Li-Qiao Entanglement Constraints Confirming the Entanglement Probability of $\frac{13}{27}$ for the Two-Qutrit Hiesmayr-Löffler Magic Simplex of Bell States

Paul B. Slater

Kavli Institute for Theoretical Physics,
University of California,
Santa Barbara, CA 93106-4030

(Dated: April 16, 2020)

Abstract

By implementing the pair of Li-Qiao necessary and sufficient conditions for separability of the Hiesmayr-Löffler two-qutrit magic simplex of Bell states, we are able to confirm its Hilbert-Schmidt entanglement probability of $\frac{13}{27}$. The constraints ensuring entanglement take the form $S > \frac{16}{9} \approx 1.7777$ and $P > \frac{134217728}{239100338226160487651} = \frac{227}{315.214.13} \approx 5.61324 \cdot 10^{-15}$. Here, $S$ is the square of the sum (the Ky Fan norm) of the eight singular values of the $8 \times 8$ correlation matrix in the Bloch representation, and $P$, the square of the product of these singular values. In the two-ququart Hiesmayr-Löffler scenario, one constraint is $S > \frac{9}{4} \approx 2.25$, while $\frac{324}{2356000} \approx 1.2968528306 \cdot 10^{-29}$ serves as an upper bound on the appropriate $P$ value, with the entanglement probability $\approx 0.607698$. The $S$ constraints, in both cases, prove equivalent to the well-known CCNR/realignment criteria.

Further, we are able to detect and verify—using software provided by A. Mandilara—pseudo-one-copy undistillable (POCU) negative partial transposed two-qutrit states distributed over the surface of the separable states. Further, we investigate the best separable approximation problem within this two-qutrit setting.

PACS numbers: Valid PACS 03.67.Mn, 02.50.Cw, 02.40.Ft, 02.10.Yn, 03.65.-w

*Electronic address: slater@kitp.ucsb.edu
I. INTRODUCTION

In our recent preprint “Jagged Islands of Bound Entanglement and Witness-Parameterized Probabilities” [1], we reported a PPT (positive partial transpose) Hilbert-Schmidt probability of \( \frac{8\pi}{27\sqrt{3}} \approx 0.537422 \) for the Hiesmayr-Löffler two-qutrit magic simplex of Bell states (and \( \frac{1}{2} + \frac{\log(2-\sqrt{3})}{8\sqrt{3}} \approx 0.404957 \) for the two-ququart such model) [2]. Additionally, we utilized their mutually unbiased bases (MUB) test and the Choi \( W(+) \) witness test [3, 4], obtaining entanglement (bound and “non-bound”/“free”) probabilities for both tests individually of \( \frac{1}{6} \approx 0.16667 \), while their union and intersection gave \( \frac{2}{9} \approx 0.22222 \) and \( \frac{1}{9} \approx 0.11111 \), respectively. The same bound-entangled probability \( \frac{4}{9} + \frac{4\pi}{27\sqrt{3}} + \frac{\log(2)}{6} \approx 0.00736862 \) was achieved with both these witnesses—the sets (“jagged islands”) detected having void intersection.

Further, application of the realignment (CCNR) test for entanglement [5, 6] yielded an entanglement probability of \( \frac{2}{81} (27 + \sqrt{3} \log (97 + 56\sqrt{3})) \approx 0.445977 \) and an exact bound-entangled probability of \( \frac{2}{81} (4\sqrt{3}\pi - 21) \approx 0.0189305 \). (Thus, the total entanglement probability equals \( (1 - \frac{8\pi}{27\sqrt{3}}) + \frac{2}{81} (4\sqrt{3}\pi - 21) = \frac{13}{27} \approx 0.481481 \). This is a result we are able—in our main advance here—to reproduce through independent means. In the two-ququart Hiesmayr-Löffler case, the analogous target entanglement probability appears to be \( (1 - (\frac{1}{2} + \frac{\log(2-\sqrt{3})}{8\sqrt{3}})) + 0.012654 \approx 0.607698 \).

Also, in a pair of recent reprints “Archipelagos of Total Bound and Free Entanglement” [7] and “Archipelagos of Total Bound and Free Entanglement. II” [8], we implemented the necessary and sufficient conditions recently put forth by Li and Qiao [9, 10] for the three-parameter qubit-ququart model,

\[
\rho_{AB}^{(1)} = \frac{1}{2} \cdot \frac{1}{4} \otimes 1 + \frac{1}{4} (t_1 \sigma_1 \otimes \lambda_1 + t_2 \sigma_2 \otimes \lambda_{13} + t_3 \sigma_3 \otimes \lambda_3),
\]

(1)

where \( t_\mu \neq 0, t_\mu \in \mathbb{R} \), and \( \sigma_i \) and \( \lambda_\nu \) are SU(2) (Pauli matrix) and SU(4) generators, respectively (cf. [11]). We also examined there, certain three-parameter two-ququart and two-qutrit scenarios.

Here, we seek—in two different manners—to extend these procedures developed by Li and Qiao to the Hiesmayr-Löffler two-qutrit magic simplex of Bell states [2], earlier studied by us in [1]. To do so, constitutes a substantial challenge, since now the associated correlation matrix of the Bloch representation of the bipartite state

\[
\rho_{HL} = \frac{1}{9} \otimes 1 + \frac{1}{4} (t_9 \lambda_3 \otimes \lambda_8 + t_{10} \lambda_8 \otimes \lambda_3 + \Sigma_{i=1}^{8} t_i \lambda_i \otimes \lambda_i).
\]

(2)
is eight-dimensional, rather than two- or three-dimensional as in our previous studies and those
of Li and Qiao. (Interestingly, in the three-dimensional matrix [Gell-mann] representation of
$SU(3)$, the Cartan subalgebra is the set of linear combinations [with real coefficients] of the
two matrices $\lambda_3$ and $\lambda_8$, which commute with each other.) In the simplifying parameterization
of the Hiesmayr–Löffler states introduced in [1, sec. II.A],

$$
\rho_{HL} = \begin{pmatrix}
\gamma_1 & 0 & 0 & 0 & \gamma_2 & 0 & 0 & 0 & \gamma_2 \\
0 & Q_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \gamma_3 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \gamma_3 & 0 & 0 & 0 & 0 & 0 \\
\gamma_2 & 0 & 0 & 0 & \gamma_1 & 0 & 0 & 0 & \gamma_2 \\
0 & 0 & 0 & 0 & 0 & Q_2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & Q_2 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \gamma_3 & 0 \\
\gamma_2 & 0 & 0 & 0 & \gamma_2 & 0 & 0 & 0 & \gamma_1
\end{pmatrix},
$$

(3)

where $\gamma_1 = \frac{1}{3} (Q_1 + 2Q_3), \gamma_2 = \frac{1}{3} (Q_1 - Q_3)$, and $\gamma_3 = \frac{1}{3} (-Q_1 - 3Q_2 - 2Q_3 + 1)$, we have
$t_1 = t_4 = t_6 = \frac{2}{3} (Q_1 - Q_3), t_2 = t_5 = -\frac{2}{3} (Q_1 - Q_3), t_3 = t_8 = -(\frac{1}{3} + Q_1 + 2Q_3)$. Further,
$t_9 = \frac{Q_1 + 6Q_2 + 2Q_3 - 1}{\sqrt{3}}$ and $t_{10} = -t_9$.

The requirement that $\rho_{HL}$ be a nonnegative definite density matrix—ensured by requiring
that its nine leading nested minors all be nonnegative [12]—takes the form [11 eqs. (29)],

$$
Q_1 > 0 \land Q_2 > 0 \land Q_3 > 0 \land Q_1 + 3Q_2 + 2Q_3 < 1.
$$

(4)

Additionally, the constraint that the partial transpose of the $9 \times 9$ density matrix be
nonnegative definite is

$$
Q_1 > 0 \land Q_3 > 0 \land Q_1 + 3Q_2 + 2Q_3 < 1 \land Q_1^2 + 3Q_2Q_1 + (3Q_2 + Q_3)^2 < 3Q_2 + 2Q_1Q_3.
$$

(5)

Further, the Hiesmayr-Löffler mutually-unbiased-bases (MUB) criterion for bound entangle-
ment, $I_4 = \Sigma_{k=1}^4 C_{A_k,B_k} > 2$, where $C_{A_k,B_k}$ are correlation functions for observables $A_k, B_k$
[13 Fig. 1] is

$$
Q_1 > 3Q_2 + 4Q_3.
$$

(6)

In the Hiesmayr-Löffler $d = 3$ two-qutrit density-matrix setting, the Choi-witness entangle-
ment requirement that $\text{Tr}[W \rho_{HL}] < 0$ assumes the form

$$
2Q_3 + 1 - 2Q_1 - 3Q_2 < 0.
$$

(7)
The realignment constraint that, if satisfied, ensures entanglement is

$$\frac{2}{3} \sqrt{-9Q_2 - 6Q_3 + 3 (Q_1^2 + (3Q_2 + 4Q_3 - 1) Q_1 + 9Q_2^2 + 4Q_3^2 + 6Q_2 Q_3) + 1 + \frac{1}{3} + |Q_1 - Q_3|} > 1.$$  \hspace{1cm} (8)

II. TWO-QUTRIT ANALYSES

The pair of entanglement constraints in the Li-Qiao framework, for which we seek the appropriate bounds, would be based on the eight singular values of the $8 \times 8$ correlation matrix for the Hiesmayr–Löffler model–bipartite in nature–under examination. (We should note that the correlation matrix for this two-qutrit model is non-diagonal in nature, since there are terms in the expansion $[2]$ of the form $\lambda_3 \otimes \lambda_8$ and $\lambda_8 \otimes \lambda_3$. The coefficients of these terms in the indicated reparameterization being $\frac{Q_1 + 6Q_2 + 2Q_3}{\sqrt{3}}$ and $-\frac{Q_1 + 6Q_2 + 2Q_3}{\sqrt{3}}$, respectively, as noted earlier.)

Entanglement is achieved if either the square ($P$) of the product of the eight singular values exceeds a certain threshold, or the square ($S$) of the sum (the Ky Fan norm) of the singular values exceeds a corresponding threshold. Our research here is focused on determining the appropriate thresholds to employ.

To so proceed, we found that six of the eight singular values of the correlation matrix of $[2]$ are $\frac{2}{3} \sqrt{(Q_1 - Q_3)^2}$ and the remaining two are $\frac{2}{3} \sqrt{-9Q_2 - 6Q_3 + 3 (Q_1^2 + (3Q_2 + 4Q_3 - 1) Q_1 + 9Q_2^2 + 4Q_3^2 + 6Q_2 Q_3) + 1}$. The square of the product of the eight values is, then,

$$P = \frac{65536 (Q_1 - Q_3)^{12} (3Q_1^2 + 3 (3Q_2 + 4Q_3 - 1) Q_1 + 27Q_2^2 + 9Q_2 (2Q_3 - 1) + 6Q_3 (2Q_3 - 1) + 1)^2}{43046721}$$  \hspace{1cm} (9)

and the square of their sum is

$$\left( \frac{4\sqrt{\zeta}}{3} + 4\sqrt{(Q_1 - Q_3)^2} \right)^2$$  \hspace{1cm} (10)

where (cf. [8])

$$\zeta = -9Q_2 - 6Q_3 + 3 (Q_1^2 + (3Q_2 + 4Q_3 - 1) Q_1 + 9Q_2^2 + 4Q_3^2 + 6Q_2 Q_3) + 1.$$  \hspace{1cm} (11)

These are the two quantities—in the Li-Qiao framework—for which we must find suitable lower bounds. If a particular Hiesmayr-Löffler state exceeds either bound it is necessarily entangled.
We, preliminarily, found that the maxima—over the entire magic simplex (of both entangled and separable states)—of $P$ is \( \frac{65536}{43046721} = \left(\frac{2}{3}\right)^{16} \approx 0.00152 \) and of $S$, \( \frac{256}{9} \approx 28.4444 \). But, we desire the maxima over solely the separable states.

Thus, we now restrict the search for the maxima to the Hiesmayr–Löffler states with positive partial transpose, but which are \textit{not} bound-entangled according to the realignment test. Then, our numerics indicated that the maxima are \( \frac{134217728}{23910933822616040487651} = 2^{27} \cdot 3^{18} \cdot 7^{15} \cdot 13 \approx 5.61324 \cdot 10^{-15} \) for $P$ and \( \frac{16}{9} \approx 1.7777 $ for $S$ (at \( Q_1 = \frac{1}{3}, Q_2 = 0, Q_3 = \frac{1}{3} \)). (This last maximum can also be achieved at \( Q_1 = \frac{1}{4}, Q_2 = \frac{1}{24} (3 - \sqrt{5}), Q_3 = 0 \)—which in the original Hiesmayr-Löffler coordinates, converts to \( q_1 = \frac{5}{24} (\sqrt{5} - 3), q_2 = -1 - \frac{\sqrt{5}}{3}, q_3 = -\frac{\sqrt{5}}{4} \). If, on the other hand, we simply search for the maxima over the Hiesmayr–Löffler states with positive partial transpose—within which all the separable states must lie—but now do \textit{not} omit those states that are bound-entangled based on the realignment test—we obtain as the maximum for $S$, \( \frac{25}{9} \approx 2.7777 $, and \( \frac{228}{3^{16} \cdot 7^{15}} \approx 9.194481490 \cdot 10^{-12} $ for $P$ (at \( Q_1 = \frac{2}{7}, Q_2 = \frac{4}{21}, Q_3 = 0 \)).

Enforcement of the constraint $S > \frac{16}{9}$ proves, interestingly, fully equivalent to the application of the realignment (CCNR) test for entanglement \cite{5,6} in yielding a total entanglement probability of \( \frac{1}{81} \left( 27 + \sqrt{3} \log \left( 97 + 56 \sqrt{3} \right) \right) \approx 0.445977 $ and a bound-entanglement probability of \( \frac{2}{81} \left( 4 \sqrt{3} \pi - 21 \right) \approx 0.0189035 $. (The realignment bound-entangled ”island” completely contains the corresponding Choi and MUB islands, with an additional probability of \( \frac{1}{27} \left( 10 - 9 \log(3) \right) \approx 0.00416627 \) \cite{1, Fig. 25}.)

\textbf{A. Graphic representations}

Now, in a series of figures, let us attempt to gain insight into the specific relations between the constraints and the geometric structure of entanglement. To begin, in Fig. 1 we show a sampling of just those entangled Hiesmayr–Löffler two-qutrit states that \textit{do} satisfy the $P > \frac{2^{27}}{3^{16} \cdot 7^{15} \cdot 13}$ constraint, but do \textit{not} satisfy the $S > \frac{16}{9}$ constraint. (The sampling is based on use of the Mathematica FindInstance command to generate points satisfying the basic constraint \cite{4}, which points are, then, employed to test further constraints. We so proceed, although we are not aware of any particular associated measure [Hilbert-Schmidt, Bures, \ldots].) The bound-entangled states correspond to the green points, and the free-entangled states to the red. There appear to be \textit{two} islands of entanglement.

In Fig. 2 we reverse the role of the two constraints.
FIG. 1: A sampling of just those entangled Hiesmayr–Löffler two-qutrit states that do satisfy the $P > \frac{2^{27}}{3^{18} \cdot 7^{15}}$ constraint, but do not satisfy the $S > \frac{16}{9}$ constraint. The bound-entangled states correspond to the green points, and the free-entangled states to the red. There appear to be two islands of entanglement.

Now, in Fig. 3, we present a sampling of those states which satisfy neither of the entanglement constraints. The (predominantly) green points are separable in nature, while the red ones appeared to be pseudo-one-copy undistillable (POCU) negative partial transposed states \[15\]. (“Our results are disclosing that for the two-qutrit system the BE [bound-entangled] states have negligible volume and that these form tiny islands sporadically distributed over the surface of the polytope of separable states. The detected families of BE states are found to be located under a layer of pseudo-one-copy undistillable negative partial transposed states with the latter covering the vast majority of the surface of the separable polytope” \[15\]. The term “pseudo” is used to emphasize that although a single copy of the
FIG. 2: A sampling of just those entangled Hiesmayr–Löffler two-qutrit states that do not satisfy the $P > \frac{27}{3^{18},11,13}$ constraint, but do satisfy the $S > \frac{16}{9}$ constraint. The bound-entangled states correspond to the green points, and the free-entangled states to the red. There appear to be multiple islands of entanglement.

A state is undistillable, a collection of more than one might be.) A Mathematica program is available for testing for the POCU property [16]. (One instance of such a point to be so tested is $Q_1 = \frac{201}{634}, Q_2 = \frac{1}{148}, Q_3 = \frac{69}{305}$, while another is $Q_1 = \frac{761}{2702}, Q_2 = \frac{3}{422}, Q_3 = \frac{47}{290}$.) In fact, employing the indicated program on a sample of ten candidate POCU states, we were able to confirm that they all possess this property. (Also, all ten $9 \times 9$ density matrices were of full rank.)

Numerical analyses indicated that for these POCU states, an upper bound on the lowest value that $S$ can attain is 0.47742 (at $Q_1 = \frac{16022}{89351}, Q_2 = \frac{28}{185}, Q_3 = \frac{101}{551}$). In Figs. 4, 5 and 6
FIG. 3: A sampling of those Hiesmayr–Löffler two-qutrit states which satisfy neither of the entanglement constraints. The green points are separable in nature, while the red ones are pseudo-one-copy undistillable negative partial transposed states. Numerical analyses indicated that for these POCU states, an upper bound on the lowest value that $S$ can attain is 0.47742.

we show plots based on additional Boolean combinations of the two constraints. (Note that there are some differences in scaling among the several figures in the paper.)

1. States on the boundary of separability

The points in the next two figures (Figs. 7 and 8) all saturate the $S$ entanglement constraint, i.e., $S = \frac{16}{9}$. The points in the former lie, in general, within the PPT states, while in the latter, they lie on the boundary of the PPT states. Efforts of ours to produce a
FIG. 4: A sampling of those Hiesmayr–Löffler two-qutrit states which do not satisfy at least one of the entanglement constraints. The green points are separable in nature, while the red ones appear to be *pseudo-one-copy undistillable negative partial transposed states*. The highest value of $S$ for the red points in this plot is 3.11447.

A companion pair of figures to these last two, in which instead of the $S$ entanglement constraint being saturated, the $P$ constraint would be, proved much more computationally challenging. However, we were able to obtain a fewer-point analogue of Fig. 8 that is, Fig. 9. In Fig. 10 we jointly plot the two curves (Fig. 8 and Fig. 9), showing the intersection of the PPT boundary with points saturating the $S$ and $P$ constraints, respectively.
FIG. 5: A sampling of those Hiesmayr–Löffler two-qutrit states which satisfy at least one of the entanglement constraints. The bound-entangled states correspond to the green points, and the free-entangled states to the red.

B. Analyses employing Li-Qiao variables $\alpha_i, \beta_i$

As a matter of analytical interest, we had initially concentrated upon attempting to construct the proper entanglement bounds—now reported above—for $P$ and $S$ applicable to the Hiesmayr–Löffler two-qutrit model, but strictly within the Li-Qiao framework. In so doing, we follow [8], in which we employed the well-known necessary and sufficient conditions for nonnegative-semidefiniteness that all leading minors be nonnegative [12]. There are twenty-two sets of such minors of $3 \times 3$ density matrices to so consider, since the Li-Qiao algorithm expands $\rho_{HL}$ into eleven separable two-qutrit states. (We were able to obtain this explicit expansion, lending us confidence in our further analyses. In the Li-Qiao setup, we initially have twenty parameters, ten $\alpha_i$ and ten $\beta_i$, with $t_i = \alpha_i/\beta_i$. Then, the solution yielding the correct expansion was expressible as $\beta_i = \frac{2(Q_1-Q_3)}{3\alpha_i}, i = 1, 4, 6$ and $\beta_i = -\frac{2(Q_1-Q_3)}{3\alpha_i}, i = 2, 5, 7$, and $\beta_i = -\frac{1+3Q_1+6Q_3}{3\alpha_i}, i = 3, 8$, and $\beta_i = -\frac{1+Q_1+6Q_2+2Q_3}{3\alpha_i}, i = 9, 10$.)

Then, using numerical integration in a thirteen-dimensional setting ($Q_1, Q_2, Q_3$ and the
ten $\alpha_i$’s), our highest estimate of the (multiplicative) quantity was $P = 8.91229 \times 10^{-22}$, and of the (additive-type) quantity was $S = 0.155322$. Requiring that $P > 8.91229 \times 10^{-22}$, yields an entanglement probability estimate of 0.764984, and enforcing $S > 0.155322$, gives 0.972243. So, these bounds are disappointingly small, leading to entanglement probability estimates clearly too large, given the PPT probability $\frac{8\pi}{27\sqrt{3}} \approx 0.537422$, all but only $\frac{2}{81} (4\sqrt{3}\pi - 21) \approx 0.0189305$ of which is bound-entangled, through enforcement of the realignment test.

So, while we are confidently able to claim knowledge of the proper bounds for the pair of Li-Qiao entanglement constraints on the singular-value-based terms $S$ and $P$ for the Hiesmayr-Löffler two-qutrit magic simplex of Bell states, this was only achievable in the first of our two lines of two-qutrit analysis, employing simply the trivariate $(Q_1, Q_2, Q_3)$ set of constraints (4)-(8)). The second line of 13-variable $(Q_1, Q_2, Q_3$ and ten Li-Qiao parameters $\alpha_i, i = 1, \cdots, 10$) analyses, conducted within the Li-Qiao framework, has not similarly yet succeeded.
FIG. 7: Hiesmayr–Löffler two-qutrit states on the boundary of the separable states for which the $S$ entanglement constraint is saturated, i.e. $S = \frac{16}{9}$.

C. Best separable approximations

In their pair of recent skillful papers [9, 10], Li and Qiao presented necessary and sufficient conditions for separability, the implementation of which we have investigated above. They did not, however, discuss the apparently related best separable approximation problem [17]. To begin a study of the possible application of the Li-Qiao analytical framework to this problem of major interest, we sought a best separable approximation for the entangled Hiesmayr-Löffler two-qutrit density matrix [3] with its parameters having been set to $Q_1 = \frac{4235}{5001}, Q_2 = \frac{1}{166}, Q_3 = \frac{30}{113}$. Then, we obtained a value of $B = 0.195662$, where $B$ is the parameter one seeks to minimize $0 \leq B \leq 1$, in the equation [15, eq. (2)]

$$\hat{\rho} = (1 - B)\hat{\rho}_{sep} + B\hat{\rho}_{ent}.$$  

(12)

Now, the minimum $B = 0.195662$ for the indicated choice of $Q$'s for $\hat{\rho}$ is obtained if we choose for the parameterization of $\hat{\rho}_{ent}$, the values $Q_1 = 1.50726 \times 10^{-7}, Q_2 = 1.95701 \times 10^{-8}$ and $Q_3 = 0.5$. Then, from [12], we can obtain the desired $\hat{\rho}_{sep}$—for which $Q_1 = 0.10754, Q_2 = 0.0074895$ and $Q_3 = 0.208439$. 

12
FIG. 8: Hiesmayr–Löffler two-qutrit states on the boundaries of both the separable states and PPT states for which the $S$ entanglement constraint is saturated, i.e. $S = \frac{16}{9}$. 
FIG. 9: Hiesmayr–Löfller two-qutrit states on the boundaries of both the separable states and PPT states for which the $P$ entanglement constraint is saturated, i.e. $P = \frac{134217728}{2390003382260000487651} = \frac{2^{27}}{3^{18} \cdot 7^{15} \cdot 13} \approx 5.61324 \cdot 10^{-15}$. There are three curves, one much smaller than the other two.
FIG. 10: A joint plot of the two curves (Fig. 8 and Fig. 9), showing the intersection of the PPT boundary of the Hiesmayr–Löfﬂer two-qutrit states with points for which $S = \frac{16}{9}$ and $P = \frac{227}{315.315.315.13}$, respectively.
III. TWO-QUQUART ANALYSES

For the $d = 4$ two-ququart Hiesmayr-Löffler magic simplex states, $
\rho_{HL}^{2qq} = \begin{pmatrix}
\kappa_1 & 0 & 0 & 0 & \kappa_2 & 0 & 0 & 0 & \kappa_2 & 0 & 0 & 0 & \kappa_2 \\
0 & Q_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & Q_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \kappa_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & \kappa_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\kappa_2 & 0 & 0 & 0 & \kappa_1 & 0 & 0 & 0 & \kappa_2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & Q_2 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & Q_3 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & Q_3 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \kappa_3 & 0 & 0 & 0 \\
\kappa_2 & 0 & 0 & 0 & \kappa_1 & 0 & 0 & 0 & \kappa_2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & Q_2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & Q_2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \kappa_3 & 0 & 0 & 0 \\
\kappa_2 & 0 & 0 & 0 & \kappa_1 & 0 & 0 & 0 & \kappa_2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & Q_2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & Q_2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \kappa_3 & 0 & 0 & 0 \\
\kappa_2 & 0 & 0 & 0 & \kappa_1 & 0 & 0 & 0 & \kappa_2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & Q_2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & Q_2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \kappa_3 & 0 & 0 & 0 \\
\kappa_2 & 0 & 0 & 0 & \kappa_1 & 0 & 0 & 0 & \kappa_2 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & Q_2 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & Q_2 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \kappa_3 & 0 & 0 & 0 \\
\kappa_2 & 0 & 0 & 0 & \kappa_1 & 0 & 0 & 0 & \kappa_2 & 0 & 0 & 0
\end{pmatrix},
\tag{13}

where, $\kappa_1 = \frac{1}{4} (Q_1 + 3Q_4)$, $\kappa_2 = \frac{1}{4} (Q_1 - Q_4)$ and $\kappa_3 = \frac{1}{4} (-Q_1 - 4Q_2 - 4Q_3 - 3Q_4 + 1)$. The requirement that $\rho_{HL}^{2qq}$ is a nonnegative definite density matrix—or, equivalently, that its sixteen leading nested minors are nonnegative—takes the form [1, eq. (29)]

$$Q_1 > 0 \land Q_4 > 0 \land Q_2 > 0 \land Q_3 > 0 \land Q_1 + 4(Q_2 + Q_3) + 3Q_4 < 1.\tag{14}$$

The constraint that the partial transpose of $\rho_{HL}^{2qq}$ is nonnegative definite is [1, eq. (30)]

$$Q_3 > 0 \land Q_1 + 3Q_4 > 0 \land Q_1 + 4(Q_2 + Q_3) + 3Q_4 < 1 \land Q_1^2 + 4Q_2Q_1 + Q_4^2 \tag{15} + 16Q_2(Q_2 + Q_3) + 12Q_2Q_4 < 4Q_2 + 2Q_1Q_4 \land (Q_1 - Q_4)^2 < 16Q_3^2.$$  

With these formulas, we are able to establish that the corresponding PPT-probability is

$$\frac{1}{2} + \frac{\log(2 - \sqrt{3})}{8\sqrt{3}} \approx 0.404957$$  

(again, quite elegant, but seemingly of a different analytic form than the $d = 3$ counterpart of $\frac{8\pi}{27\sqrt{3}}$).
As in the \( d = 3 \) case \([3]\), the \( d = 4 \) (16 × 16) density matrix \([13]\) is of normal form \([10]\) eq. (12)], in which “the Bloch representation of \( \rho_{AB} \) has \( \textbf{a}^* = 0 \) and \( \textbf{b}^* = 0 \), that is, the local density matrices would be maximally mixed”. (A constructive way of bringing a single copy of a quantum state into normal form under local filtering operations was presented in \([18]\).) The Li-Qiao framework requires such normal forms.

Then, our 4-variable (as opposed to 32-variable [in Li-Qiao framework]) computations show that—if we maximize over simply the PPT states—we have \( P = \frac{\sqrt{24}}{2 \times 134} \approx 1.2968528306 \times 10^{-29} \) (for \( Q_1 = \frac{3}{16} \), \( Q_2 = \frac{9}{64} \), \( Q_3 = \frac{3}{64} \), \( Q_4 = 0 \)) and \( S = \frac{49}{16} \approx 3.0625 \) for the same four parameters. Now, if we exclude from the PPT states those that are bound-entangled according to the realignment criterion, we obtain \( S = \frac{9}{4} \approx 2.25 \) (for \( Q_1 = 0 \), \( Q_2 = \frac{1}{4} \), \( Q_3 = 0 \), \( Q_4 = 0 \)), while \( P \) appears to be unchanged. If we enforce the \( P > \frac{\sqrt{24}}{2 \times 134} \) constraint, our estimate of the associated entanglement probability is 0.31711552, while the \( S > \frac{9}{4} \) constraint gives us 0.39717107. Unfortunately, at this point in time, we do not have an exact entanglement probability—such as \( \frac{13}{27} \), as in the two-qutrit case studied above—to which to fit the Li-Qiao entanglement constraint bounds.

IV. CONCLUDING REMARKS

In our analyses here, the CCNR (computable cross-norm realignment) criterion \([5, 6]\) for entanglement proves to be equivalent to the properly enforced constraint—involving the square of the Ky Fan norm (the sum of the singular values) \([10\) eq. (32)] of the correlation matrix in the Bloch representation—on \( S \). Whether this equivalence is true, in general, is a question to be addressed. (In certain auxiliary analyses, we concluded that in the Hiesmayr-Loffler \( d = 3 \) [two-qutrit] magic simplex model, the CCNR is equivalent—and not inferior, as can be the case \([6\] to the ESIC [SIC POVMs] test \([6\), in yielding the same sets of entangled and bound-entangled states. Efforts to similarly compare these two criteria in the \( d = 4 \) [two-ququart] version have so far proved too computationally challenging to complete.)

Acknowledgments

This research was supported by the National Science Foundation under Grant No. NSF PHY-1748958. I thank A. Mandilara for providing me with the Mathematica code by which
I was able to corroborate the nature of the pseudo-one-copy undistillable states generated.

[1] P. B. Slater, arXiv preprint arXiv:1905.09228 (2019).
[2] B. C. Hiesmayr and W. Löffler, Physica Scripta **2014**, 014017 (2014).
[3] K.-C. Ha and S.-H. Kye, Physical Review A **84**, 024302 (2011).
[4] D. Chruściński, M. Marciniak, and A. Rutkowski, Acta Mathematica Vietnamica **43**, 661 (2018).
[5] K. Chen and L.-A. Wu, arXiv preprint quant-ph/0205017 (2002).
[6] J. Shang, A. Asadian, H. Zhu, and O. Gühne, Physical Review A **98**, 022309 (2018).
[7] P. B. Slater, arXiv preprint arXiv:2001.01232 (2020).
[8] P. B. Slater, arXiv preprint arXiv:2002.04084 (2020).
[9] J.-L. Li and C.-F. Qiao, Scientific reports **8**, 1442 (2018).
[10] J.-L. Li and C.-F. Qiao, Quantum Information Processing **17**, 92 (2018).
[11] A. Singh, A. Gautam, K. Dorai, et al., Physics Letters A **383**, 1549 (2019).
[12] J. E. Prussing, Journal of Guidance, Control, and Dynamics **9**, 121 (1986).
[13] B. C. Hiesmayr and W. Löffler, New journal of physics **15**, 083036 (2013).
[14] *Find parameter value for which sharply-peaked constrained 3d-integral equals 1*, URL https://mathematica.stackexchange.com/questions/218459/find-parameter-value-for-which-sharply-peaked-constrained-3d-integral-equals-1
[15] A. Gabdulin and A. Mandilara, Physical Review A **100**, 062322 (2019).
[16] *Quantum virtual lab*, URL http://www.qubit.kz/?page=Qutrits.php
[17] V. Akulin, G. Kabatiansky, and A. Mandilara, Physical Review A **92**, 042322 (2015).
[18] F. Verstraete, J. Dehaene, and B. De Moor, Physical Review A **68**, 012103 (2003).