Density matrix :

Definition and some properties

QUANTUM state can be characterized by a density matrix. this is a more general description, usefull principally in the case of mixed states which cannot be written as vectors

$$\rho = \sum_\lambda p_\lambda |\Psi_\lambda\rangle\langle\Psi_\lambda|$$

→ outer product

→ not necessarily orthogonal

↓ describes a statistical mixture of vector $|\Psi_\lambda\rangle$ with probability p_λ and $\sum p_\lambda = 1$

- $\rho = \rho^+$ hermitian
- spectral representation $\rho = \sum_i \lambda_i |\varphi_i\rangle\langle\varphi_i|$ where $|\varphi_i\rangle$ are ON vectors, $\lambda_i > 0$, $\sum \lambda_i = 1$
- positive definite $\langle\Psi_\lambda|\rho|\Psi_\lambda\rangle \geq 0$ → probability of finding the syst in the state $|\Psi_\lambda\rangle$
- $tr(\rho) = 1$
- $\langle \mathcal{O}\rangle = tr(\rho\,\mathcal{O})$ expectation values

  if $\mathcal{O} = \mathbb{I} \Rightarrow tr(\rho) = 1$

Mixed state ≠ superposition of pure states.

- if the p_λ are all 0, except one ⇒ ρ represents a pure state.

  $\rho = |\alpha\rangle\langle\alpha|$ which is a projector over $|\alpha\rangle$

  $\rho^2 = \rho$ for pure states.

2

- In general for any hermitian, positive definite and tr 1 operator

$$\mathrm{tr}\,\rho^2 \leq 1$$

Obviously for pure states $\mathrm{tr}\,\rho^2 = 1$ ✓

REDUCED DENSITY MATRIX (Introduced by Dirac in 1930)

two syst $A, B \rightarrow \mathcal{H}_A, \mathcal{H}_B$

$\rightarrow$ the global state $|\psi\rangle \in \underbrace{\mathcal{H}_A \otimes \mathcal{H}_B}$

$\mathcal{H}$ is a bipartite tensor product

We introduce a base $|i,j\rangle = |i\rangle \otimes |j\rangle$ of the complete space $\mathcal{H}$ $\Rightarrow$ $|\psi\rangle = \sum \lambda_{k\ell} |k,\ell\rangle$

with $\sum |\lambda_{k\ell}|^2 = 1$

The density matrix is $\rho = |\psi\rangle\langle\psi|$

$= \lambda_{ij} \lambda^*_{k\ell} |ij\rangle\langle k\ell|$

We define $\boxed{\rho_A = \mathrm{tr}_B\, \rho}$ $\Rightarrow$ $\rho_A = \sum_\ell \lambda_{k\ell} \lambda^*_{i\ell} |k\rangle\langle i|$

Any operator $\mathcal{O} : H_A \rightarrow H_A$

$$\langle \mathcal{O} \rangle = \mathrm{tr}\,(\rho_A \mathcal{O})$$

the VON NEUMANN ENTROPY (1927)

NUMBER OF MICROSTATES FOR A GIVEN MACROSTATE

$$S = -\mathrm{tr}\,\rho \log \rho$$

$\longrightarrow$ QUANTUM generalization of the statistical entropy

$$S = k_B \ln(\Omega)$$

Properties

- $S(\rho) = 0 \Rightarrow \rho$ is pure
- $S(\rho)$ is maximal $S(\rho) = \ln N$ for a maximally mixed state, N being the dim. of the Hilbert space

- $S(\rho)$ is concave

- $S(\rho)$ is additive for independent systems

$$+ S$$

$$S(\rho_A \otimes \rho_B) = S(\rho_A) \otimes (\rho_B)$$

but in general $S(\rho)$ is strongley subadditive for any three systems $\mathcal{H} = \mathcal{H}^1 \otimes \mathcal{H}^2 \otimes \mathcal{H}^3$

$$S(\rho_{ABC}) + S(\rho_B) \leq S(\rho_{AB}) + S(\rho_{BC})$$

Lieb - Ruskai 1973.

A	B	C

- $S(\rho_A)$ can be ,

ENTANGLEMENT ENTROPY: $S_A = -\mathrm{tr}\,\rho_A \log \rho_A$

- Any ρ can be thought or expressed as a reduced state of a pure density operator. "purification" in a bigger space

- two syst A, B and ρ_{AB} pure $\Rightarrow$ ρ_A and ρ_B have equal eigenvalues. $\Rightarrow$ $S_A = S_B$

- Simple example

(Einstein - Podolsky - Rosen 1935)

system: two particles with spin 1/2 (EPR pairs)

one of the Bell states (*)

state with spin 0 $\Rightarrow$ $|\chi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right)$

ENTANGLED PURE ENSEMBLE

$|\uparrow\rangle_A \otimes |\downarrow\rangle_B$

$S(\rho) = 0$

mixed ENSEMB

$S(\rho_A) = S(\rho_B) \neq 0$? $\rho_A = \frac{1}{2}\left(|\uparrow\rangle_A\langle\uparrow|_A + |\downarrow\rangle_A\langle\downarrow|_A\right)$

Alice measures $\uparrow$ $\Rightarrow$ system collapses to $|\uparrow\downarrow\rangle$ $\rightarrow$ Bob measures $\downarrow$

" " $\downarrow$ $\rightarrow$ " " " $|\downarrow\uparrow\rangle$ $\rightarrow$ " " $\uparrow$

(*) Alices measurement result is random $\Rightarrow$ she cannot transmit inf $\Rightarrow$ causality is preserved

- ENTANGLEMENT

DEF: A state in $\mathcal{H}_{AB}$ bipartite system is <u>NOT</u> entangled

if $$\rho_{AB} = \sum p_i\, \rho_A^i \otimes \rho_B^i$$

- if the global state is not entangled and pure $\Rightarrow$ $\rho_{AB} = \rho_A \otimes \rho_B$.

- if the global state is pure but entangled $\Rightarrow$ $S_A = S_B$

EXAMPLES in spin-1/2 system

$$\rho_1 = |\uparrow\rangle\langle\uparrow| \longrightarrow \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{pure}$$

$$\rho_2 = \frac{1}{\sqrt{2}}\left(|\uparrow\rangle + |\downarrow\rangle\right)\left(\langle\uparrow| + \langle\downarrow|\right) \rightarrow \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

pure

$$\rho_3 = \frac{3}{4}|\uparrow\rangle\langle\uparrow| + \frac{1}{4}|\downarrow\rangle\langle\downarrow| \rightarrow \begin{pmatrix} \frac{3}{4} & 0 \\ 0 & \frac{1}{4} \end{pmatrix}$$

TOTALLY mixed

- pure states → only one eigenvalue equal to unity. (already mentioned!)

- two different mixed states can have the same ρ

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} (1 \ 0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \checkmark$$

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} (0 \ 1) = \begin{matrix} 0 & 1 \\ 0 & 0 \end{matrix}$$

- the off diagonals are a measure of the "coherence" between any two of the basis states.

Maximal coherence

$$\rho_{mn}\rho_{nm} = \rho_{mm}\rho_{nn}$$

• ¿ connected to thermodynac entropy?

syst in thermal equilibrium → canonical ensemble

$\begin{cases} N \text{ particles} \\ \text{Temperature } T = 1/\beta \end{cases}$

if the eigenstate $|i\rangle$ of the Hamiltonian has energy E_i ⟹ the probability

$$P_{E_i} = \frac{e^{-\beta E_i}}{\sum_i e^{-\beta E_i}} = \frac{e^{-\beta E_i}}{Z}$$ is the probability of the system being in that state.

$$\underbrace{S = k_B \ln \Omega}$$

Boltzmann formula (only when microstates are equally probable)

or more generally $\underbrace{S = -k_B \sum p_i \ln p_i}$

Gibbs formula or general Boltzmann formula.

$$\Rightarrow \hat{\rho} = \frac{e^{-\beta \hat{H}}}{Z} \longrightarrow S = -\mathrm{tr}\,\rho \log \rho = \beta \langle H \rangle + \log$$

$$\left(\frac{1}{Z}\sum_i e^{-\beta E_i} |i\rangle\langle i|\right)$$

From thermodynamics $F = E - TS$

$-T \log Z = E - TS$ ✓

ρ analogous to the operator $U(t) = e^{-iHt/\hbar}$ with imaginary time $t = -i\hbar\beta$

↓

EE is more general

$$\longrightarrow \hat{\rho} = N e^{-\hat{H}}$$

$\hat{H}$ → MODULAR HAMILTONIAN or ENTANGLEMENT HAMILTONIAN (hermitian)

At zero temperature ($\beta = \infty$) the probability coeff are all zero except for the ground state ⟹ ρ has every element zero except for a single element on the diag ⟹ pure state.

At ∞ temp. all probabilities are equal ⟹ $\rho = \frac{1}{N}\mathbb{I}$

(*)1 $|\phi^{\pm}\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_A \otimes |0\rangle_B \pm |1\rangle_A \otimes |1\rangle_B\right)$

$|\psi^{\pm}\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle_A \otimes |1\rangle_B \pm |1\rangle_A \otimes |0\rangle_B\right)$

ON basis of the Hilbert space of two qubits.

qubit $\rightarrow$ vector in a bidimensional vect. space

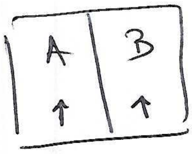
$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle$

$|\alpha|^2 + |\beta|^2 = 1$

¿Can be measured?

Measuring S implies to measure ρ: this means the complete knoledge of the state and the space of states $\mathcal{H}$ where it acts.

For example: $|\psi_{AB}\rangle$ pure



ρ_A gives the same expectation values as ρ

$\mathrm{tr}\, \rho_A \mathcal{O}_A = \langle \psi_{AB} | \mathcal{O}_A | \psi_{AB} \rangle \Rightarrow$

it cannot be distinguish from exp. values!

¿? Nevertheles there are less operators in $\mathcal{H}_A$ than in $\mathcal{H}_{AB}$ and $S_A \geq 0$ while $S_{AB} = 0$!!

one of the Bell states.

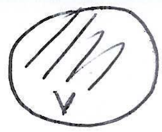
$$|\psi_{AB}\rangle = \frac{1}{\sqrt{2}} \left(|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle \right) \rightarrow \rho_A = \frac{1}{2} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

- Now suppose a system of N spins $\Rightarrow \dim \mathcal{H} = 2^N$

$\Rightarrow \rho$ is $2^N \times 2^N$ matrix !

as N grows, ρ has an "ugly" growing!!

$\Rightarrow$ ¿how to calculate?

Gaussian systems. $\rightarrow$ spatial region  $\mathcal{H}_V \otimes \mathcal{H}_{-V}$

for example the vacuum state of a free theory

(scalars or fermions)

canonical commutation relations $\rightarrow$ a collection of operator ϕ_i and π_i

$$[\phi_i, \pi_j] = i\,\delta_{ij} \qquad [\phi_i\, \phi_j] = [\pi_i, \pi_j] = 0$$

$$\langle \phi_i\, \phi_j \rangle = X_{ij} \qquad \langle \pi_i\, \pi_j \rangle = P_{ij}$$

$$\langle \phi_i\, \pi_j \rangle = \langle \pi_j\, \phi_i \rangle^* = \frac{i}{2}\delta_{ij}$$

Gaussian $\rightarrow$ ~~from~~ the two point functions contains all the information.

$$\langle \phi_1, \cdots, \phi_4 \rangle = \langle \phi_1 \phi_2 \rangle \langle \phi_3 \phi_4 \rangle + \langle \phi_1 \phi_3 \rangle \langle \phi_2 \phi_4 \rangle + \cdots$$

- Wick

$\Rightarrow$ Introducing the anzats

$$\rho = e^{-[\phi_i N_{ij} \phi_j + \pi_i M_{ij} \pi_j]}$$

$\downarrow$ quadratic exponential.

(which it reproduces Wick)

New variables

$$\phi_i = \alpha_{ij}^* a_j^+ + \alpha_{ij} a_j \quad ; \quad \pi_i = -i\,\beta_{ij}^* a_j^+ + i\,\beta_{ij} a_j$$

with $[a_i\, a_j^+] = \delta_{ij} \Rightarrow \alpha^* \beta^T + \alpha\, \beta^+ = -1$

$$\rho = \prod_\ell e^{-\varepsilon_\ell a_\ell^+ a_\ell} \underbrace{(1 - e^{-\varepsilon_\ell})}_{\text{normalization.}}$$

From the two point functions we obtain $\alpha, \beta, \varepsilon$

$$i/2\ \delta_{ij} = tr(\rho\, \phi_i \pi_j) \Rightarrow 1/2 = \alpha^* n \beta^T - \alpha (n+1) \beta^T$$

$$X_{ij} = tr(\rho\, \phi_i \phi_j) = \alpha^* n\, \alpha^T + \alpha (n+1) \alpha^+$$

$$P_{ij} = tr(\rho\, \pi_i \pi_j) = \beta^* n\, \beta^T + \beta (n+1) \beta^T$$

In particular

$$\frac{1}{2}\coth(\varepsilon_k/2) = \nu_k = \text{eigenvalue of } C_V = \sqrt{X_V P_V}$$

region V

$\Rightarrow$ the entropy is given by the entropy contributions of the decoupled armonic oscilators with $\beta\omega \equiv \varepsilon_k$

$$S = \sum_e \left(-\log(1-e^{-\varepsilon_e}) + \frac{\varepsilon_e e^{-\varepsilon_e}}{1-e^{-\varepsilon_e}} \right)$$

$$\boxed{= \operatorname{tr}\left[(C+1/2)\log(C+1/2) - (C-1/2)\log(C-1/2) \right]}$$

- $C \geq 1/2$ always
- $C = 1/2$ when ρ_V is pure
- C is an $N \times N$ matrix !

$\Downarrow$

for a gaussian state

$$\boxed{\text{two point correlators} \Updownarrow \text{Entropy}}$$

this can be extended to different theories.

For fermions: $\langle \psi_i \psi_j^+ \rangle = C_{ij}$ $\quad \langle \psi_i^+ \psi_j \rangle = \delta_{ij} - C_{ij}$

$$H = -\log(C^{-1} - 1)$$

$$S(V) = \sum_e \cdots\cdots =$$

$$-\operatorname{tr}\left((1-C)\log(1-C) + C\log C\right)$$

Examples in QFT:

Free boson

- $H = \frac{1}{2}\sum \pi_i^2 + \sum_{ij} \phi_i K_{ij} \phi_j$ discrete version lattice version

- fundamental state.

- $X_{ij} = \langle \phi_i \phi_j \rangle = \frac{1}{2}\left(K^{-1/2}\right)_{ij}$

- $P_{ij} = \langle \pi_i \pi_j \rangle = \frac{1}{2}\left(K^{1/2}\right)_{ij}$.

In two spatial dimensions

$$H = \frac{1}{2}\sum \epsilon^2 \left(\pi_{m,n}^2 + \frac{(\phi_{n+1,m} - \phi_{n,m})^2}{\epsilon^2} + \frac{(\phi_{n,m+1} - \phi_{n,m})^2}{\epsilon^2} + M^2 \phi_{n,m}^2 \right)$$

$$\circledast\ \langle \phi_{00}, \phi_{ij} \rangle = \frac{1}{8\pi^2} \int_{-\pi}^{\pi} dp_x \int_{\pi}^{\pi} dp_y \frac{\cos(i p_x)\cos(j p_y)}{\sqrt{2(1-\cos p_x) + 2(1-\cos p_y) + \ldots}}$$

Details of the integrals. References to our work

$\boxed{\text{10 - 15 digits.}}$ (300 × 300)

first integ. analyt.
* polynomial × elliptic functions
the second integral numerically

For circles → radial discretization
Srednicki 1992

Some results:

$⊛_2$

$$\langle \phi_{00}\,\phi_{ij} \rangle = \frac{1}{8\pi^2} \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} dx\,dy\, \frac{\cos(x(i-1))\cos(y(j-1))}{\sqrt{2(1-\cos(x))+2(1-\cos y)}}$$

$$\langle \Pi_{00}, \Pi_{ij} \rangle = \frac{1}{8\pi^2} \int_{-\pi}^{\pi}\int_{-\pi}^{\pi} dx\,dy\, \cos(x(i-1))\cos y(j-1)) ⊗ \sqrt{2(1-\cos x)+2(1-\cos y)}$$

$$\Theta^{-1} \underline{\underline{K}}\, \Theta = K_d$$

↳ eigenvalues in the diagonal

eigenvectors as columns

$\boxed{\text{Mathematica Subroutine}}$

$$P = \frac{1}{2}\, \Theta \sqrt{K_d}\, \Theta^{-1}$$

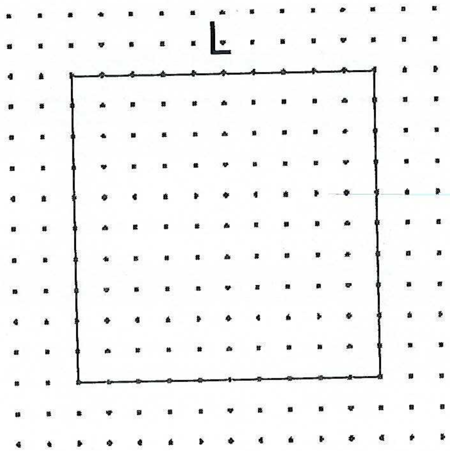
$$X = \frac{1}{2}\, \Theta\, (K_d)^{-1/2}\, \Theta^{-1}$$

P_v ; X_v

$$C = (X_v . P_v)^{1/2}$$

↳ eigenvalues

Massless (gapless) scalar field model. Vacuum (fundamental) state in a square lattice
Similar to phonons in a solid

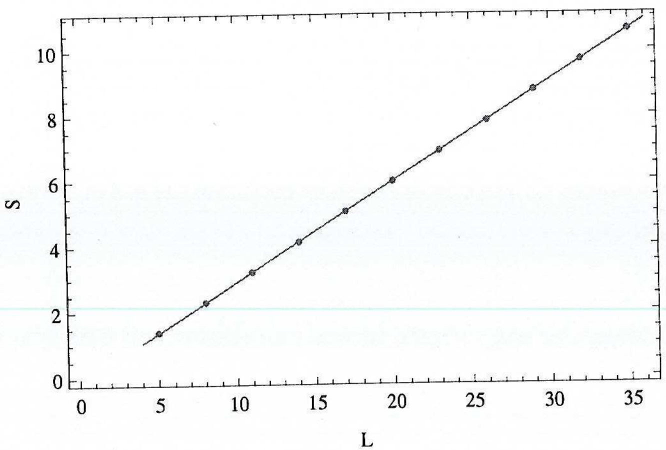


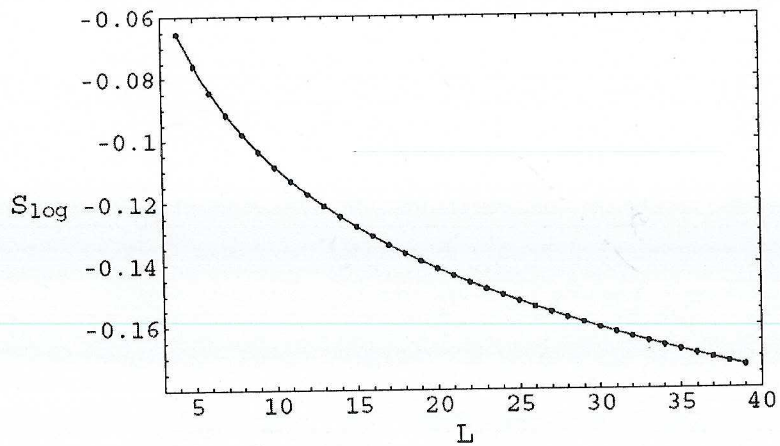
$$H = \frac{1}{2}\int d^2x \left(\dot{\phi}(x)^2 + (\nabla\phi(x))^2\right)$$

$$\rightarrow H = \frac{1}{2}\sum_i \epsilon^2 \left(\dot{\phi_i}^2 + \sum_{j\sim i}\frac{(\phi_i-\phi_j)^2}{\epsilon^2}\right)$$

For interacting spin systems the Hilbert space dimension grows as 2^N

For coupled Harmonic oscillators we have only to diagonalize matrices of $N \times N$

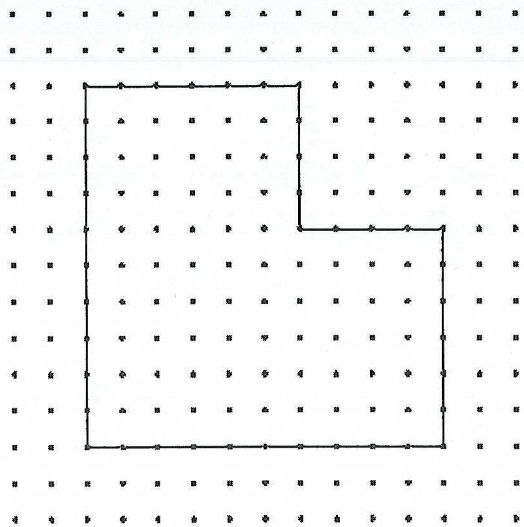




S = .075 (4 L/ε) - 0.047 Log[L/ε] + const=.075 (perimeter/ε) - 0.047 Log[L/ ε] + const

We have an «area» term and a logarithmic correction. These are divergent as $\varepsilon \longrightarrow 0$

S = .075 (perimeter/ε) - (6/4) 0.047 Log[L/ε] + const

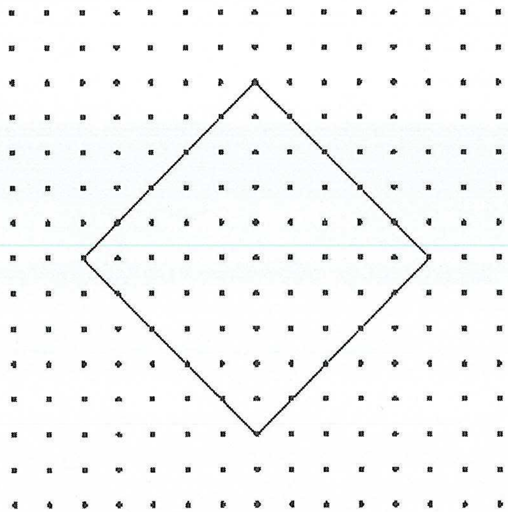


The same «area» term. A logarithmic coefficient growing with the number of vertices.
(All vertices have the same angle S(A)=S(-A) for a global pure state)

In general:

$$S(A) = c_1\,(\text{perimeter}/\epsilon) - \sum_{\text{vertices}} c_{\log}(\theta)\log(R/\epsilon) + \text{const}$$

S = .085 (perimeter/ε) - 0.047 Log[L/ε] + const



Bad: area term does not have the rotational symmetry of the theory in the continuum limit

Good: the logarithmic term does not notice the lattice