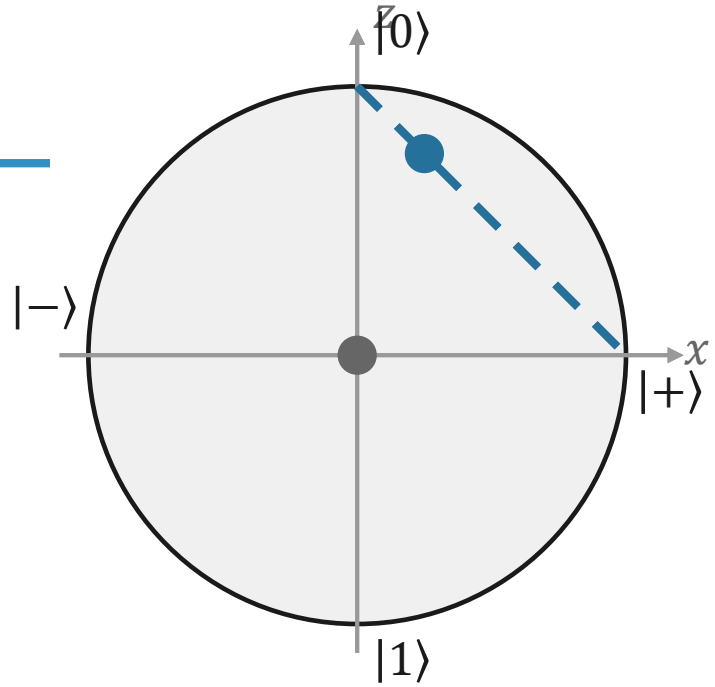
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EEE 6516 · QUANTUM COMPUTING

Density Matrices

Ensembles, the Bloch ball, the partial trace and how close two states are

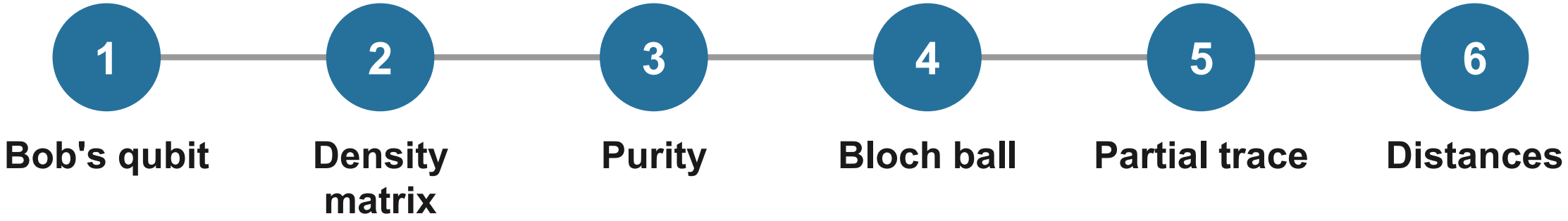
Chapter 7 · Lecture 15



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Today



By the end of this lecture you can

- construct the density matrix of an ensemble and compute probabilities and mean values from it
- tell a mixture from a superposition, and convert between ρ and the Bloch vector
- compute reduced states with the partial trace and restate no-signalling
- compute fidelity and trace distance, and say which fidelity a tool reports

YOUR TURN · PREDICT

Which state does Bob hold?

Think · 45 seconds

Alice and Bob share $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$. Bob gets each outcome with probability ½ in every basis. Which ket describes his qubit?

A $|0\rangle$

B $|+\rangle$

C $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ up to a phase

D no single ket does

ANSWER

D: no ket reproduces ½, ½ along every axis

A pure state has a Bloch vector of length 1: measured along that vector, it gives one outcome every time.

Bob's qubit gives ½, ½ along every axis, so no $|\varphi\rangle$ fits.

The same holds for a coin-toss source: $|0\rangle$ or $|1\rangle$, each with probability ½.

We need a description that carries classical uncertainty: the density matrix.

1 Ensembles and the density matrix

How do we describe a source we only know statistically?

The density matrix of an ensemble

Ensemble $\{p_i, |\psi_i\rangle\} \rightarrow$ density matrix

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$$

$$\text{pure: } \rho = |\psi\rangle\langle\psi|; \quad \text{otherwise mixed}$$

The trace, recalled

$$\mathrm{Tr}(AB) = \mathrm{Tr}(BA), \qquad \mathrm{Tr}|a\rangle\langle b| = \langle b|a\rangle$$

$$\langle\psi|A|\psi\rangle = \mathrm{Tr}(A|\psi\rangle\langle\psi|)$$

An ensemble emits the normalised state $|\psi_i\rangle$ with probability p_i.

ρ is a weighted sum of projectors: a 2×2 matrix for one qubit.

The trace turns a sandwich $\langle\psi|A|\psi\rangle$ into a trace of a product.

Coin toss: $\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = I/2$.

DERIVATION

The Born rule becomes a trace

Outcome m of a measurement with projector Π_m; the source emits $|\psi_i\rangle$ with probability p_i.

$\Pr(m) = \sum_i p_i \langle\psi_i\|\Pi_m\|\psi_i\rangle$	law of total probability over the ensemble
$= \sum_i p_i \mathrm{Tr}(\Pi_m \|\psi_i\rangle\langle\psi_i\|)$	sandwich as a trace
$= \mathrm{Tr}(\Pi_m \sum_i p_i \|\psi_i\rangle\langle\psi_i\|)$	the trace is linear
$= \mathrm{Tr}(\Pi_m \rho)$	every prediction depends only on ρ

Same steps: ⟨A⟩ = Tr(ρA); a gate acts as ρ ↦ UρU†; after outcome m, ρ ↦ Π_mρΠ_m/Pr(m).

COMMON MISTAKE

“Any Hermitian matrix with trace 1 is a state”

✗ Hermitian, trace 1, entries ≤ 1

$$\begin{bmatrix} 0.5 & 0.6 \\ 0.6 & 0.5 \end{bmatrix}$$

passes the obvious checks

Its eigenvalues are 1.1 and −0.1.

✓ Also positive semidefinite

$\text{eigenvalues} \geq 0; \quad \text{qubit: } |r| \leq 1$

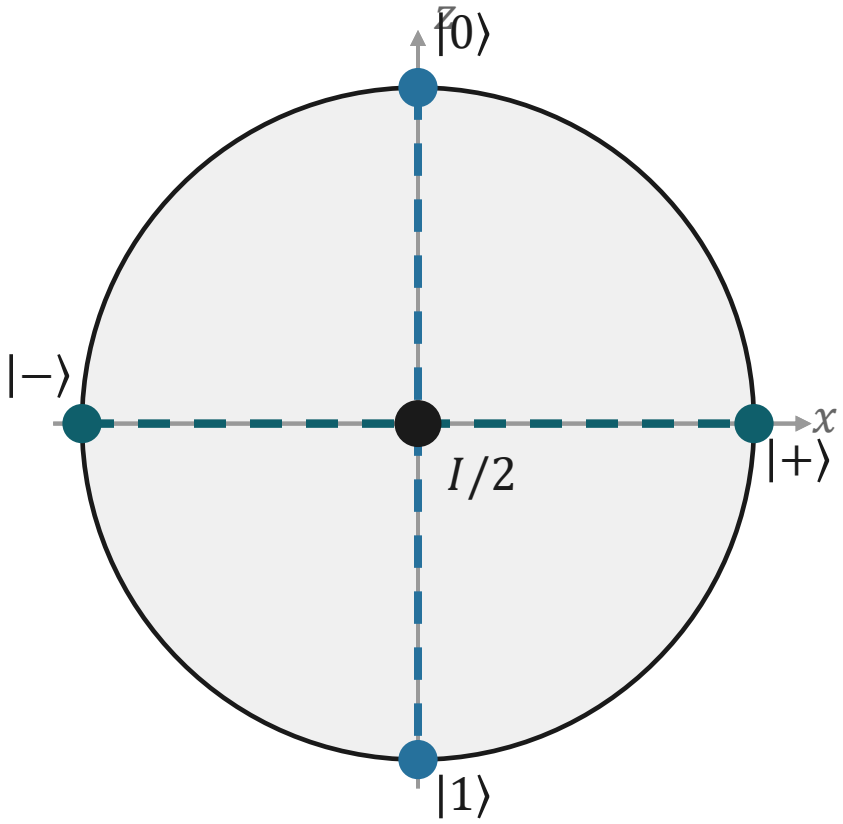
a −0.1 'probability' in its eigenbasis

Density matrices = Hermitian, ≥ 0, trace 1.

Check positivity: the eigenvalues (or, for a qubit, the length of the Bloch vector).

WORKED EXAMPLE · STEP 1 OF 2

Two ensembles and their density matrices



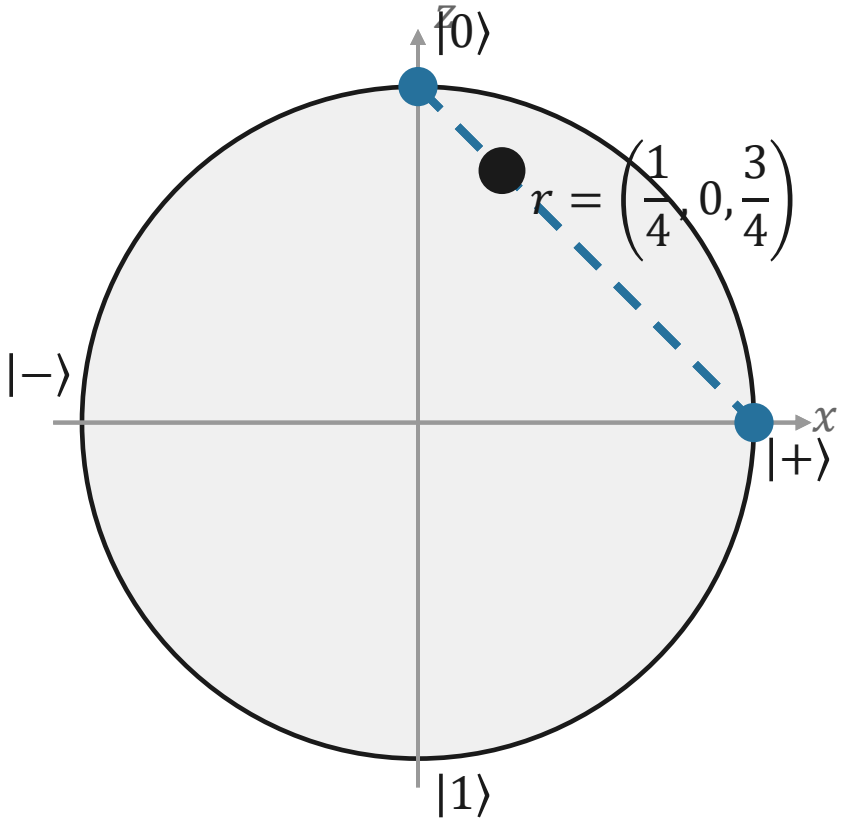
1 ½|0⟩⟨0| + ½|1⟩⟨1| = I/2, and ½|+⟩⟨+| + ½|−⟩⟨−| = I/2 too: two ensembles, one ρ.

Before the next slide

Now {¾, |0⟩; ¼, |+⟩}: ρ, Pr in Z and X, and Tr ρ²?

WORKED EXAMPLE · STEP 2 OF 2

Two ensembles and their density matrices



1 ½|0⟩⟨0| + ½|1⟩⟨1| = I/2, and ½|+⟩⟨+| + ½|−⟩⟨−| = I/2 too: two ensembles, one ρ.

2 $\rho = \frac{3}{4}\begin{bmatrix}1 & 0\\ 0 & 0\end{bmatrix} + \frac{1}{8}\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix} = \begin{bmatrix}7/8 & 1/8\\ 1/8 & 1/8\end{bmatrix}$

2 Purity: a mixture is not a superposition

Can any measurement tell $|+\rangle$ from a coin toss?

YOUR TURN · PREDICT

Which measurement separates $|+\rangle\langle+|$ from $I/2$?

Think · 45 seconds

Compare $|+\rangle\langle+| = \frac{1}{2}\begin{bmatrix}1 & 1\\ 1 & 1\end{bmatrix}$ with $I/2 = \frac{1}{2}\begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$.

A a Z measurement

B an X measurement

C both

D neither: they are the same state

ANSWER

B: only the X measurement tells them apart

Z basis: both diagonals are $\left(\frac{1}{2}, \frac{1}{2}\right)$: identical statistics.

X basis: $\langle + | \rho | + \rangle = 1$ for |+⟩, but ½ for I/2.

The off-diagonal entries (coherences) are what X detects. Purity $\mathrm{Tr}\rho^2$: 1 against ½.

Purity Tr ρ² ≤ 1, with equality exactly for pure states; ½ ≤ Tr ρ² for a qubit.

SIMULATION

Simulation 7.1: a superposition and a mixture

```
qc.h(1)
qc.h(0)
qc.measure(0, 0)
with qc.if_test((qc.clbits[0], 1)):
    qc.x(1)
```

Line 1 makes |+⟩. Lines 2–5: a coin qubit is measured; its result decides whether X is applied to the data qubit.

An H before the final measurement gives the X basis; 2000 shots per row.

source	basis	0	1
|+⟩	Z	973	1027
|+⟩	X	2000	0
mixture	Z	998	1002
mixture	X	1025	975

2000 shots per row; binomial σ ≈ 22

COMMON MISTAKE

“A 50/50 mixture is the state (|0⟩ + |1⟩)/√2”

✗ Same Z statistics, so same state

½, ½ in the Z basis for both

$$\Rightarrow \quad \frac{1}{2} I = |+\rangle\langle +| \quad ?$$

Only one basis was checked.

✓ Different states

mixture: is |0⟩ or |1⟩, we do not know which

|+⟩: is neither; certain outcome + in X

No measurement makes the mixture behave like a pure state.

Agreement in one basis is not equality: compare ρ (or the Bloch vectors), not one set of probabilities.

DERIVATION

Every qubit state has a Bloch vector

$$\rho = \frac{1}{2}\left(I + r_x X + r_y Y + r_z Z\right)$$

I, X, Y, Z span the 2×2 Hermitian matrices

$$= \frac{1}{2}\begin{bmatrix} 1 + r_z & r_x - i r_y \\ r_x + i r_y & 1 - r_z \end{bmatrix}, \qquad r_k = \mathrm{Tr}(\rho \sigma_k)$$

Paulis traceless, $\mathrm{Tr}(\sigma_j \sigma_k) = 2\delta_{jk}$

r = (⟨X⟩, ⟨Y⟩, ⟨Z⟩): the Bloch vector is the list of mean values.

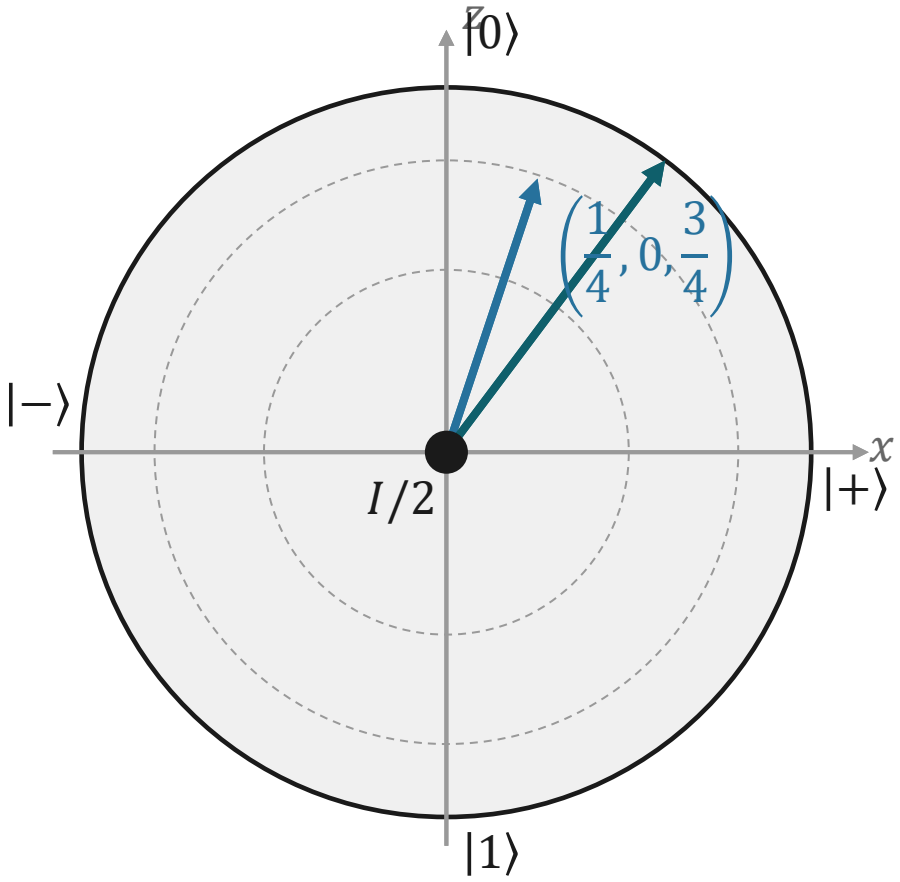
DERIVATION

Positivity and purity in terms of |r|

eigenvalues: $\frac{1}{2}(1 \pm \lvert r \rvert)$	Problem PRB-0187
$\rho \geq 0 \;\Leftrightarrow\; \lvert r \rvert \leq 1$	positivity becomes a length
$\mathrm{Tr}\rho^2 = \frac{1}{2}(1 + \lvert r \rvert^2)$	purity from the length

Pure: |r| = 1 (the Bloch sphere of Chapter 2). Mixed: inside. I/2: the centre, r = 0.

The Bloch ball



Surface: pure states (|r| = 1). Inside: mixed. Centre: I/2, nothing known.

Dashed circles: equal purity ½(1 + |r|²).

Mixing averages Bloch vectors: r = Σ p_i r_i, a point on the chord between members.

A point inside lies on many chords: ρ does not remember how it was made.

3 Subsystems and the partial trace

What does Bob's half of the pair look like on its own?

The partial trace: discarding a qubit

Partial trace (linear)

$$\mathrm{Tr}_A(C \otimes D) = (\mathrm{Tr}\, C)\, D$$

$$\mathrm{Tr}_B(C \otimes D) = C\, (\mathrm{Tr}\, D)$$

Reduced state of B

$$\rho_B = \mathrm{Tr}_A \rho_{AB}$$

$$\mathrm{Tr}(\rho_B M) = \mathrm{Tr}\big(\rho_{AB}(I \otimes M)\big)$$

Bob can only measure observables $I \otimes M$: his statistics are $\mathrm{Tr}\big(\rho_{AB}(I \otimes M)\big)$.

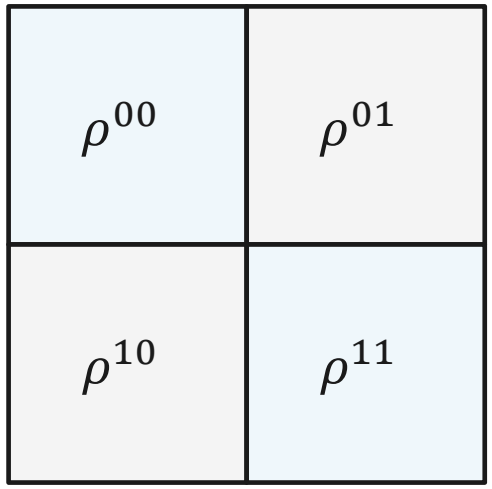
ρ_B is the 2×2 matrix that reproduces all of them.

Tracing out A is what discarding (ignoring) qubit A means.

Textbook order: qubit 0 = A is the first tensor factor.

Computing it: the block recipe

ρ_{AB} (4×4)



qubit A (first) selects the block

$$\mathrm{Tr}_A\colon \rho_B = \rho^{00} + \rho^{11}$$

$$\mathrm{Tr}_B\colon \rho_A = \begin{bmatrix} \mathrm{Tr}\rho^{00} & \mathrm{Tr}\rho^{01} \\ \mathrm{Tr}\rho^{10} & \mathrm{Tr}\rho^{11} \end{bmatrix}$$

Write $\rho_{AB} = \sum |a\rangle\langle a'| \otimes \rho^{aa'}$: the first Kronecker factor selects the block (Chapter 3).

Tr_A adds the diagonal blocks; Tr_B replaces every block by its trace.

Worked example: reduced states and no-signalling

$$|\Phi^+\rangle\langle\Phi^+| = \frac{1}{2}\begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

1 (a) |Φ⁺⟩: blocks ½|a⟩⟨a′|. Tr_A gives I/2; Tr_B gives I/2 (off-diagonal blocks are traceless).

$$\rho_B = \frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \frac{I}{2}, \qquad \rho_A = \frac{I}{2}$$

Before the next slide

And a product state |ψ⟩|φ⟩?

Worked example: reduced states and no-signalling

$$|\psi\rangle\langle\psi| \otimes |\varphi\rangle\langle\varphi|$$

$$\rho_B = \langle\psi|\psi\rangle\,|\varphi\rangle\langle\varphi| = |\varphi\rangle\langle\varphi|$$

1 (a) |Φ⁺⟩: blocks ½|a⟩⟨a′|. Tr_A gives I/2; Tr_B gives I/2 (off-diagonal blocks are traceless).

2 (b) Product |ψ⟩|φ⟩: ρ_B = |φ⟩⟨φ|, pure.

Before the next slide

Alice measures in Z and tells no one. Bob's ρ_B?

Worked example: reduced states and no-signalling

$$\frac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 11|) = \frac{1}{2}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$\rho_B = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1| = \frac{I}{2}$$

1 (a) $|\Phi^+\rangle$: blocks $\frac{1}{2}|a\rangle\langle a'|$. Tr_A gives I/2; Tr_B gives I/2 (off-diagonal blocks are traceless).

2 (b) Product $|\psi\rangle|\varphi\rangle$: $\rho_B = |\varphi\rangle\langle\varphi|$, pure.

3 (c) After Alice's untold measurement: $\frac{1}{2}|00\rangle\langle 00| + \frac{1}{2}|11\rangle\langle 11|$, so $\rho_B = I/2$ — unchanged.

DERIVATION

No-signalling: nothing done to A changes ρ_B

$$\mathrm{Tr}_A[(U \otimes I)(C \otimes D)(U^\dagger \otimes I)] = \mathrm{Tr}(UCU^\dagger)\, D$$

a unitary on A, applied to one product term

$$= \mathrm{Tr}(U^\dagger UC)\, D = (\mathrm{Tr}\, C)\, D$$

cyclic property of the trace

measurement: $\sum_m \mathrm{Tr}(\Pi_m C \Pi_m)\, D = (\mathrm{Tr}\, C)\, D$

$\sum_m \Pi_m = I$; linearity covers every ρ_{AB}

No unitary on A and no untold measurement of A changes ρ_B.

Same halves, different pairs

Bell pair

$$|\Phi^+\rangle\langle\Phi^+|$$

$$\rho_A = \rho_B = I/2$$

purity 1

$$\langle X \otimes X \rangle = 1$$

coin-toss pair

$$\frac{1}{2}(|00\rangle\langle 00| + |11\rangle\langle 11|)$$

$$\rho_A = \rho_B = I/2$$

purity ½

$$\langle X \otimes X \rangle = 0$$

Neither Alice nor Bob alone can tell the two sources apart: both halves are I/2.

Together they can: X ⊗ X is perfectly correlated only for the Bell pair.

For a pure joint state, a mixed half is the signature of entanglement.

4 How close are two states?

How do we score a state that should have been $|\psi\rangle$?

Fidelity and trace distance

Fidelity to a pure target (squared)

$$F(\rho,\psi) = \langle\psi|\rho|\psi\rangle; \quad \text{pure: } |\langle\psi|\varphi\rangle|^2$$

Trace distance

$$D(\rho,\sigma) = \frac{1}{2}\mathrm{Tr}|\rho-\sigma| = \frac{1}{2}\sum_k |\lambda_k|$$

$$\text{qubits: } D = |r-s|/2$$

F: the probability that ρ passes the test “is the state |ψ⟩?”.

D: the largest difference in any outcome probability; best single-shot guess is right with ½(1 + D).

Conventions differ: this book and Qiskit's state_fidelity use the squared F; Nielsen–Chuang and Watrous its square root.

0.99 (square-root) is 0.98 squared; 0.99 squared is ≈ 0.995 square-root. Ask which one a number uses.

YOUR TURN · PAIRS

Your turn: F and D between |0⟩ and |+⟩

Pairs · 1 minute

Use $F = |\langle 0| +\rangle|^2$ and $D = |r - s|/2$ with the Bloch vectors.

A $F = \frac{1}{2}, D = \frac{\sqrt{2}}{2}$

B $F = \frac{1}{\sqrt{2}}, D = \frac{1}{2}$

C $F = \frac{1}{2}, D = \frac{1}{2}$

D $F = 0, D = 1$

ANSWER

A: F = ½, D = √2/2 ≈ 0.707

$$F = |\langle 0| +\rangle|^2 = \frac{1}{2}; \quad D = \frac{1}{2}|(0,0,1) - (1,0,0)| = \frac{\sqrt{2}}{2}$$

A noisy Bell source $\rho = 0.9|\Phi^+\rangle\langle\Phi^+| + 0.1\, I/4$:

$$F = 0.9 + 0.1 \times \frac{1}{4} = 0.925, \qquad D = 0.075$$

For pure states D = √(1 − F): one number fixes the other. For mixed states they differ.

LIVE DEMO

Simulation 7.2 (live): density matrices in Qiskit

```
a = 0.5 * dm("0") + 0.5 * dm("1")
b = 0.5 * dm("+") + 0.5 * dm("-")
bell.h(0)
bell.cx(0, 1)
rho = DensityMatrix(bell)
```

The script then calls partial_trace(rho, [0]), which discards qubit 0 — the same qubit in both qubit orders.

Purities and Bloch vectors come from DensityMatrix methods.

printed by density.py	value
two ensembles of WE 7.1(a) equal	True
Bell pair: purity	1.0
Bob's half ρ_B: purity	0.5
half of |+⟩|0⟩: purity	1.0
WE 7.1(b): purity	0.8125

$\rho_B = I/2$; WE 7.1(b): r = (0.25, 0., 0.75)

Recap

1

Density matrix

$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$; Pr(m) = Tr($\Pi_m \rho$); ρ ↦ UρU†

2

Mixture ≠ superposition

same Z statistics, different X statistics; purity Tr ρ² ≤ 1

3

Bloch ball

$\rho = \frac{1}{2}(I + r \cdot \sigma), |r| \leq 1$; mixing averages r

4

Partial trace and distances

half of |Φ⁺⟩ is I/2; F = ⟨ψ|ρ|ψ⟩, D = |r − s|/2

After the break: Lecture 16

Channels and noise: what does noise do to the Bloch vector?

Read: handout 7.1–7.4 before next week; Problems PRB-0187 and PRB-0189.

Exit ticket

Find the Bloch vector and purity of $\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|+\rangle\langle +|$. Is it closer to $|0\rangle$ or to $|+\rangle$ in trace distance?

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