Excitonic qubit dynamics on complex networks in presence of a local phonon environment : perturbative approach vs. exact calculations.

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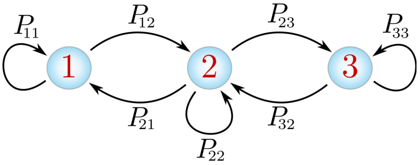
I) "Walk on network" : a powerful paradigm for information science

Classical walk on network : the MCMC example

The base of a network : **nodes** and **bonds**.



The **transition matrix** of the network :

$$\Longrightarrow P = \begin{pmatrix} P_{11} & P_{12} & 0 \\ P_{21} & P_{22} & P_{23} \\ 0 & P_{32} & P_{33} \end{pmatrix}$$

In classical information theory :

- Research time in a database
- Nodes ranking
- Monte Carlo algorithms ...

In quantum information theory :

- Grover's research algorithm
- Quantum "Hitting time"
- Quantum state transfer ...

Question : *How can we concretely generate a quantum walk ?*

II) A realistic quantum walk : model and Hamiltonian

Complex network as supports : a geometrical approach

Polymer chemistry

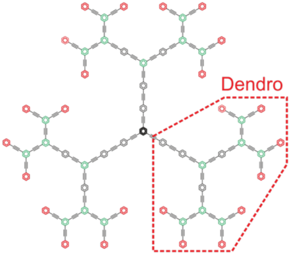


FIGURE : polyphenylacetylene dendrimer (hyperbranched macromolecule)

Real physical networks !

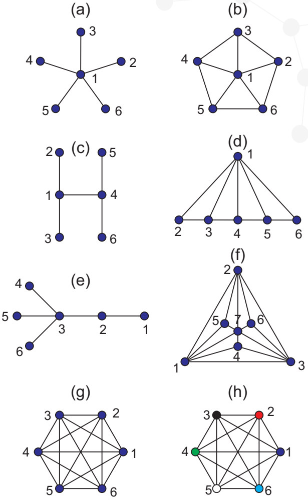


FIGURE : (a) The star graph, (b) the wheel graph, (c) the H graph, (d) the hat graph, (e) the fork graph, (f) the Apollonian network, (g) the complete graph, and (h) the random complete graph.

Excitonic quantum transport

Exciton : Local excited state (electronical, vibrationnal . . .) able to delocalize accross a molecule.

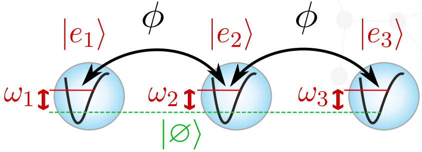


FIGURE : Three molecular subunits interacting with a hopping constant ϕ.

Tight Binding Model

- Each node ⇔ a two level system
- The i^{th} node is associated to the local excited state $|e_i\rangle$
- Global void state $|\varnothing\rangle$ (absence of exciton)

One network ⇔ One Hamiltonian
This "molecular graph" is associated with the following matrix :

$$H_{exc} = \begin{pmatrix} \omega_1 & \Phi & 0 \\ \Phi & \omega_2 & \Phi \\ 0 & \Phi & \omega_3 \end{pmatrix}$$

A local phonon environment : the Holstein model

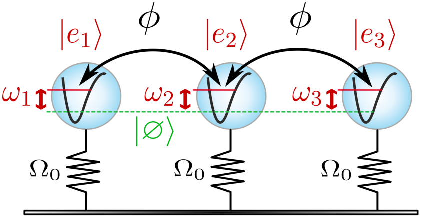


FIGURE : Each site has his own local phononic mode

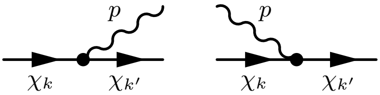
Holstein model : The environment is composed of **local phononic modes**

$$H_{\text{pho}} = \sum_{l=1}^{N} \Omega_0 a_l^\dagger a_l$$

where $a_l/a_l^\dagger$ are the annihilation/creation operators of the "l^{th}" local mode.

Potential deformation model : a local phonon mode interacts with its respective local two level system (with an amplitude Δ_0)

$$\Delta H_{\text{exc-pho}} = \sum_{l=1}^{N} \Delta_0 |e_l\rangle\langle e_l|(a_l^\dagger + a_l)$$



Phonon emission/absorption process

The quantum state transfer problem

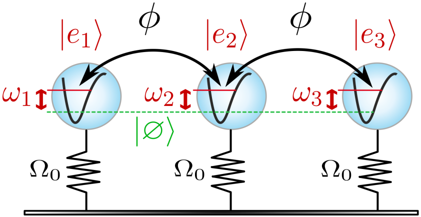


FIGURE : Each site has his own local phononic mode

Problem : estimation of $\mathcal{G}_{fi}(t)$? $\Longleftarrow$

Our task : the quantum state transfer

We study the **excitonic-qubit transmission from a site** i **to a site** f with the elements of an effective propagator $\mathcal{G}$ such as

$$\mathcal{G}_{fi}(t) = \mathrm{Tr}_{\text{pho}}[e^{iH_{\text{pho}}t}\langle e_f|e^{-iHt}|e_i\rangle\rho_{\text{pho}}(0)]$$

with the global hamiltonian

$$H = H_{\text{exc}} + H_{pho} + \Delta H_{\text{exc-pho}}$$

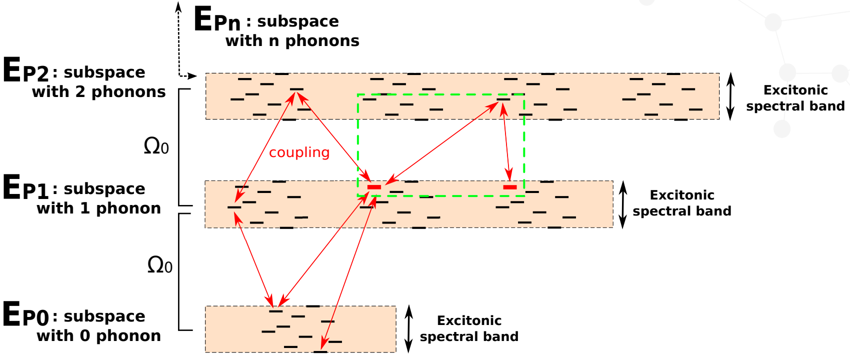
and the initial phonon density matrix

$$\rho_{\text{pho}} = \exp(-\beta H_{\text{pho}})/\mathcal{Z}_{\text{pho}}$$

$\hookrightarrow$ **Numerical way**
A raw method : One builds the hamiltonian matrix H to diagonalize it !

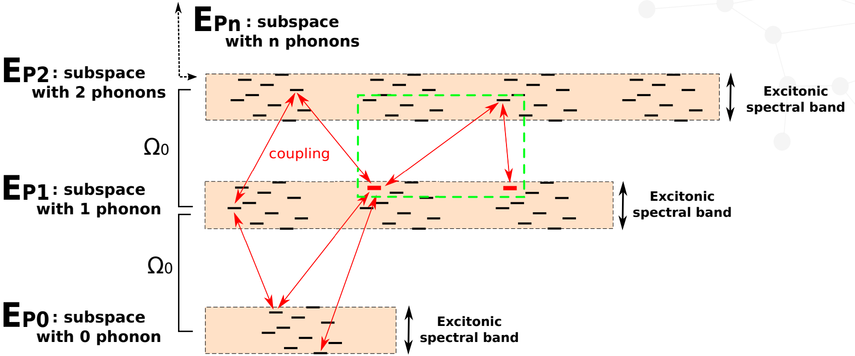
$\hookrightarrow$ **Theoretical way**
A subtile method : One treats H with a judicious perturbative approach

The numerical way : let's build H !



For a network of N sites, we generate **a truncated phonon basis** by fixing the total number of $\mathcal{N}_{\text{pho}}$ phonons
$\hookrightarrow$ "Just enough states" **to obtain a good statistics**

$$\dim(H) = \frac{(\mathcal{N}_{\text{pho}} + N)!}{\mathcal{N}_{\text{pho}}!\,(N-1)!} \longrightarrow \dim(H) = 30030 \text{ if } N = 6, N_b = 9$$



Weak coupling $\Longrightarrow \Delta H_{\text{exc-pho}} \ll H_{\text{exc}} + H_{pho}$, and we introduce a transformation $U = e^{S}$ to bloc diagonalize H according each E_P subspace

$$H = \begin{pmatrix} \blacksquare & \blacksquare \\ \blacksquare & \ddots \end{pmatrix} \longrightarrow \tilde{H} = UHU^{\dagger} = \begin{pmatrix} E_{P0} & 0 & 0 & \dots \\ 0 & E_{P1} & 0 & \dots \\ 0 & 0 & E_{P2} & \dots \\ \vdots & \vdots & \vdots & E_{P\dots} \end{pmatrix}$$

We introduce an **"ansazt"** for the new global Hamiltonian

$$\tilde{H} \simeq \tilde{H}_{\text{exc}} + \sum_k \tilde{H}_{\text{pho}}^{(\tilde{\chi}_k)} |\tilde{\chi}_k\rangle\langle\tilde{\chi}_k|$$

A new **excitonic Hamiltonian :**

$$\tilde{H}_{\text{exc}} = \sum_k \omega_{\tilde{\chi}_k} |\tilde{\chi}_k\rangle\langle\tilde{\chi}_k|$$

In the new point of view, we obtain new excitonic eigenstates with the spectrum of the excitonic Hamiltonian are slighlty modified.

A **new Phonon Hamiltonian :**

$$\tilde{H}_{\text{pho}}^{(\tilde{\chi}_k)} = \sum_{l,p} (\Omega_0 \delta_{lp} + \Lambda_{lp}^{(\tilde{\chi}_k)}) a_l^\dagger a_p$$

$\Longrightarrow$ When the exciton is in a state $|\tilde{\chi}_k\rangle$ a phonon **can jump from a local mode to another one** !

If $|\tilde{\chi}_k\rangle$ is degenerated we set

$$\tilde{H}_{\text{pho}}^{(\tilde{\chi}_k)} \equiv H_{\text{pho}}$$

We introduce an **"ansazt"** for the new global Hamiltonian

$$\tilde{H} \simeq \tilde{H}_{\text{exc}} + \sum_k \tilde{H}_{\text{pho}}^{(\tilde{\chi}_k)} |\tilde{\chi}_k\rangle\langle\tilde{\chi}_k|$$

Thanks to the **diagonalization of the quadratic Hamiltonians** $\tilde{H}_{\text{pho}}^{(\tilde{\chi}_k)}$ we get

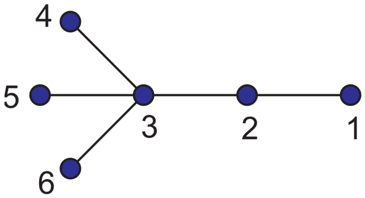
$$\mathcal{G}_{fi}(t) \simeq \sum_k \frac{Z_{\text{pho}}^{(\tilde{\chi}_k)}(t)}{Z_{\text{pho}}} \; e^{-i\omega_{\tilde{\chi}_k} t} \langle f|\tilde{\chi}_k\rangle\langle\tilde{\chi}_k|i\rangle$$

Where we introduce a temporal function of partition $Z_{\text{pho}}^{(\tilde{\chi}_k)}(t)$ depending on the **eigenpulsations** $\{\delta\Omega_q^{(\tilde{\chi}_k)}\}$ of the **phononic jump matrix** $\Lambda^{(\tilde{\chi}_k)}$ as

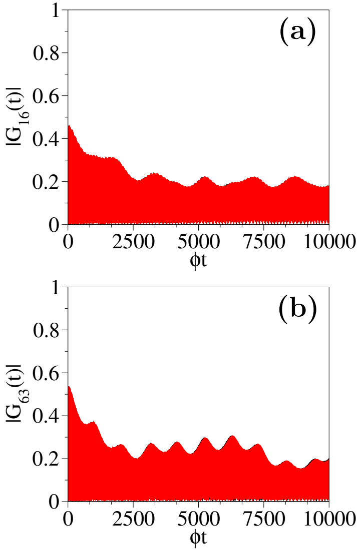
$$Z_{\text{pho}}^{(\tilde{\chi}_k)}(t) = \begin{cases} \prod_q (1 - e^{-(\frac{1}{\alpha} + i\delta\Omega_q^{(\tilde{\chi}_k)} t)})^{-1} & \text{if } |\tilde{\chi}_k\rangle \text{ is not degenerated} \\ 1 & \text{otherwise.} \end{cases}$$

III) Application : comparison of the two methods

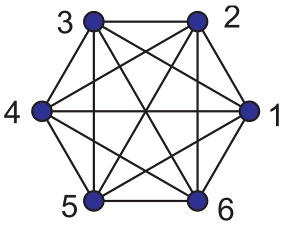
The fork graph : low degeneracy



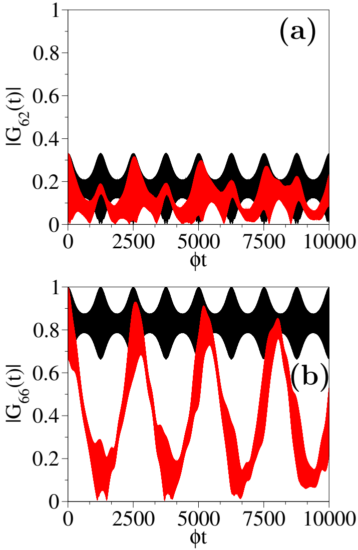
The results are very good ! The two approachs give the same dynamics.



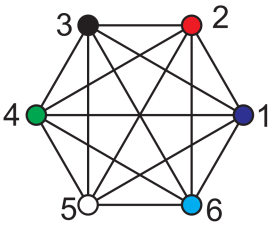
The complete graph : important degeneracy

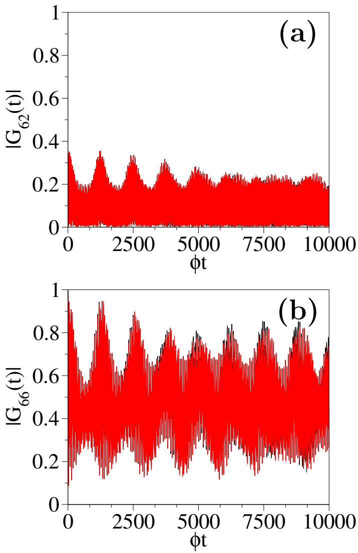


The results are not good at all . . . because of the degeneracy of lot of $|\tilde{\chi}_k\rangle$.



The random complete graph : lift of degeneracy





The results are good ! Thanks to the lift of degeneracy generated by the disorder.

CONCLUSIONS

Numerical way

- Treating HUGE MATRICES (only little networks . . .)
- Needs an efficient truncated basis to get a good statistics
- No real insight on the internal physics (size of the basis . . .)
- Very long simulation : for $N = 6$ sites with $N_b = 9$ phonons (on 16 threads, INTEL MKL, OPEN MP)

$$\Rightarrow \mathbf{T_{sim}} \sim \mathbf{36h}$$

Theoretical way

- Treating $N \times N$ matrices (every networks !)
- Doesn't need any numerical phonon basis
- Real insight on the internal physics : phonon hoping matrices . . .
- Very short simulations : for $N = 6$ sites without any optimization in the code (on 1 thread)

$$\Rightarrow \mathbf{T_{sim}} \sim \mathbf{10s}$$

Thanks for your attention !