A lower bound on the C-numerical radius of nilpotent matrices appearing in coherent spectroscopy

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Abstract

We provide a lower bound for the efficiency of polarization or coherence transfer between quantized states under unitary transformations. Mathematically the problem is the determination of the C-numerical radius of A for certain nilpotent matrices C and A. The presented lower bound is conjectured to be exact as it coincides with numerical data provided in [U. Helmke et al., *J. Global Opt.* **23** (2002), 283-308].

1 Introduction

In the study of the efficiency of polarization or coherence transfer between quantized states under unitary transformations (see [1, 2, 3, 5, 6]), one is interested in determining or estimating the quantity

$$b(A_n, C_n) := \max_{UU^*=\mathbb{I}} |\mathrm{tr}(C_n^* U A_n U^*)|, \tag{1.1}$$

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where U^* denotes the Hermitian transpose of U, and A_n and C_n are given matrices derived from a spin system, defined as follows:

$$A_n = \begin{pmatrix} N_n & 0 \\ 0 & N_n \end{pmatrix}, \quad C_n = \begin{pmatrix} 0 & 0 \\ \mathbb{I}_{2^n} & 0 \end{pmatrix}, \tag{1.2}$$

with $\mathbb{I}_m$ the $m \times m$ identity matrix and N_n given inductively by

$$N_0 = (0), \quad N_n = \begin{pmatrix} N_{n-1} & 0 \\ \mathbb{I}_{2^{n-1}} & N_{n-1} \end{pmatrix}.$$

Note that the matrices A_n and C_n are of size $2^{n+1} \times 2^{n+1}$. In matrix analysis literature, the quantity $b(A_n, C_n)$ is called the C_n^*-*numerical radius* of A_n. In [3] the authors proved that $b(A_1, C_1) = 2$ and $b(A_2, C_2) = 4$. By numerical methods, they have the following conjectured values:

n	3	4	5	6
$b(A_n, C_n)$	$4(1+\sqrt{3})$	$8(1+\sqrt{3})$	$16(1+\sqrt{3})+4\sqrt{5}$	$32(1+\sqrt{3})+8\sqrt{5}$

In this note, we show that there is a systematic way to extrapolate these values for general n, and construct unitary matrices U_n such that $\operatorname{tr}(C_n^* U_n A_n U_n^*)$ attains these values. The key idea in our proof is a reduction of A_n to a weighted Jordan form $\tilde{A}_n$ using unitary similarity transforms. One can then get our proposed bounds using the off-diagonal entries of $\tilde{A}_n$.

In the next section we present our main result, and in the last section we discuss some open problems.

2 Main result

Recall that two matrices A and $\widetilde{A}$ are unitarily similar (notation: $A \sim \widetilde{A}$) if there is a unitary matrix U so that $A = U^* \widetilde{A} U$. Clearly, when $A \sim \widetilde{A}$ and $C \sim \widetilde{C}$, then $b(A, C) = b(\widetilde{A}, \widetilde{C})$. If we let $\widetilde{C}_n$ be the direct sum of 2^n copies of $\begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$, then $C_n \sim \widetilde{C}_n$. Thus, to compute $b(A_n, C_n) = b(A_n, \widetilde{C}_n)$, we need to find a unitary U_n to maximize the quantity

$$\left| \operatorname{tr}(\tilde{C}_n^* U_n^* A_n U_n) \right| = \left| \sum_{j=1}^{2^n} a_{2j,2j-1} \right|, \quad \text{where } U_n^* A_n U_n = (a_{ij}). \tag{2.1}$$

Therefore, we need to focus on those unitary matrices U such that $U^* A_n U$ has large positive values on the subdiagonal. Proposition 2.1 will give the right tools. We need some notation to describe the result.

Consider the $(j+1)\times(j+1)$ matrices B_j, S_j, J_j, and the $(j+1)\times j$ matrix Z_j:

$$B_j = \begin{pmatrix} 0 & 0 & 0 & \dots & 0 \\ \sqrt{j}\sqrt{1} & 0 & 0 & \dots & 0 \\ 0 & \sqrt{j-1}\sqrt{2} & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & \sqrt{1}\sqrt{j} & 0 \end{pmatrix},$$

$$S_j = \begin{pmatrix} \sqrt{0} & & & \bigcirc \\ & \sqrt{1} & & \\ & & \ddots & \\ \bigcirc & & & \sqrt{j} \end{pmatrix}, \quad J_j = \begin{pmatrix} \bigcirc & & 1 \\ & 1 & \\ & . & \\ 1 & & \bigcirc \end{pmatrix}, \quad Z_j = \begin{pmatrix} 0 & \cdots & 0 \\ 1 & & \bigcirc \\ \bigcirc & \ddots & \\ & & 1 \end{pmatrix}.$$

Note that $B_0 = (0)$.

Proposition 2.1 *The $(2j+2)\times(2j+2)$ matrix*

$$U_j = \frac{1}{\sqrt{j+1}} \begin{pmatrix} -S_j Z_j & J_j Z_{j+1}^* S_{j+1} J_{j+1} \\ J_j S_j Z_j J_{j-1} & Z_{j+1}^* S_{j+1} \end{pmatrix} \tag{2.2}$$

is unitary and the following equality holds:

$$\begin{pmatrix} B_j & 0 \\ \mathbb{I} & B_j \end{pmatrix} = U_j \begin{pmatrix} B_{j-1} & 0 \\ 0 & B_{j+1} \end{pmatrix} U_j^*. \tag{2.3}$$

Note that U_j is a real matrix with a simple structure. For instance,

$$U_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & \sqrt{2} & 0 & 0 \\ -1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & \sqrt{2} \end{pmatrix}, \quad U_2 = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 & 0 & \sqrt{3} & 0 & 0 & 0 \\ -1 & 0 & 0 & \sqrt{2} & 0 & 0 \\ 0 & -\sqrt{2} & 0 & 0 & 1 & 0 \\ \sqrt{2} & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & \sqrt{3} \end{pmatrix}.$$

Proof of Proposition 2.1. Note that each column of U_j has at most two nonzero entries. It is straightforward to check the columns of U_j form an orthoromal family. Also, it is straightforward to check that

$$\begin{pmatrix} B_j & 0 \\ \mathbb{I} & B_j \end{pmatrix} U_j = U_j \begin{pmatrix} B_{j-1} & 0 \\ 0 & B_{j+1} \end{pmatrix}. \qquad \square$$

As $B_1 = N_1$, equation (2.3) yields that

$$N_2 = \begin{pmatrix} N_1 & 0 \\ \mathbb{I} & N_1 \end{pmatrix} \sim B_0 \oplus B_2.$$

Here $A \oplus B$ stands for the direct sum of A and B, i.e., $A \oplus B = \begin{pmatrix} A & 0 \\ 0 & B \end{pmatrix}$. Clearly, $A \oplus B \sim B \oplus A$, but in general $A \oplus B \neq B \oplus A$. Next, again using (2.3), we have

$$N_3 = \begin{pmatrix} N_2 & 0 \\ \mathbb{I} & N_2 \end{pmatrix} \sim \begin{pmatrix} B_0 \oplus B_2 & 0 \\ \mathbb{I} & B_0 \oplus B_2 \end{pmatrix} \sim \begin{pmatrix} B_0 & 0 \\ \mathbb{I} & B_0 \end{pmatrix} \oplus \begin{pmatrix} B_2 & 0 \\ \mathbb{I} & B_2 \end{pmatrix} \sim B_1 \oplus (B_1 \oplus B_3).$$

We shall abbreviate $B_1 \oplus B_1 \oplus B_3$ as $2B_1 \oplus B_3$. In other words,

$$nB_j := B_j \oplus \cdots \oplus B_j,$$

where B_j appears n times in the right hand side. Continuing this way, we get

$$N_4 \sim 2 \begin{pmatrix} B_1 & 0 \\ \mathbb{I} & B_1 \end{pmatrix} \oplus \begin{pmatrix} B_3 & 0 \\ \mathbb{I} & B_3 \end{pmatrix} \sim 2(B_0 \oplus B_2) \oplus (B_2 \oplus B_4) \sim 2B_0 \oplus 3B_2 \oplus B_4,$$

$$N_5 \sim 2 \begin{pmatrix} B_0 & 0 \\ \mathbb{I} & B_0 \end{pmatrix} \oplus 3 \begin{pmatrix} B_2 & 0 \\ \mathbb{I} & B_2 \end{pmatrix} \oplus \begin{pmatrix} B_4 & 0 \\ \mathbb{I} & B_4 \end{pmatrix} \sim$$
$$\sim 2B_1 \oplus 3(B_1 \oplus B_3) \oplus (B_3 \oplus B_5) \sim 5B_1 \oplus 4B_3 \oplus B_5,$$

etc. In general, we have

$$N_{2m+1} \sim a_1^{(2m+1)} B_1 \oplus a_3^{(2m+1)} B_3 \oplus \cdots \oplus a_{2m+1}^{(2m+1)} B_{2m+1} \tag{2.4}$$

and

$$N_{2m} \sim a_0^{(2m)} B_0 \oplus a_2^{(2m)} B_2 \oplus \cdots \oplus a_{2m}^{(2m)} B_{2m}, \tag{2.5}$$

where for $j \geq i \geq 0$ the numbers $a_i^{(j)}$ are integers satisfying

$$a_j^{(j)} = 1, \quad a_i^{(j)} = a_{i-1}^{(j-1)} + a_{i+1}^{(j-1)}, \quad \text{if } \ i+j \text{ is even.} \tag{2.6}$$

$$a_i^{(j)} = 0 \quad \text{if } \ i+j \text{ is odd.}$$

The numbers $a_i^{(j)}$ are uniquely determined by the above conditions. We can tablilize the values as follows.

Table for $a_i^{(j)}$

$j \setminus i$	0	1	2	3	4	5	6	7	$\cdots$
1		1							
2	1		1						
3		2		1					
4	2		3		1				
5		5		4		1			
6	5		9		5		1		
7		14		14		6		1	
8	14		28		20		7		1
$\vdots$									

We derive the following closed formula for the numbers $a_i^{(j)}$ in terms of binomial coefficients $\binom{r}{s}$. As usual we let $\binom{r}{s} = 0$ when $s < 0$ or $s > r$, and $\binom{0}{0} = 1$.

Proposition 2.2 *For $j \geq i \geq 0$, the following formulas hold:*

$$a_i^{(j)} = \binom{j-1}{\frac{j-i}{2}} - \binom{j-1}{\frac{j-i}{2}-2}, \quad i+j \text{ is even}, \tag{2.7}$$

and $a_i^{(j)} = 0$, otherwise.

Proof. First observe that $a_j^{(j)} = 1 = \binom{0}{0} - \binom{0}{-2}$. Since the numbers $a_i^{(j)}$ are uniquely determined by the recurrence relation (2.6), it suffices to show that our proposed formula in (2.7) satisfy (2.6) if $i+j$ is even. Using the Pascal identity on binomial coefficients $\binom{k}{l-1} + \binom{k}{l} = \binom{k+1}{l}$, we have

$$\begin{aligned} a_{i-1}^{(j-1)} + a_{i+1}^{(j-1)} &= \binom{j-2}{\frac{j-i}{2}} - \binom{j-2}{\frac{j-i}{2}-2} + \binom{j-2}{\frac{j-i}{2}-1} - \binom{j-2}{\frac{j-i}{2}-3} = \\ &= \binom{j-1}{\frac{j-i}{2}} - \binom{j-1}{\frac{j-i}{2}-2} = a_i^{(j)}. \end{aligned}$$

□

Our main result is the following.

Theorem 2.3 *Suppose n is a positive integer. We have*

$$b(A_{n+1}, C_{n+1}) \geq 2b(A_n, C_n). \tag{2.8}$$

Moreover, if $n = 2m+1$ is odd, then $b(A_n, C_n)$ is not less than

$$2\sum_{k=0}^{m} \left\{ \left(\binom{2m}{k} - \binom{2m}{k-2} \right) \left(\sum_{q=1}^{m+1-k} \sqrt{2(m+1-k-q)+1}\sqrt{2q-1} \right) \right\}. \tag{2.9}$$

Proof. Suppose $U = \begin{pmatrix} U_{11} & U_{12} \\ U_{21} & U_{22} \end{pmatrix}$ is a $2^{n+1} \times 2^{n+1}$ unitary matrix such that $U_{11}, U_{12}, U_{13}, U_{14}$ are $2^n \times 2^n$ matrices, and $b(A_n, C_n) = |\mathrm{tr}\,(C_n^* U A_n U^*)|$. Let

$$\tilde{U} = \begin{pmatrix} U_{11} & 0 & U_{12} & 0 \\ 0 & U_{11} & 0 & U_{12} \\ U_{21} & 0 & U_{22} & 0 \\ 0 & U_{21} & 0 & U_{22} \end{pmatrix}.$$

Then

$$b(A_{n+1}, C_{n+1}) \geq |\mathrm{tr}\,(C_{n+1} \tilde{U} A_{n+1} \tilde{U}^*)| = 2b(A_n, C_n).$$

So, (2.8) holds.

Next, consider the $2r \times 2r$ matrix

$$L_r = \begin{pmatrix} 0 & 0 \\ \mathbb{I}_r & 0 \end{pmatrix}.$$

Then $C_n = L_{2^n}$ is unitarily similar to $L_{r_1} \oplus \cdots \oplus L_{r_k}$ as long as $r_1 + \ldots + r_k = 2^n$. In particular, we have

$$C_n \sim C_{n-1} \oplus C_{n-1}$$

and

$$C_{n-1} \sim a_1^{(2m+1)} L_1 \oplus a_3^{(2m+1)} L_2 \oplus \cdots \oplus a_{2m+1}^{(2m+1)} L_{m+1}.$$

Thus, combining this with (2.4),

$$b(A_n, C_n) \geq 2b(N_n, C_{n-1}) \geq$$

$$\geq 2[(a_1^{(2m+1)} b(B_1, L_1) + a_3^{(2m+1)} b(B_3, L_2) + \ldots + a_{2m+1}^{(2m+1)} b(B_{2m+1}, L_{m+1})]. \quad (2.10)$$

Also, observe that by a permutation

$$B_{2m+1} \sim \begin{pmatrix} 0 & S_m \\ T_m & 0 \end{pmatrix}, \quad (2.11)$$

where T_m and S_m are the $(m+1) \times (m+1)$ matrices

$$T_m = \begin{pmatrix} \sqrt{2m+1}\sqrt{1} & & & \bigcirc \\ & \sqrt{2m-1}\sqrt{3} & & \\ & & \ddots & \\ \bigcirc & & & \sqrt{1}\sqrt{2m+1} \end{pmatrix},$$

$$S_m = (0) \oplus \begin{pmatrix} \sqrt{2m}\sqrt{2} & & & \bigcirc \\ & \sqrt{2m-2}\sqrt{4} & & \\ & & \ddots & \\ \bigcirc & & & \sqrt{2}\sqrt{2m} \end{pmatrix}.$$

Thus

$$b(B_{2m+1}, L_{m+1}) \geq \sum_{q=1}^{m+1} \sqrt{2(m+1-q)+1}\sqrt{2q-1}. \quad (2.12)$$

Combining (2.10) with (2.12) yields the lower bound in (2.9). □

An alternative way to compute the quantity on the right hand side of (2.9) is the following: Compute the singular values of the matrix A_n. These numbers are square roots of even and odd integers. When one adds up all the singular values that are square roots of odd integers, one arrives at the quantity on the right hand side of (2.9). For the unitary matrix one may take either the unitary matrix consisting of the left singular vectors of A_n or the unitary matrix consisting of the right singular vectors of A_n. As it turns out, a permutation connects the left and right singular vectors. Indeed, this follows immediately from the fact that A_n is unitarily similar to a direct sum decomposition of B_j's (see (2.4) and (2.5)) and from the unitary similarity given in (2.11).

Keeping track of the unitary similarities to achieve the bound in (2.9) gives a way to construct the corresponding unitary U. For instance, when $n = 3$, we have $N_3 = \begin{pmatrix} N_2 & 0 \\ \mathbb{I} & N_2 \end{pmatrix}$. As

$$N_2 = \begin{pmatrix} B_1 & 0 \\ \mathbb{I} & B_1 \end{pmatrix} = U_1(B_0 \oplus B_2)U_1^*,$$

we get that

$$N_3 = (U_1 \oplus U_1) \begin{pmatrix} B_0 & 0 & 0 & 0 \\ 0 & B_2 & 0 & 0 \\ \mathbb{I} & 0 & B_0 & 0 \\ 0 & \mathbb{I} & 0 & B_2 \end{pmatrix} (U_1^* \oplus U_1^*) =$$

$$= (U_1 \oplus U_1)Y_2 \begin{pmatrix} B_0 & 0 & 0 & 0 \\ \mathbb{I} & B_0 & 0 & 0 \\ 0 & 0 & B_2 & 0 \\ 0 & 0 & \mathbb{I} & B_2 \end{pmatrix} Y_2^*(U_1^* \oplus U_1^*) =$$

$$= (U_1 \oplus U_1)Y_2(U_0 \oplus U_2)(2B_1 \oplus B_3)(U_0^* \oplus U_2^*)Y_2^*(U_1^* \oplus U_1^*),$$

where

$$Y_k = \begin{pmatrix} \mathbb{I}_k & 0 & 0 & 0 \\ 0 & 0 & \mathbb{I}_k & 0 \\ 0 & \mathbb{I}_k & 0 & 0 \\ 0 & 0 & 0 & \mathbb{I}_k \end{pmatrix}.$$

Furthermore, $C_3 = Y_4(C_2 \oplus C_2)Y_4^*$, $C_2 = V(2L_1 \oplus L_2)V^*$, $Y_1 L_2 Y_1^* = L_1 \oplus L_1$, where

$$V = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

So

$$\operatorname{tr}(C_3^* U A_3 U^*) = 4\sqrt{3} + 4$$

for

$$U = Y_4(V \oplus V)(\mathbb{I}_4 \oplus Y_1^* \oplus \mathbb{I}_4 \oplus Y_1^*)(U_0^* \oplus U_2^* \oplus U_0^* \oplus U_2^*)(Y_2^* \oplus Y_2^*)4U_1^*.$$

It is still a challenge to give an easy formula for the unitary matrix in the general case. By the way, it is interesting to note that in [4] the matrix $2B_1 \oplus B_3$ appears (up to a permutation) as the matrix O_-.

3 Open problems

As mentioned in the introduction, the right hand side of (2.9) coincides with the numerical computation of $b(A_n, C_n)$, $n = 1, \ldots, 6$, in [3]. In addition, it is straightforward to check that the U attaining the right hand side of (2.9) satisfies the optimality condition of Lagrange multipliers that

$$C_n U A_n U^* - U A_n U^* C_n$$

is Hermitian. These observations lead us to believe that equality holds in (2.9). Thus the inequality $\leq$ in Theorem 2.3 remains to be proven (if our conjecture is true).

From a practical NMR viewpoint it is a very important question whether the optimal U_n can actually be realized in experiments. Indeed, in NMR spectroscopy there are a limited number of manipulations that one can perform that mathematically result in a unitary transformation. In other words, only a limited number of unitary matrices corresponds to physically possible experiments. The possible unitaries are formed by cascades of operations e^{iH}, where the selfadjoint matrix H can be one of the following:

$$H_{rf} = aI_{kx} + bI_{ky}, H_{Jhe} = 2cI_{kz}S_z, H_{Jho} = c(I_{kz}S_z + I_{kx}S_x + I_{ky}S_y),$$

$$H_{shift} = dI_{kz} + eS_z, H_{dihe} = 2fI_{kz}S_z, H_{diho} = g(2I_{kz}S_z - I_{kx}S_x - I_{ky}S_y),$$

$$H_{planar} = h(2I_{kx}S_x + sI_{ky}S_y), H_{iso} = i(2I_{kx}S_x + 2I_{ky}S_y + 2I_{kz}S_z),$$

with

$$S_\alpha = I_\alpha \otimes \mathbb{I} \otimes \cdots \otimes \mathbb{I}, I_{k\alpha} = \mathbb{I} \otimes \cdots \otimes \mathbb{I} \otimes I_\alpha \otimes \mathbb{I} \otimes \cdots \mathbb{I}, \alpha \in \{x, y, z\},$$

where in the last equality I_α apears in the $k+1$st position. Here $\otimes$ stands for the Kronecker product, and

$$I^+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, I^- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, I_x = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, I_y = \frac{i}{2}\begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, I_z = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

These choices of H correspond to typical experiments, but other experiments may be possible as well. Note that the above operations yield a subgroup of the unitaries.

We also would like to mention the problem of finding a physical explanation for our result. As remarked earlier, the matrices A_n have singular values that are square roots of integers. In the case that n is odd, half of them are square roots of odd integers, and one simply needs to add all of these to obtain the right hand side of (2.9). Is there a physical explanation for this phenomenon?

Finally, the physical problem we discussed in this paper concerns the transformation from the so-called -1 quantum coherence of the I spins to the -1 quantum coherence of the S spin (see [2]). Other transformations are of interest as well, namely in [2] the transfer between $A = F^-$ and $C = 2F_z S^-$ is mentioned. This leads to the same A_n's as before, but now C_n is given by

$$C_n = \begin{pmatrix} 0 & 0 \\ M_n & 0 \end{pmatrix},$$

where $M_0 = 0$ and

$$M_j = M_{j-1} \otimes \mathbb{I}_2 + \mathbb{I}_{2^{j-1}} \otimes \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Also in this case one would like to determine $b(A_n, C_n)$.

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