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*, PRL**83**, 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)   PRA **71**, 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), PRA **71**, 032341 (2005)

thermal states (separable) → **quantum gates** → ρ **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 !)

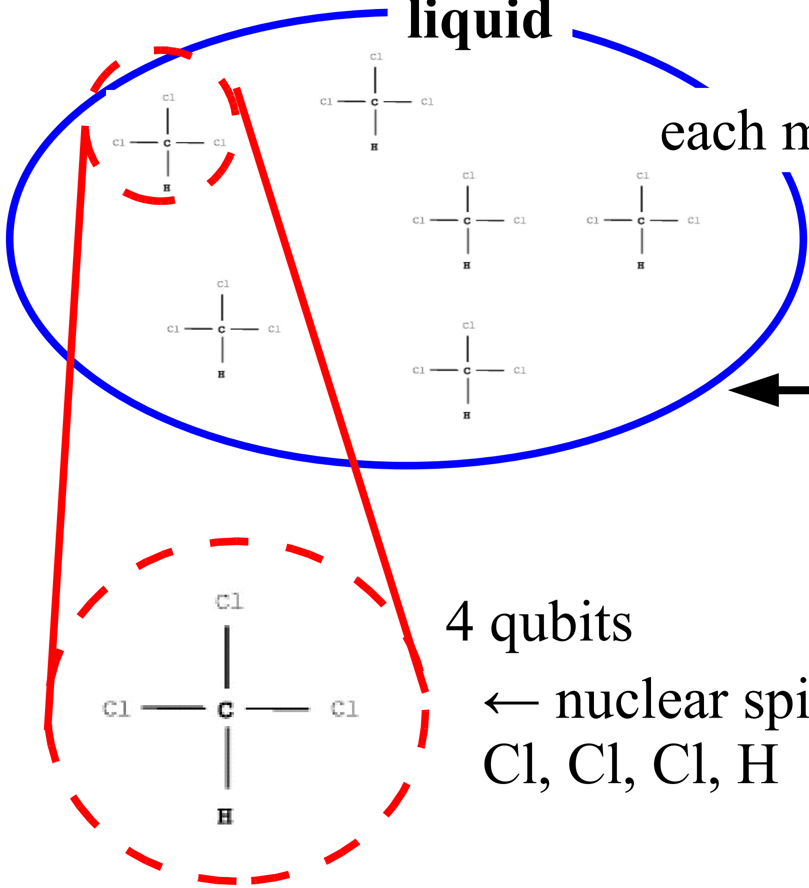
  system's symmetry + quantum dynamics →? **entanglement generation**

- their (indirect) method for evaluating entanglement → **(probably) don't work**
  → **directly and correctly evaluate**

Model

ex. chloroform

liquid



each molecule is independent

4 qubits

← nuclear spins for Cl, Cl, Cl, H

room temperature

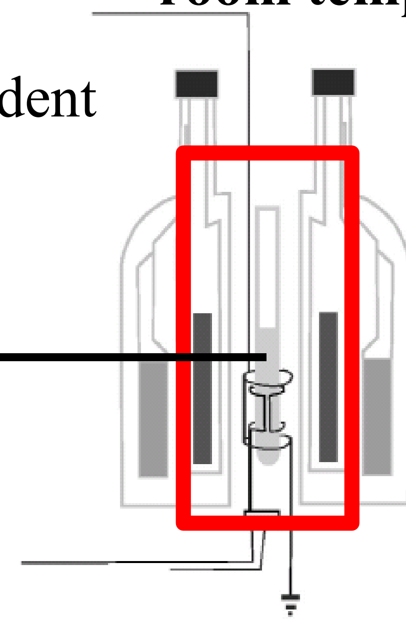


FIG. 50. Schematic setup of a NMR experiment. The liquid sample is in the middle tube surrounded by a radio-frequency cavity that produces a strong, homogeneous magnetic field. The apparatus is connected to electronic control devices not shown. From Cory *et al.* (2000).

RMP**74**, 347

RMP**76**, 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 ith qubit

assumption

- J-coupling: omitting ← smaller than Zeeman energy

- the computational basis

$$|0\rangle_i \ , \ |1\rangle_i$$

$$I_i = |0\rangle_i\langle 0| + |1\rangle_i\langle 1| \quad Z_i = |0\rangle_i\langle 0| - |1\rangle_i\langle 1|$$

$$X_i = |0\rangle_i\langle 1| + |1\rangle_i\langle 0| \quad H_i = (Z_i + X_i)/\sqrt{2}$$

Model

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

thermal state in liquid-state NMR

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

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

- 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-

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

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

$$\alpha_i \neq \alpha_j$$

chemical shift

in YBC → α_i : common value →

- **not realistic model !!**
- **with high symmetry**

$$\rho_{\rm th} = \frac{1}{\mathcal{Z}} \exp\left(-2\alpha J_z\right) \qquad J_z = \frac{1}{2}\sum_{i=1}^{N} Z_i$$

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

Unitary transformed thermal states

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

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

what kind of unitary transformation ??

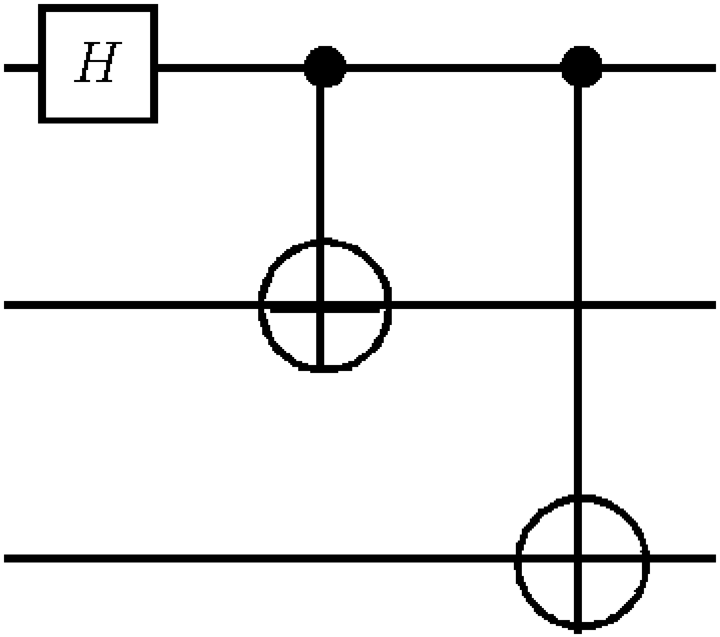
- entanglement generators (e.g., Hadamard + CNOT)
- important quantum gates in Quantum Algorithms (e.g. QFT ...)

☆ trial (the same as YBC)

1. CH op. $U_{\rm CH} = U_{\rm fan}(H_1 \otimes I) \rightarrow \rho_{\rm CH}$
2. CH-fanout op. $U_{\rm CF} = U_{\rm CH} U_{\rm fan} \rightarrow \rho_{\rm CF}$

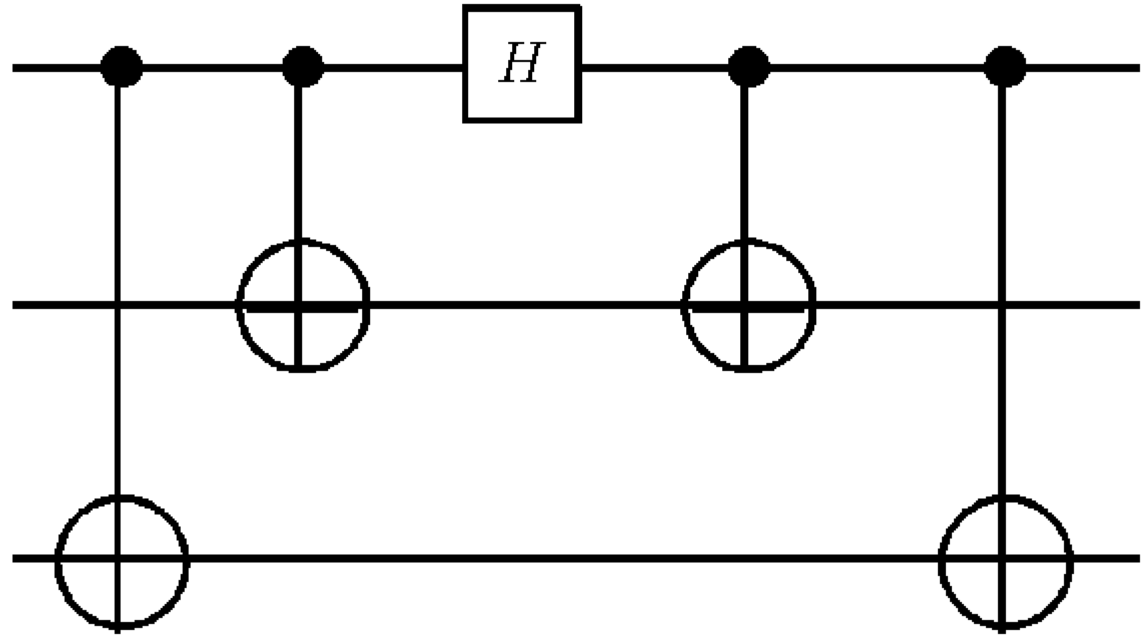
$$U_{\rm fan} = |0\rangle_1\langle 0| \otimes I + |1\rangle_1\langle 1| \otimes X \qquad I = \bigotimes_{i=2}^{N} I_i, \quad X = \bigotimes_{i=2}^{N} X_i$$

N=3



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

controlled-NOT-Hadamaed op.



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

CH-fanout op.

ex. N=3, input:|000>

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

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

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, $\rho \longrightarrow \rho_N$:**more easily evaluated the entanglement**

↑

local operations: not increasing the entanglement

proper entanglement measure →

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

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)

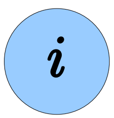
CH: not working, CH-fanout: working

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

Notation & Method

- specification of a bipartition

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

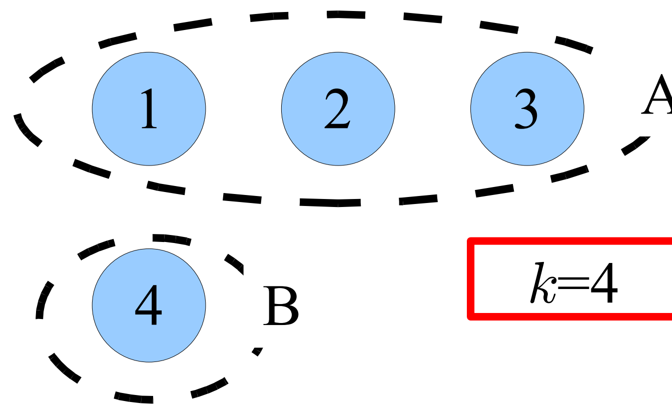


the ith qubit

$k_i = 0$ → party A

$k_i = 1$ → party B

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



k=4

the first qubit: always in party A

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

→ specifying the bipartition k

Notation & Method

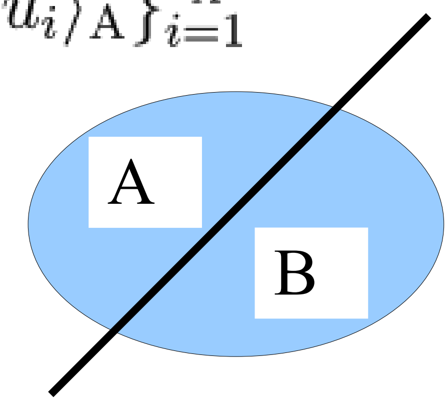
- PPT criterion: simple and computable way to evaluate entanglement

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

  total sys. → divided into two subsystems, A and B

$$\rho = \sum_{i,j=1}^{d_{\rm A}} \sum_{k,l=1}^{d_{\rm B}} \underline{C(ik|jl)}\, |u_i\rangle_{\rm A}\langle u_j| \otimes |v_k\rangle_{\rm B}\langle v_l|$$

$$\{|u_i\rangle_{\rm A}\}_{i=1}^{d_{\rm A}}$$



$$\{|v_j\rangle_{\rm B}\}_{i=1}^{d_{\rm B}}$$

↓ partial transpose w.r.t. party B

$$\rho^{\rm T_B} = \sum_{i,j=1}^{d_{\rm A}} \sum_{k,l=1}^{d_{\rm B}} \underline{C(il|jk)}\, |u_i\rangle_{\rm A}\langle u_j| \otimes |v_k\rangle_{\rm B}\langle v_l|$$

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

$$\rho^{T_B} \geq 0 \overset{\text{def}}{\Longleftrightarrow} \rho\text{: positive partial transposition (PPT)}$$

$$\rho^{T_B} \ngeq 0 \overset{\text{def}}{\Longleftrightarrow} \rho\text{: negative partial transposition (NPT)}$$

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 $\rho_{\mathrm{B}}^{\mathrm{T_B}}$

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

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

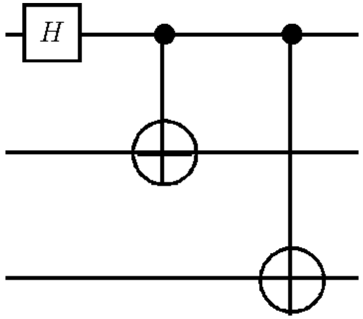
$\xi_* = \frac{1}{N-w}\sum_{i\in A_k}\alpha_i$ mean value of the state of polarization for party A

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

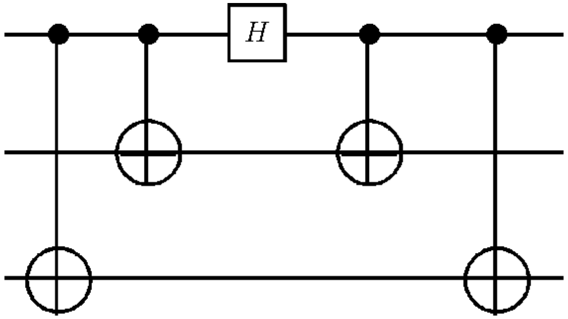
$N\bar{\alpha} = \sum_{i=1}^{N}\alpha_i = (N-w)\xi_* + w\eta_*$ w: # of the elements in party B

if α_i : **a common vale,** α ⟶ **Yu-Brown-Chuang's result !**

CH



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



CF

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

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

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

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_* party A

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

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. $\cosh\left[(N-w)\xi_* - w\eta_*\right] \geq \sinh\left(N\bar{\alpha}\right)$

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. $$\cosh\left[(N-w)\xi_* - w\eta_*\right] = \sinh\left(N\bar{\alpha}\right)$$

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

toy model for chemical shift

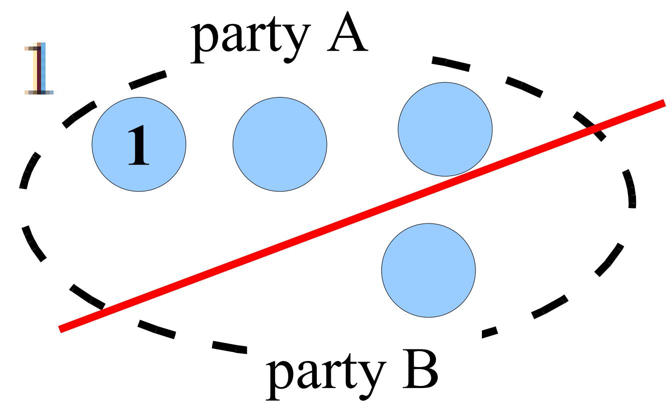
$$\alpha_i = \alpha(1 + x_i) \quad , \qquad x_i$$: uniform random variable in $[-\delta, \delta]$

w: number of elements in party B

For example, ...

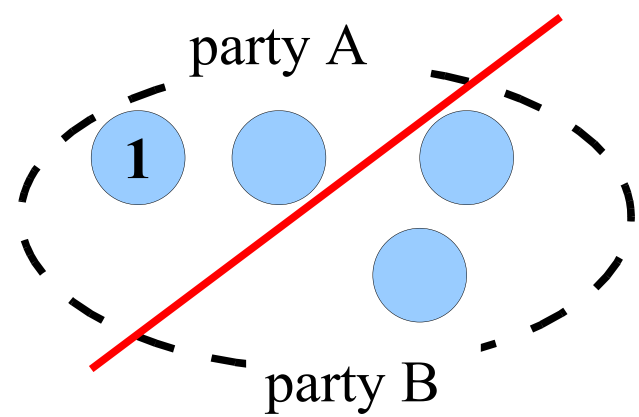
- CH op. $k = 2^{N-1} - 1$

$w = 1$



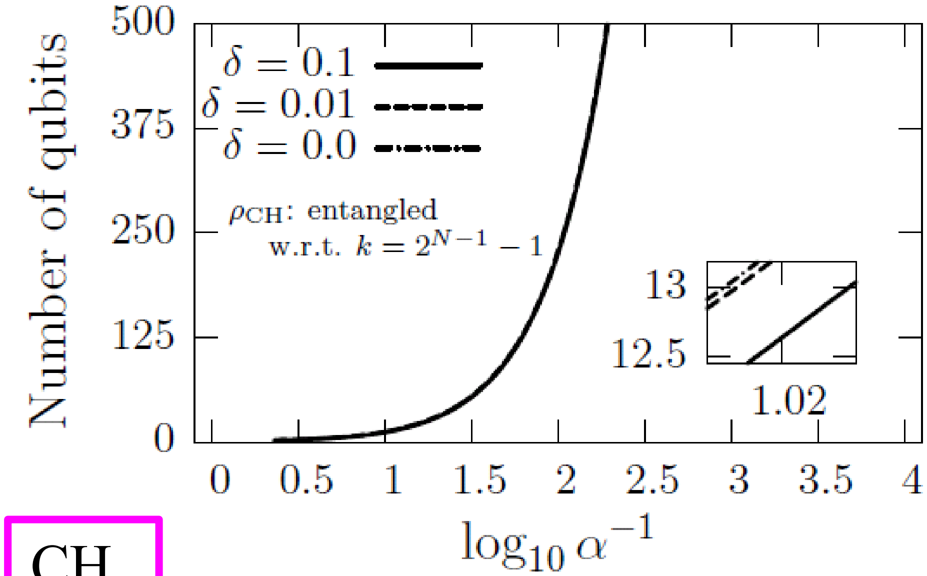
- CH-fanout op. $k = 2^{N-1} - 2^{\lfloor N/2 \rfloor - 1}$

$w = \lfloor N/2 \rfloor$



⋆ **boundary between separability and nonseparability**

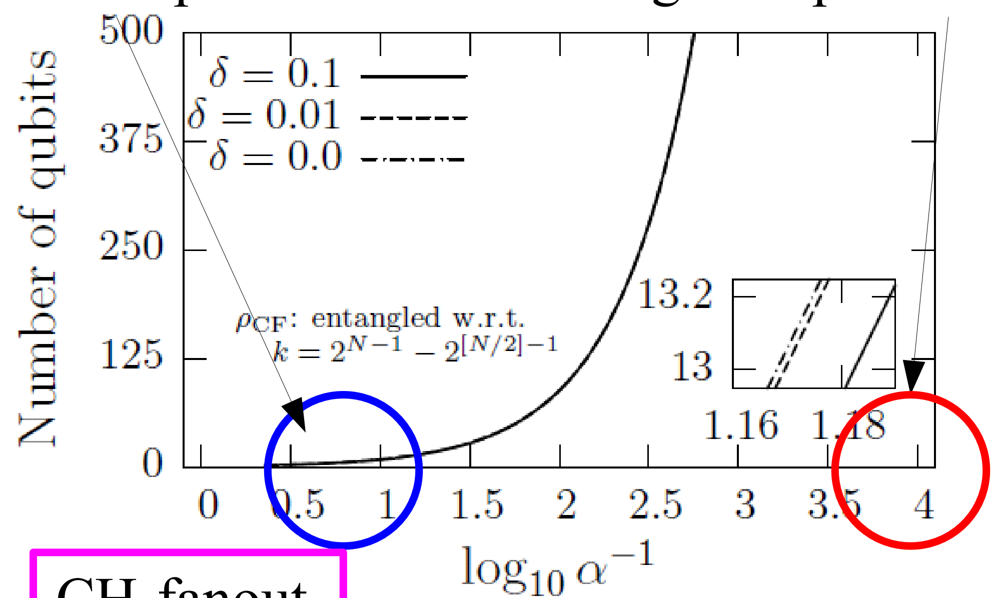
``effect of chemical shift''



CH

low temperature

high temperature



CH-fanout

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

why?? conditions for separability or nonseparablity

→ 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 → negligible !

- connection between entanglement generation and symmetry → not clear ...

→ need to study other model of chemical shift

ex. $\alpha_i \not> 0$, 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

→ application to solid-state NMR experiments ??

★ ability to generate entanglement

Yu-Brown-Chuang:

With respect to the thermal state,

$\rho_{\rm CF}$ **generate entanglement more effectively than** $\rho_{\rm CH}$

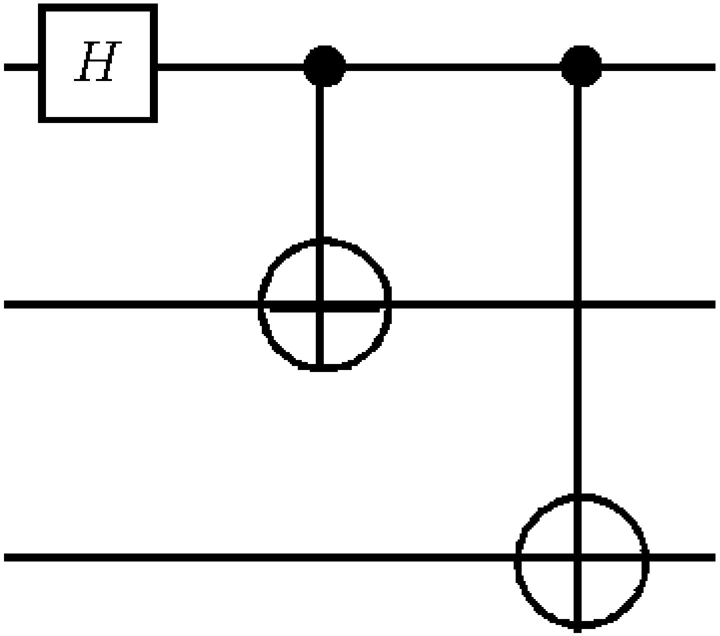
for more detail classification of the ability, ...

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

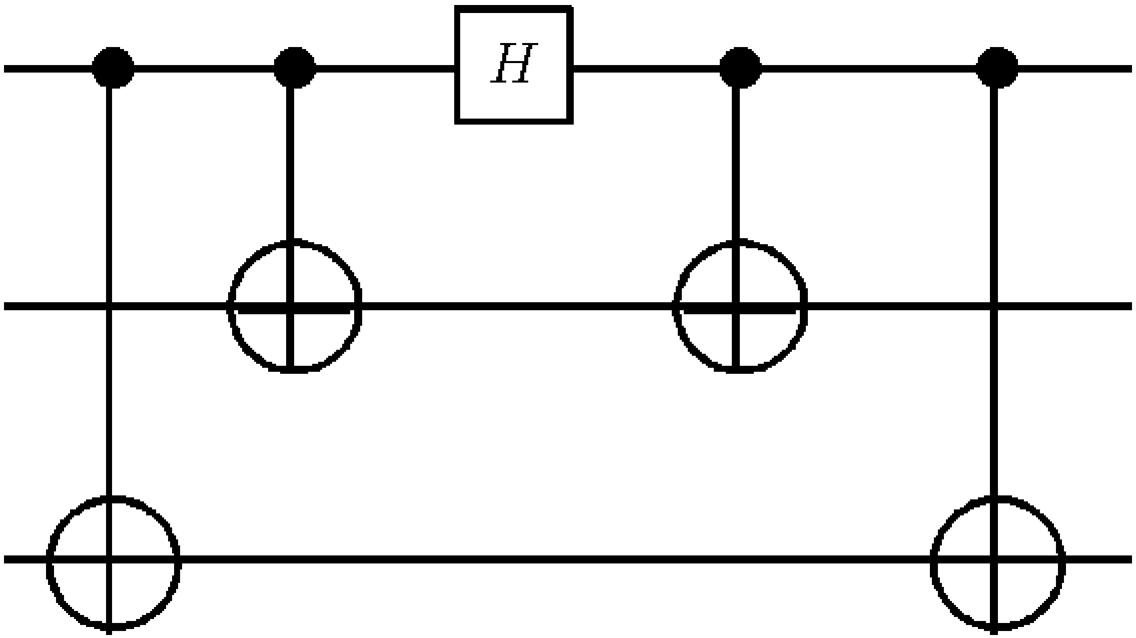
ability of quantum gates to generate entanglement

two quantum gates

N=3



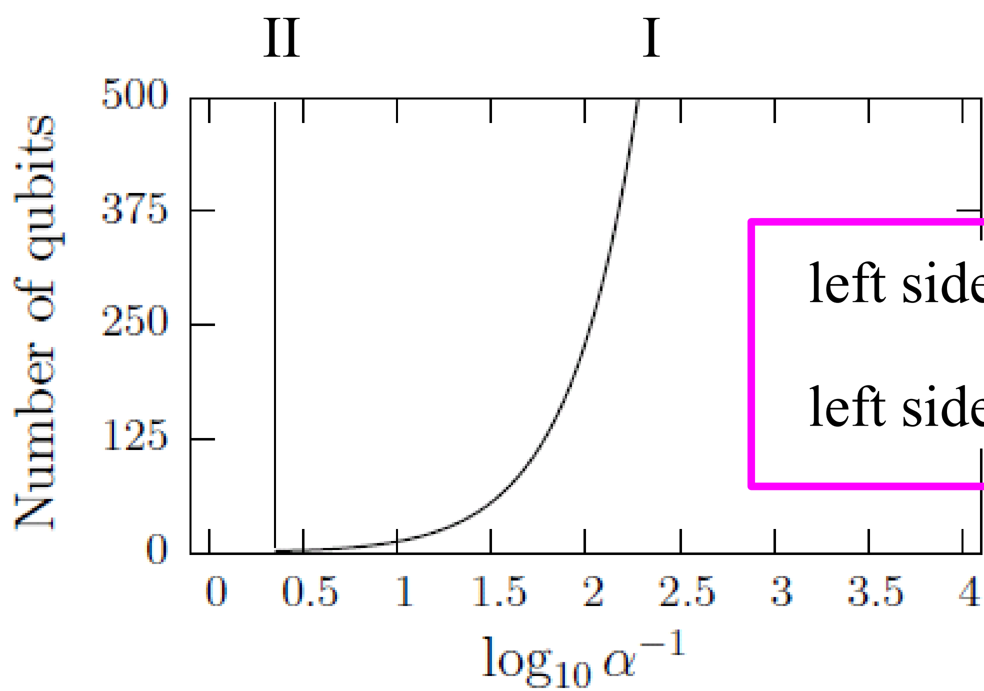
$$U_{\rm CH} = U_{\rm fan}(H_1 \otimes I)$$



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

ability to generate entanglement from thermal state

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



$$\alpha_i = \alpha$$

left side of line I: ρ_{CF} is fully distillable

left side of line II: ρ_{CH} is fully distillable

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, ... → trial !!

logarithmic negativity $E_N(\rho) = \log_2 \|\rho^{T_B}\|_1$ PRA**65**, 032314

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

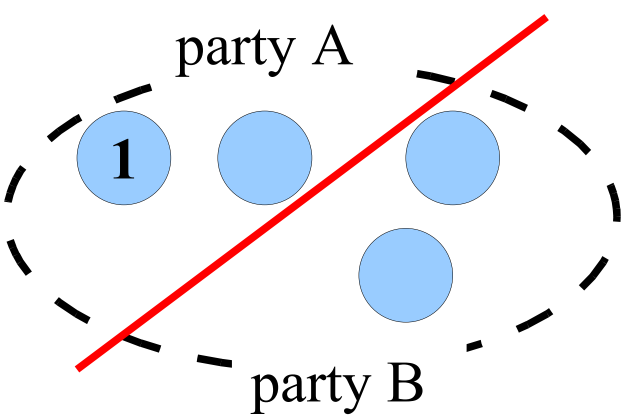
separable: 0
maximal entangled state: 1

hereafter $\alpha_i = \alpha$

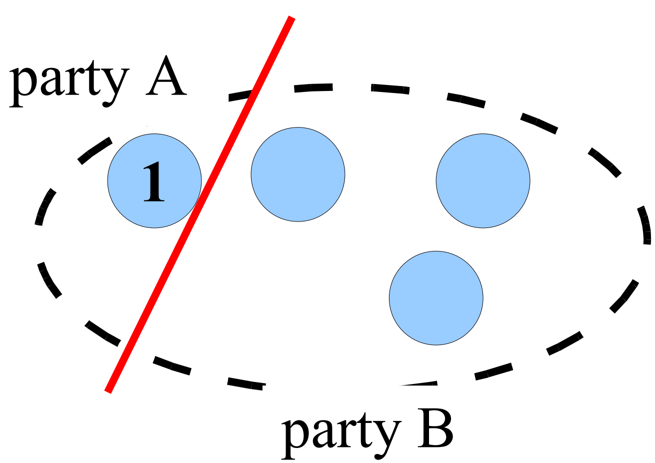
showing results for three types of w

w: number of elements in party B

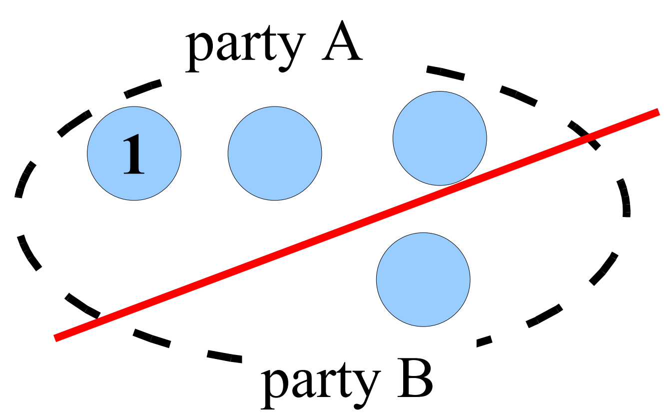
$w = \lfloor N/2 \rfloor$



$w = N - 1$



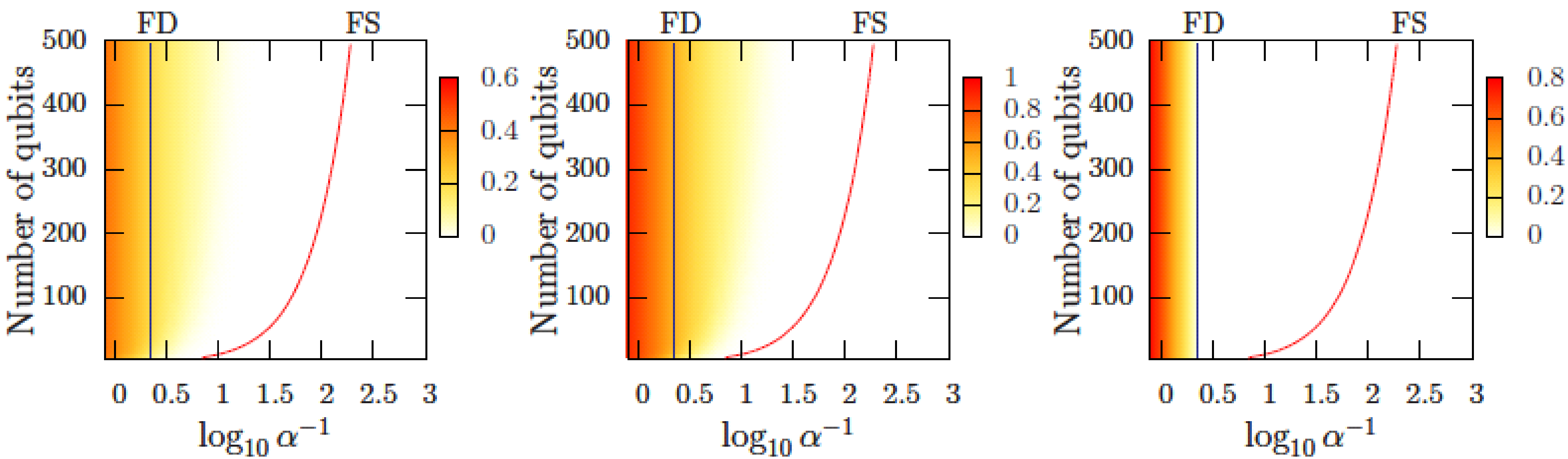
$w = 1$



Result II: logarithmic negativity

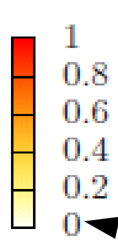
ρ_{CH}

$w = \lfloor N/2 \rfloor$ $\quad$ $w = N - 1$ $\quad$ $w = 1$



left side of FD ⟺ full distillable $\quad$ right side of FS ⟸ full separable

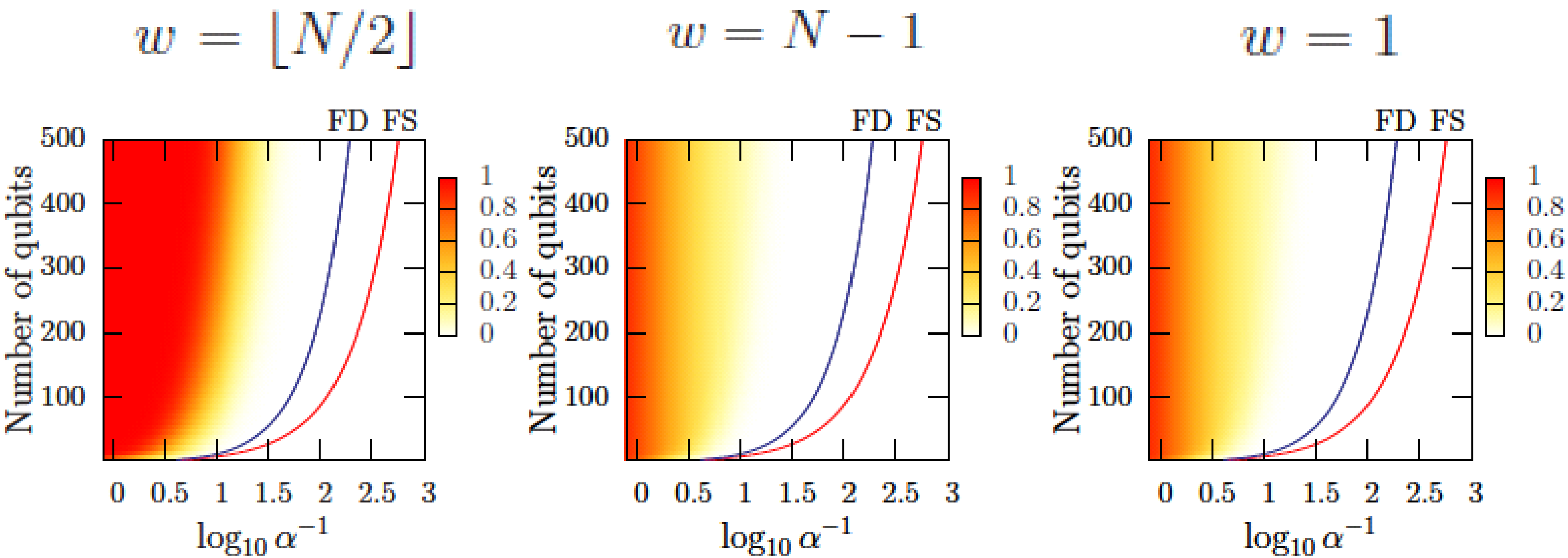
value of $E_{\mathcal{N}}(\rho)$



maximal entangled state

separable state

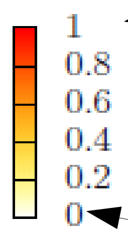
ρ_{CF}



left side of FD ⟺ full distillable

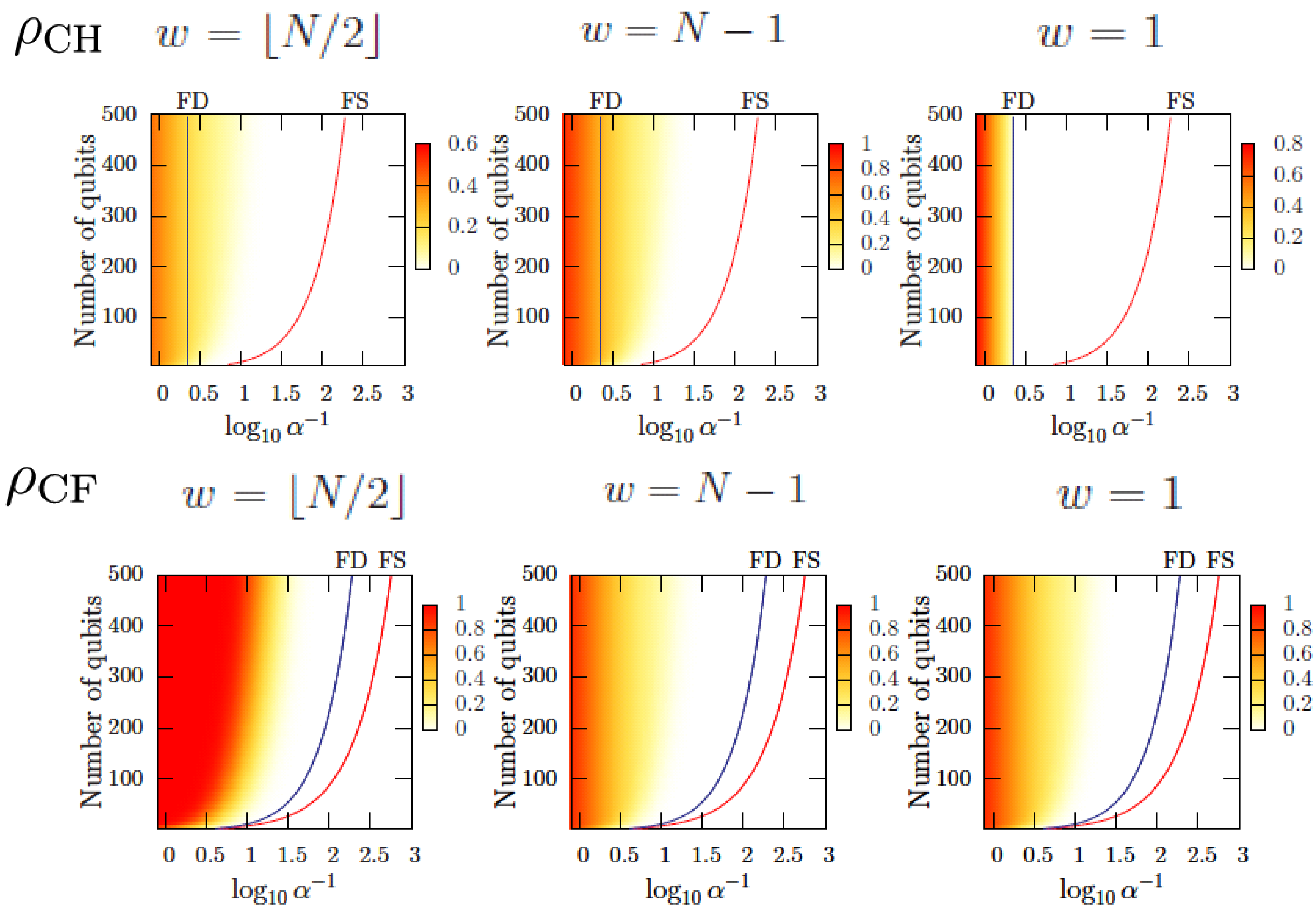
right side of FS ⟸ full separable

value of $E_{\mathcal{N}}(\rho)$



maximal entangled state

separable state



increasing rate → 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

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

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

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

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

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

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!! Δ , $2\lambda_k$

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

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

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

1. simultaneous spin-flip operation

$$\mathcal{L}_1\,\rho = \frac{1}{2}\rho + \frac{1}{2}\left(\sigma_x^1 \otimes \ldots \otimes \sigma_x^N\right)\rho\left(\sigma_x^1 \otimes \ldots \otimes \sigma_x^N\right)$$

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 kth qubit

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

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

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

3. local random phase operation

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

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

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

in summary, ...

$$\rho_N = \underbrace{\mathcal{L}_{\mathrm{LRP}}\mathcal{L}_N \ldots \mathcal{L}_2\mathcal{L}_1}\, \rho$$

$$\lambda_0^{\pm} = \langle \Psi_0^{\pm} | \rho | \Psi_0^{\pm} \rangle$$

$$2\lambda_j = \langle \Psi_j^{+} | \rho | \Psi_j^{+} \rangle + \langle \Psi_j^{-} | \rho | \Psi_j^{-} \rangle$$

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 $\longrightarrow$ ρ_{iso}: entangled $\Longleftrightarrow$ $f > 1/3$

($\Rightarrow$, because $N = 2$)

on the other hand,

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

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

$\longrightarrow$ $f > 1/3 \Rightarrow \rho_{iso}$: entangled   consistent !

Example 2: NOT WORK !!

slightly different from the previous example ...

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

PPT criterion $\longrightarrow$ ρ'_{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

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

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

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

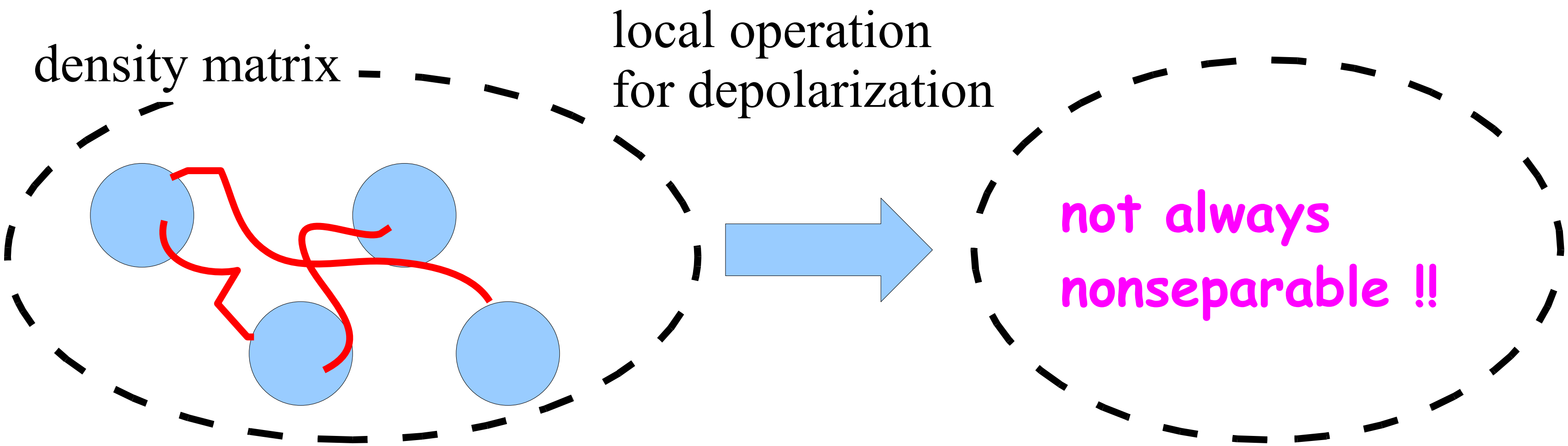
$$\begin{aligned}\mathcal{L}_{LRP}\rho'_{iso} \;=\; & \frac{1-f}{4}|0\rangle_1\langle 0| \otimes |0\rangle_2\langle 0| + \frac{1-f}{4}|1\rangle_1\langle 1| \otimes |1\rangle_2\langle 1| \\ & + \frac{1+f}{4}|0\rangle_1\langle 0| \otimes |1\rangle_2\langle 1| + \frac{1+f}{4}|1\rangle_1\langle 1| \otimes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

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 (?)

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