Exploring Entanglement with Molecules

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I. Introduction : definition and characterization of bipartite entanglement

II. Entanglement characterization with molecular orientation correlations

III. Molecular Chain

Pure and mixed state

Pure state :

We know with certainty the state of the system

$$\cancel{e^{i\phi}}\, |\psi\rangle \in \mathcal{H} \quad \text{with } \langle\psi|\psi\rangle = 1$$

or

Density operator $\rho = |\psi\rangle\langle\psi|$ with $\mathrm{tr}[\rho] = \mathrm{tr}[\rho^2] = 1$

For a pure state, ρ is the projector on $|\psi\rangle$

Pure and mixed state

Mixed state :

Probabilistic description of our knowledge about the system $\rho : \mathcal{H} \to \mathcal{H} \quad \rho = \rho^\dagger \quad \rho > 0 \quad \mathrm{tr}[\rho] = 1$

$$\mathrm{tr}[\rho^2] < 1$$

example: $\rho = \sum_i p_i |\phi_i\rangle\langle\phi_i| \quad p_i > 0 \quad \sum_i p_i = 1$

von Neumann entropy: $S = -\mathrm{tr}[\rho \ln \rho]$

Pure state $S = 0$

Mixed state $S > 0$

Expectation value of an observable

Let O hermitian operator

ρ state of the system

The expectation of O : $\langle O \rangle_\rho$

$$\langle O \rangle_\rho \equiv \mathrm{tr}\left[O\rho \right]$$

If ρ is pure, $\rho = |\psi\rangle\langle\psi|$

$$\langle O \rangle_\rho = \langle \psi | O | \psi \rangle$$

Entanglement Definition

for a pure state

Two Quantum sub-systems a and b of S:

$$|\phi\rangle_a \in \mathcal{H}_a; \quad |\phi\rangle_b \in \mathcal{H}_b \quad |\Psi\rangle \in \mathcal{H}_a \otimes \mathcal{H}_b$$

The state of the system is entangled if it is not a product

Examples :

$|\Psi\rangle = |\phi\rangle_a \otimes |\psi\rangle_b$ is separable

$|\Psi\rangle = |\phi\rangle_a \otimes |\psi\rangle_b + |\psi\rangle_a \otimes |\phi\rangle_b$ is entangled

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Entanglement characterization
for a bipartite pure state

A pure state is entangled $\Leftrightarrow$ reduced state is a mixed state

$$\rho = |\Psi\rangle\langle\Psi|; \quad \rho_a = \mathrm{tr}_b[\rho] \equiv \sum_i {}_b\langle\phi_i|\rho|\phi_i\rangle_b$$

$|\Psi\rangle$ is entangled $\Leftrightarrow$ ρ_a mixed state $\Leftrightarrow$ $S[\rho_a] > 0$

$S[\rho_a]$ is the von Neumann entropy

Conclusion:

Answering the question : « is $|\Psi\rangle$ entangled ? »

is a simple task

Entanglement Definition
for a mixed state

The state of the system is entangled if it is not separable

Separable state : $\rho = \sum_i p_i \rho_i^a \otimes \rho_i^b; \quad p_i > 0; \quad \sum_i p_i = 1$

OPEN PROBLEM :

Necessary and sufficient condition for the separability of mixed states with dim>2x3

Motivation : Entanglement between N>3 levels systems

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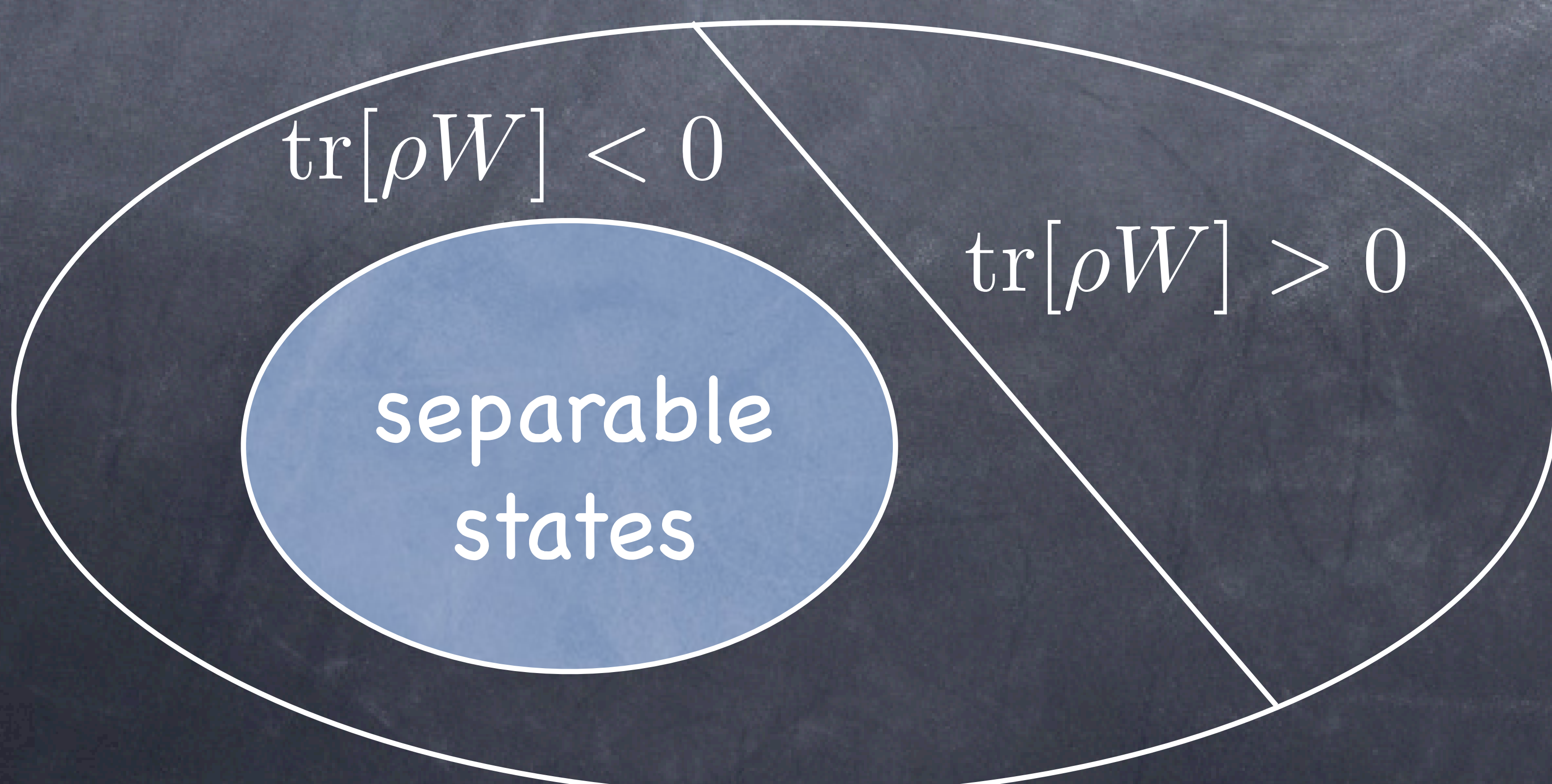
Entanglement witness

W operator such that:

$\mathrm{tr}[\rho W] > 0 \Rightarrow$ state ρ is entangled

$\mathrm{tr}[\rho W] < 0$ nothing can be concluded

Sufficient but not necessary entanglement criterion



Entanglement witness

Example CHSH inequality 2-levels system

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \qquad \sigma(\theta) = \cos\theta\sigma_z + \sin\theta\sigma_x$$

Correlator : $C(\theta, \theta') = \sigma^a(\theta) \otimes \sigma^b(\theta')$

$$W(\theta, \theta') \equiv \quad C(0,0) + C(\theta, 0) + C(0, \theta') - C(\theta, \theta')$$

If ρ is separable then $|\mathrm{tr}\,[\rho W(\theta, \theta')]| \leq 2$

But $\sup\limits_{\theta, \theta', \rho} |\mathrm{tr}\,[\rho W(\theta, \theta')]| = 2\sqrt{2} > 2$

Motivation

Molecules as a tool for exploring entanglement in N-levels systems

- Molecular orientation correlation based CHSH inequality, for detecting entanglement
- Molecular chains
  - Thermal entanglement
  - Information transfer

N levels systems = rotational levels

$$H = BJ^2 \qquad U(t) = e^{-iBJ^2 t}$$

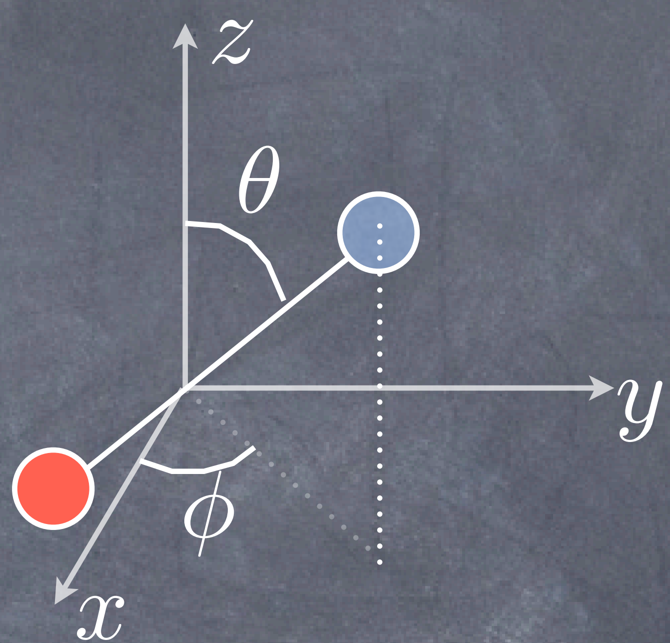
$$J^2|j,m\rangle = j(j+1)|j,m\rangle$$

$$\langle \theta, \phi | jm \rangle = Y_{jm}(\theta, \phi)$$

$$J_z|j,m\rangle = m|j,m\rangle$$

$$m = -j, -j+1, \cdots, j$$

$$E_{Jm} = Bj(j+1)$$



$j = 3$

$j = 2$

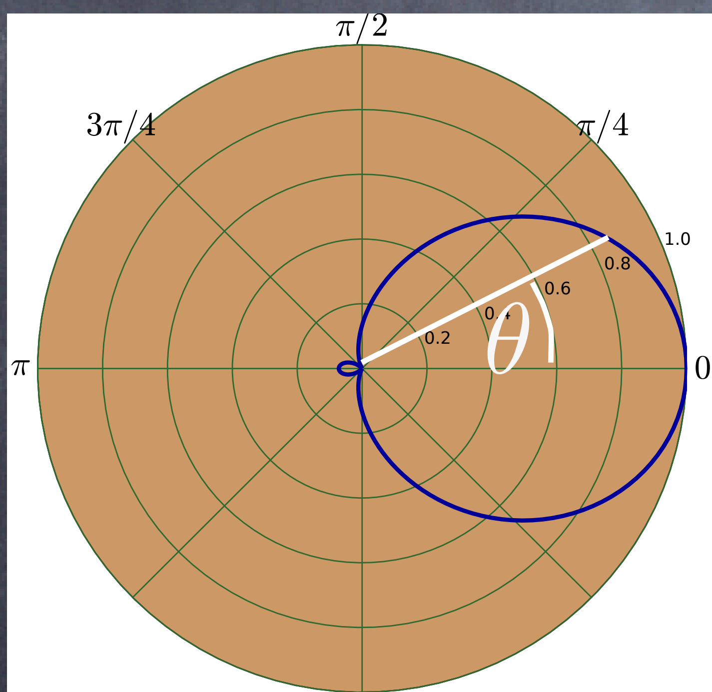
$j = 1$

$j = 0$

Oriented states

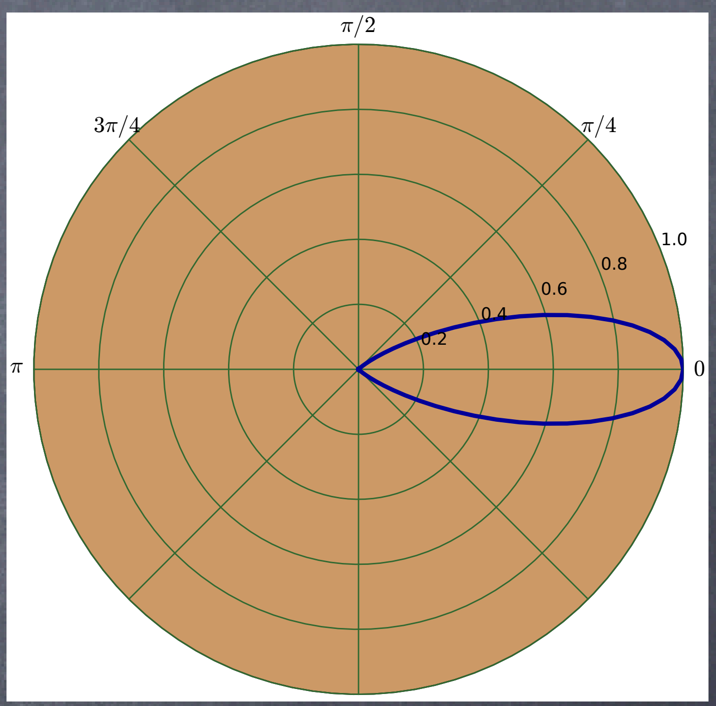
Orientation observable: $\hat{O} \equiv \cos(\hat{\theta})$

Orientation of a state : $O = \langle \hat{O} \rangle_\rho \equiv \mathrm{tr}[\rho \hat{O}]$



$$|\lambda_{j_{\max}}\rangle = \sum_{j=|m|}^{j_{\max}} C_j |j, m\rangle$$

$$\hat{O}|\lambda_{j_{\max}}\rangle = \lambda_{j_{\max}} |\lambda_{j_{\max}}\rangle$$



$j_{\max} = 1$
$O = 0.57$

$j_{\max} = 5$
$O = 0.96$

Oriented state are not stationary :

$$O(t) = \langle U^{-1}(t) \hat{O} U(t) \rangle_\rho$$

Orientation correlations

Correlator: $\hat{C}(t_1,t_2)=\hat{O}_1(t_1)\otimes\hat{O}_2(t_2)$

$$\hat{O}_i(t)\equiv U^{-1}(t)\hat{O}_iU(t),\ \hat{O}_i\equiv\cos(\hat{\theta}_i)$$

Witness: $\hat{W}(t_1,t_2)=\hat{C}(0,0)+\hat{C}(t_1,0)+\hat{C}(0,t_2)-\hat{C}(t_1,t_2)$

- if $\left|\langle\hat{W}(t_1,t_2)\rangle_\rho\right|>2$ then ρ is entangled

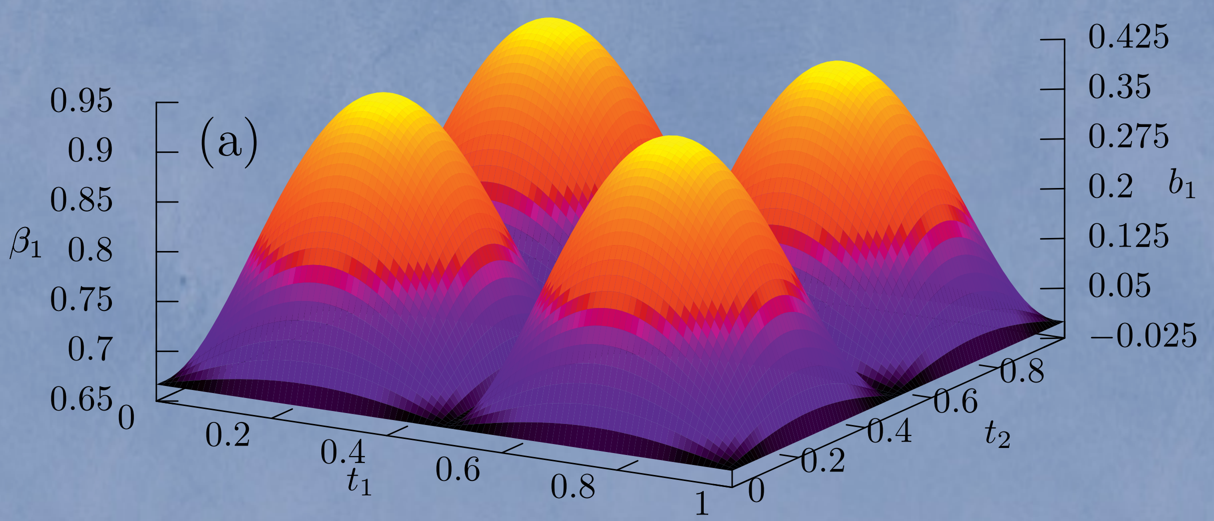
- if we know that $j\leq j_{\max}$ then:

  if $\left|\langle\hat{W}(t_1,t_2)\rangle_\rho\right|>2\lambda^2_{j_{\max}}$ then ρ is entangled

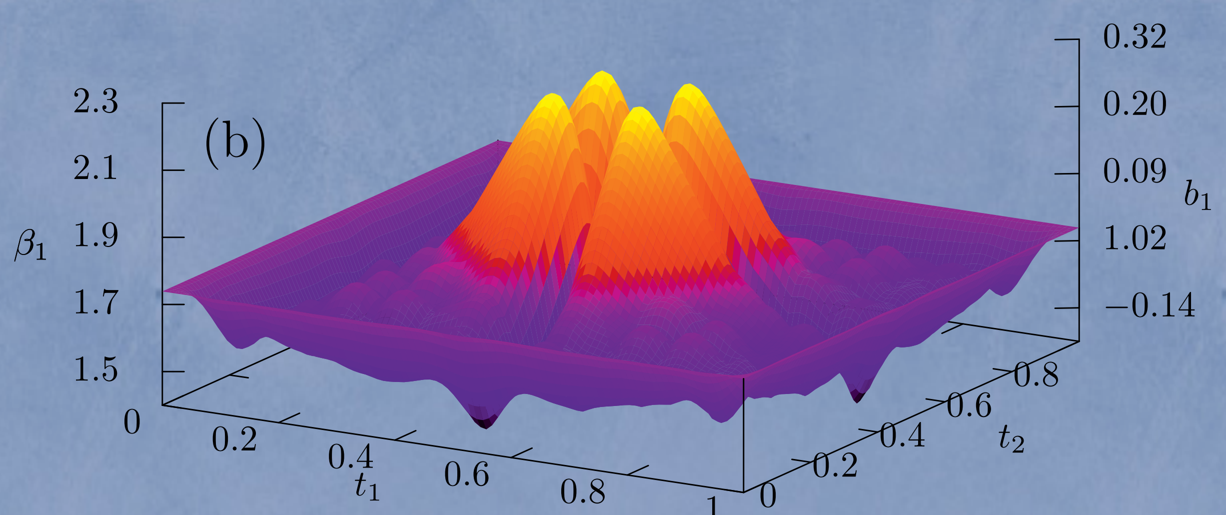
II-Entanglement characterization

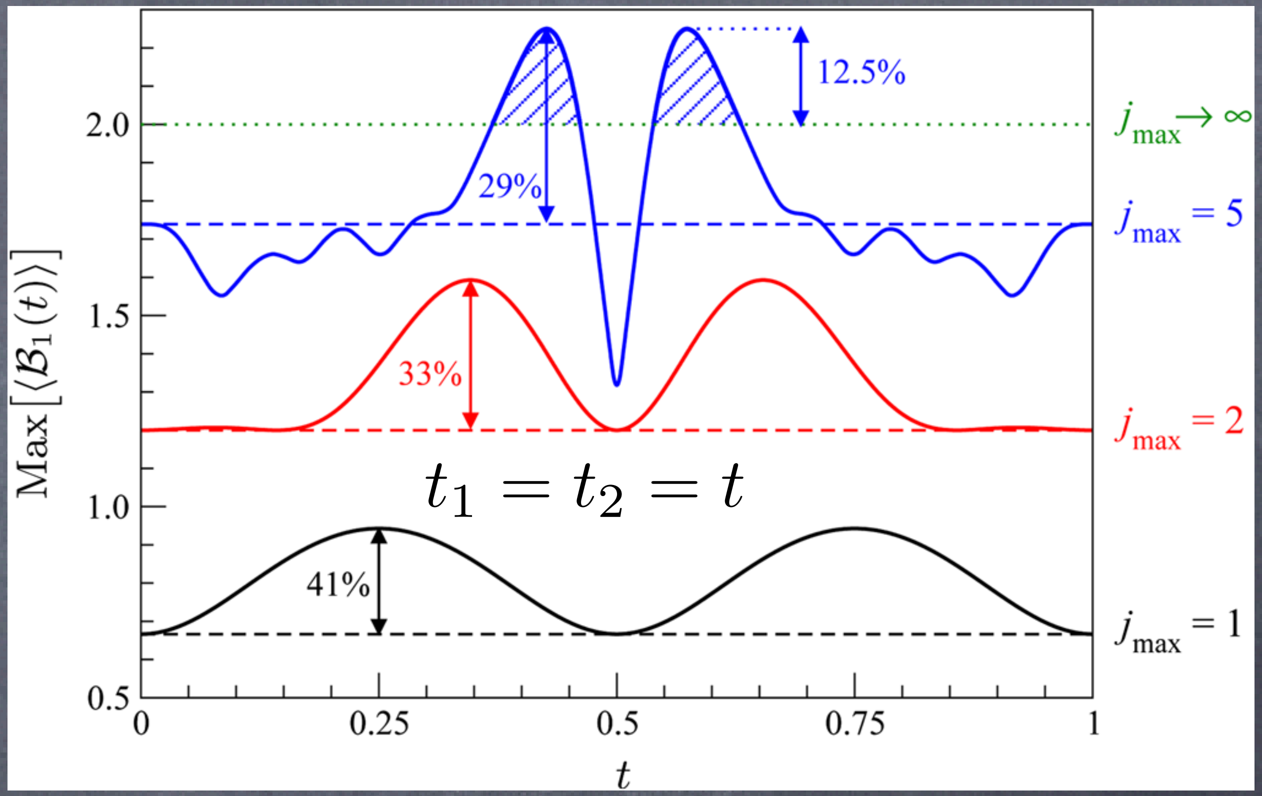
$$\max_{|\psi\rangle} \langle\psi|\hat{W}(t_1, t_2)|\psi\rangle$$

$j_{\max} = 1$



$j_{\max} = 5$





$$\exists(t_1, t_2), \hat{W}(t_1, t_2)$$

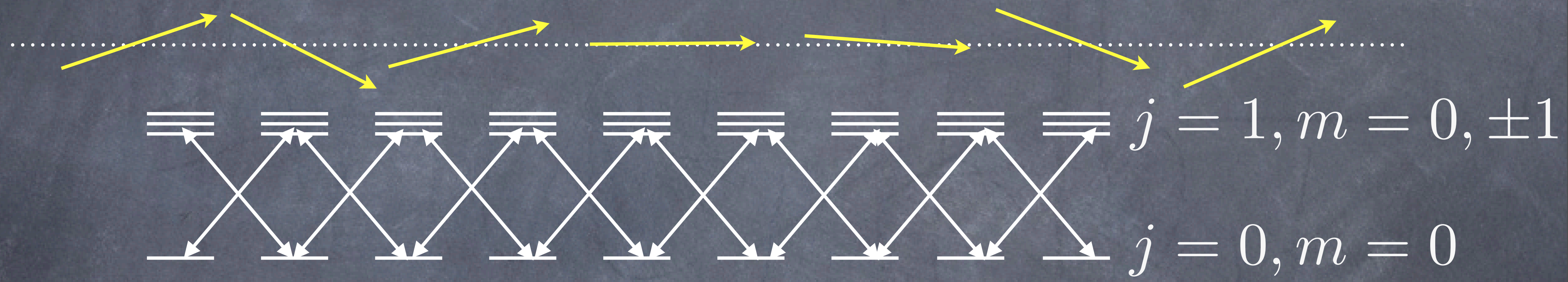
is an entanglement witness

P. Milman et al. Phys. Rev. Lett. (2007)

P. Milman, et al. Eur. Phys. J. (2009)

Entanglement in many body systems

Finite chain of N polar molecules

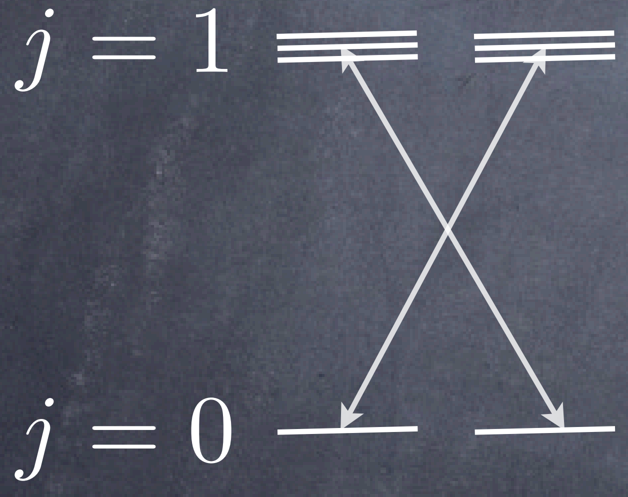


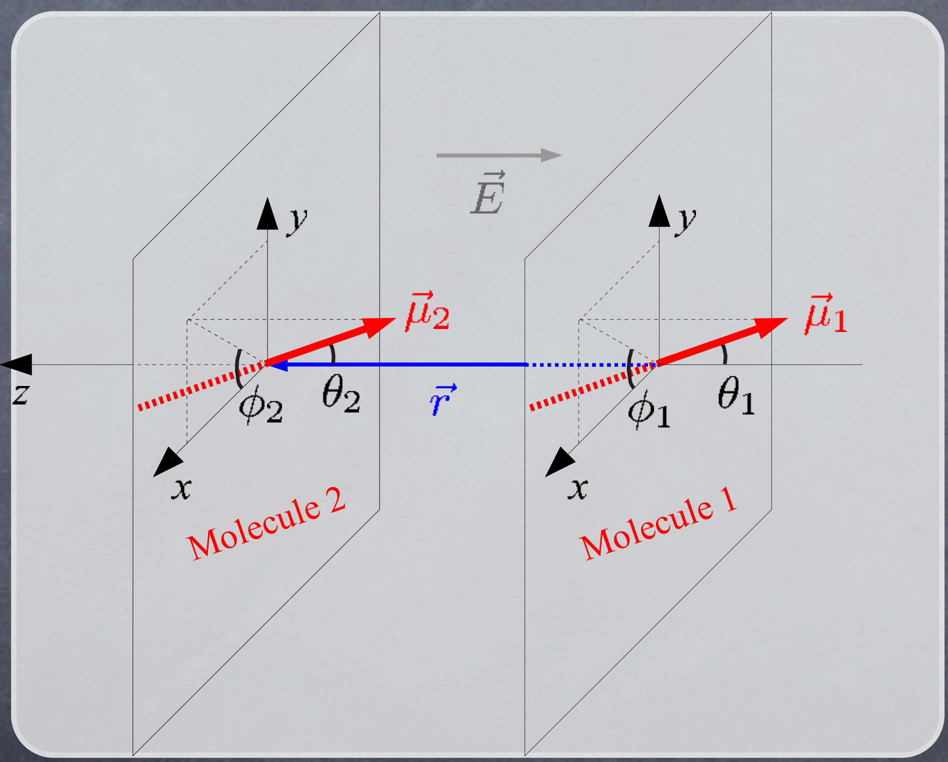
Questions:

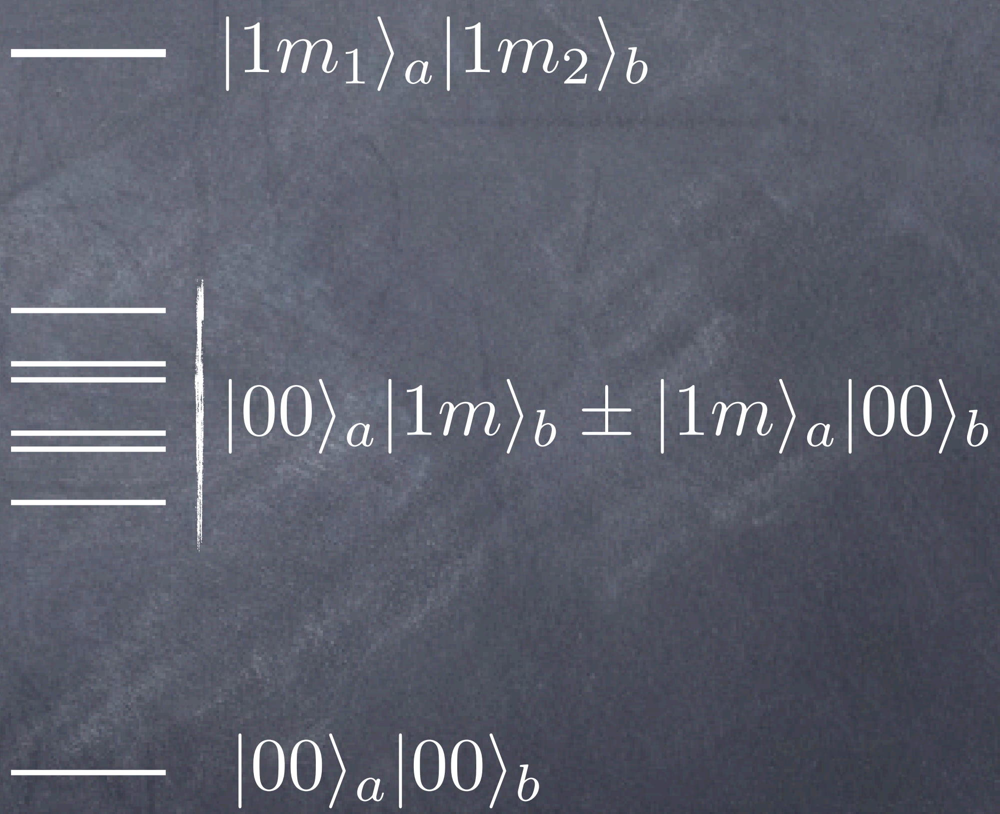
- Entanglement as a function of temperature
- Information transmission along the chain

Dipole-Dipole interaction

$$V_\mathrm{d}(\vec{r}) = \frac{\mu_1 \mu_2}{4\pi\epsilon_0 r^3}\left[-2\cos\theta_1\cos\theta_2 + \sin\theta_1\sin\theta_2\cos(\phi_1 - \phi_2)\right]$$







Dipole-Dipole interaction creates entanglement

Hamiltonian of the chain

$$H = \sum_{m=0\pm1} H^{(m)} \qquad \sigma_i^{+(m)} = |1_i m_i\rangle\langle 0_i 0_i| \qquad \sigma_i^{-(m)} = |0_i 0_i\rangle\langle 1_i m_i|$$

$$H^{(m)} = 2B\sum_{i=1}^{N}\sigma_i^{+(m)}\sigma_i^{-(m)} + v^{(|m|)}\sum_{i=1}^{N-1}\left[\sigma_i^{+(m)}\otimes\sigma_{i+1}^{-(m)} + \sigma_i^{-(m)}\otimes\sigma_{i+1}^{+(m)}\right]$$

$$\left[H^{(m)}, \sum_{i=1}^{N}\sigma_i^{+(m)}\sigma_i^{-(m)}\right] = 0$$

In the mono-excited subspace: $\langle\sum_{i=1}^{N}\sigma_i^{+(m)}\sigma_i^{-(m)}\rangle \leq 1$

$$[H^{(m)}, H^{(m')}] = 0$$

3 indépendents XX-Heisenberg Chains $(m = 0 \pm 1)$

$$E_{k_m}^{(|m|)} = 2B + 2v^{|m|}\cos(\frac{k_m\pi}{N+1}); (k_m = 1, 2, \cdots, N)$$

$$|\psi_{k_m}\rangle = \sqrt{\frac{2}{N+1}}\sum_{j=1}^{N}\sin(\frac{jk_m\pi}{N+1})|00\rangle_1\otimes\cdots\otimes|1m\rangle_j\otimes\cdots\otimes|00\rangle_N$$

Entanglement Measure

let $\rho = \sum_{ijkn} \rho_{ijkn} |i\rangle_a \langle j| \otimes |k\rangle_b \langle n|$

Partial transpose $\rho^{T_a} = \sum_{ijkn} \rho_{jikn} |i\rangle_a \langle j| \otimes |k\rangle_b \langle n|$

Diagonalisation $= \sum_{m} r_m |\Psi_m\rangle \langle \Psi_m|$

$$\mathcal{N}(\rho) = \sum_{r_m<0} |r_m|$$

Negativity

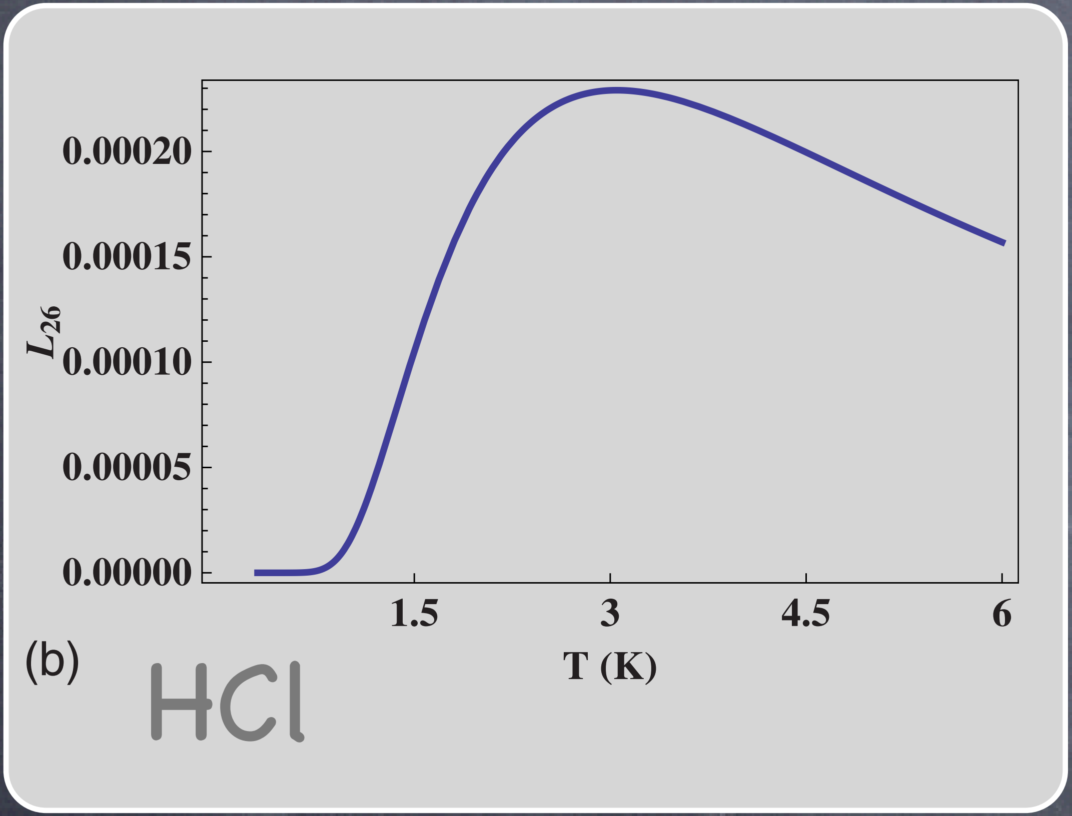
$$E_N(\rho) = \log_2(2\mathcal{N} + 1)$$

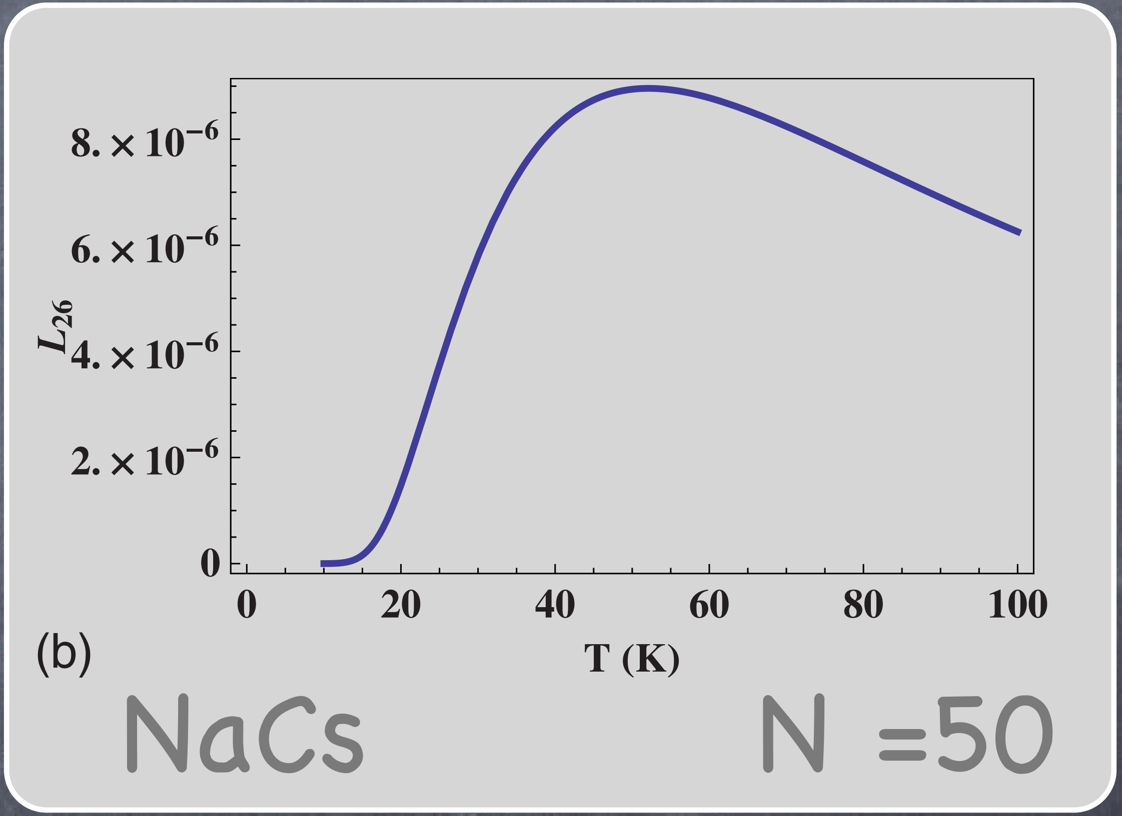
Logarithmic negativity

measures by how much ρ^{T_A} fails to be positive definite

Thermal entanglement

$$\rho = \frac{1}{Z}\exp - \frac{H}{k_B T}$$



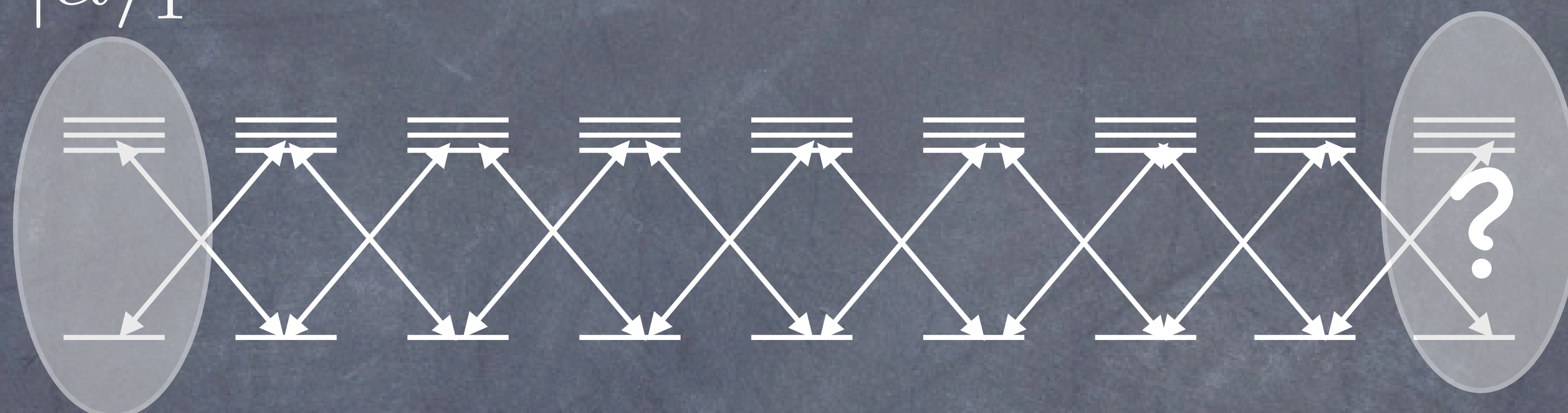


Entanglement of a molecule with the rest of the chain increases with the temperature.

P. Milman, A. Keller, Phys. Rev. A. **79**, 52303 (2009).

Information transmission along the chain

$t = 0 \;\; |\alpha\rangle_1$ $\qquad\qquad$ $|\alpha\rangle_N$



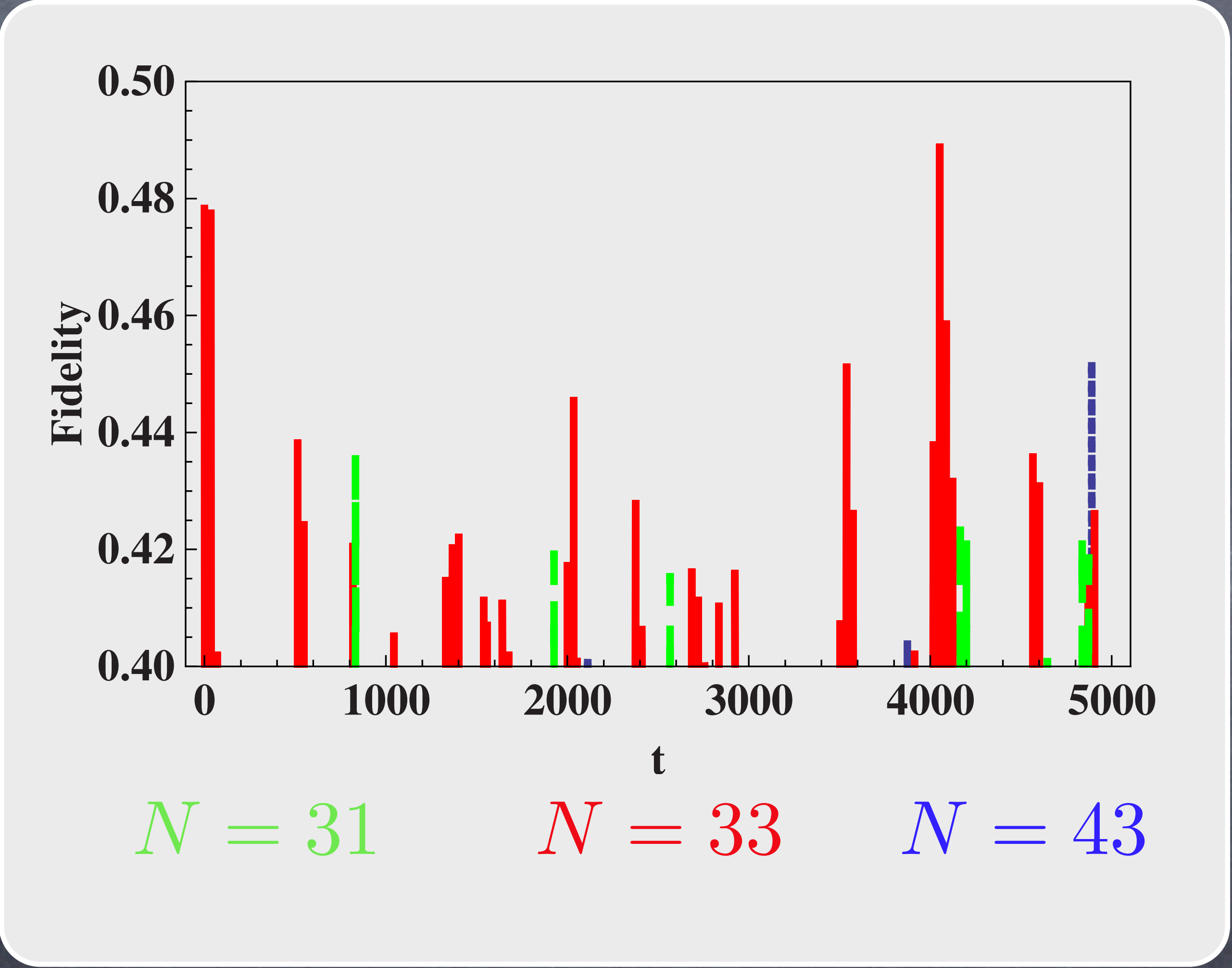
$$t > 0 \quad \rho(t) = \mathrm{tr}_{1\ldots N-1}\left[U(t)|\alpha\rangle_1\langle\alpha|U^{-1}(t)\right]$$

Fidelity : $F(t) = \mathrm{tr}\left[\rho(t)|\alpha\rangle_N\langle\alpha|\right] = \langle\alpha|\rho(t)|\alpha\rangle_N$

$\langle F(t)\rangle \equiv$ averaged over all input states

Classical communication $\langle F(t)\rangle \leq \dfrac{2}{d+1} = \dfrac{2}{5}$

Information transmission along the chain



$$\langle F(t) \rangle > \frac{2}{5}$$ Quantum transmission

Perfect state transfer with 2 levels systems

$$\sigma_i^+ = |1\rangle_i\langle 0| \qquad \sigma_i^- = |0\rangle_i\langle 1|$$

$$H = \sum_{i<j=1}^{N-1} \left[h_{ij}\sigma_i^+ \otimes \sigma_j^- + h_{ij}^* \sigma_j^+ \otimes \sigma_i^- \right]$$

Objective : find $h_{j'j}$ such that perfect transfer occurs at a time t>0

Perfect state transfer with 2 levels systems

Dynamics takes place in the mono-excited subspace

$$|j\rangle \equiv |0\rangle_1 \otimes |0\rangle_2 \otimes \cdots \otimes |1\rangle_j \otimes |0\rangle_{j+1} \otimes \cdots \otimes |0\rangle_N \; (j = 1, \cdots, N)$$

$$|0\rangle \equiv |0\rangle_1 \otimes |0\rangle_2 \otimes \cdots \otimes |0\rangle_j \otimes |0\rangle_{j+1} \otimes \cdots \otimes |0\rangle_N$$

$$|\psi(t=0)\rangle = \alpha|0\rangle + \beta|1\rangle \longrightarrow |\psi(t>0)\rangle = e^{-iHt}\left[\alpha|0\rangle + \beta|1\rangle\right] = \alpha|0\rangle + \beta e^{-iht}|1\rangle$$

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

$$\rho(t) = \mathrm{tr}_{1\dots N-1}|\psi(t>0)\rangle\langle\psi(t>0)|$$

$$F(t) = \langle\psi(0)|\rho(t)|\psi(0)\rangle = \left(|\alpha|^4 + |\beta|^4\right)|U_{N1}(t)|^2 + 2\,|\alpha|^2\,|\beta|^2\,\Re\left[U_{N1}(t)\right]$$

$$F(t) = \mathrm{cte} \neq 0 \forall \alpha, \beta \Leftrightarrow F(t) = 1 \forall \alpha, \beta \Leftrightarrow U_{N1}(t) = 1$$

where $U_{N1}(t) = \langle N|e^{-iht}|1\rangle$ h is a $N \times N$ hermitian matrix

Perfect state transfer with 2 levels systems

Finally the problem reduces to:

We look for the hermitian $N \times N$ matrix h

with $h_{nn} = 0 \quad (n = 1, \cdots, N)$

such that $\exists t \in \mathbb{R}^+ \langle 1|e^{-iht}|N\rangle = 1$

Perfect state transfer with 2 levels systems

One Solution: (M. Christandl et all Phys. Rev. Lett 2004)

nearest neighbors $h_{nn'} = (K_n \delta_{n'n-1} + K_n^* \delta_{n'n+1})$

Mapping to angular momentum states $|n\rangle \leftrightarrow |J,m\rangle$

N odd $J = \frac{N-1}{2}$ $m = -J + n - 1;\; n \in [1, N]$ $m \in [-J, J]$

$$J_y = \frac{1}{2i}\Big[\sqrt{J(J+1) - m(m+1)}|J, m+1\rangle\langle J, m|$$
$$\sqrt{J(J+1) - m(m-1)}|J, m-1\rangle\langle J, m|\Big]$$

$h \leftrightarrow J_y$: $U_{N1}(t) \leftrightarrow \langle J, J| \exp^{-iJ_y t}|J, -J\rangle = D^J_{J,-J}(0,t,0) = \left(\sin\frac{t}{2}\right)^{2J}$

Perfect transfer $t = \pi$ $U_{N1}(t) = 1$

Perspectives

- Detecting entanglement measuring correlation of photons orbital angular momentum instead of molecules.

- How to find others chains with perfect transfer
- How to explore all the solutions in the mono-excited subspace
- Explore the relation between entanglement and quantum state transfer
- Extension to multi-excited subspace