpha})^{1/\alpha}P \right\} = h(1).$$

Considering the restriction 0 ≤ B ≤ A ≤ I we will show the following two particular cases of (1.1):

• The first particular case of (1.1) is

(1.11)
$$H(1) \le H(2)$$
, that is $BAB \le (BA^2B)^{1/2}$.

Remark 1.3. Although we have $BA^2B \leq (BA^2B)^{1/2}$ and $BA^2B \leq BAB$ (since $0 \leq A, B \leq I$) we cannot conclude from these two operator inequalities that $BAB \leq (BA^2B)^{1/2}$.

• We can derive the operator inequality (1.11) based on the following result in Kamei [10] which is a variation of [5]:

(1.12)
$$0 \le B \le A \text{ assures } (B^{s/2}A^pB^{s/2})^{\frac{1+s}{p+s}} \ge B^{s/2}AB^{s/2} \text{ for } p \ge 1 \text{ and } s \ge 0.$$

To understand this, take p = s = 2 in (1.12), namely, we obtain

$$\left(BA^2B\right)^{\frac{3}{4}} \ge BAB$$

On the other hand,

$$\left(BA^2B\right)^{\frac{1}{2}} \ge \left(BA^2B\right)^{\frac{3}{4}}$$

because $BA^2B \leq BIB \leq I$ since $0 \leq A, B \leq I$.

• The second particular case of (1.1) is a generalization of the first one. More precisely

(1.13) $H(1) \le H(p), \text{ that is, } BAB \le (BA^pB)^{1/p} \text{ for}$

$$H(1) \leq H(p)$$
, that is, $BAB \leq (BA^{p}B)^{1/p}$ for all $p \geq 1$.

We can obtain the above operator inequality using the following result (see [6]) which is also a variant of [5] and a more precise estimation than (1.12):

...

(1.14) The function
$$F_r(p) = (B^r A^p B^r)^{\frac{1+2r}{p+2r}}$$
 for $p \ge 1, r \ge 0$
is operator increasing as a function of p whenever $0 \le B \le A$.

Now the operator inequality $H(1) \leq H(p)$ follows from (1.14) setting r = 1, that is,

$$(BA^{p}B)^{\frac{3}{p+2}} = F_{1}(p) \ge F_{1}(1) = BAB.$$

On the other hand,

$$(BA^{p}B)^{\frac{1}{p}} \ge (BA^{p}B)^{\frac{3}{p+2}}$$

because $BA^pB \leq BIB \leq I$ $(0 \leq A, B \leq I)$ and $3/(p+2) \geq 1/p$ for $p \geq 1$.

We shall state the following couterexamples associated with Theorem 1.1.

Counterexamples. In order to show that we cannot generally drop "Tr" from the inequality (1.5) apart from the cases a) $1 \le \alpha \le \beta$ or b) $1/2 \le \alpha \le \beta$ and $\beta \ge 1$, consider the following concrete example of 2×2 matrices: Let be $B := \begin{pmatrix} 1 & 0 \\ 0 & 1/2 \end{pmatrix}$ and A := 64P + Q with $P := 1/2 \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$ and Q := I - P orthogonal projections. Since we are working with 2×2 matrices, we observe that $\text{Det} [H(\beta) - H(\alpha)] < 0$ implies $H(\beta) \ne H(\alpha)$. Based on this observation we calculate the following determinants:

1) Det $[H(1) - H(1/3)] = -81/16 \approx -5.06 < 0$ 2) Det $[H(2/3) - H(1/2)] = 12 - \frac{63}{26}\sqrt{26} \approx -0.36 < 0$ 3) Det $[H(2/3) - H(1/3)] = 9 - \frac{2115}{832}\sqrt{26} \approx -3.96 < 0$ 4) Det $[H(1/3) - H(1/6)] = -9446625/2097152 \approx -4.5045 < 0$ 5) Det $[H(1/2) - H(1/3)] = -225/128 \approx -1.76 < 0$ 6) Det $[H(4/3) - H(1/3)] \approx -3.5 < 0$

and conclude that the respective affirmatives:

- 1) $H(\beta) \ge H(\alpha)$ holds for all $0 < \alpha < 1/2$ and $\beta = 1$
- 2) $H(\beta) \ge H(\alpha)$ holds for all $1/2 \le \alpha < \beta < 1$
- 3) $H(\beta) \ge H(\alpha)$ holds for all $0 < \alpha < 1/2 < \beta < 1$
- 4) $H(\beta) \ge H(\alpha)$ holds for all $0 < \alpha < \beta < 1/2$
- 5) $H(\beta) \ge H(\alpha)$ holds for all $0 < \alpha < \beta = 1/2$
- 6) $H(\beta) \ge H(\alpha)$ holds for all $0 < \alpha < 1/2$ and $\beta > 1$

are false.

2. **PROOF OF THEOREM 1.1**

Definition 2.1. We say that a real function f is operator concave on the interval I when for all real numbers $0 \le \lambda \le 1$,

$$f((1-\lambda)X + \lambda Y) \ge (1-\lambda)f(X) + \lambda f(Y)$$

for every pair $X, Y \in M_n$ whose spectra lie in the interval *I*. Likewise we say that *f* is operator monotone when $f(X) \leq f(Y)$ for every pair $X, Y \in M_n$ with $X \leq Y$.

Lemma 2.1. [Operator concavity, monotony and contractions, part of Theorems 2.1 and 2.5 of *F*. Hansen and G. K. Pedersen [9]]. Let $f : [0, \infty) \to [0, \infty)$ be a continuous function then the following conditions are equivalent:

- (i) f is operator concave on $[0, \infty)$.
- (ii) f is operator monotone.
- (iii) $Kf(X)K^* \leq f(KXK^*)$ for every contraction K (i.e. $||K|| \leq 1$, where $||\cdot||$ is the operator norm) and for every matrix $X \geq 0$.
- (iv) $Pf(X)P \le f(PXP)$ for all projections P and matrices $X \ge 0$.

A function f is called operator convex if the function -f is operator concave.

As an example of a contraction we have a matrix $B \in M_n$ with $0 \le B \le I$.

Lemma 2.2. Let be $R, S \in M_n$ with $0 \le R$ and $0 \le S \le I$ then the following estimate holds for all $\alpha > 0$

(2.1)
$$\operatorname{Tr}\left\{\left(SRS\right)^{1/\alpha}\right\} \leq \operatorname{Tr}\left\{R^{1/\alpha}\right\}$$

In order to give a proof of Lemma 2.2 and c) of Theorem 1.1, we state the following Lemma 2.3 which is derived from *the minimax principle* for the sake of convenience for readers:

Lemma 2.3. [[7], Lemma 1.1]. If A and B are $n \times n$ positive semidefinite matrices such that $A \ge B \ge 0$, then their eigenvalues of A and B are ordered as

$$\lambda_j(A) \ge \lambda_j(B)$$
 for $j = 1, 2, \dots, n$.

Proof of Lemma 2.2. First we observe that matrices XY and YX have the same eigenvalues with the same multiplicities for $X, Y \in M_n$. Let be $0 \le R$ and $0 \le S \le I$ and using this observation with $X = SR^{1/2}$ and $Y = R^{1/2}S$ we have

(2.2)
$$\lambda_i(SRS) = \lambda_i(SR^{1/2}R^{1/2}S) = \lambda_i(R^{1/2}S^2R^{1/2})$$

for i = 1, 2, ..., n. Since $S^2 \leq S \leq I$ we have that $R^{1/2}S^2R^{1/2} \leq R^{1/2}R^{1/2} = R$. From the last operator inequality it follows from Lemma 2.3 that the eigenvalues of $R^{1/2}S^2R^{1/2}$ and R are ordered as

(2.3)
$$0 \le \lambda_i (R^{1/2} S^2 R^{1/2}) \le \lambda_i(R)$$

for $i = 1, 2, \ldots, n$. From (2.2) and (2.3) we have for all $\alpha > 0$ that

$$\operatorname{Tr}\{(SRS)^{1/\alpha}\} = \sum_{i=1}^{n} \lambda_i (SRS)^{1/\alpha} \\ = \sum_{i=1}^{n} \lambda_i (R^{1/2} S^2 R^{1/2})^{1/\alpha} \\ \leq \sum_{i=1}^{n} \lambda_i (R)^{1/\alpha} = \operatorname{Tr}\{R^{1/\alpha}\},$$

which proves the Lemma 2.2.

Proof of a) of (1.1) in Theorem 1.1. Defining $r := \alpha/\beta$ we have $0 < r \le 1$ since $0 < \alpha \le \beta$. Since the function $f(t) = t^r$, $0 \le r \le 1$ is operator concave (and monotone) on $[0, \infty)$ and the matrix *B* is a contraction we conclude by Lemma 2.1, setting $X = A^{\beta}$ and K = B that

(2.4)
$$BA^{\alpha}B = B(A^{\beta})^{r}B \le (BA^{\beta}B)^{r}.$$

holds for all $0 < \alpha \leq \beta$.

On the other hand using the fact that the function $f(t) = t^s$, $0 \le s \le 1$ is operator monotone and taking $s = 1/\alpha \le 1$ (since $1 \le \alpha$), it follows from (2.4) that

(2.5)
$$(BA^{\alpha}B)^{1/\alpha} \le (BA^{\beta}B)^{r/\alpha} = (BA^{\beta}B)^{1/\beta},$$

which proves a).

Proof of b') and b") in Theorem 1.1. In the case $1/2 \le \alpha \le 1$ and $\beta = 1$ we have $1 \le r := 1/\alpha \le 2$. Based on the fact that the function $f(t) = t^r$ is operator convex on $[0, \infty)$ if and only if $1 \le r \le 2$ (see [4] Theorem V.2.9) it follows by Lemma 2.1 setting $X := A^{1/r}$ with $r := 1/\alpha$ and K := B that

$$H(\alpha) := (BA^{\alpha}B)^{1/\alpha} = (BA^{1/r}B)^r = (KXK^*)^r$$
$$\leq KX^r K^* = BAB := H(\beta = 1) ,$$

which proves b').

In the case $0 < \alpha < 1/2$ and $\beta = 1$ we have $r = 1/\alpha > 2$ which means that the function $f(t) = t^r$ is not operator convex. It follows from Lemma 2.1 that we can find a matrix $X \ge 0$ and a projection P such that $(PXP)^{1/\alpha} \not\leq PX^{1/\alpha}P$. Taking $A = X^{1/\alpha}$ and B = P we have

$$H(\alpha) := (BA^{\alpha}B)^{1/\alpha} = (PXP)^{1/\alpha}$$
$$\nleq PX^{1/\alpha}P = BAB = H(\beta = 1) ,$$

which proves b").

Proof of c) in Theorem 1.1. First we recall that the operator inequality (2.4),

$$BA^{\alpha}B \le \left(BA^{\beta}B\right)^{\alpha/\beta}$$

holds for all $0 < \alpha \le \beta$. From (2.6) it follows from Lemma 2.3 that the eigenvalues of $BA^{\alpha}B$ and $(BA^{\beta}B)^{\alpha/\beta}$ are ordered as

(2.7)
$$\lambda_i(BA^{\alpha}B) \le \lambda_i((BA^{\beta}B)^{\alpha/\beta})$$

for i = 1, ..., n.

From (2.6), (2.7) and since the function $f(t) = t^{1/\alpha}$ is increasing we obtain

$$\operatorname{Tr}\left\{ \left(BA^{\alpha}B\right)^{1/\alpha} \right\} = \sum_{i=1}^{n} \lambda_{i} \left(BA^{\alpha}B\right)^{1/\alpha}$$
$$\leq \sum_{i=1}^{n} \lambda_{i} \left(\left(BA^{\beta}B\right)^{\alpha/\beta} \right)^{1/\alpha}$$
$$= \operatorname{Tr}\left\{ \left(BA^{\beta}B\right)^{1/\beta} \right\} ,$$

which proves c).

Proof of d) in Theorem 1.1. Setting $r = \alpha/\beta$, $S := B^{1-r}$ and $R := B^r A^{\alpha} B^r$ we have $0 \le S \le I$ (because $0 < r \le 1$) and $0 \le R$. Applying the inequality (2.1) for this choice of R and S we obtain

(2.8)
$$\operatorname{Tr}\left\{ \left(BA^{\alpha}B\right)^{1/\alpha}\right\} = \operatorname{Tr}\left\{ \left(B^{1-r}\left(B^{r}A^{\alpha}B^{r}\right)B^{1-r}\right)^{1/\alpha}\right\} \\ \leq \operatorname{Tr}\left\{ \left(B^{r}A^{\alpha}B^{r}\right)^{1/\alpha}\right\} ,$$

which proves d).

Proof of e) in Theorem 1.1. First we note that we can express $\operatorname{Tr}\left\{\left(B^{r}A^{\alpha}B^{r}\right)^{1/\alpha}\right\}$ as a norm, namely:

(2.9)
$$\operatorname{Tr}\left\{\left(B^{r}A^{\alpha}B^{r}\right)^{1/\alpha}\right\} = \|B^{r}A^{\alpha}B^{r}\|_{1/\alpha}^{1/\alpha} = \|B^{r}(A^{\beta})^{r}B^{r}\|_{1/\alpha}^{1/\alpha}$$

where $\|\cdot\|_{1/\alpha}$ is the $1/\alpha$ -trace norm which is an unitarily invariant norm (note that $1/\alpha \ge 1$ since in our hypothesis $0 < \alpha \le 1$).

On the other hand a result from [4] (Theorem IX.2.10) states that for every unitarily invariant norm $\| \cdot \|$ we have

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$$(2.10) |||B^{r}A^{r}B^{r}||| \le |||(BAB)^{r}|||$$

for all $0 \le r \le 1$ if A and B are positive matrices. It follows from (2.10) that

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(2.11)
$$\begin{aligned} \left\| B^{r} (A^{\beta})^{r} B^{r} \right\|_{1/\alpha}^{1/\alpha} &\leq \left\| \left(BA^{\beta}B \right)^{r} \right\|_{1/\alpha}^{1/\alpha} \\ &= \operatorname{Tr} \left\{ \left| \left(BA^{\beta}B \right)^{r} \right|^{1/\alpha} \right\} \\ &= \operatorname{Tr} \left\{ \left(BA^{\beta}B \right)^{r/\alpha} \right\} \\ &= \operatorname{Tr} \left\{ (BA^{\beta}B)^{1/\beta} \right\} \end{aligned}$$

where we could drop the $|\cdot|$ within the trace in the above estimate because $BA^{\beta}B$ is a positive matrix. Now the proof of e) in Theorem 1.1 follows directly from (2.9) and (2.11).

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The Hubbard model describes electrons in solids and poses several mathematical challenges (e.g. [12]). In this model, the extreme points of the set $\{B \in M_n | 0 \le B \le I\}$ correspond to many-electron functions (Slater Determinants). We searched for extreme points that minimize the functional energy of the model. Applying the trace inequality (1.5) for the case $\beta = 1$ V. Bach and the author could reproduce a special result from V. Bach and J. Poelchau [2] for the Hubbard model. Details on the Hubbard model and this application of the trace inequality on it go beyond the scope of this study and will be published separately.

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 \square

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