

# Numerical simulation of randomly generated states for two-qubit system according to the LHVMM paradigm and entropy measure


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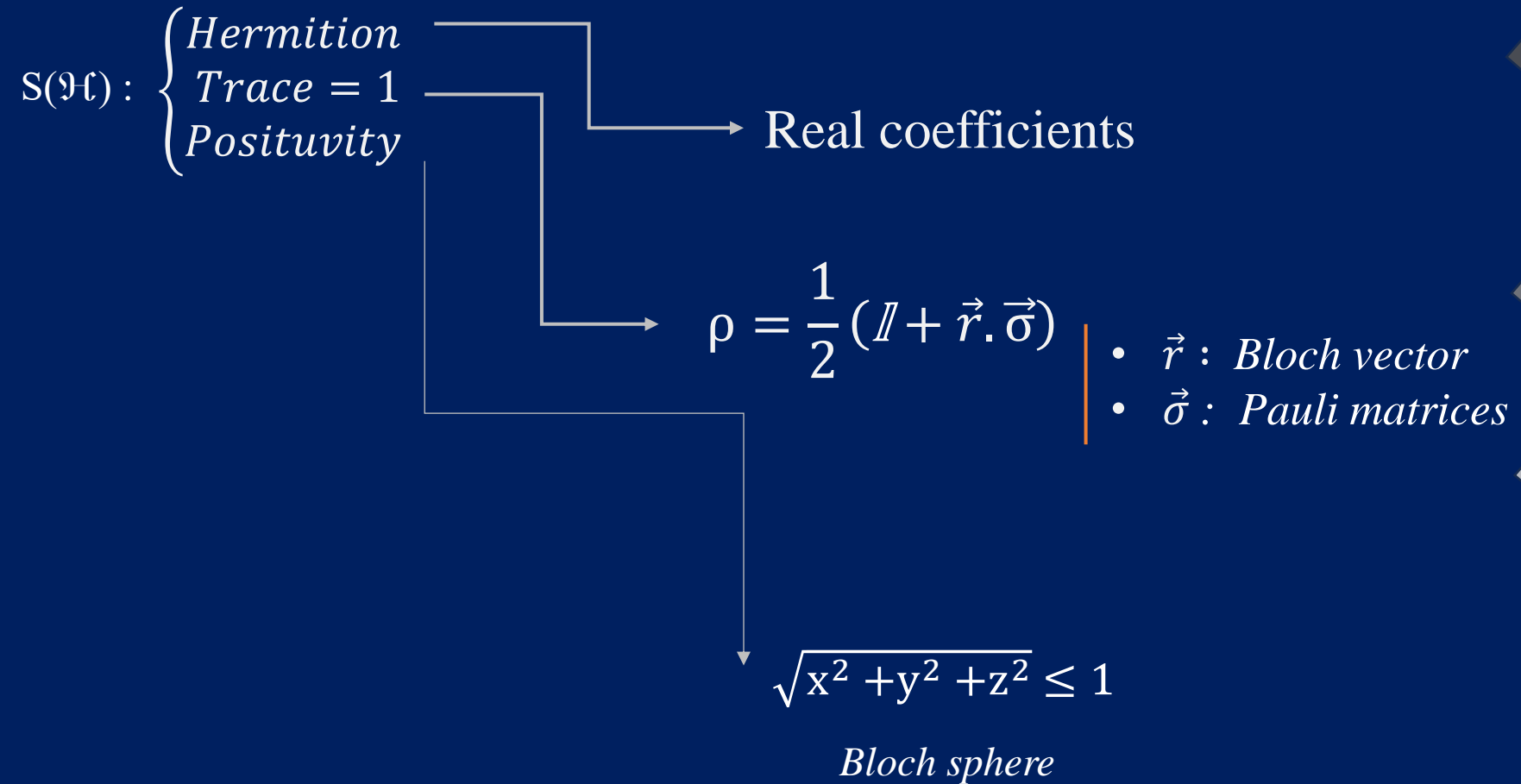
*By* **Arash T. Jamshidi**

*September 2024*

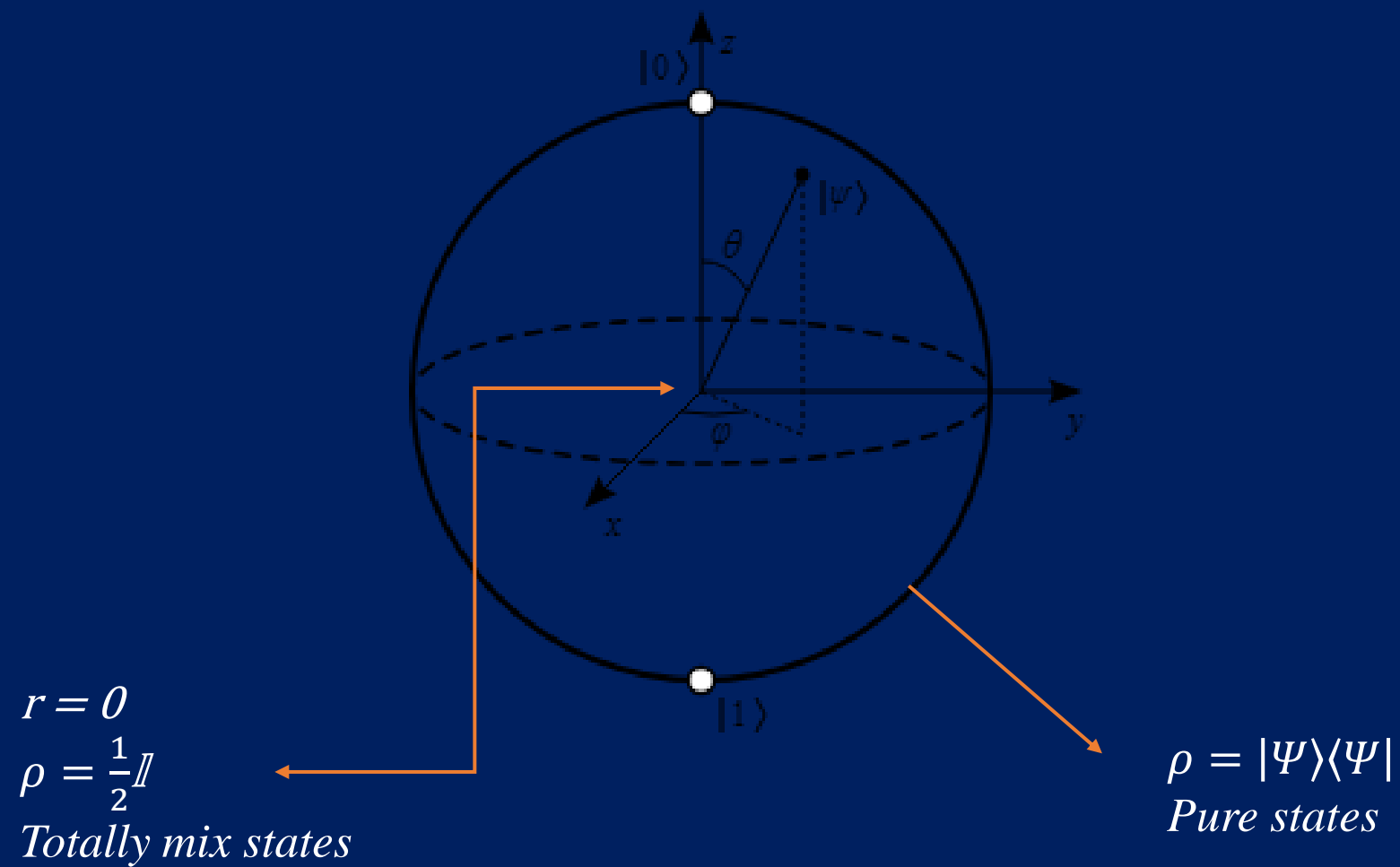


- 
- *State space*
  - *Hilbert-Schmidt form of density matrix*
  - *Two-qubit system and defining  $s_j$   $r_i$   $t_{ij}$*
  - *Generating random uniform states*
  - *Problems that we have faced!*
  - *Separability and entanglement*
  - *EPR – Bell inequalities*
  - *Horodecki's theorem*
  - *Results*
  - *Entropic Manifestation of Entanglement*
  - *MEMS and Results*

## *“State Space”*



## *“ Bloch sphere*



## *“Hilbert-Schmidt*

*Qudit !*

$$\rho = \frac{1}{d} (\mathbb{I} + \vec{r} \cdot \vec{\lambda})$$

•  $\vec{\lambda}$  : Gell-Mann matrices

$$2^d - 1$$

For two-qubit system :  $\mathcal{H} = \mathbb{C}^2 \otimes \mathbb{C}^2$

$$\rho = \frac{1}{4} (\mathbb{I} \otimes \mathbb{I} + (\vec{r} \cdot \vec{\sigma}) \otimes \mathbb{I} + \mathbb{I} \otimes (\vec{s} \cdot \vec{\sigma}) + t_{ij} (\vec{\sigma}_i \otimes \vec{\sigma}_j))$$

$$\rho = \frac{1}{4} (\mathbb{I} \otimes \mathbb{I} + (\vec{r} \cdot \vec{\sigma}) \otimes \mathbb{I} + \mathbb{I} \otimes (\vec{s} \cdot \vec{\sigma}) + t_{ij} (\vec{\sigma}_i \otimes \vec{\sigma}_j))$$

$$\text{Tr}(\sigma_i \sigma_j) = 2\delta_{ij}$$

$$r_i = \text{Tr}[\rho(\vec{\sigma}_i \otimes \mathbb{I})]$$

$$t_{ij} = \text{Tr}[\rho(\vec{\sigma}_i \otimes \vec{\sigma}_j)]$$

$$s_j = \text{Tr}[\rho(\mathbb{I} \otimes \vec{\sigma}_j)]$$

## *“How we generate random states*

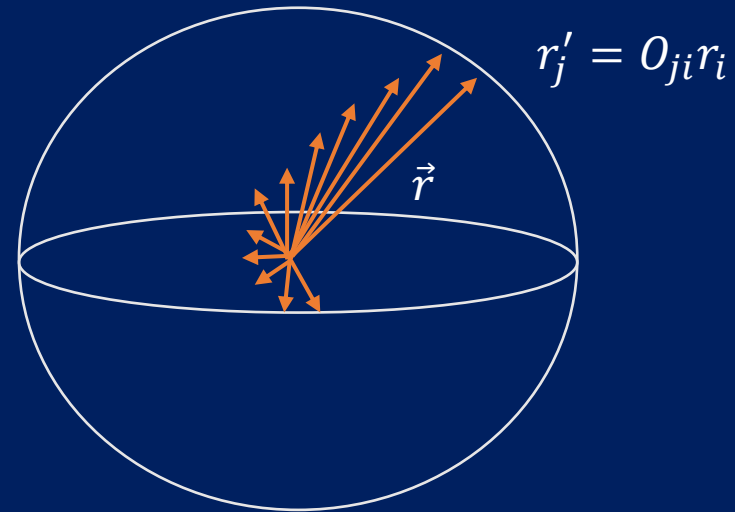
$$\rho = \frac{1}{d}(\mathbb{I} + \vec{r} \cdot \vec{\lambda}) \quad SO(3) \leftrightarrow SU(2)$$

$$\rho' = \frac{1}{d}(\mathbb{I} + \vec{r}' \cdot \vec{\lambda}) \rightarrow \rho' = \frac{1}{d} \left( \mathbb{I} + \sum_{i,j} O_{ji} r_i \lambda_j \right)$$

$$u \lambda_i u^\dagger = \sum_{j=1}^{N^2-1} O_{ji} \lambda_j \quad \rho' = \frac{1}{d} \left( \mathbb{I} + \sum_{i,j} u \lambda_i u^\dagger r_i \right)$$

$$\rightarrow \rho' = \frac{1}{d}(\mathbb{I} + u(\vec{r} \cdot \vec{\lambda})u^\dagger) = u \left\{ \frac{1}{d}(\mathbb{I} + (\vec{r} \cdot \vec{\lambda})) \right\} u^\dagger$$

$$\rho \rightarrow \rho' = u \rho u^\dagger$$



## *“How we generate random uniform probability*

$$\rho' = u\rho_d u^\dagger$$

$$\rho_d = \begin{bmatrix} P_1 & 0 & 0 & 0 \\ 0 & P_2 & 0 & 0 \\ 0 & 0 & P_3 & 0 \\ 0 & 0 & 0 & P_4 \end{bmatrix} \quad \sum_i P_i = 1$$

Which  $P_i$  are randomly generated with Dirichlet distribution, from NumPy package in python.

it worth to notice that this function uniformly generate initial probabilities.

```
for i in range(num_denmet):
    def generate_diagonal_elements(d):
        # Generate n random numbers following Dirichlet distribution
        random_numbers = np.random.dirichlet(np.ones(d))
        return random_numbers

    diagonals = generate_diagonal_elements(d)

    set_ro_d.append(diagonals*np.identity(d))
```



## “How we generate random Unitary matrix

$$\rho' = u\rho u^\dagger$$

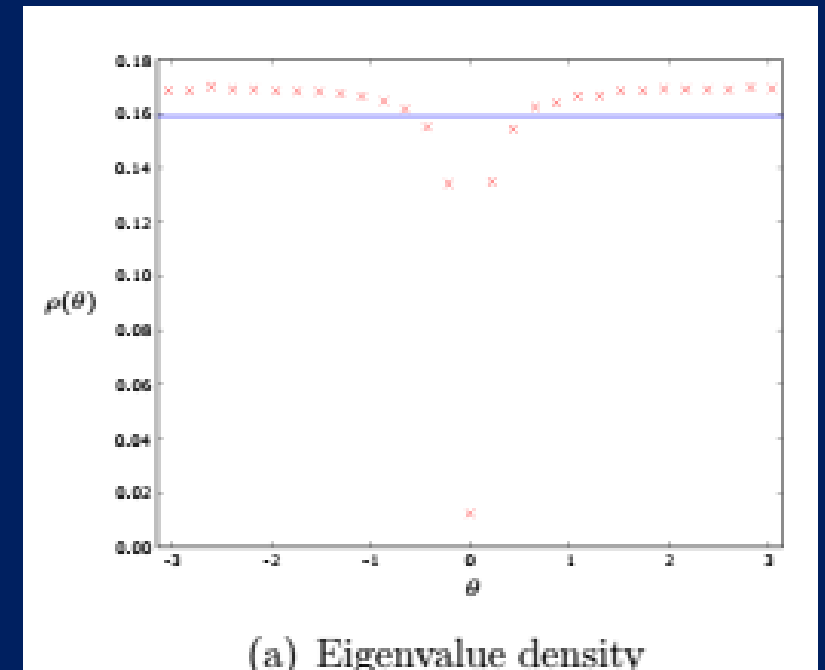
“steps

- Uniform, random unitary matrix
  - 1. First we generate a random complex matrix
  - 2. We use QR decomposition to decompose our random complex matrix to one unitary matrix (Q) and one upper-triangular (R)
- But the output is not distributed with Haar measure.

in the case of unitary matrices distributed according to the Haar measure:

(large matrices)  
random matrix theory

1. eigenvalues tend to repel each other (level repulsion)
2. average density of eigenvalues around the unit circle is approximately constant



- F. Mezzadri, "How to generate random matrices from the classical compact groups," Notices of the American Mathematical Society, 54 (5), 592-604 (2007).

## *“Our problem with random unitary matrix distribution*

The main problem is that QR decomposition is not unique !

$Z \in GL(N, \mathbb{C})$ ,  $Z = QR$  which  $Q$  is unitary and  $R$  is upper triangular matrices.

$$Z = Q\Lambda\Lambda^{-1}R \quad \text{let } \Lambda = \begin{pmatrix} e^{i\theta_1} & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & e^{i\theta_N} \end{pmatrix} = \text{diag}(e^{i\theta_1}, \dots, e^{i\theta_N}) \quad \Lambda \in \Lambda(N)$$

"unitary diagonal matrices group"

$Q' = Q\Lambda$  and  $R' = \Lambda^{-1}R$  are still unitary and upper triangular respectively.

QR decomposition defines a multi valued map:  $Z = QR = Q'R'$

$$QR: GL(N, \mathbb{C}) \rightarrow U(N) \times T(N)$$

- F. Mezzadri, "How to generate random matrices from the classical compact groups," Notices of the American Mathematical Society, 54 (5), 592-604 (2007).

## *“Our problem with random unitary matrix distribution*

$$QR: GL(N, \mathbb{C}) \rightarrow U(N) \times T(N) \quad QR = Q'R'$$

$\Lambda(N) = U(N) \cap T(N)$  so we should consider one-to-one map:

$$\overline{QR}: GL(N, \mathbb{C}) \rightarrow U(N) \times \Gamma(N)$$

where  $\Gamma(N) = T(N)/\Lambda(N)$  is the right coset space of  $\Lambda(N)$  in  $T(N)$

can be chosen by fixing the arguments of the elements of the main diagonal of  $R \in T(N)$

$$\Lambda = \begin{pmatrix} \frac{r_{11}}{|r_{11}|} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & \frac{r_{NN}}{|r_{NN}|} \end{pmatrix}$$

$r_{jj}$

- F. Mezzadri, "How to generate random matrices from the classical compact groups," Notices of the American Mathematical Society, 54 (5), 592-604 (2007).

## “How we generate random Unitary matrix

$$\rho' = u\rho u^\dagger$$

The  $Q' = Q\Lambda$  is distributed with Haar measure

```
for i in range(num_state):
    def random_unitary(d):
        # Generate a random complex matrix
        X = np.random.randn(d, d) + I * np.random.randn(d, d)

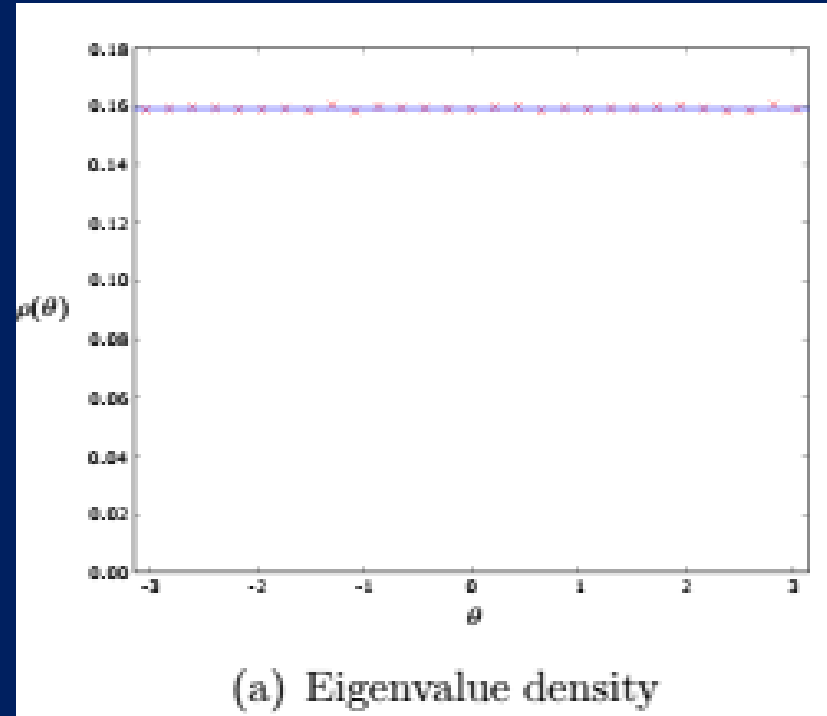
        # QR decomposition
        Q, R = np.linalg.qr(X)

        # Create a diagonal matrix with phase factors
        D = np.diag(np.diag(R) / np.abs(np.diag(R)))

        # Construct the unitary matrix
        U = np.dot(Q, D)

        return U

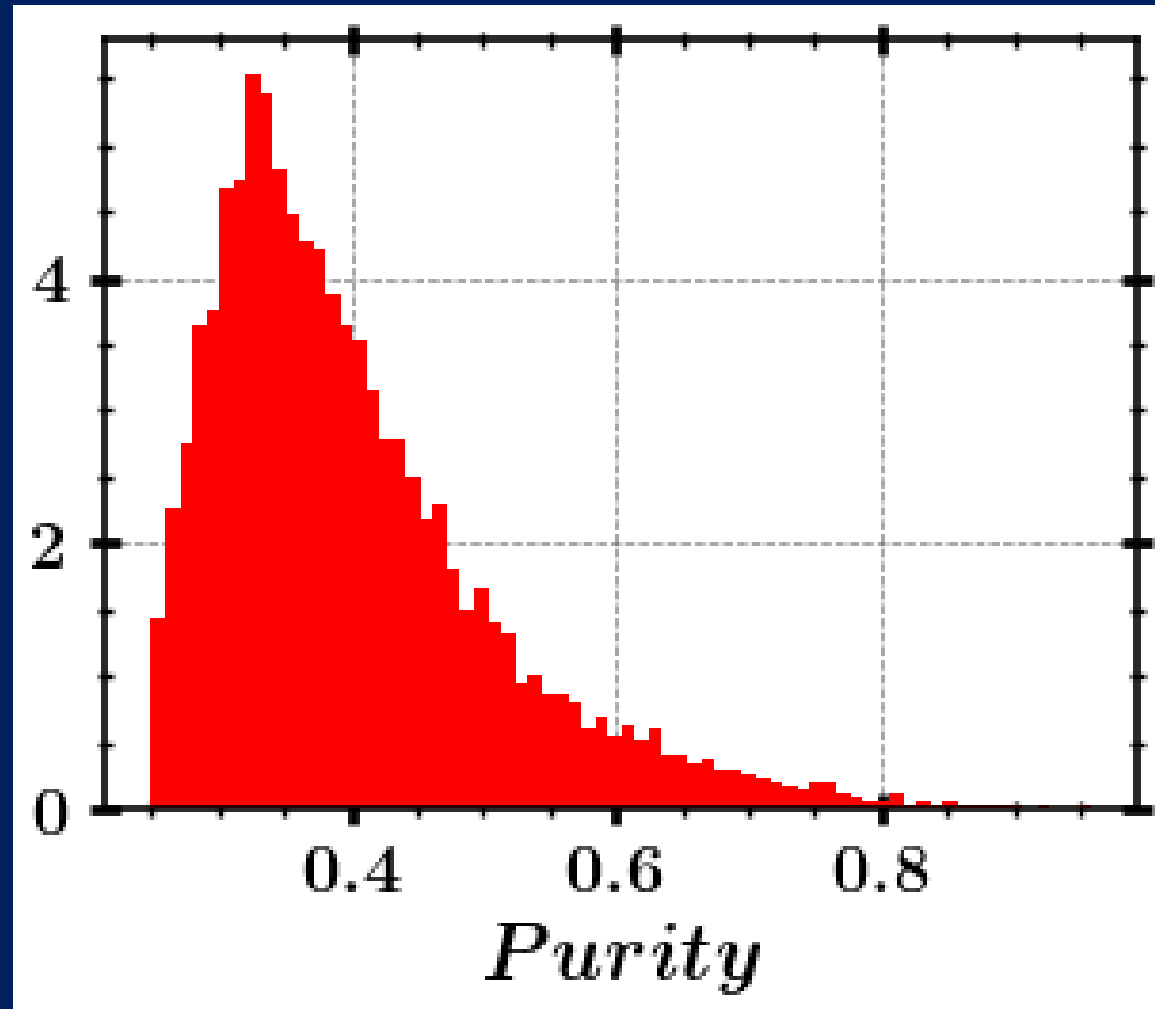
    set_state.append(random_unitary(d))
```



- small fluctuations due to the repulsion effect

- F. Mezzadri, "How to generate random matrices from the classical compact groups," Notices of the American Mathematical Society, 54 (5), 592-604 (2007).

*“Purity of randomly generated states*



## *“Separability and Entanglement*

$$\rho = \sum P_k (\rho_A^k \otimes \rho_B^k)$$



*If it can't be written as convex sum of pure states,  $\rho$  is Entangled !*

## *“EPR - Bell - CHSH*

$$P(a, b) = \int A(a, \lambda) B(b, \lambda) \rho(\lambda) d\lambda$$

$$\langle B \rangle \leq \beta_{LR}$$

## *“CHSH*

$$\mathbf{B}_{CHSH} = \mathbf{A} \otimes [\mathbf{B} + \mathbf{B}'] + \mathbf{A}' \otimes [\mathbf{B} - \mathbf{B}']$$

$$\langle \mathbf{B}_{CHSH} \rangle = \text{Trac}[\rho \mathbf{B}_{CHSH}]$$

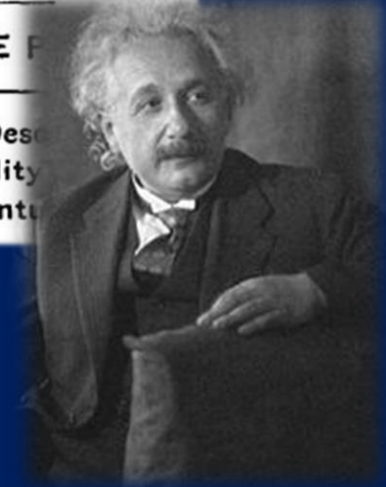
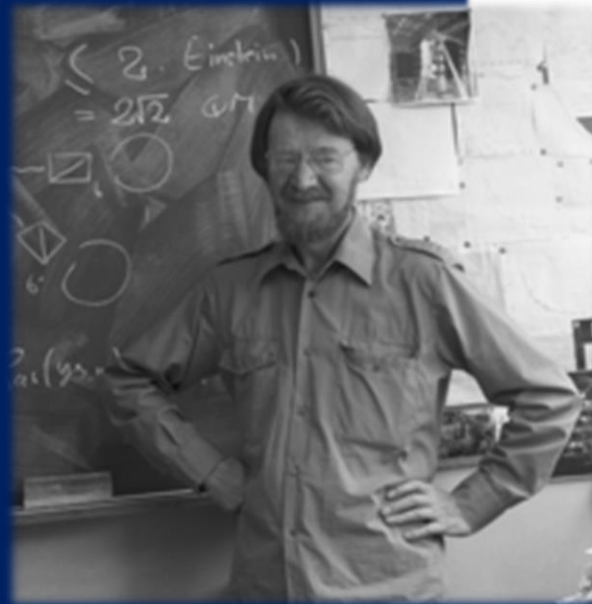
$$|\langle \mathbf{B}_{CHSH} \rangle| \leq 2$$

## EINSTEIN ATTACKS QUANTUM THEORY

Scientist and Two Colleagues  
Find It Is Not 'Complete'  
Even Though 'Correct.'

LLER ONE P

a Whole Des  
ysical Reality  
vided Eventu



- *Locality*
- *Realism*

1935

1964

1969

- A. Einstein, B. Podolsky, and N. Rosen, "Can quantum-mechanical description of physical reality be considered complete?" *Physical Review*, 47 (10), 777-780 (1935)
- J. S. Bell, "On the Einstein Podolsky Rosen Paradox," *Physics Physique Физика*, 1 (3), 195-200 (1964).
- J. F. Clauser, M. A. Horne, A. Shimony, and R. A. Holt, "Proposed experiment to test local hidden-variable theories," *Physical Review Letters*, 23 (15), 880-884 (1969)

$$\mathbf{B}_{CHSH} = \mathbf{A} \otimes [\mathbf{B} + \mathbf{B}'] + \mathbf{A}' \otimes [\mathbf{B} - \mathbf{B}']$$

$$\rho = \frac{1}{4} (\mathbb{I} \otimes \mathbb{I} + (\vec{r} \cdot \vec{\sigma}) \otimes \mathbb{I} + \mathbb{I} \otimes (\vec{s} \cdot \vec{\sigma}) + t_{ij} (\vec{\sigma}_i \otimes \vec{\sigma}_j))$$

$$\langle \mathbf{B}_{CHSH} \rangle = \text{Trac}[\rho \mathbf{B}_{CHSH}]$$

$$\text{Tr}(\sigma_i \sigma_j) = 2\delta_{ij} \rightarrow r_i \text{ \& \; } s_j \quad \langle \mathbf{B}_{CHSH} \rangle \propto t_{ij}$$

$$\langle \mathbf{B}_{CHSH} \rangle = \text{Tr} \left[ \frac{1}{4} t_{ij} (\vec{\sigma}_i \otimes \vec{\sigma}_j) [\mathbf{B}_{CHSH}] \right] \rightarrow \langle \mathbf{B}_{CHSH} \rangle = \sum a_i t_{ij} (b + b')_j + a'_i t_{ij} (b - b')_j$$

$$t_{ij} = \begin{bmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{bmatrix}$$

“Correlation tensor”

- $A' = \sigma \cdot a'$
- $A = \sigma \cdot a$
- $B' = \sigma \cdot b'$
- $B = \sigma \cdot b$



## *“Horodecki’s measure of maximum Bell’s operator expectation value*

$$T = \begin{bmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{bmatrix} \longrightarrow \text{We cannot necessarily diagonalize the matrix } T \text{ but we can calculate the matrix } T^\dagger T \text{ which is both diagonal and positive.}$$

***Horodecki’s theorem :*** The maximum expectation value of the Bell operator is equal to:

$$\text{Max}\{\langle \mathbf{B}_{CHSH} \rangle\} = 2\sqrt{u_1 + u_2}$$

Where  $u_i$  are the non-negative eigenvalues of the positive and real matrix  $T^\dagger T$ , such that :

$$u_1 \geq u_2 \geq u_3 \geq 0$$

- R. Horodecki, P. Horodecki, and M. Horodecki, "Violating Bell inequality by mixed spin-1/2 states: necessary and sufficient condition," Physical Review Letters, 74 (20), 414-417 (1995)

*“steps*

*random*  $4 \times 4 \rho_i$

$$\rho = \frac{1}{4} (\mathbb{I} \otimes \mathbb{I} + (\vec{r} \cdot \vec{\sigma}) \otimes \mathbb{I} + \mathbb{I} \otimes (\vec{s} \cdot \vec{\sigma}) + t_{ij} (\vec{\sigma}_i \otimes \vec{\sigma}_j))$$

$$t_{ij} = \text{Tr}[\rho(\vec{\sigma}_i \otimes \vec{\sigma}_j)]$$

$$T = \begin{bmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{bmatrix}$$

$$\text{eig}(T^\dagger T)$$

$$u_1 \geq u_2 \geq u_3 \geq 0$$

$$\text{Max}\{\langle \mathbf{B}_{CHSH} \rangle\} = 2\sqrt{u_1 + u_2}$$

$$|\langle \mathbf{B}_{CHSH} \rangle| \leq 2$$

$$\text{if } \sqrt{u_1 + u_2} \geq 1 \rightarrow \rho \text{ is Entagled}$$

## *“Main loop for checking the Bell’s inequality*

```
for q in range(num_denmet):
    for j in range(num_state):

        TT = []
        ro = set_state[j]@set_ro_d[q]@Dagger(set_state[j])
        density_matrix.append(ro)
        puty = np.trace(density_matrix[q]@(density_matrix[q].conj()).T)
        purity.append(abs(puty))
        for i in range(len(sig_prdct)):
            t = np.trace(density_matrix[q]@sig_prdct[i])
            TT.append(t)
        T = np.array([[TT[0],TT[1],TT[2]],
                      [TT[3],TT[4],TT[5]],
                      [TT[6],TT[7],TT[8]]])

        eigval , eigvec = np.linalg.eig(Dagger(T)@T)
        eeg = abs(eigval)
        g = np.trace(np.diag(eeg))-min(eeg)

        max_Exp = 2 * np.sqrt(g)
        Expectation_sum.append(max_Exp)
        if max_Exp > 2:
            Entangled_state.append(set_state[j])
            purity_ents = np.trace(abs(density_matrix[q]@density_matrix[q].conj()).T)
            good_ro_purity.append(purity_ents)
            Expectation_sum_notBell.append(g)

        else:
            Separable_state.append(set_state[j])
            Expectation_sum_Bell.append(g)
```

## “Main loop for checking the Bell’s inequality

```
for q in range(num_denmet):
    for j in range(num_state):

        TT = []
        ro = set_state[j]@set_ro_d[q]@Dagger(set_state[j])
        density_matrix.append(ro)
        puty = np.trace(density_matrix[q]@(density_matrix[q].conj().T))
        purity.append(abs(puty))
        for i in range(len(sig_prdct)):
            t = np.trace(density_matrix[q]@sig_prdct[i])
            TT.append(t)
        T = np.array([[TT[0],TT[1],TT[2]],
                      [TT[3],TT[4],TT[5]],
                      [TT[6],TT[7],TT[8]]])

        eigval , eigvec = np.linalg.eig(Dagger(T)@T)
        eeg = abs(eigval)
        g = np.trace(np.diag(eeg))-min(eeg)

        max_Exp = 2 * np.sqrt(g)
        Expectation_sum.append(max_Exp)
        if max_Exp > 2:
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            purity_ents = np.trace(abs(density_matrix[q]@density_matrix[q].conj().T))
            good_ro_purity.append(purity_ents)
            Expectation_sum_notBell.append(g)

        else:
            Separable_state.append(set_state[j])
            Expectation_sum_Bell.append(g)
```

```
sigma_x = np.array([[0,1],
                    [1,0]])
sigma_y = np.array([[0,-1],
                    [1,0]])
sigma_z = np.array([[1,0],
                    [0,-1]])

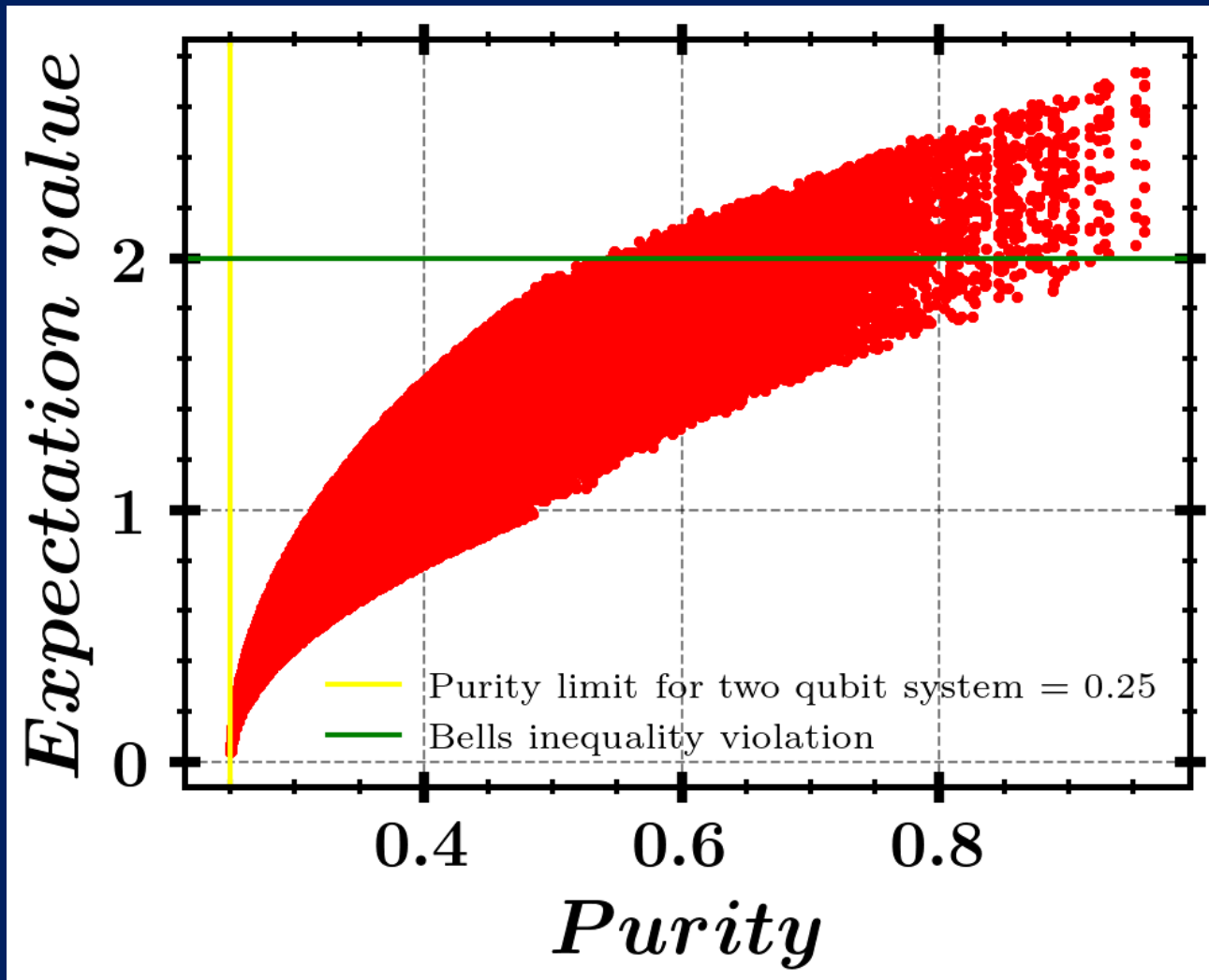
sigma = [sigma_x ,sigma_y ,sigma_z]
#-----
for i in range(0,3):
    for j in range(0,3):
        tt = np.kron(sigma[i],sigma[j])
        sig_prdct.append(tt)
```

$$t_{ij} = \text{Tr}[\rho(\vec{\sigma}_i \otimes \vec{\sigma}_j)]$$

- $\rho_d : 100000$
- $u_i : 10$

Example run

*Bell's inequality as witness suggest that we have 27880  
Entangled state out of 696700 possible ones.*



4.002 % of the randomly  
generated states are  
Entangled state as far as  
Bell's inequality can tell.

## *“Entropic Manifestation of Entanglement”*

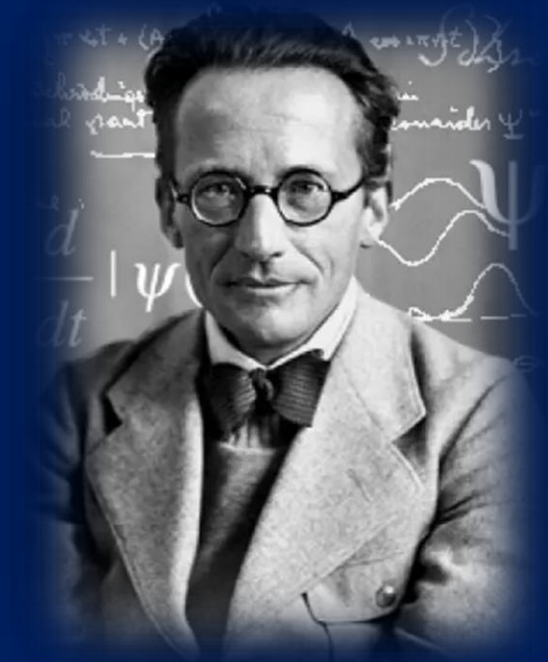
$$\text{Classic} : I(x|y) = I(x, y) - I(y) \geq 0$$

$$\text{QM} : I(A|B) = S(\rho_{AB}) - S(\rho_A) !$$

If  $\rho_{AB}$  is separable then  $\rightarrow I(A|B) \geq 0$

$$\rho = \sum P_k (\rho_A^k \otimes \rho_B^k)$$

$$\begin{cases} S(\rho_{AB}) \geq S(\rho_A) \\ S(\rho_{AB}) \geq S(\rho_B) \end{cases}$$



*“The best possible knowledge of a whole does not include the best possible knowledge of its parts and this is what keeps coming back to haunt us”*

- 
- Horodecki and Horodecki, 1996: R. Horodecki and M. Horodecki, "Information-theoretic aspects of quantum inseparability of mixed states," Physical Review A, 54 (3), 1838-1843 (1996)
  - R. Horodecki et al., 1996: R. Horodecki, M. Horodecki, and P. Horodecki, "Separability of mixed states: necessary and sufficient conditions," Physics Letters A, 223 (1-2), 1-8 (1996)
  - Terhal, 2002: B. M. Terhal, "Detecting quantum entanglement," Theoretical Computer Science, 287 (1), 313-335 (2002)
  - Vollbrecht and Wolf, 2002: K. G. H. Vollbrecht and M. M. Wolf, "Conditional entropies and their relation to entanglement criteria," Journal of Mathematical Physics, 43 (9), 4299-4306 (2002)


*“calculating the partial trace*

```
# calculating partial trace
density_A = []
density_B = []
for i in range(len(density_matrix)):
    BB = np.split(density_matrix[i], 2, axis=1)
    BB0 = np.split(BB[0], 2, axis=0)
    BB1 = np.split(BB[1], 2, axis=0)
    B00 = BB0[0]
    B01 = BB1[0]
    B10 = BB0[1]
    B11 = BB1[1]
    P_Tr_B = np.array([[np.trace(B00), np.trace(B01)],
                       [np.trace(B10), np.trace(B11)]])
    density_A.append(P_Tr_B)
    P_Tr_A = np.array([[B00[0][0]+B11[0][0], B00[0][1]+B11[0][1]],
                       [B00[1][0]+B11[1][0], B00[1][1]+B11[1][1]]])
    density_B.append(P_Tr_A)
```

*“Calculating the Von Neumann entropy*

```
#calculating of Von Neumann entropy
import math
Entropy_A = []
Entropy_AB = []
for i in range(len(density_A)):
    eigval, eigvec = np.linalg.eig(density_A[i])
    eg = abs(eigval)
    s = -(eg[0]*(math.log(eg[0])) + eg[1]*(math.log(eg[1])))
    Entropy_A.append(s)

for i in range(len(density_matrix)):
    eigval, eigvec = np.linalg.eig(density_matrix[i])
    eg = abs(eigval)
    s = -(eg[0]*(math.log(eg[0])) + eg[1]*(math.log(eg[1])) + eg[2]*(math.log(eg[2])) + eg[3]*(math.log(eg[3])))
    Entropy_AB.append(s)
```




```
# calculating entropy witness
separables_S = []
entangleds_S = []
for i in range(len(Entropy_AB)):
    if Entropy_AB[i] >= Entropy_A[i]:
        separables_S.append(density_matrix[i])
    else:
        entangleds_S.append(density_matrix[i])
```



Entropy as witness suggest that we have 16535 Entangled state.

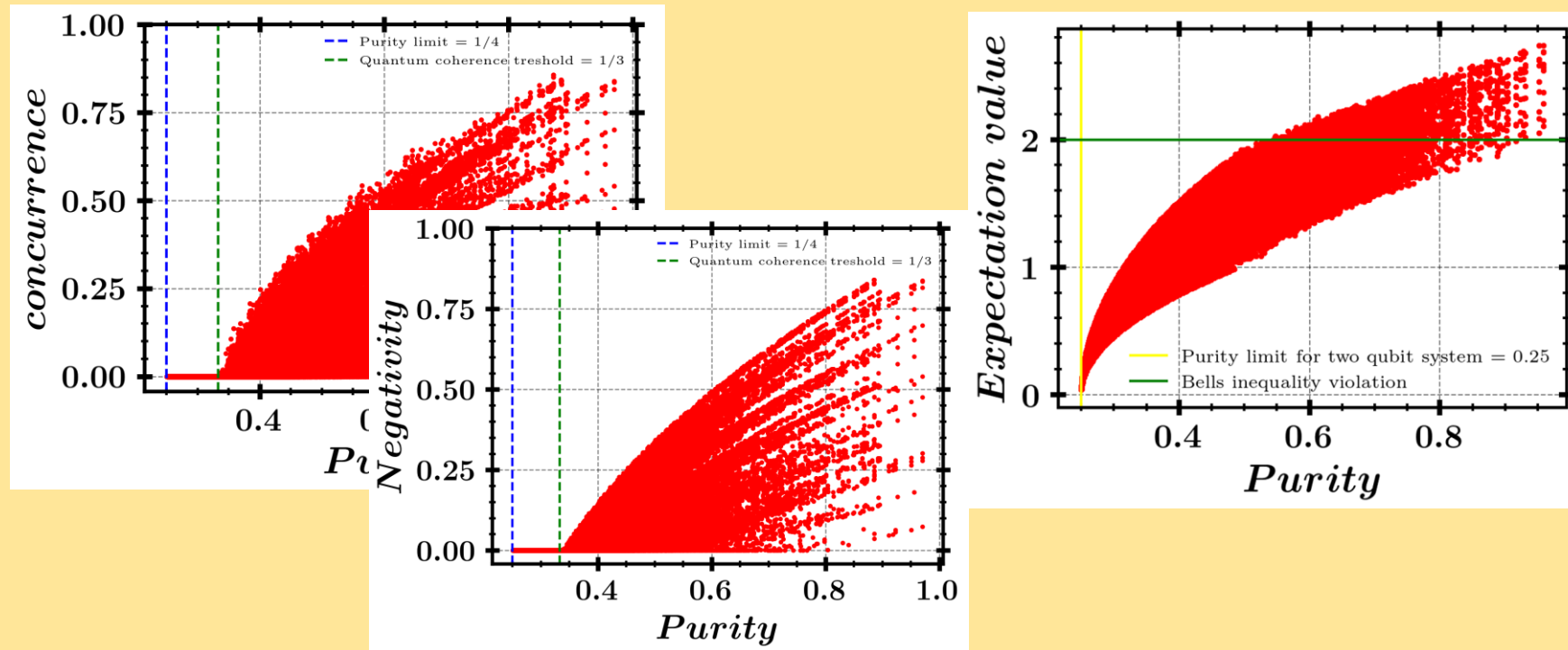
1.6535 % of the generated random states are Entangled state as far as Entropy as witness can tell.



**Thanks for your attention !**  
**To be continued ...**



As we saw in previous presentation we investigate different entanglement measures  
different entanglement measures can give different orderings for pairs of mixed states.

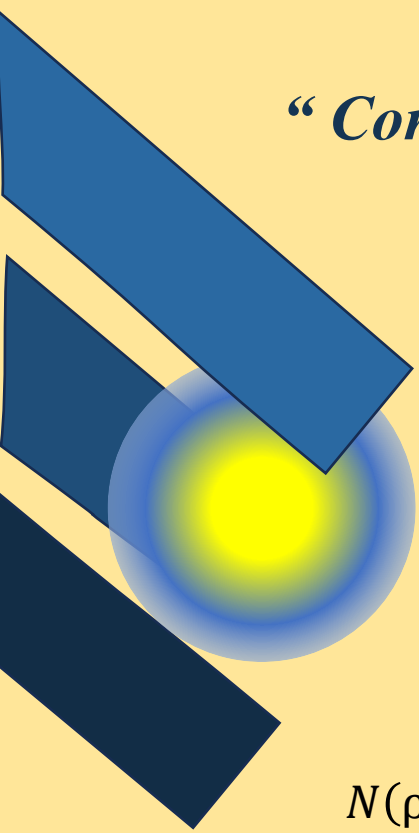


Now we investigate the highest possible entanglement for a given level of mixedness

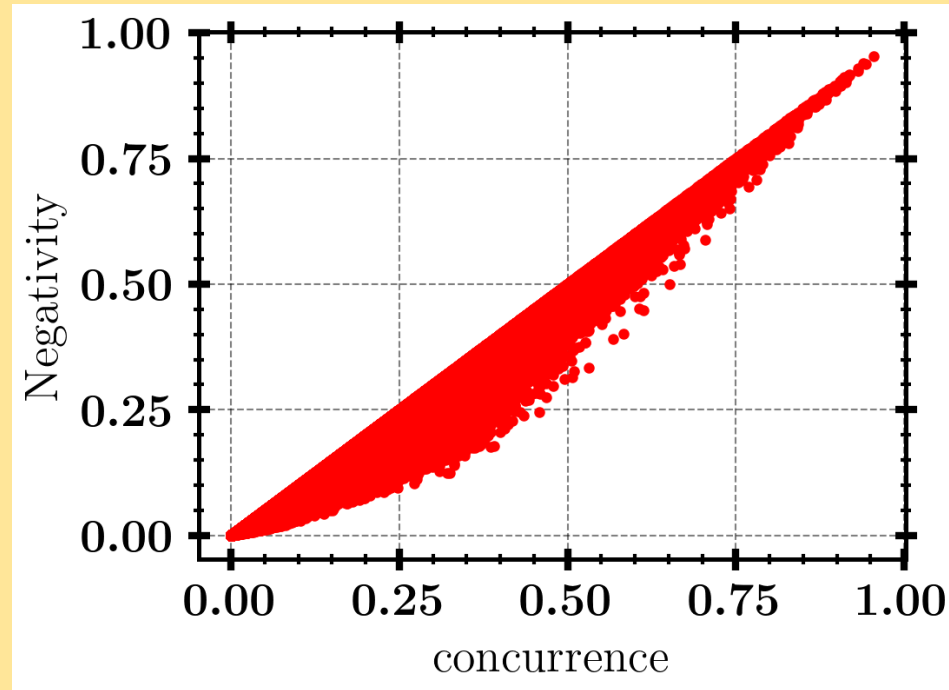
### ***“MEMS”***

- G. Vidal and R. F. Werner, 2002: G. Vidal and R. F. Werner, "A computable measure of entanglement," Physical Review Letters, 89 (17), 170401 (2002)
- K. Zyczkowski, P. Horodecki, A. Sanpera, and M. Lewenstein, 1998: K. Zyczkowski, P. Horodecki, A. Sanpera, and M. Lewenstein, "Volume of the set of separable states," Physical Review Letters, 85 (17), 2961-2964 (1998)
- A. Peres, 1996: A. Peres, "Separability criterion for density matrices," Physical Review Letters, 77 (8), 1413-1415 (1996)
- M. Horodecki, P. Horodecki, and R. Horodecki, 1996: M. Horodecki, P. Horodecki, and R. Horodecki, "Separability of mixed states: necessary and sufficient conditions," Physics Letters A, 223 (1-2), 1-8 (1996)

## “Concurrence vs Negativity”

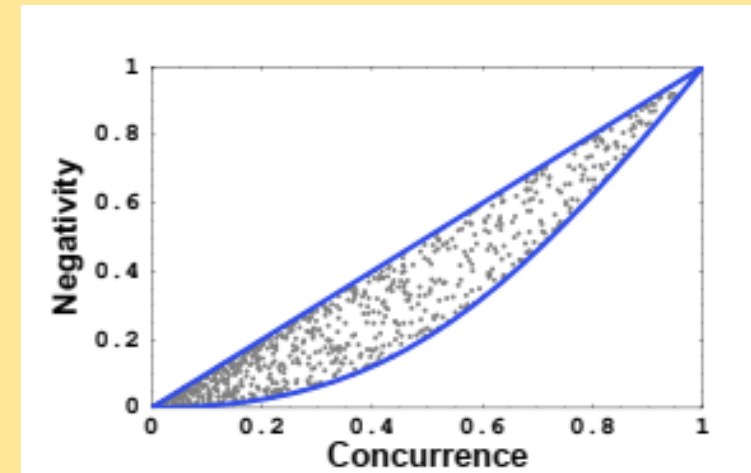


$$N(\rho) = \frac{\|\rho^{T_B}\|_1 - 1}{2}$$



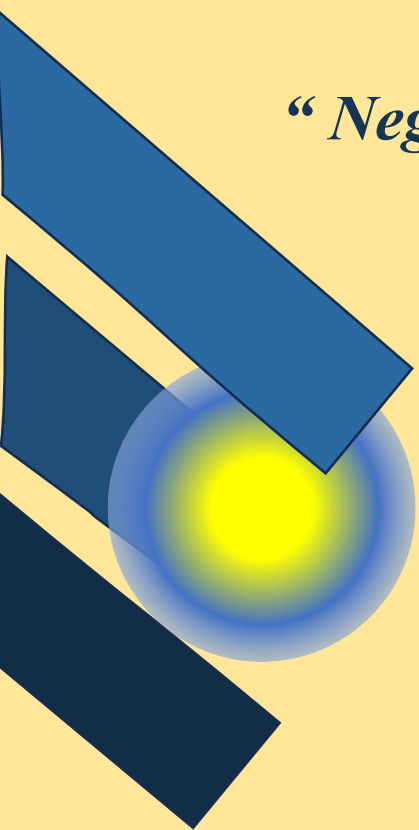
- Maximum negativity for a given value of concurrence using **Lagrange optimization techniques**.

$$\mathcal{L} = N(\rho) + \lambda(C(\rho) - C_0)$$



- F. Verstraete, K. Audenaert, J. Dehaene, and B. De Moor, 2001: F. Verstraete, K. Audenaert, J. Dehaene, and B. De Moor, "A comparison of the entanglement measures negativity and concurrence," *Journal of Physics A: Mathematical and General*, 34 (47), 10327-10332 (2001)
- Tzu-Chieh Wei et al.: T.-C. Wei, K. Nemoto, P. M. Goldbart, P. G. Kwiat, W. J. Munro, and F. Verstraete, "Maximal entanglement versus entropy for mixed quantum states," *Physical Review A*, 67 (2), 022110 (2003)

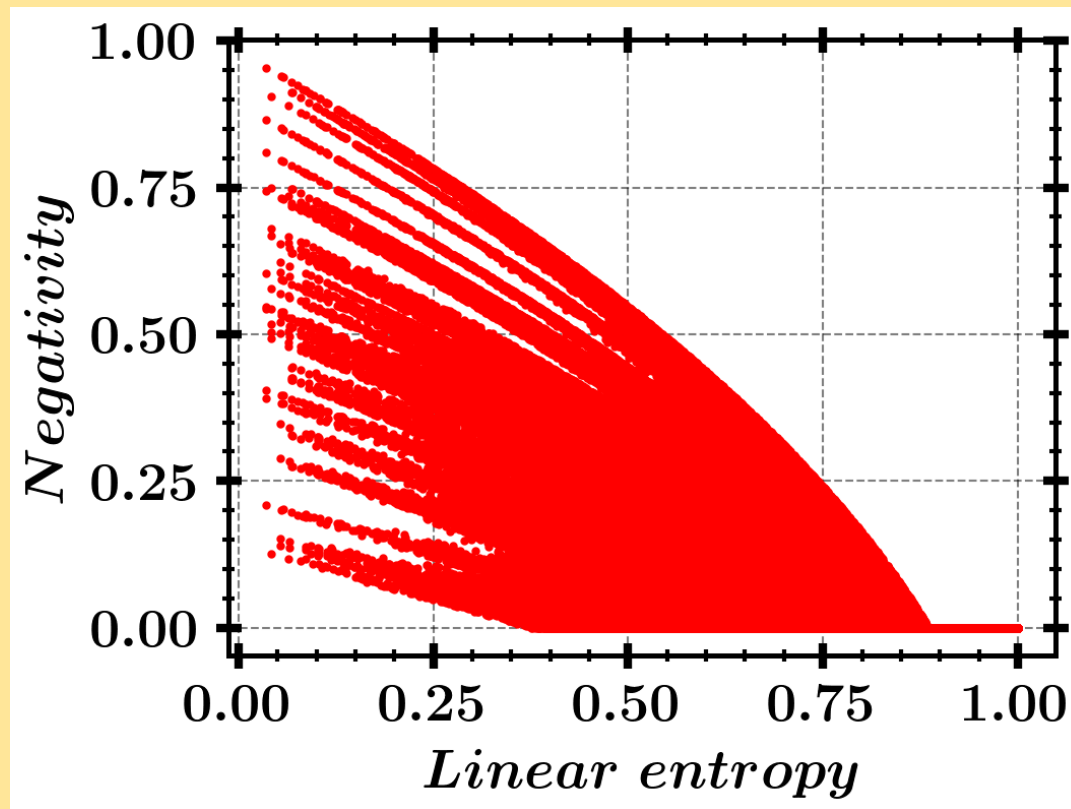
## “Negativity vs Linear Entropy”



Example (Werner states):

$$\rho_W(P) = P|\Psi^-\rangle\langle\Psi^-| + (1-p)\frac{I}{4}$$

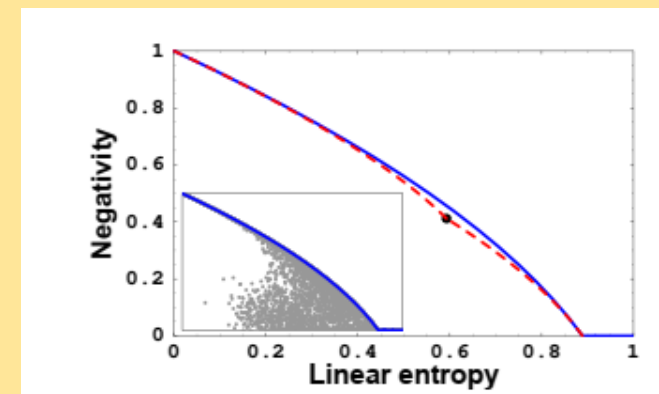
$$S_L(\rho_W(P)) = \frac{3P^2}{2} \quad N(\rho) = \text{Max}(0, \frac{P}{2})$$



$$S_L(\rho) = \frac{N}{N-1} [1 - \text{Tr}(\rho^2)]$$

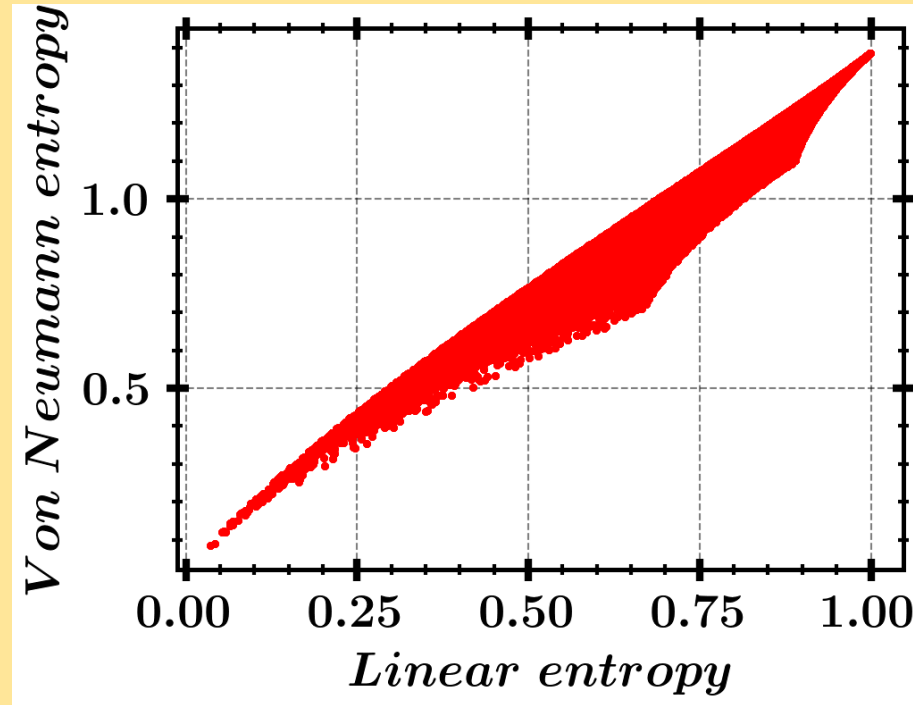
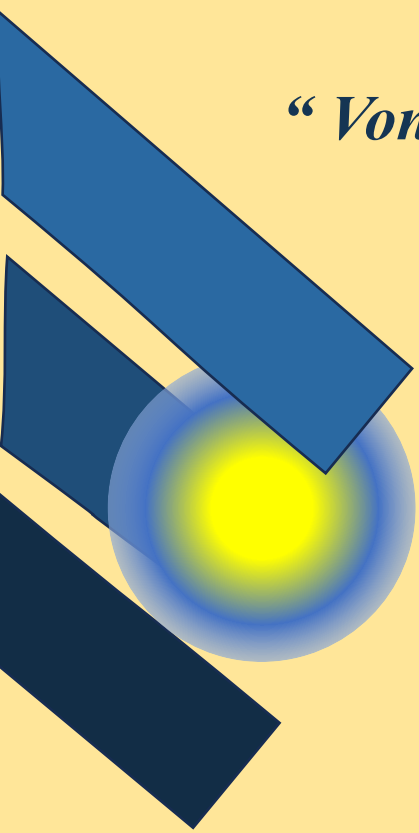
$$N(\rho) = \frac{\|\rho^{T_B}\|_1 - 1}{2}$$

$$\mathcal{L} = N(\rho) + \lambda(S_L(\rho) - S_0)$$



- Tzu-Chieh Wei et al.: T.-C. Wei, K. Nemoto, P. M. Goldbart, P. G. Kwiat, W. J. Munro, and F. Verstraete, "Maximal entanglement versus entropy for mixed quantum states," Physical Review A, 67 (2), 022110 (2003)

# “ Von Neumann Entropy vs Linear Entropy



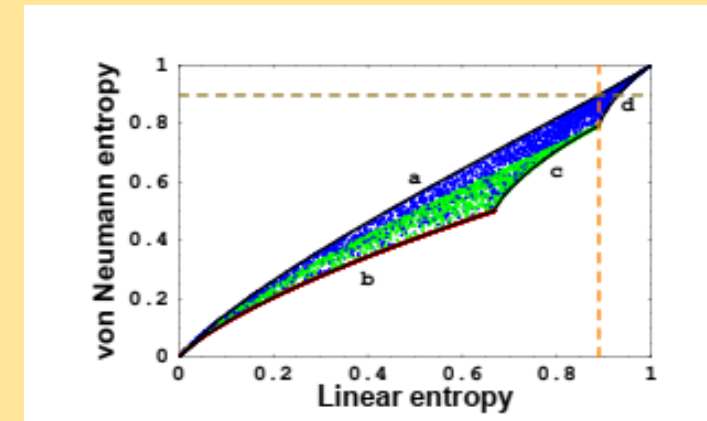
Maximize von Neumann entropy for a fixed linear entropy using Lagrange multipliers

$$\mathcal{L} = - \sum_i \lambda_i \text{Log}(\lambda_i) + \lambda(1 - \sum_i \lambda_i^2 - S_0)$$

$$S_L(\rho) = \frac{N}{N-1} [1 - \text{Tr}(\rho^2)]$$

$$S_{VN}(\rho) = -\text{Tr}(\rho \text{Log}(\rho))$$

$$\mathcal{L} = -\text{Tr}(\rho \text{Log}(\rho)) + \lambda(1 - \text{Tr}(\rho^2) - S_L)$$



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**THANKS FOR YOUR ATTENTION**

