

Entanglement generation from thermal state with low symmetry by quantum gates in liquid-state nuclear magnetic resonance

Quantum **M**echanics: from **F**undamental **P**roblems to **A**pplications

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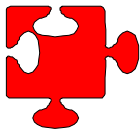
Liquid-state nuclear magnetic resonance QC



successful physical model for a Quantum Computer (QC)

→ not (maybe) practical, but useful and important **prototype of QC**

By the way, ...



entanglement

← key property for the power of quantum computing (not fully understood)

Braunstein, *et. al*, PRL83, 1054 (1999)

effective pure state is **separable**, in current experiments

typical states
in a liquid-state NMR QC

- NMR QC: genuine QC ?
- Entanglement : necessary for QC?

★ Yu, Brown, Chuang (YBC) PRA71, 032341 (2005)

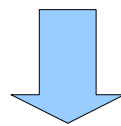
**entanglement attainable from thermal state by quantum gates
in liquid-state NMR !!**

thermal state: elementary state in liquid-state NMR

the most natural (liquid state NMR ← very high temperature !)

effective pure state ← **thermal state + quantum gates + ensemble average**

" unitary transformed thermal states are **entangled
more easily** than effective pure states"



(even if the unitary transformed thermal state is separable in the current experiment, ...)

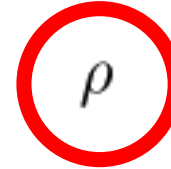
- insight into role of entanglement in liquid state NMR
- understanding of mixed-state entanglement in QC
- entanglement generation by quantum dynamics

Today's Talk

Yu, Brown, and Chuang (YBC), PRA71, 032341 (2005)

**thermal states
(separable)**

— quantum gates —▶



**separable
or entangled ?**

**entanglement attainable from thermal state by quantum gates
in liquid-state NMR !!**

our results

- ★ the model is a rather special case —▶ **no chemical shift ! (high symmetry)**
—▶ get rid of **this limitation** (no such symmetry !)
?
system's symmetry + quantum dynamics —▶ entanglement generation
- ★ their (**indirect**) method for evaluating entanglement —▶ **(probably) don't work**
—▶ **directly and correctly evaluate**

Model

ex. chloroform

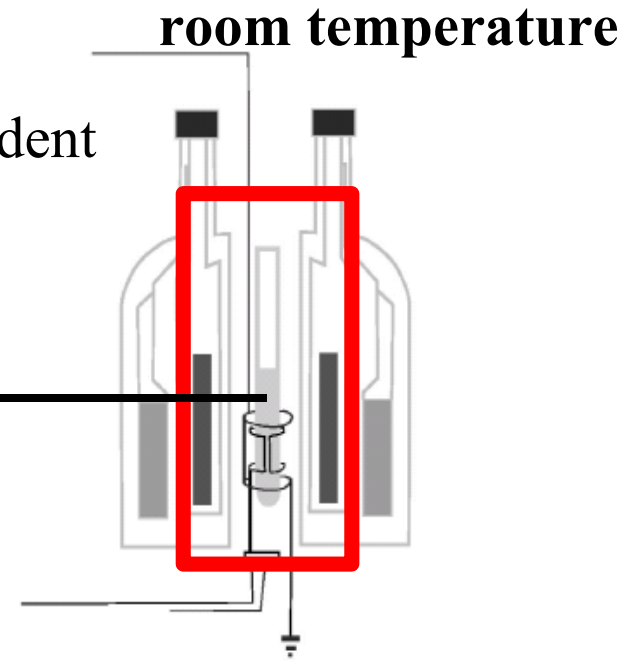
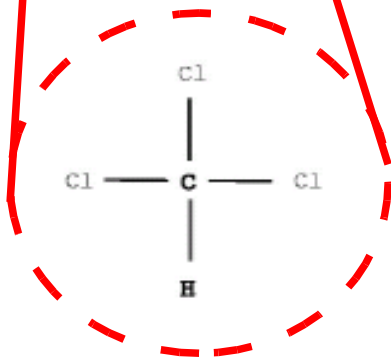
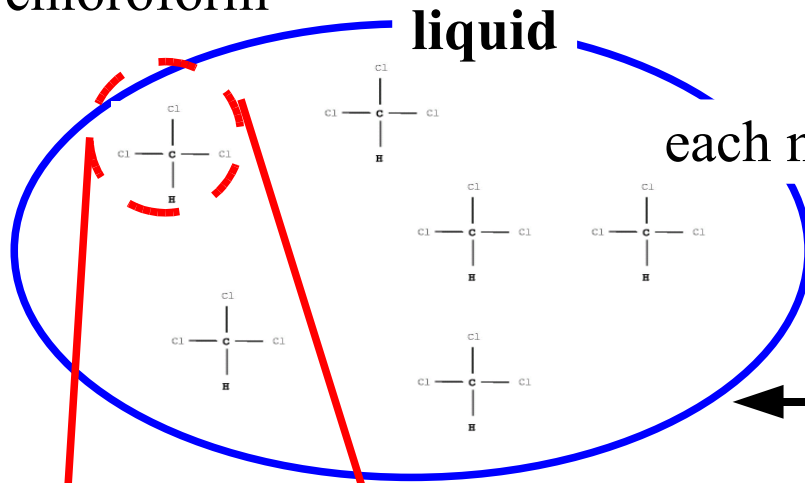


FIG. 50. Schematic setup of a NMR experiment. The liquid sample is in the middle tube surrounded by a radio-frequency cavity that produces a strong, homogeneous magnetic field. The apparatus is connected to electronic control devices not shown. From Cory *et al.* (2000).

RMP74, 347

RMP76, 1037

ensemble of individual quantum systems (computers)

restrict on one molecule (N-qubit system)



Hamiltonian for describing the thermal state ?

Model

Hamiltonian (for one molecule) in liquid-state NMR

$$\mathcal{H} = \sum_{i=1}^N \frac{h\nu_i}{2} Z_i$$

N : number of qubits $h\nu_i$: Zeeman energy for the i th qubit

assumption

- J -coupling: omitting ← smaller than Zeeman energy

- the computational basis

$|0\rangle_i, |1\rangle_i$

$$\begin{aligned} I_i &= |0\rangle_i\langle 0| + |1\rangle_i\langle 1| & Z_i &= |0\rangle_i\langle 0| - |1\rangle_i\langle 1| \\ X_i &= |0\rangle_i\langle 1| + |1\rangle_i\langle 0| & H_i &= (Z_i + X_i)/\sqrt{2} \end{aligned}$$

Model

typically, $\sim 10^{-5}$

thermal state in liquid-state NMR

$$\rho_{\text{th}} = \frac{1}{\mathcal{Z}} \exp \left(- \sum_{i=1}^N \alpha_i Z_i \right)$$

$$\alpha_i = h\nu_i / 2k_B T (> 0) \quad \alpha_i \neq \alpha_j$$

- characteristic physical parameters
above thermal state: always **separable**

$$N, \{\alpha_i\}_{i=1}^N$$

polarization

★ assumption: **all polarizations are positive !!**

Thermal state with low symmetry - chemical shift-

$$\rho_{\text{th}} = \frac{1}{\mathcal{Z}} \exp \left(- \sum_{i=1}^N \alpha_i Z_i \right)$$

$$\alpha_i = h\nu_i / 2k_B T \quad (> 0)$$

$$\alpha_i \neq \alpha_j$$

chemical shift

in YBC $\rightarrow \alpha_i$: common value \rightarrow

- not realistic model !!
- with high symmetry

$$\rho_{\text{th}} = \frac{1}{\mathcal{Z}} \exp(-2\alpha J_z) \quad J_z = \frac{1}{2} \sum_{i=1}^N Z_i$$

$$[\rho_{\text{th}}, J_z] = 0$$

Unitary transformed thermal states

in liquid-state NMR, all types of quantum gates are available ...

unitary transformed thermal state $\rho_B = U_B \rho_{\text{th}} U_B^\dagger$

what kind of unitary transformation ??

- entanglement generators (e.g., Hadamard + CNOT)
- important quantum gates in Quantum Algorithms (e.g. QFT ...)

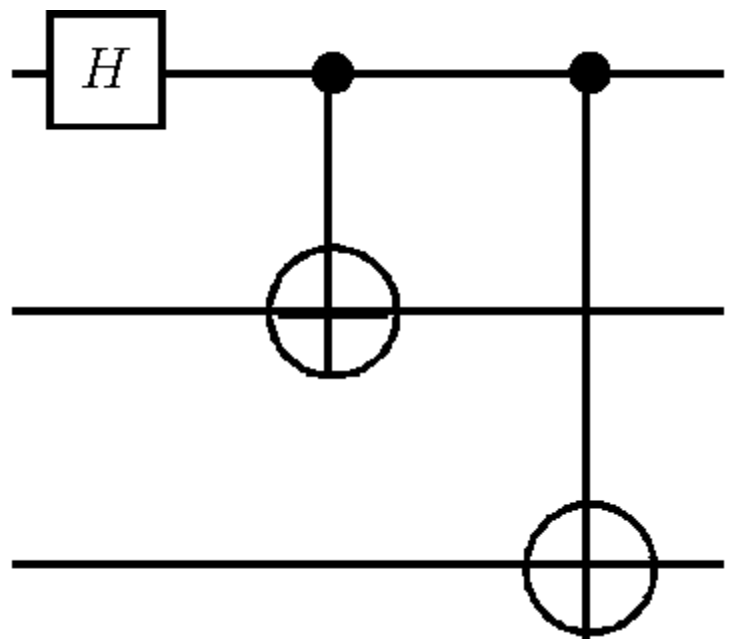
★ trial (the same as YBC)

1. CH op. $U_{\text{CH}} = U_{\text{fan}}(H_1 \otimes I) \rightarrow \rho_{\text{CH}}$

2. CH-fanout op. $U_{\text{CF}} = U_{\text{CH}} U_{\text{fan}} \rightarrow \rho_{\text{CF}}$

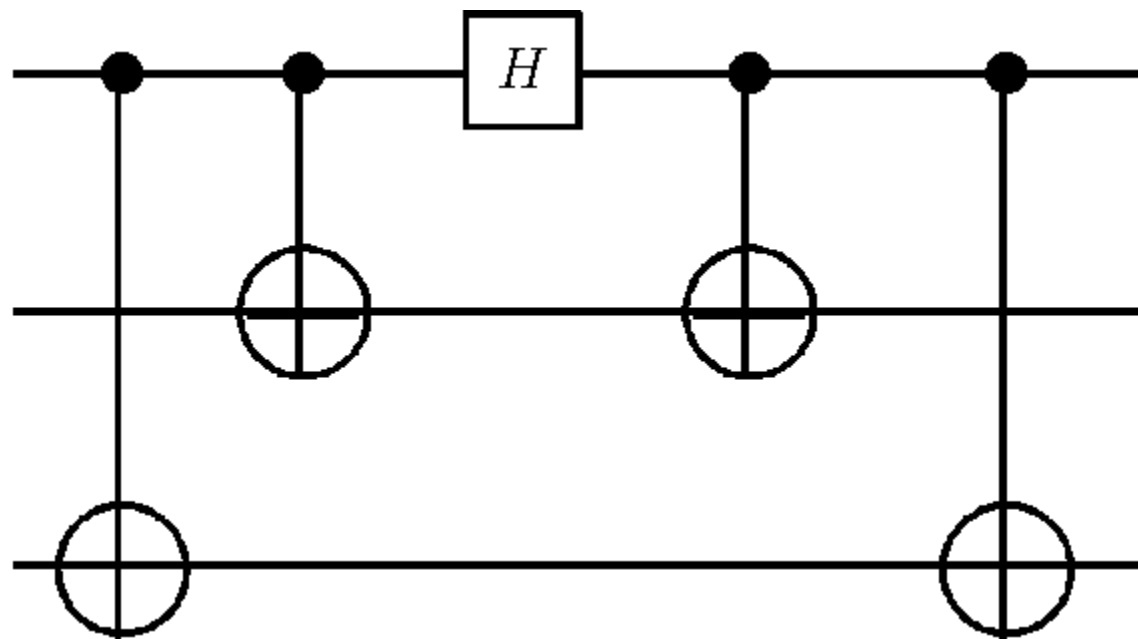
$$U_{\text{fan}} = |0\rangle_1 \langle 0| \otimes I + |1\rangle_1 \langle 1| \otimes X \quad I = \bigotimes_{i=2}^N I_i, \quad X = \bigotimes_{i=2}^N X_i$$

$N=3$



$$U_{\text{CH}} = U_{\text{fan}}(H_1 \otimes I)$$

controlled-NOT-Hadamard op.



$$U_{\text{CF}} = U_{\text{CH}}U_{\text{fan}}$$

CH-fanout op.

ex. $N=3$, input: $|000\rangle$

$$U_{\text{CH}}|000\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$$

$$U_{\text{CF}}|000\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$$

evaluation of nonseparable physical parameter region

for unitary transformed thermal states with the chemical shift

Dür-Cirac classification

Before showing our results, ...

Dür-Cirac classification [PRA**61**, 042314 (2000)]:

← YBC use it !!

very effective, (widely) used

entanglement of either pure or mixed state in a multiqubit system

★ main idea:

state interested, $\rho \rightarrow \rho_N$: **more easily evaluated the entanglement**



local operations: **not increasing the entanglement**

proper

entanglement measure

$$\rightarrow E(\rho) \geq E(\rho_N)$$

Dür-Cirac classification

- does it always work ???-

In our opinion, ...

not always obtain the information of the entanglement !!



transformed state is not always nonseparable (entangled)

CH: not working, CH-fanout: working

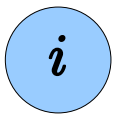
need to revisit the evaluation of nonseparability without the above method!

Notation & Method

- specification of a bipartition

a set of binary numbers: $\{k_i\}_{i=1}^N$ ($k_i = 0, 1$)

ex. $N=4, k_1=0, k_2=0, k_3=0, k_4=1$

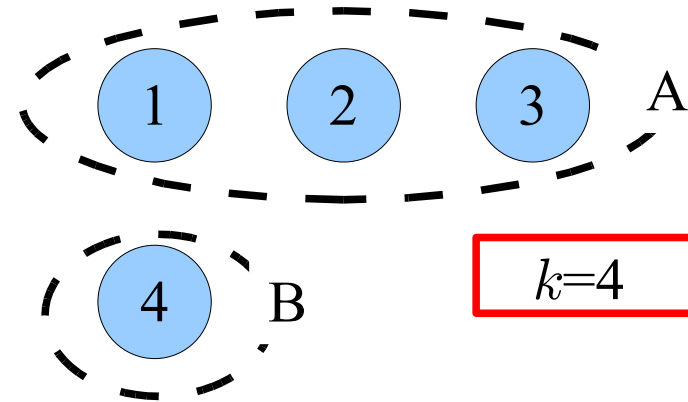


$k_i = 0 \rightarrow$ party A

$k_i = 1 \rightarrow$ party B

the i th qubit

the first qubit: always in party A



$$k = \sum_{i=2}^N k_i 2^{i-2}$$

\rightarrow specifying the bipartition k

Notation & Method

★ PPT criterion: **simple and computable way to evaluate entanglement**

[PRL 77, 1413 (1996); PLA 223, 8 (1996)]

total sys. \longrightarrow divided into **two subsystems**, A and B

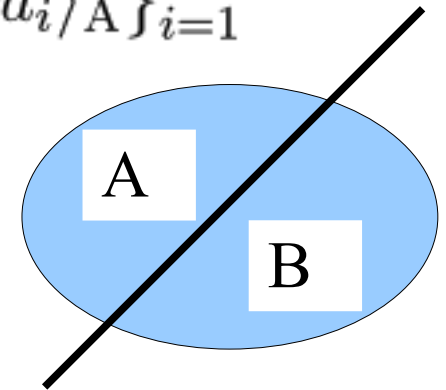
$$\rho = \sum_{i,j=1}^{d_A} \sum_{k,l=1}^{d_B} \underline{C(ik|jl)} |u_i\rangle_A \langle u_j| \otimes |v_k\rangle_B \langle v_l|$$

$$\{|u_i\rangle_A\}_{i=1}^{d_A}$$

partial transpose w.r.t. party B

$$\rho^{T_B} = \sum_{i,j=1}^{d_A} \sum_{k,l=1}^{d_B} \underline{C(il|jk)} |u_i\rangle_A \langle u_j| \otimes |v_k\rangle_B \langle v_l|$$

$$\{|v_j\rangle_B\}_{i=1}^{d_B}$$



Now, let us investigate the positivity of ρ^{T_B} ...

$$\rho^{\text{T}_B} \geq 0 \stackrel{\text{def}}{\iff} \rho: \text{positive partial transposition (PPT)}$$

$$\rho^{\text{T}_B} \not\geq 0 \stackrel{\text{def}}{\iff} \rho: \text{negative partial transposition (NPT)}$$

The most important thing...

$$\rho: \text{separable} \Rightarrow \rho: \text{PPT}$$

$$\rho: \text{NPT} \Rightarrow \rho: \text{nonseparable (i.e., entangled)}$$

moreover $\rho: \text{distillable} \Rightarrow \rho: \text{NPT}$

[see, G. Alber *et al.*, Quantum Information (Springer,2001), Chap.5]

Result: Nonseparable regions

analytically calculate the eigenvalues of $\rho_B^{\text{T}_B}$

★ sufficient conditions for the nonseparability w.r.t. a bipartition, k

- | | |
|-----------------|--|
| 1. CH op | $e^{-2w\eta_*} < \tanh \alpha_1$ |
| 2. CH-fanout op | $\cosh [(N - w)\xi_* - w\eta_*] < \sinh (N\bar{\alpha})$ |

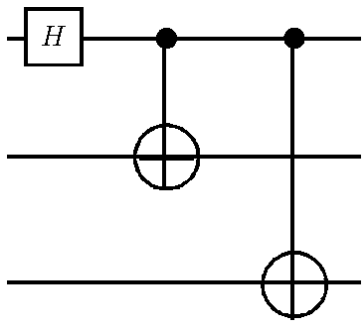
$$\xi_* = \frac{1}{N - w} \sum_{i \in A_k} \alpha_i \quad \text{mean value of the state of polarization for party A}$$

$$\eta_* = \frac{1}{w} \sum_{i \in B_k} \alpha_i \quad \text{mean value of the state of polarization for party B}$$

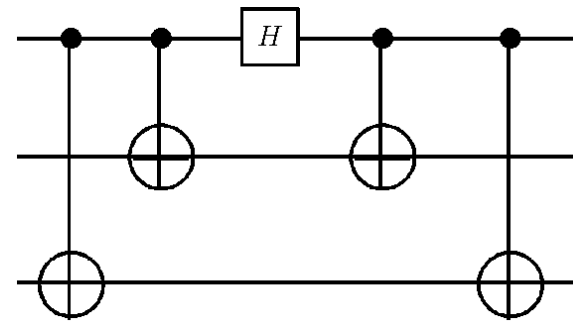
$$N\bar{\alpha} = \sum_{i=1}^N \alpha_i = (N - w)\xi_* + w\eta_* \quad w: \# \text{ of the elements in party B}$$

if α_i : a common value, $\alpha \longrightarrow$ Yu-Brown-Chuang's result !

CH



$$U_{\text{CH}} = U_{\text{fan}}(H_1 \otimes I)$$



CF

$$U_{\text{CF}} = U_{\text{CH}}U_{\text{fan}}$$

1. CH op

$$e^{-2w\eta_*} < \tanh \alpha_1$$

2. CH-fanout op

$$\cosh [(N - w)\xi_* - w\eta_*] < \sinh (N\bar{\alpha})$$

polarization-dependence

CH: α_1 and η_*
 (independent of mean value of polarization of party A)

CH-fanout: ξ_* and η_*

mean value
of polarization

ξ_*

η_*

party A

party B

clear difference about polarization-dependence

Boundary between nonsep. and sep.

- sufficient condition for nonseparability w.r.t. a bipartition, k

- | | |
|-----------------|--|
| 1. CH op | $e^{-2w\eta_*} < \tanh \alpha_1$ |
| 2. CH-fanout op | $\cosh [(N - w)\xi_* - w\eta_*] < \sinh (N\bar{\alpha})$ |

by using the PPT criterion...

- necessary condition for separability w.r.t. a bipartition, k

- | | |
|------------------|---|
| 1. CH op. | $e^{-2w\eta_*} \geq \tanh \alpha_1$ |
| 2. CH-fanout op. | $\cosh [(N - w)\xi_* - w\eta_*] \geq \sinh (N\bar{\alpha})$ |

Boundary between nonsep. and sep.

- boundary between nonseparability and separability by the PPT criterion

1. CH op. $e^{-2w\eta_*} = \tanh \alpha_1$

2. CH-fanout op. $\cosh [(N - w)\xi_* - w\eta_*] = \sinh (N\bar{\alpha})$

★ boundary between separability and nonseparability
 ``effect of chemical shift''

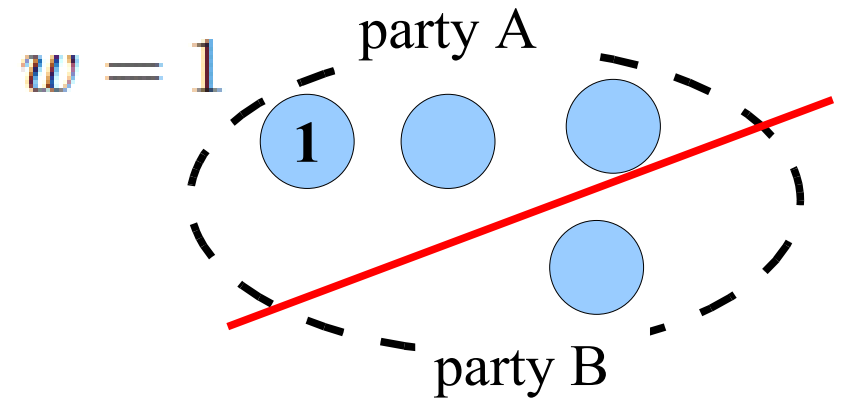
toy model for chemical shift

$$\alpha_i = \alpha(1 + x_i) \quad , \quad x_i : \text{uniform random variable} \\ \text{in } [-\delta, \delta]$$

w : number of elements
in party B

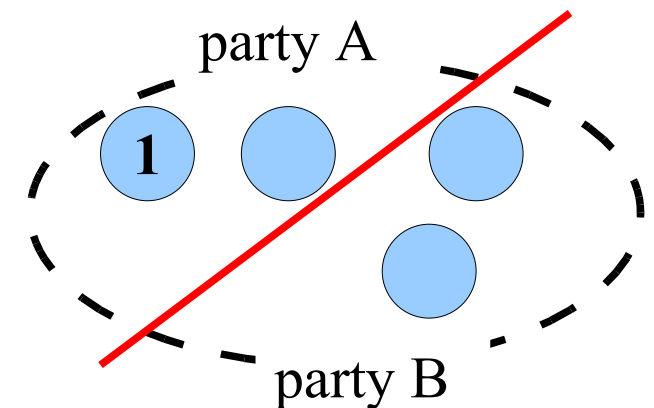
For example, ...

• CH op. $k = 2^{N-1} - 1$

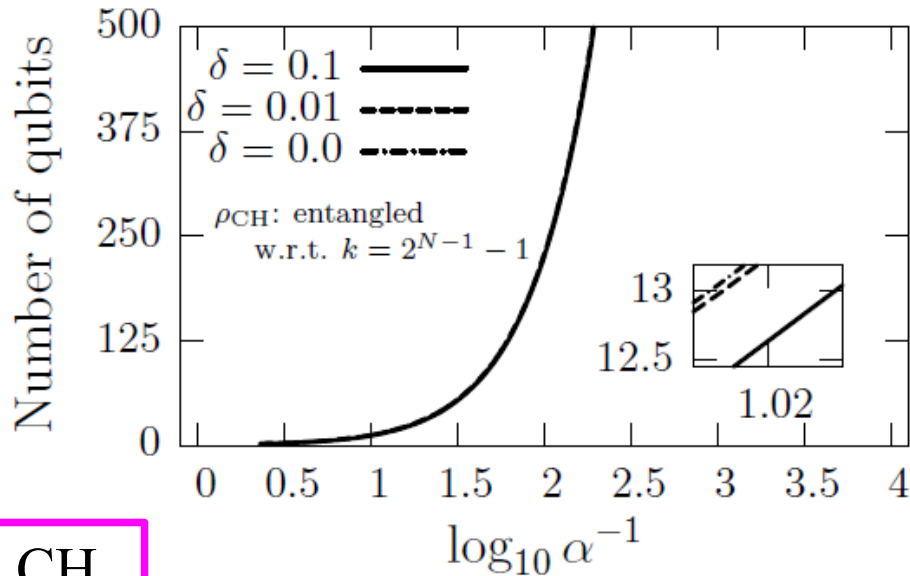


• CH-fanout op. $k = 2^{N-1} - 2^{\lfloor N/2 \rfloor - 1}$

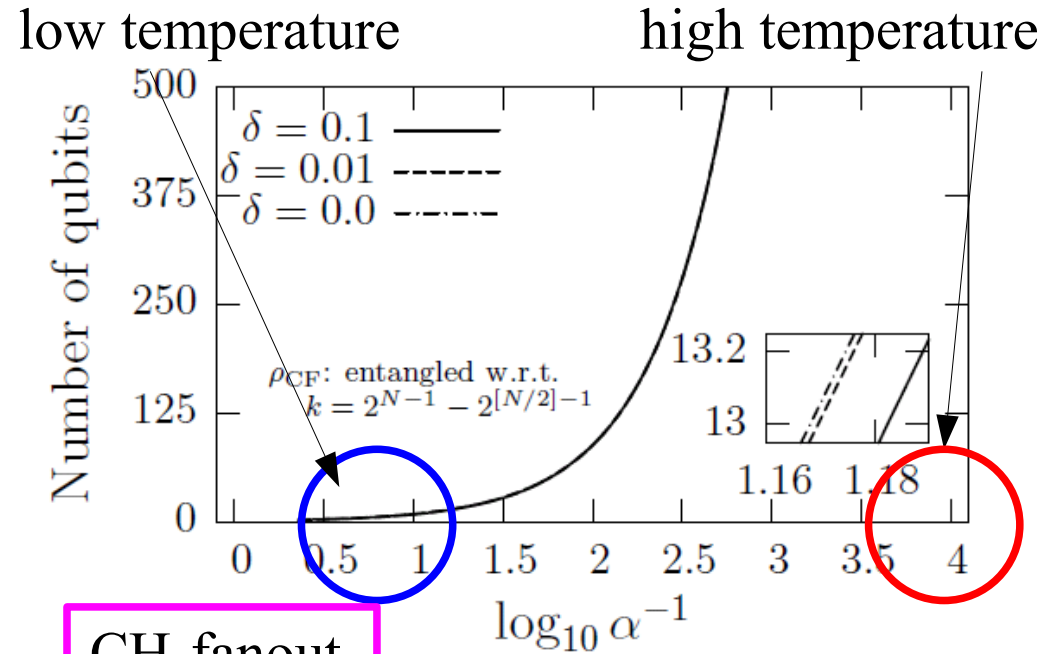
$w = \lfloor N/2 \rfloor$



★ boundary between separability and nonseparability
 ``effect of chemical shift''



CH



CH-fanout

difference: invisible (as N is large, the difference goes to zero)

why??

conditions for separability or nonseparability

→ mainly depended on the mean value of α_i for each party

Unfortunately, ...

- boundary: region difficult to achieve in the current liquid-state NMR experiment
- not reveal the connection between symmetry and entanglement generation

On the other hand,

- experimental check of entangled state: easy !!

only two parameters!

the number of qubits

N

mean value of polarization

α

Summary

★ **sufficient condition for the nonseparability of ρ_B w.r.t. any bipartition**

chemical shift exists, direct evaluating method

generalization of YBC's result

effect of chemical shift \rightarrow negligible !

- connection between entanglement generation and symmetry \rightarrow not clear ...
 - \longrightarrow need to study other model of chemical shift
 - ex. $\alpha_i \not\approx 0$, more complex distribution of α_i
- experimental check of entangled state: easy !!

only two parameters!

the number of qubits

N

mean value of polarization

α

\longrightarrow application to solid-state NMR experiments ??

★ **ability to generate entanglement**

Yu-Brown-Chuang:

With respect to the thermal state,

ρ_{CF} generate entanglement more effectively than ρ_{CH}

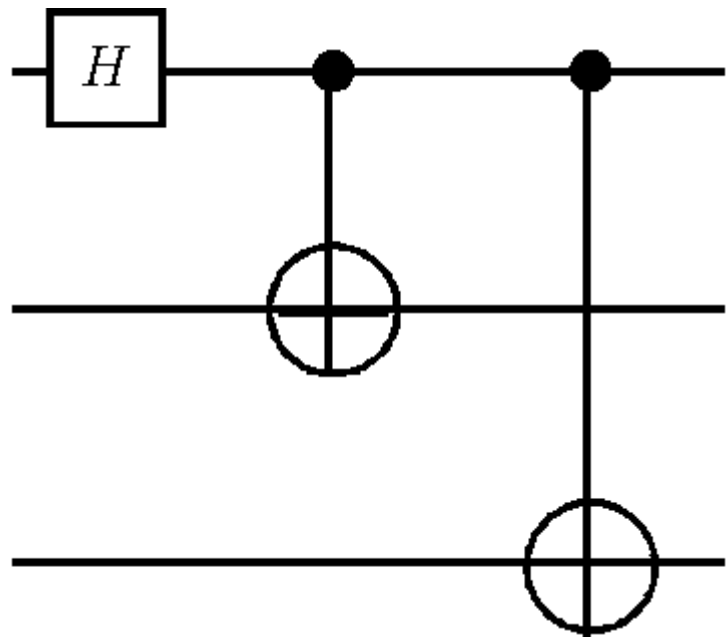
for more detail classification of the ability, ...

evaluation of entanglement measure: logarithmic negativity (in progress ...)

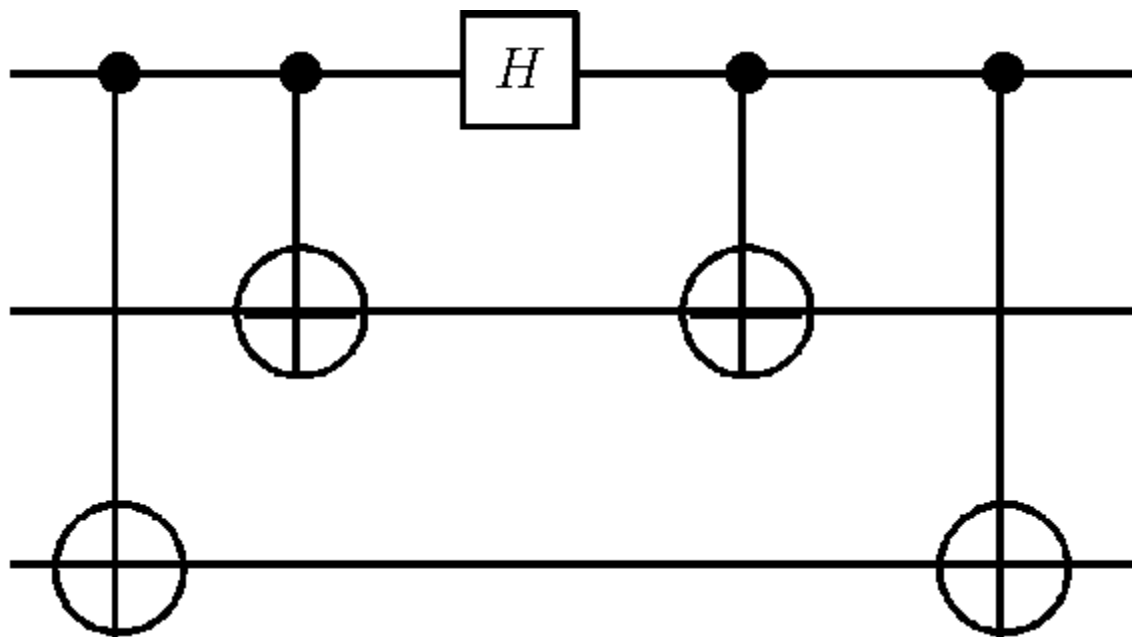
ability of quantum gates to generate entanglement

two quantum gates

$N=3$



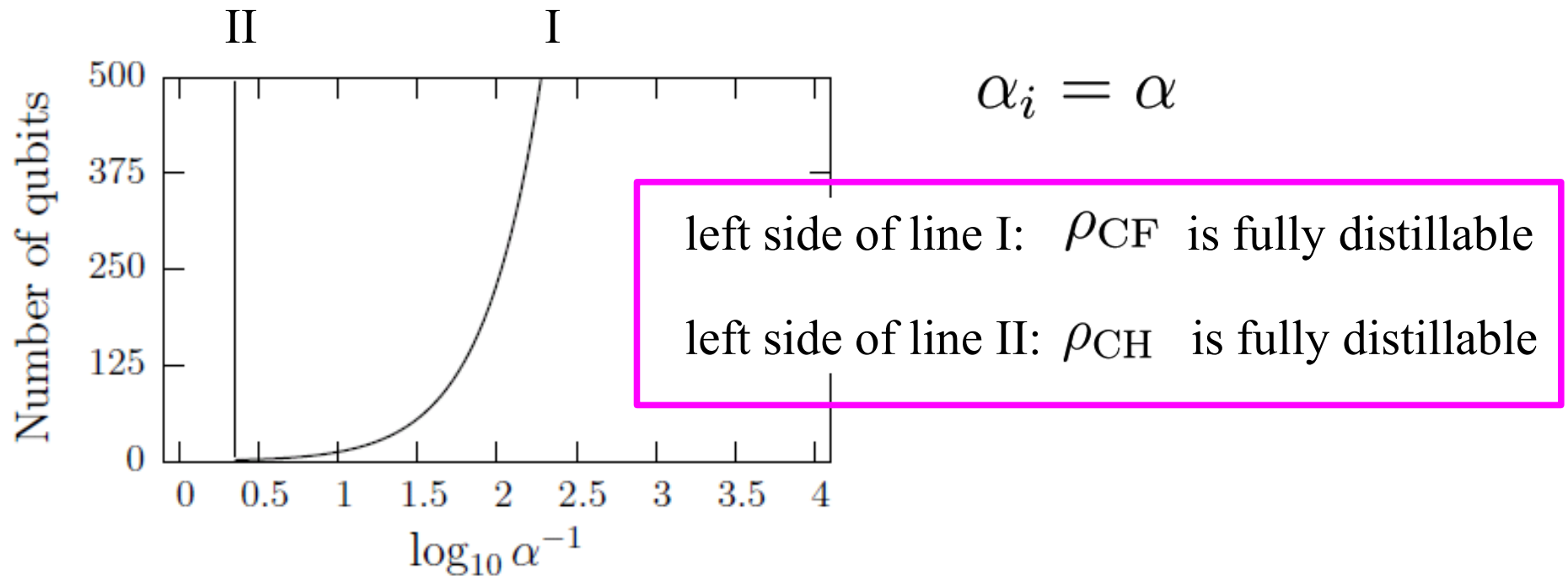
$$U_{\text{CH}} = U_{\text{fan}}(H_1 \otimes I)$$



$$U_{\text{CF}} = U_{\text{CH}}U_{\text{fan}}$$

ability to generate entanglement from thermal state

- ability fully distillable (i.e., distillable with respect to any bipartition)



With respect to the thermal state,

ρ_{CF} generate entanglement more effectively than ρ_{CH}

(YBC have already pointed out it)

Calculation of an entanglement measure

for more detail classification of the ability, ... \rightarrow trial !!

logarithmic negativity $E_N(\rho) = \log_2 \|\rho^{T_B}\|_1$ PRA65, 032314

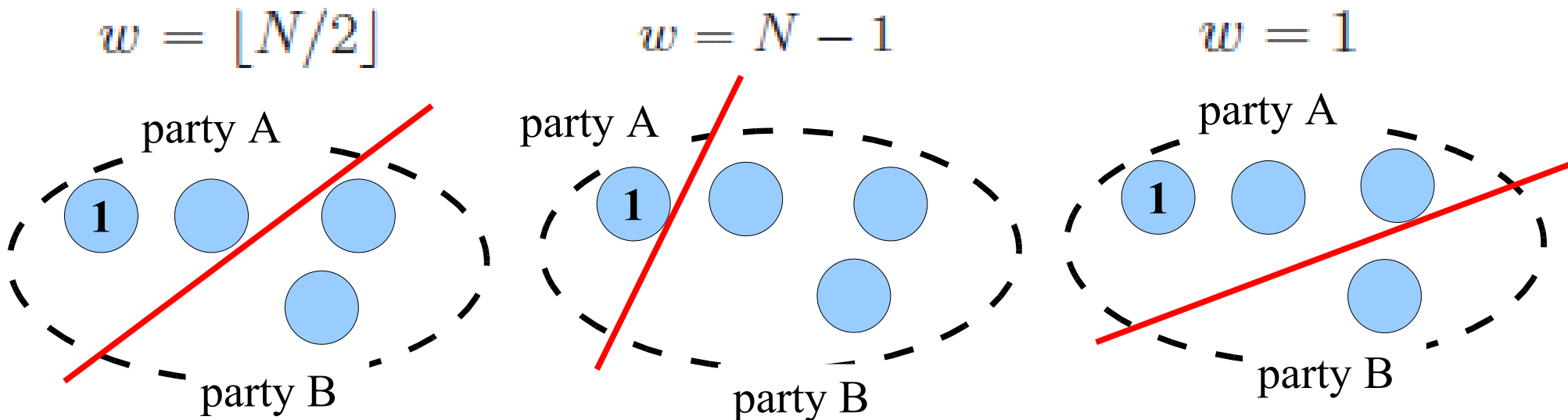
- **simple and computable**
- monotonicity under LOCC
- additivity
- upper bound to entanglement distillation

separable: 0
maximal entangled state: 1

hereafter $\alpha_i = \alpha$

showing results for three types of w

w : number of elements
in party B



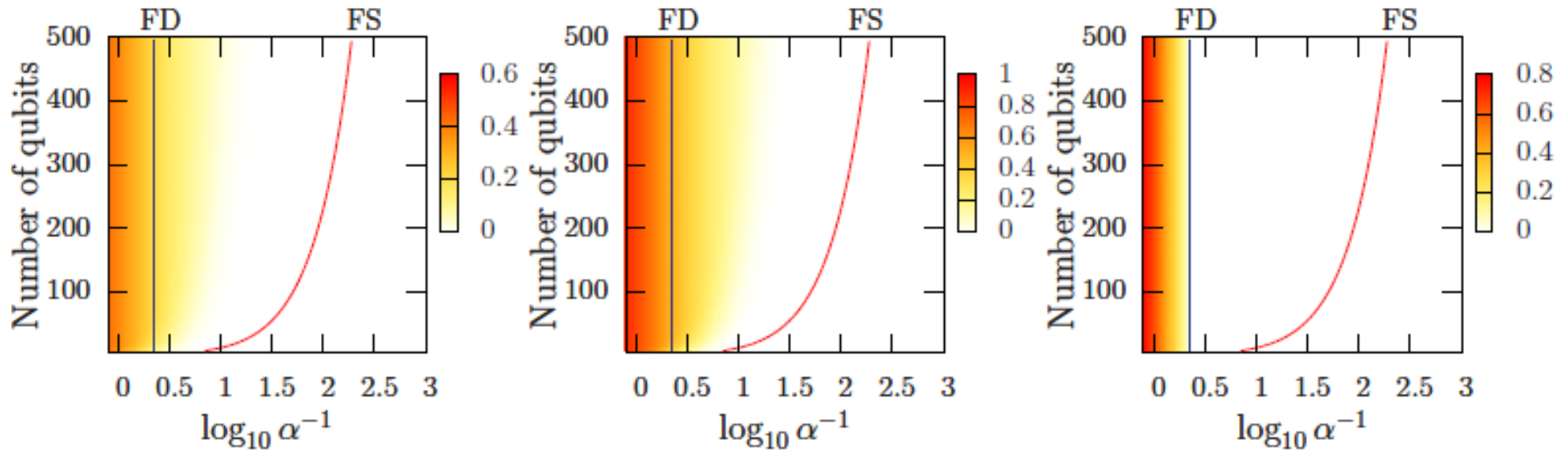
Result II: logarithmic negativity

ρ_{CH}

$w = \lfloor N/2 \rfloor$

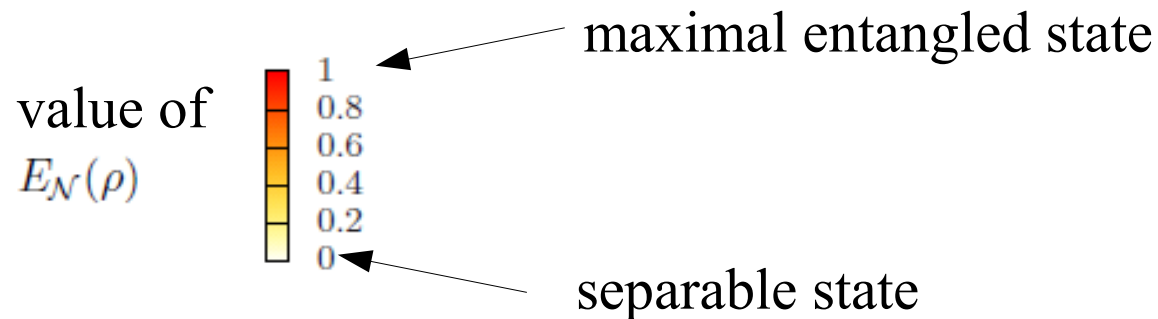
$w = N - 1$

$w = 1$



left side of FD \longleftrightarrow full distillable

right side of FS \longleftarrow full separable

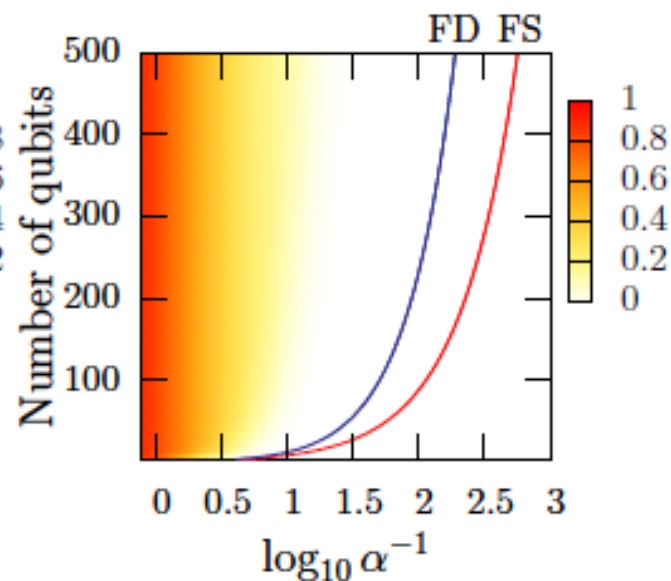
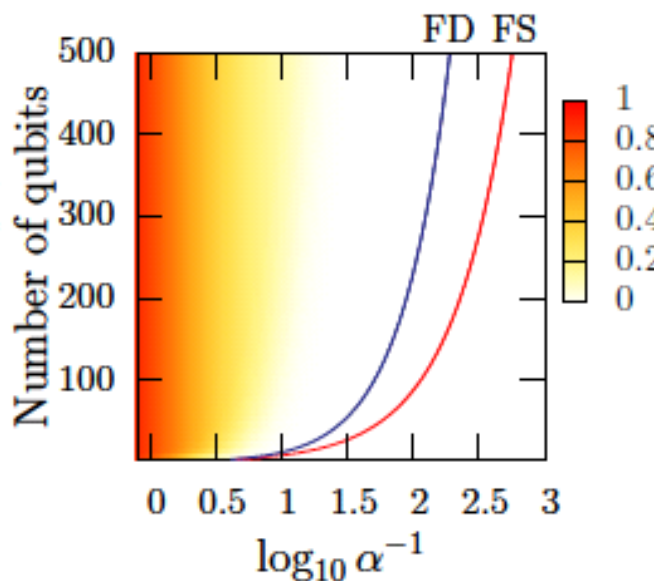
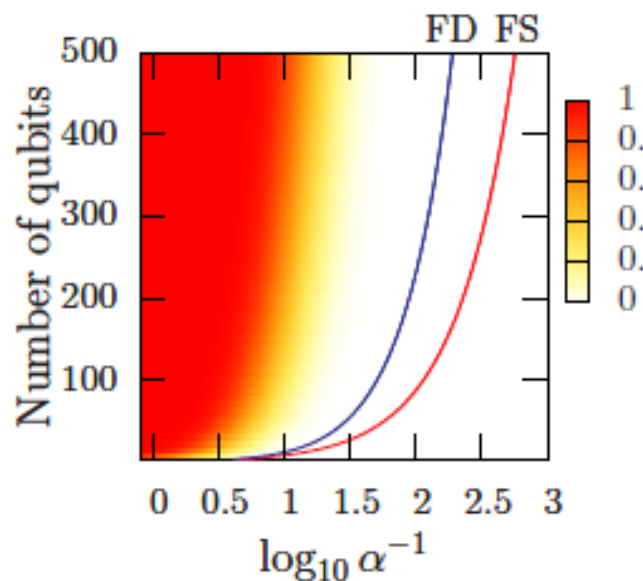


ρ_{CF}

$w = \lfloor N/2 \rfloor$

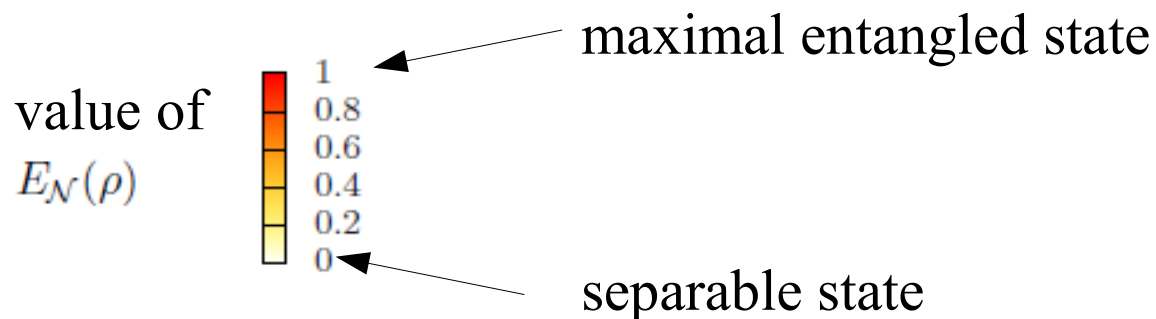
$w = N - 1$

$w = 1$

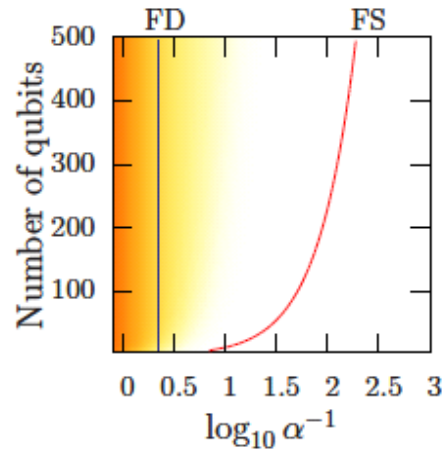


left side of FD \longleftrightarrow full distillable

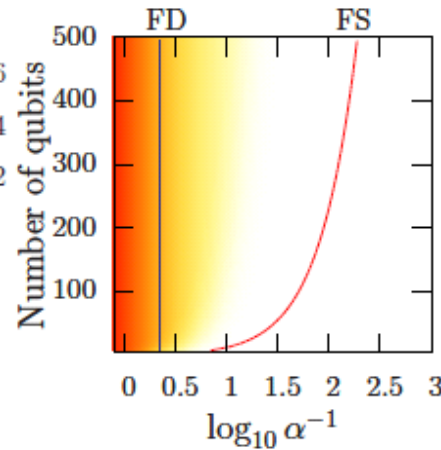
right side of FS \longleftarrow full separable



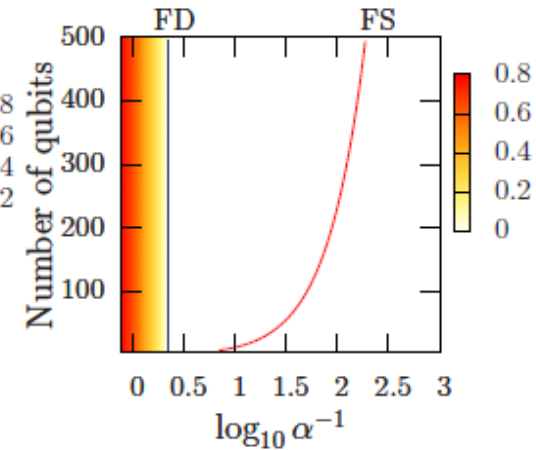
ρ_{CH} $w = \lfloor N/2 \rfloor$



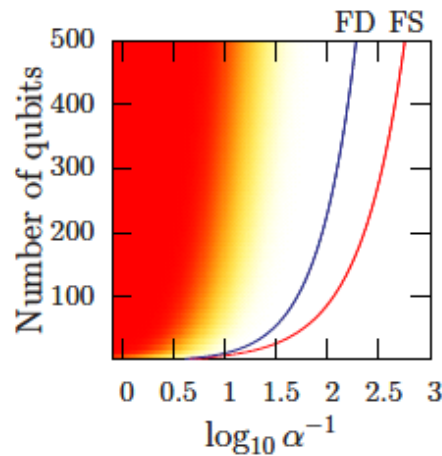
$w = N - 1$



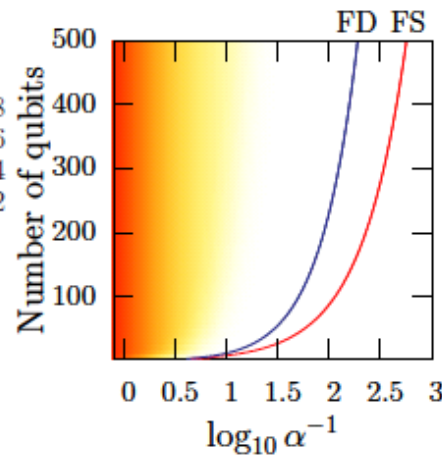
$w = 1$



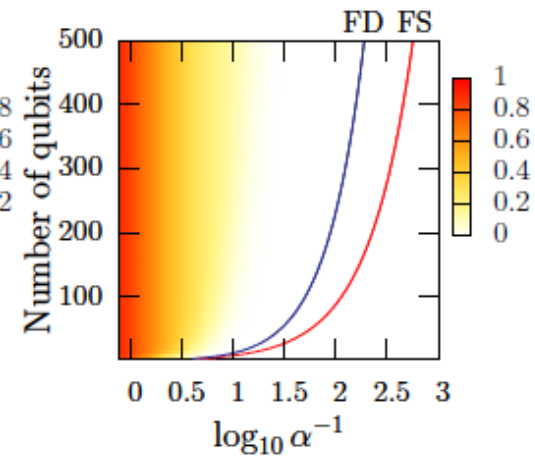
ρ_{CF} $w = \lfloor N/2 \rfloor$



$w = N - 1$



$w = 1$



increasing rate \longrightarrow difference exists (?)

need further investigation

useful for the characterization of quantum gates?

Dür-Cirac Classification

★ main idea

ρ : density matrix concerned

$\tilde{\rho}$: density matrix whose property is easily obtained

$\exists \mathcal{L}$: linear map which cannot increase the entanglement of a state

$$\tilde{\rho} = \mathcal{L}(\rho)$$

\Rightarrow investigate $\tilde{\rho}$ instead of ρ

candidate for $\tilde{\rho}$: ρ_N

★ property of the density matrix ρ_N

$$\rho_N = \lambda_0^+ |\Psi_0^+\rangle\langle\Psi_0^+| + \lambda_0^- |\Psi_0^-\rangle\langle\Psi_0^-| + \sum_{j=1}^{2^{N-1}-1} \lambda_j (|\Psi_j^+\rangle\langle\Psi_j^+| + |\Psi_j^-\rangle\langle\Psi_j^-|)$$

$$\rho_N: \text{PPT with a bipartition } k \iff \Delta \leq 2\lambda_k$$

$$\rho_N: \text{NPT with a bipartition } k \iff \Delta > 2\lambda_k$$

$$\Delta = |\lambda_0^+ - \lambda_0^-|$$

$$\lambda_0^\pm = \langle\Psi_0^\pm|\rho|\Psi_0^\pm\rangle \quad 2\lambda_j = \langle\Psi_j^+|\rho|\Psi_j^+\rangle + \langle\Psi_j^-|\rho|\Psi_j^-\rangle$$

to use Peres criterion w.r.t. a specific bipartition k ,

in general, need to know all eigenvalues,

in addition, search the minimum value out of 2^N entries !!

ρ_N : characterized by only two parameters!!

$$\Delta, 2\lambda_k$$

moreover, results independent of the choice of k

necessary and sufficient condition for fully separability or fully distillability

★ how construct such a \mathcal{L} ?

0. expansion of ρ using generalized GHZ state

$$\rho = \sum_{j=0}^{2^N-1} (\lambda_j^+ |\Psi_j^+\rangle \langle \Psi_j^+| + \lambda_j^- |\Psi_j^-\rangle \langle \Psi_j^-|) + \sum_{\sigma, \sigma'} \sum_{j \neq j'} \langle \Psi_j^\sigma | \rho | \Psi_{j'}^{\sigma'} \rangle |\Psi_j^\sigma\rangle \langle \Psi_{j'}^{\sigma'}|$$

note: $\lambda_j^+ + \lambda_j^- = 2\lambda_j$

1. simultaneous spin-flip operation

$$\mathcal{L}_1 \rho = \frac{1}{2} \rho + \frac{1}{2} (\sigma_x^1 \otimes \dots \otimes \sigma_x^N) \rho (\sigma_x^1 \otimes \dots \otimes \sigma_x^N)$$

a local operation randomly performed with prob. 1/2

$$\tilde{\rho}_1 = \mathcal{L}_1 \rho$$

getting rid of the term on $|\Psi_j^\sigma\rangle \langle \Psi_{j'}^{\sigma'}|$ ($\sigma \neq \sigma'$) from ρ

2. phase-shift op. w.r.t. the 1st qubit and k th qubit

$$\mathcal{L}_k \rho = \frac{1}{2} \rho + \frac{1}{2} (\sigma_z^1 \otimes \dots \sigma_z^k \otimes \dots) \rho (\sigma_z^1 \otimes \dots \sigma_z^k \otimes \dots) \quad k=2, 3, \dots, N$$

$$\tilde{\rho}_N = \mathcal{L}_N \mathcal{L}_{N-1} \dots \mathcal{L}_2 \tilde{\rho}_1$$

getting rid of the term on $|\Psi_j^\pm\rangle\langle\Psi_{j'}^\pm|$ ($j \neq j'$) from $\tilde{\rho}_1$

3. local random phase operation

$$\mathcal{L}_{\text{LRP}} \rho = \prod_{\alpha=1}^N \left[\int_0^{2\pi} \frac{d\phi_\alpha}{2\pi} \right] 2\pi \delta(\{\phi_\alpha\}) R(\{\phi_\alpha\}) \rho R^\dagger(\{\phi_\alpha\})$$

$$R(\{\phi_\alpha\}) = \bigotimes_{\alpha=1}^N e^{i\phi_\alpha/2} e^{i\phi_\alpha \sigma_z^\alpha/2} \quad \delta(\{\phi_\alpha\}) = \begin{cases} 1 & \left(\sum_{\alpha=1}^N \phi_\alpha - 2\pi \equiv 0 \pmod{2\pi} \right) \\ 0 & \text{(others)} \end{cases}$$

$$\rho_N = \mathcal{L}_{\text{LRP}} \tilde{\rho}_N$$

in summary, ...

$$\rho_N = \underbrace{\mathcal{L}_{LRP} \mathcal{L}_N \dots \mathcal{L}_2 \mathcal{L}_1}_{\text{composed of a sequence of local operations}} \rho$$
$$\lambda_0^\pm = \langle \Psi_0^\pm | \rho | \Psi_0^\pm \rangle$$
$$2\lambda_j = \langle \Psi_j^+ | \rho | \Psi_j^+ \rangle + \langle \Psi_j^- | \rho | \Psi_j^- \rangle$$

composed of a sequence of local operations

—► not increasing the entanglement !!

Accordingly, ...

tions. Accordingly, if ρ_N is a nonseparable state with a bipartition, ρ is also such a state. It should be noticed that we obtain the information on the entanglement of ρ only if ρ_N is a nonseparable state.

transformed state is always nonseparable (entangled) ?

Example 1: work

$N=2, k=1$

$$\rho_{iso} = (1 - f) \frac{1}{4} (I_1 \otimes I_2) + f |\Psi_0^+\rangle \langle \Psi_0^+| \quad (-1/3 \leq f \leq 1)$$

PPT criterion $\longrightarrow \rho_{iso}$: entangled $\iff f > 1/3$
(\implies , because $N = 2$)

on the other hand,

$$\langle \Psi_0^+ | \rho_{iso} | \Psi_0^+ \rangle = (1 + 3f)/4, \quad \langle \Psi_0^- | \rho_{iso} | \Psi_0^- \rangle = (1 - f)/4$$

$$\langle \Psi_1^+ | \rho_{iso} | \Psi_1^+ \rangle + \langle \Psi_1^- | \rho_{iso} | \Psi_1^- \rangle = (1 - f)/2$$

\longrightarrow

$$f > 1/3 \implies \rho_{iso}: \text{entangled}$$

consistent !

Example 2: NOT WORK !!

slightly different from the previous example ...

$$\rho'_{iso} = (1 - f) \frac{1}{4} (I_1 \otimes I_2) + f |\Psi_1^+\rangle \langle \Psi_1^+| \quad (-1/3 \leq f \leq 1)$$

PPT criterion $\longrightarrow \rho'_{iso}$: entangled $\iff f > 1/3$

on the other hand, ...

$$\langle \Psi_0^+ | \rho'_{iso} | \Psi_0^+ \rangle = \langle \Psi_0^- | \rho'_{iso} | \Psi_0^- \rangle = (1 - f)/4$$

$$\langle \Psi_1^+ | \rho'_{iso} | \Psi_1^+ \rangle + \langle \Psi_1^- | \rho'_{iso} | \Psi_1^- \rangle = (1 + f)/2$$

$\Delta < 2\lambda_1$ for $\forall f$ **obtain no information!!**

Why,...

Let us explicitly construct \mathcal{L} for the depolarization

need only the local random phase operation

$$\mathcal{L}_{LRP}\rho'_{iso} = \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \frac{1}{2\pi} \delta(\{\phi_1, \phi_2\}) [R(\phi_1) \otimes R(\phi_2)] \rho'_{iso} [R^\dagger(\phi_1) \otimes R^\dagger(\phi_2)]$$

$$R(\phi_a)|0\rangle_a = e^{i\phi_a}|0\rangle_a, \quad R(\phi_a)|1\rangle_a = |1\rangle_a$$

$$\phi_1 + \phi_2 = 2m\pi \quad (m \in \mathbb{Z})$$

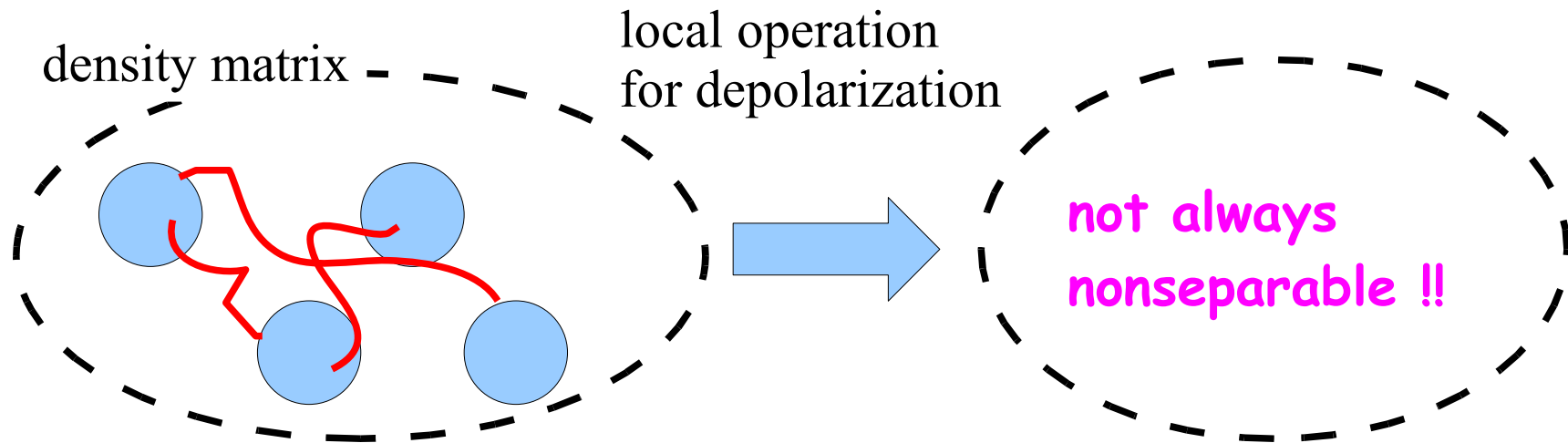
$$\begin{aligned} \mathcal{L}_{LRP}\rho'_{iso} = & \frac{1-f}{4} |0\rangle_1\langle 0| \otimes |0\rangle_2\langle 0| + \frac{1-f}{4} |1\rangle_1\langle 1| \otimes |1\rangle_2\langle 1| \\ & + \frac{1+f}{4} |0\rangle_1\langle 0| \otimes |1\rangle_2\langle 1| + \frac{1+f}{4} |1\rangle_1\langle 1| \otimes |0\rangle_2\langle 0| \end{aligned}$$

separable !!

Discussion

DC classification: very effective, simple method
for evaluating entanglement in multiqubit system

BUT, not always obtain the desired information !!



future ...

today's talk: at least exist such an example

→ general criterion?!, prescription ?

applying suitable local operations → can use such a method (?)

$$\rho_{iso} \longrightarrow \rho'_{iso}$$