Maximal vectors in Hilbert space and quantum entanglement

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Overview

Quantum Information Theory is quantum mechanics in matrix algebras - the algebras $\mathcal{B}(H)$ with $H$ finite dimensional. I’ll stay in that context for this talk; but much of the following discussion generalizes naturally to infinite dimensional Hilbert spaces.

We discuss separability of states, entanglement of states, and propose a numerical measure of entanglement in an abstract context. Then we apply that to compute maximally entangled vectors and states of tensor products $H = H_1 \otimes \cdots \otimes H_N$.

Not discussed: the physics of entanglement, how/why it is a resource for quantum computing, the EPR paradox, Bell’s inequalities, Alice and Bob, channels, qubits, philosophy.
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Separable states, entangled states

Consider states of a “composite” quantum system

\[ \mathcal{B}(H_1 \otimes \cdots \otimes H_N) \cong \mathcal{B}(H_1) \otimes \cdots \otimes \mathcal{B}(H_N), \quad N = 2, 3, \ldots. \]

A state \( \rho \) of \( \mathcal{B}(H_1 \otimes \cdots \otimes H_N) \) is said to be \textit{separable} if it is a convex combination of product states \( \sigma_1 \otimes \cdots \otimes \sigma_N \)

\[ \rho(A_1 \otimes \cdots \otimes A_N) = \sum_{k=1}^{s} t_k \cdot \sigma_1^k(A_1) \cdots \sigma_N^k(A_N), \]

with positive \( t_k \) summing to 1.

An \textit{entangled} state is one that is not separable. We will see examples shortly.
Entanglement is a noncommutative phenomenon

For commutative tensor products

\[ A = C(X_1) \otimes \cdots \otimes C(X_N) = C(X_1 \times \cdots \times X_n) \]

\(X_1, \ldots, X_N\) being finite sets, every state of \(A\) is a convex combination of pure states, pure states correspond to points of \(X_1 \times \cdots \times X_N\), and point masses are pure product states.

Hence every state is a convex combination of product states, and entangled states do not exist.

- The existence of entangled states reflects the fact that observables are operators, not functions, and operator multiplication is not commutative.
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Entangled pure states

- Factoid: for every unit vector $\xi \in H_1 \otimes \cdots \otimes H_N$, the pure state $\rho(A) = \langle A\xi, \xi \rangle$, $A \in \mathcal{B}(H_1 \otimes \cdots \otimes H_N)$ is separable iff $\xi = \xi_1 \otimes \cdots \otimes \xi_N$, for some $\xi_k \in H_k$, $1 \leq k \leq N$.

So a vector in the unit sphere $S = \{\xi \in H : \|\xi\| = 1\}$ gives an entangled pure state iff it is not decomposable. Such vectors are generic in two senses: they are a dense open subset of $S$, and they are a set whose complement has measure zero.

- The situation for mixed states is not so simple. For example, entangled states are not generic; they are not even dense in the state space.
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Examples in the “bipartite” case $N = 2$

Choose a unit vector $\zeta \in H_1 \otimes H_2$ that does not decompose into a tensor product $\xi_1 \otimes \xi_2$, and define

$$\alpha = \sup_{\|\xi_1\| = \|\xi_2\| = 1} |\langle \zeta, \xi_1 \otimes \xi_2 \rangle|^2.$$ 

Easy to see that the self-adjoint operator

$$A = \alpha \cdot 1 - \zeta \otimes \bar{\zeta}$$

has the property $(\sigma_1 \otimes \sigma_2)(A) \geq 0$ for every product state $\sigma_1 \otimes \sigma_2$ and hence $\rho(A) \geq 0$ for every separable state $\rho$.

But the choice of $\zeta$ implies that $\alpha < 1$, hence the operator $A$ is not positive.

• Conclusion: Every state $\rho$ such that $\rho(A) < 0$ is entangled.
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What are maximally entangled pure states?

The term “maximally entangled pure state" occurs frequently in the physics literature, and several “measures of entanglement" have been proposed in the bipartite case $H = H_1 \otimes H_2$. For example, when $H_1 = H_2$, everyone agrees that

$$\frac{1}{\sqrt{n}}(e_1 \otimes f_1 + \cdots + e_n \otimes f_n)$$

is a maximally entangled unit vector (here, $(e_k)$ and $(f_k)$ are orthonormal bases for $H_1 = H_2$).

But despite the attention it receives, in the multipartite case $H = H_1 \otimes \cdots \otimes H_N$ with $N \geq 3$, there does not seem to be general agreement about what properties a maximally entangled vector should have.

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Aside: the case \( N = 2 \) is too special

- The case \( H = H_1 \otimes H_2 \) has special features that are not available for higher order tensor products.

That is because vectors in \( H_1 \otimes H_2 \) can be identified with Hilbert Schmidt operators \( A : H_1 \rightarrow H_2 \), so one can access operator-theoretic invariants to analyze vectors.

Example: Using the singular value list of the operator that corresponds to a unit vector \( \xi \in H_1 \otimes H_2 \), it follows that there are orthonormal sets \( (e_k) \) in \( H_1 \) and \( (f_k) \) in \( H_2 \) and a set of nonnegative numbers \( p_1, \ldots, p_n \) with sum 1 such that

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\xi = \sqrt{p_1} \cdot e_1 \otimes f_1 + \cdots + \sqrt{p_n} \cdot e_n \otimes f_n
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Physicists call this the Schmidt decomposition of \( \xi \).
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$N = 3$ is more typical

In the case $H = H_1 \otimes H_2 \otimes H_3$, one can stubbornly identify vectors in $H$ with various Hilbert Schmidt operators, e.g.,

$$A : H_1 \rightarrow H_2 \otimes H_3, \text{ or}$$

$$B : H_2 \rightarrow H_1 \otimes H_3, \text{ or}$$

$$C : H_3 \rightarrow H_1 \otimes H_2.$$

Which one should we use? Maybe use the triple $(A, B, C)$? Unfortunately, triples don’t have singular value lists.

The cases $N > 3$ don’t get easier....

I propose giving up the idea of generalizing the “Schmidt decomposition" and starting over from scratch.
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Entanglement pairs \((H, V)\)

We will work with pairs \((H, V)\) consisting of a Hilbert space \(H\) and a norm-closed set \(V\) of unit vectors in \(H\) such that:

\[ V1: \; \lambda \cdot V \subseteq V \text{ for every } \lambda \in \mathbb{C}, \; |\lambda| = 1. \]

\[ V2: \; H \text{ is the closed linear span of } V. \]

Motivating example: a Hilbert space \(H = H_1 \otimes \cdots \otimes H_N\) presented as an \(N\)-fold tensor product of Hilbert spaces \(H_k\), where \(V\) is the set of all decomposable unit vectors

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V = \{ \xi_1 \otimes \cdots \otimes \xi_N : \xi_k \in H_k, \; \|\xi_1\| = \cdots = \|\xi_N\| = 1 \}.
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Of course there are lots of other examples of entanglement pairs, many/most of which have nothing to do with physics.
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Of course there are lots of other examples of entanglement pairs, many/most of which have nothing to do with physics.
Fix an entanglement pair \((H, V)\).

- By a maximal vector we mean a unit vector \(\xi \in H\) whose distance to \(V\) is maximum:

\[
d(\xi, V) = \max_{\|\eta\|=1} d(\eta, V),
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\(d(\xi, V)\) denoting the distance from \(\xi\) to \(V\).

If \(H\) is finite dimensional, then maximal vectors exist; and they exist in many infinite dimensional examples as well.

Maximal vectors are at the opposite extreme from the “central vector” of \(V\) described in Jesse Peterson’s talk.
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The simplest examples

Take $H = \mathbb{C}^2$, choose two unit vectors $e_1, e_2 \in H$, and let

$$V = \{ \lambda e_1 : |\lambda| = 1 \} \cup \{ \lambda e_2 : |\lambda| = 1 \}.$$ 

Calculation shows that a unit vector $\xi \in \mathbb{C}^2$ is maximal iff

$$\max(|\langle \xi, e_1 \rangle|, |\langle \xi, e_2 \rangle|)$$

is as small as possible. So taking $e_1 = (1, 0)$, $e_2 = (0, 1)$ to be the usual basis vectors, the maximal vectors turn out to be

$$\xi = \left( \frac{\lambda}{\sqrt{2}}, \frac{\lambda}{\sqrt{2}} \right), \quad |\lambda| = 1.$$ 

In general, $0 \leq d(\xi, V) \leq \sqrt{2}$. Note that since $V$ is closed,

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Measuring the entanglement of vectors

For every \( \xi \in H \) we define a preliminary norm \( \| \cdot \|_V \) by

\[
\| \xi \|_V = \sup_{v \in V} \Re \langle \xi, v \rangle = \sup_{v \in V} |\langle \xi, v \rangle|.
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The “entanglement measuring” function from \( H \) to the extended interval \([0, +\infty]\) is defined as follows:

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It is possible for \( \| \xi \|_V \) to be infinite (when \( \dim H = \infty \)); but otherwise, \( \| \cdot \|_V \) behaves like a norm on \( H \) such that

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The inner radius $r(V)$

- The *inner radius* $r(V)$ is the largest $r \geq 0$ such that
  \[ \{ \xi \in H : \|\xi\| \leq r \} \subseteq \text{convex hull } V. \]

In general, $0 \leq r(V) \leq 1$, and $r(V) = 1 \iff V$ is the entire unit sphere of $H$. More significantly for our purposes:

- If $\dim H < \infty$ then $r(V) > 0$.

**Theorem:** Each of the three formulas characterizes $r(V)$:

(i) $\inf_{\|\xi\|=1} \|\xi\|_V = r(V)$.

(ii) $\sup_{\|\xi\|=1} \|\xi\|_V = r(V)^{-1}$.

(iii) $\sup_{\|\xi\|=1} d(\xi, V) = \sqrt{2 - 2 \cdot r(V)}$. 
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Characterization of maximal vectors

**Theorem:** For every unit vector $\xi \in H$, the following are equivalent:

(i) $\|\xi\|_V = r(V)$ is minimum.
(ii) $\|\xi\|_V = r(V)^{-1}$ is maximum.
(iii) $d(\xi, V) = \sqrt{2 - 2 \cdot r(V)}$ - i.e., $\xi$ is a maximal vector.

More significantly, $\| \cdot \|_V$ measures “degree of entanglement”:

**Theorem:** If $\dim H < \infty$, then $\| \cdot \|_V$ is a norm on $H$ whose restriction to the unit sphere $S = \{ \xi \in H : \|\xi\| = 1 \}$ has the following properties:

(i) Range of values: $1 \leq \|\xi\|_V \leq r(V)^{-1}$.
(ii) Membership in $V$: $\xi \in V \iff \|\xi\|_V = 1$.
(iii) Maximal vectors: $\xi$ is maximal $\iff \|\xi\|_V = r(V)^{-1}$.
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Entanglement of mixed states

Fix \((H, V)\). A state \(\rho\) of \(\mathcal{B}(H)\) is said to be \(V\)-correlated if it is a convex combination of vector states of the form

\[ \omega(A) = \langle A\xi, \xi \rangle, \quad \xi \in V. \]

A state that is not \(V\)-correlated is said to be \(V\)-entangled, or simply entangled.

We introduce a numerical measure of entanglement of states as follows. Consider the convex subset of \(\mathcal{B}(H)\)

\[ \mathcal{B}_V = \{ A \in \mathcal{B}(H) : |\langle A\xi, \eta \rangle| \leq 1, \forall \xi, \eta \in V \}. \]

\(\mathcal{B}_V\) contains the unit ball of \(\mathcal{B}(H)\). For every \(\rho \in \mathcal{B}(H)'\) define

\[ E(\rho) = \sup_{A \in \mathcal{B}_V} |\rho(A)|. \]
Entanglement of mixed states

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Basic properties of the function $E$

According to the following result, the function $E(\cdot)$ faithfully detects entanglement of states. Moreover, it recaptures the entanglement norm $\|\xi\|^V$ of unit vectors $\xi \in H$.

**Theorem:** When $r(V) > 0$, $E$ is a norm on $\mathcal{B}(H)'$ whose restriction to the state space behaves as follows:

(i) $1 \leq E(\rho) \leq r(V)^{-2}$, for every state $\rho$.

(ii) $E(\rho) = 1$ iff $\rho$ is $V$-correlated.

(iii) $E(\rho) > 1$ iff $\rho$ is entangled.

(iv) For every pure state $\omega_\xi(A) = \langle A\xi, \xi \rangle$, $A \in \mathcal{B}(H)$,

$$E(\omega_\xi) = (\|\xi\|^V)^2.$$
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Maximally entangled mixed states

So the maximum possible value of $E(\cdot)$ on states is $r(V)^{-2}$. A state $\rho$ of $\mathcal{B}(H)$ is said to be maximally entangled if

$$E(\rho) = r(V)^{-2}.$$ 

**Theorem:** The maximally entangled pure states are the vector states $\omega_\xi$ where $\xi$ is a maximal vector.

Every maximally entangled state is a convex combination of maximally entangled pure states.
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Back to earth: Identification of $\| \cdot \|^V$ and $E(\cdot)$

Back to the formative examples $(H, V)$, in which

$$H = H_1 \otimes \cdots \otimes H_N,$$
$$V = \{\xi_1 \otimes \cdots \otimes \xi_N: \xi_k \in H_k, \|\xi_k\| = 1\}.$$

Identify the dual of $\mathcal{B}(H)$ with the Banach space $\mathcal{L}^1(H)$ of all trace class operators $A \in \mathcal{B}(H)$ in the usual way

$$\rho(X) = \text{trace}(AX), \quad X \in \mathcal{B}(H).$$

**Theorem:** $\| \cdot \|^V$ is the greatest cross norm of the projective tensor product of Hilbert spaces $H_1 \hat{\otimes} \cdots \hat{\otimes} H_N$.

$E(\cdot)$ is the greatest cross norm of the projective tensor product of Banach spaces $\mathcal{L}^1(H_1) \hat{\otimes} \cdots \hat{\otimes} \mathcal{L}^1(H_N)$. 
Back to earth: Identification of $\| \cdot \|^V$ and $E(\cdot)$

Back to the formative examples $(H, V)$, in which

$$H = H_1 \otimes \cdots \otimes H_N,$$

$$V = \{ \xi_1 \otimes \cdots \otimes \xi_N : \xi_k \in H_k, \|\xi_k\| = 1 \}. $$

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The inner radius

Continuing with the cases

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We can arrange that \( n_k = \dim H_k \) satisfies \( n_1 \leq \cdots \leq n_N \).

**Theorem:** If \( n_N \geq n_1 n_2 \cdots n_{N-1} \), then

\[ r(V) = \frac{1}{\sqrt{n_1 n_2 \cdots n_{N-1}}} \]

whereas if \( n_N < n_1 n_2 \cdots n_{N-1} \) then all I know is:

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Identification of maximal vectors

We continue to assume that $n_N \geq n_1 n_2 \cdots n_{N-1}$.

**Theorem:** A unit vector $\xi \in H_1 \otimes \cdots \otimes H_N$ is maximal iff it purifies the tracial state $\tau$ of $\mathcal{A} = \mathcal{B}(H_1 \otimes \cdots \otimes H_{N-1})$:

$$\langle (A \otimes 1_{H_N})\xi, \xi \rangle = \tau(A), \quad A \in \mathcal{A}.$$

**Corollary:** The maximal vectors of $H_1 \otimes \cdots \otimes H_N$ are:

$$\xi = \frac{1}{\sqrt{n_1 n_2 \cdots n_{N-1}}} (e_1 \otimes f_1 + \cdots + e_{n_1 n_2 \cdots n_{N-1}} \otimes f_{n_1 n_2 \cdots n_{N-1}}),$$

where $(e_K)$ is an orthonormal basis for $H_1 \otimes \cdots \otimes H_{N-1}$ and $(f_K)$ is an orthonormal set in $H_N$. 
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Unexpected stability of maximal vectors

In more physical terms, consider a tensor product $H \otimes K$ with $n = \dim H \leq m = \dim K < \infty$. The maximal vectors are

$$\xi = \frac{1}{\sqrt{n}}(e_1 \otimes f_1 + \cdots + e_n \otimes f_n), \quad (1)$$

where $(e_k)$ is an ONB for $H$ and $(f_k)$ is an ON set in $K$.

Now assume $H$ is a composite of several subsystems, so that $H = H_1 \otimes \cdots \otimes H_r$. The inner radius of $H_1 \otimes \cdots \otimes H_r \otimes K$ does not change, but the norms $\| \cdot \|^V$ and $E(\cdot)$ do change. They depend strongly on the relative sizes of $\dim H_1, \ldots, \dim H_r$.

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Significant problems remain unsolved

We have much less information about $N$-fold tensor products

$$H = H_1 \otimes \cdots \otimes H_N$$

in cases where $n_N < n_1 n_2 \cdots n_{N-1}$.

Example: $H = (\mathbb{C}^2)^{\otimes N} = \mathbb{C}^2 \otimes \cdots \otimes \mathbb{C}^2$.

- What is the inner radius?
- What are the maximal vectors?
- Which states $\rho$ of $B(H_1 \otimes \cdots \otimes H_{N-1})$ have maximal vectors as “purifications”? i.e., which $\rho$ can be written in the form

$$\rho(A) = \langle (A \otimes 1_{H_N}) \xi, \xi \rangle, \quad A \in B(H_1 \otimes \cdots \otimes H_{N-1})$$

where $\xi$ is a maximal vector in $H$? (Recently solved)
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The case $N = 3$ (in progress)

Let $H, K$ be Hilbert spaces of dimensions $p, q$. Here is an “operator space” formula for the inner radius $r(p, q, n)$ of $H \otimes K \otimes \mathbb{C}^n$ in the critical cases $n \leq pq$.

Let $M_{pq}$ be the operator space of $p \times q$ complex matrices, $M_{pq} \cong \mathcal{B}(K, H)$. We consider the following two norms on the space of linear maps $\phi : M_{pq} \to M_{pq}$:

$$\|\phi\|_{HS} = \left( \sum_{i,j=1}^{p,q} \text{trace} |\phi(E_{ij})|^2 \right)^{1/2}$$

(the Hilbert Schmidt norm of $\phi : \mathcal{L}^2(K, H) \to \mathcal{L}^2(K, H)$), and

$$\|\phi\|_{2,\infty} = \sup_{\text{trace } |A|^2 \leq 1} \|\phi(A)\|,$$

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The \textit{rank} of $\phi$ is the dimension of its range $\dim \phi(M_{pq})$.

\textbf{Theorem:} For $n \leq pq$, the inner radius of $\mathbb{C}^p \otimes \mathbb{C}^q \otimes \mathbb{C}^n$ is determined by linear maps $\phi : M_{pq} \rightarrow M_{pq}$ as follows:

$$r(p, q, n) = \inf\{\|\phi\|_{2,\infty} : \|\phi\|_{HS} = 1, \ \text{rank} \ \phi \leq n\}.$$

Let's save notation by fixing $p, q$ and writing $r_n = r(p, q, n)$ for $n = 1, 2, \ldots, pq$. We can prove that

$$r_1 = \frac{1}{\sqrt{\min(p, q)}} \geq r_2 \geq \cdots \geq r_{pq} = \frac{1}{\sqrt{pq}}.$$

\textbf{Conjecture:} $r(p, q, n) > r(p, q, n + 1)$ for $n < pq$. 

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Three qubits: \( p = q = n = 2 \)

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H = \mathbb{C}^2 \otimes \mathbb{C}^2 \otimes \mathbb{C}^2, \quad V = \{ \xi \otimes \eta \otimes \zeta : \|\xi\| = \|\eta\| = \|\zeta\| = 1 \}.
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Preceding results imply that \( \frac{1}{\sqrt{2}} \geq r(V) > \frac{1}{2} \), and we have

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This has significant consequences. For example, maximal vectors must have "unequal weights" (and entropy less than the expected value \( \log 2 \)), in the sense that

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\xi = \sqrt{\theta} \cdot e_1 \otimes f_1 + \sqrt{1-\theta} \cdot e_2 \otimes f_2
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where \( 0 < \theta < 1/2 \), \( \{ e_k \} = \text{ONB for } \mathbb{C}^2 \), \( \{ f_k \} = \text{ON set in } \mathbb{C}^4 \).

There is compelling numerical evidence (thanks to Michael Lamoureux and Geoff Price) indicating that

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r(V) \leq 0.68 < \frac{1}{\sqrt{2}} \approx 0.71.
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NEWS FLASH: \( r(2, 2, 2) < \frac{1}{\sqrt{2}}! \)

Two days ago, I received an email from Geoff Price in which he seems to prove that \( r(2, 2, 2) \leq \frac{2}{3} \approx 0.68. \)

More precisely, for the unit vector

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and with some trickery, he hand-calculates

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\|\xi\|_V = \sup_{\|v_k\|=1} |\langle \xi, v_1 \otimes v_2 \otimes v_3 \rangle| = \frac{2}{3},
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It is conceivable that \( r(2, 2, 2) = 2/3, \) but numerical evidence suggests \( r(2, 2, 2) \leq 0.65 < 2/3. \)
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Connects with the local theory of Banach spaces

Let $H_1, \ldots, H_N$ be finite dimensional Hilbert spaces, consider the two Banach spaces

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and let $c$ be the smallest constant that relates the two norms $\|\xi\|_E \leq c \cdot \|\xi\|_H$. The Banach space folks want to calculate or estimate the value of $c$, and they have many results.

Our calculations provide the following new result: Arrange that $n_N$ is the largest of $n_1, \ldots, n_N$. Then

$$c = \sqrt{n_1 \cdots n_{N-1}}, \quad \text{if } n_N \geq n_1 \cdots n_{N-1};$$

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