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Quantum Dynamical Phase Transition in NMR, Double Quantum Dots and Two Level Systems

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These are preliminary lecture notes, intended only for distribution to participants

Quantum Dynamical Phase Transition in NMR, double quantum dots and two level systems

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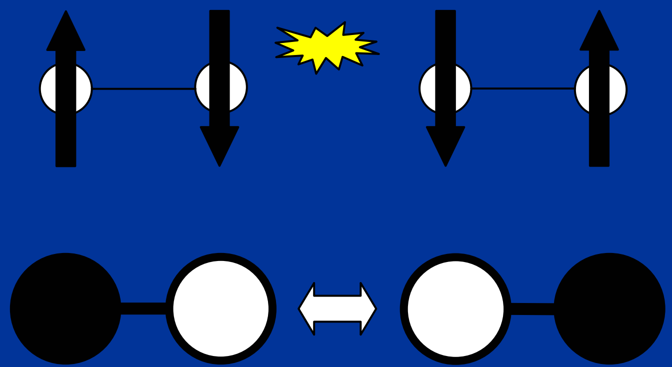
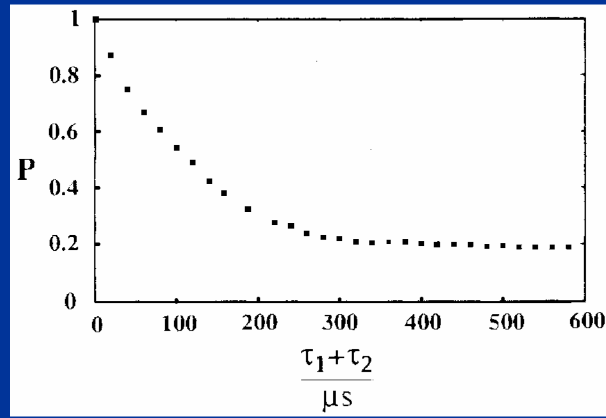
Facultad de Matemática, Astronomía y Física (50th anniversary)

Wigner-Jordan: spins → fermions

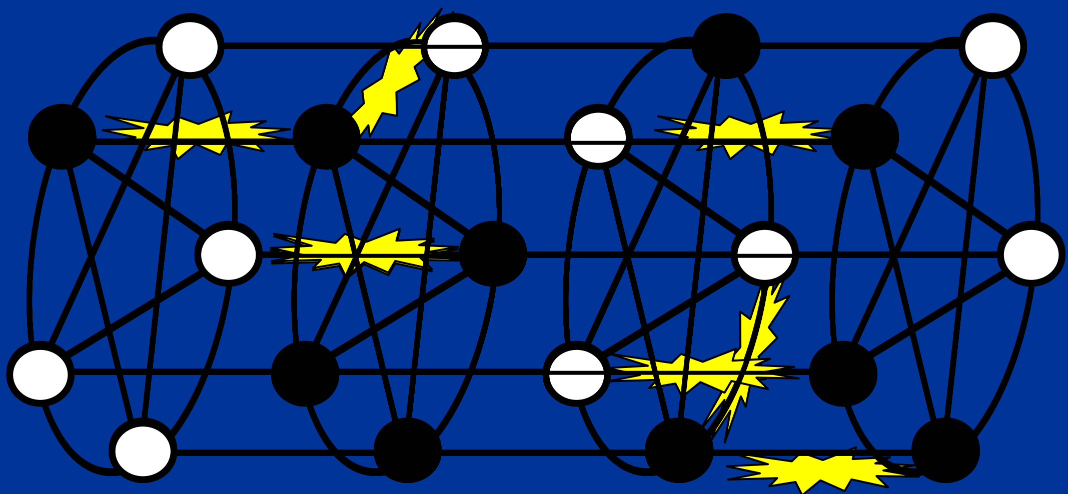
flip-flop XY →hopping of electrons

Ising → Hubbard





Zhang, Meier y Ernst *Phys.Rev.Lett.*1992



interactions

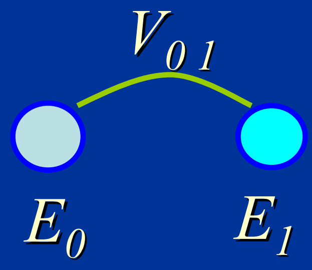
ON /OFF

and scaled

with r.f. pulses

complex many-body interactions→ spin "diffusion"

Effective Hamiltonian for CLOSED Systems



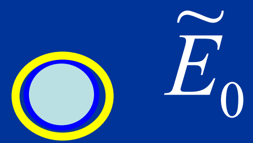
$$\begin{pmatrix} E_0 & V_{0,1} \\ V_{1,0} & E_1 \end{pmatrix} \begin{pmatrix} u_0 \\ u_1 \end{pmatrix} = \varepsilon \begin{pmatrix} u_0 \\ u_1 \end{pmatrix}$$

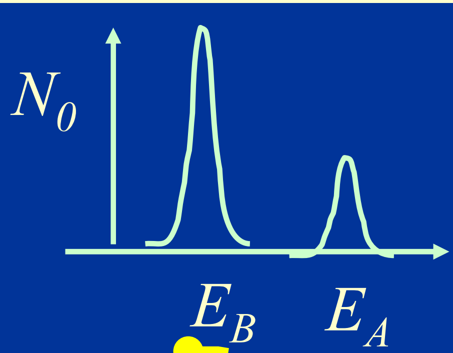
$$u_1 = V_{1,0} \frac{1}{\varepsilon - E_0} u_0$$

$$\left(E_0 + V_{0,1} \frac{1}{\varepsilon - E_1} V_{1,0} \right) u_0 = \widetilde{E}_{0(\varepsilon)} u_0 = \varepsilon u_0$$

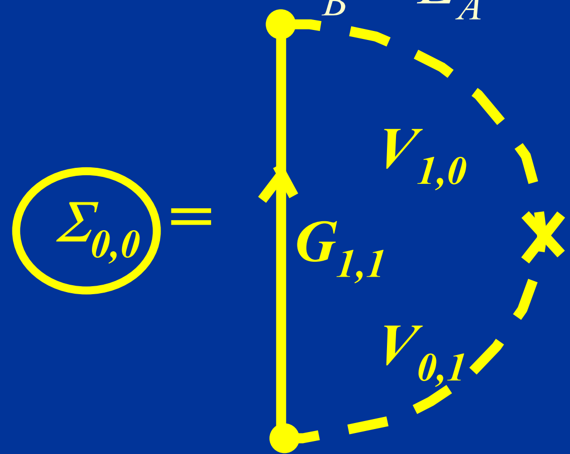
$$G_{0,0} = \frac{1}{\varepsilon - \widetilde{E}_0} = \frac{1}{\varepsilon - E_0 - V_{0,1} \frac{1}{\varepsilon - E_1} V_{1,0}}$$

Σ_0



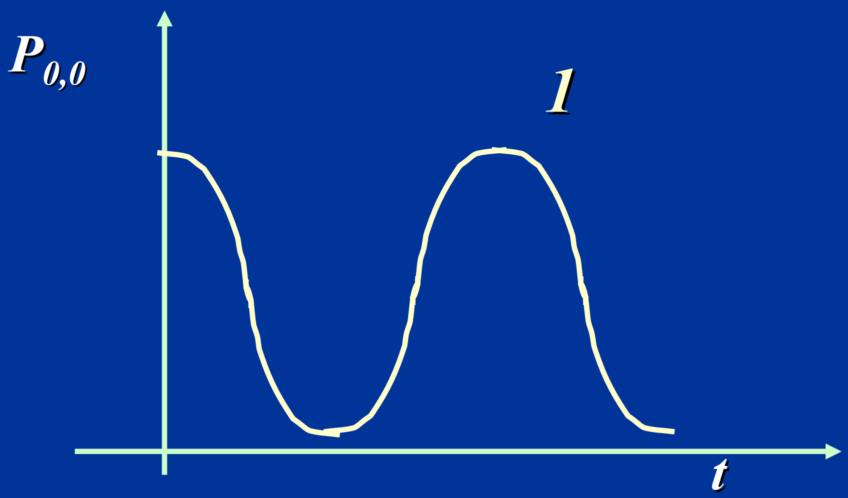


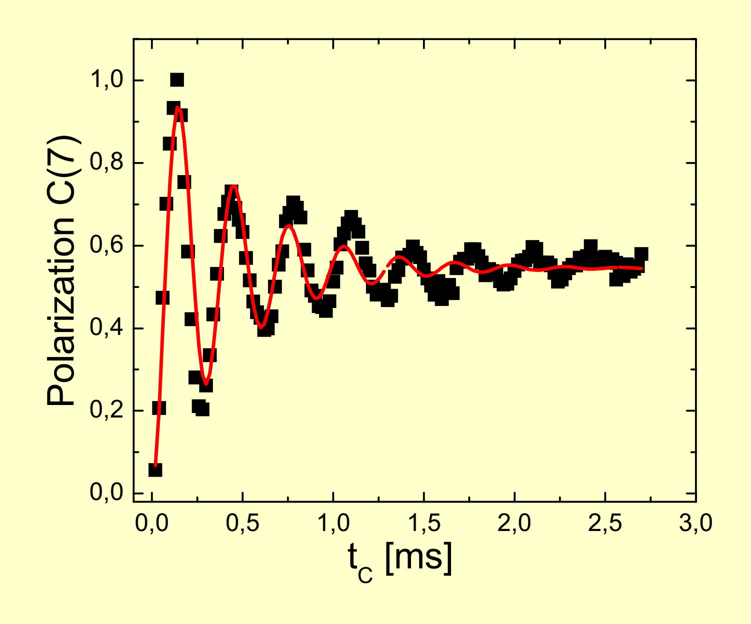
$$\begin{aligned} G^R_{0,0} &= G^{(0)R}_{00} + G^{(0)R}_{00} V_{0,1} G^{(0)R}_{1,1} V_{1,0} G^{(0)R}_{0,0} + \ldots \\ &= G^{(0)R}_{00} + G^{(0)R}_{00} \Sigma^R_0 G^{(0)R}_{0,0} + \ldots \\ &= G^{(0)R}_{00} + G^{(0)R}_{00} \Sigma^R_0 G^R_{0,0} \end{aligned}$$



Simple Quantum Dynamics

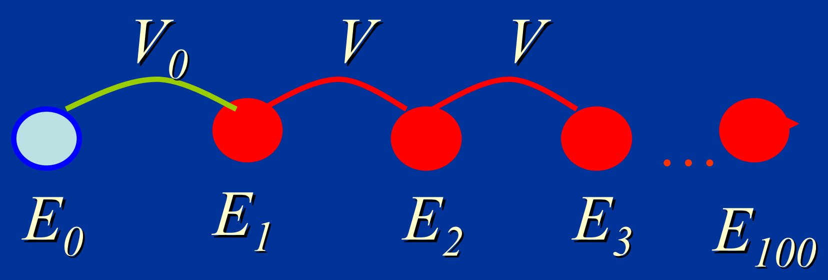
$$P_{0,0}(t) = \left| \int_{-\infty}^{\infty} \frac{d\,\varepsilon}{2\pi\hbar} e^{-i\varepsilon t/\hbar} G_{0,0}(\varepsilon) \right|^2$$





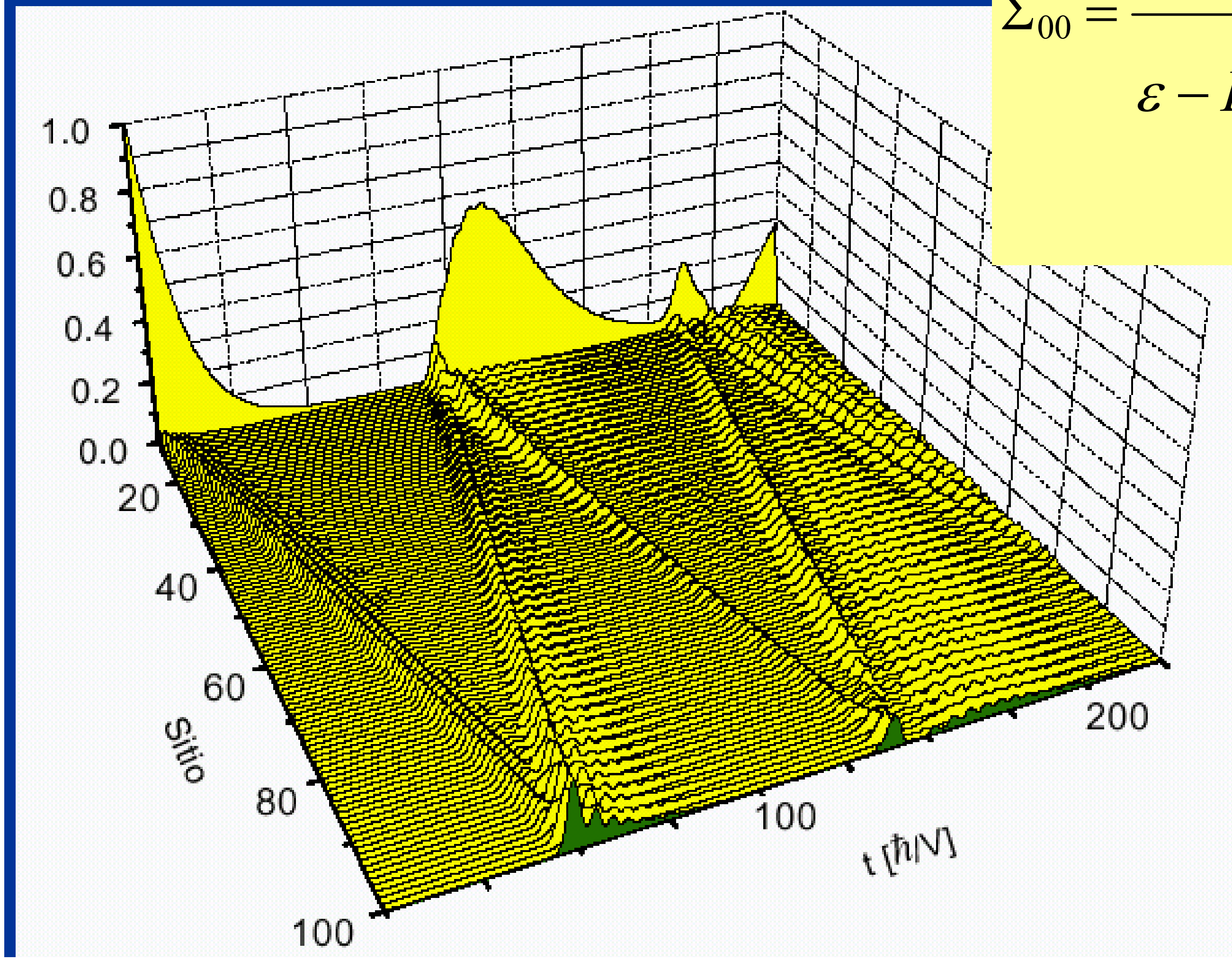
Levstein, Chattah, HMP J.Chem.Phys. **121**, 7313 (2004)

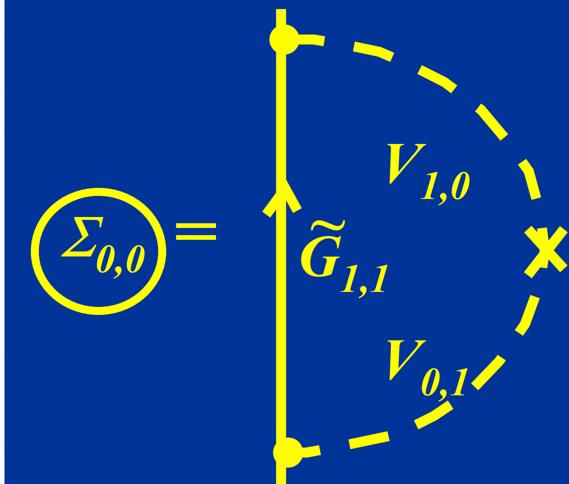
finite chain: real self-energy



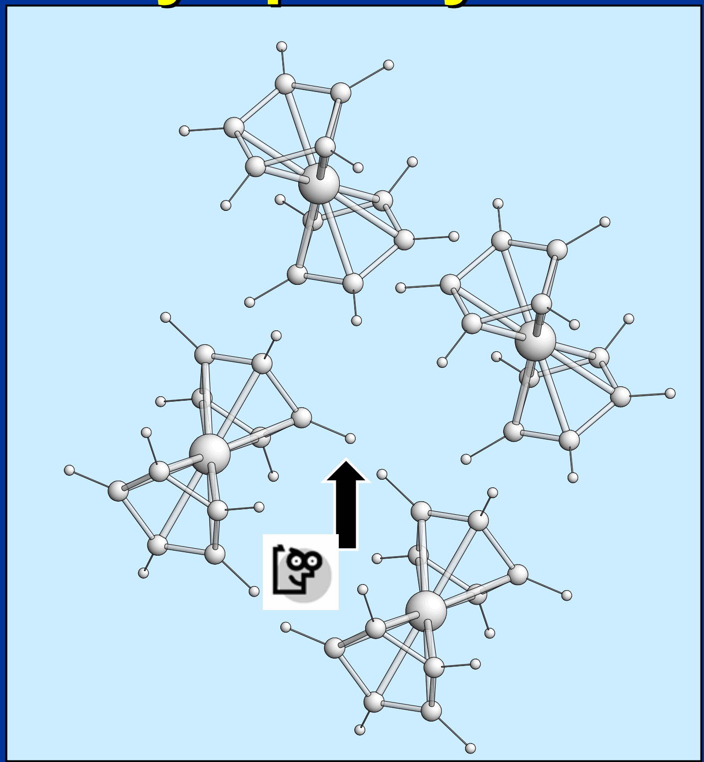
$$\widetilde{E}_0 = E_0 + \Sigma_{00}$$

$$\Sigma_{00} = \cfrac{V_0^{\,2}}{\varepsilon - E_1 - \cfrac{V^2}{\varepsilon - E_2 - \ldots\ldots \cfrac{V^2}{\varepsilon - E_{100}}}}$$





many-spin dynamics→ quantum spin “diffusion”

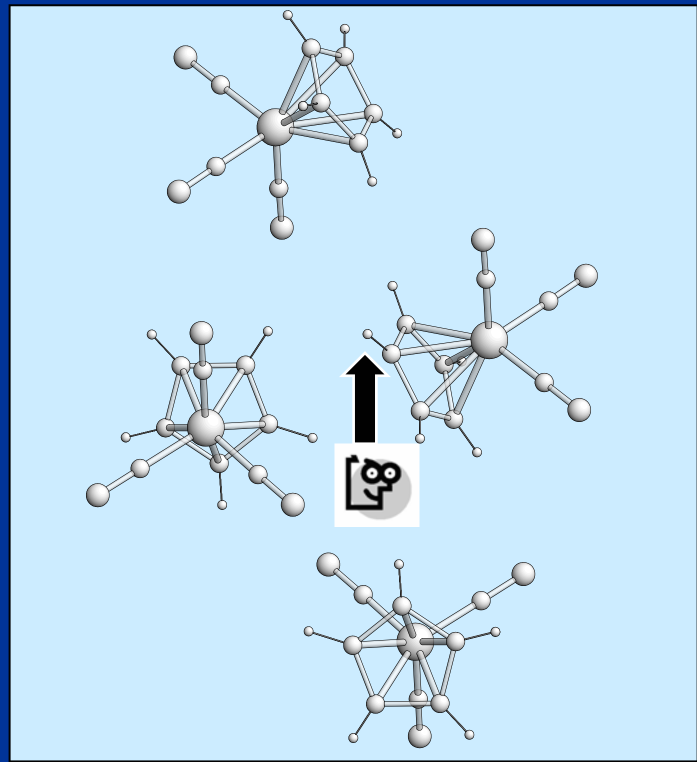


a ^{13}C

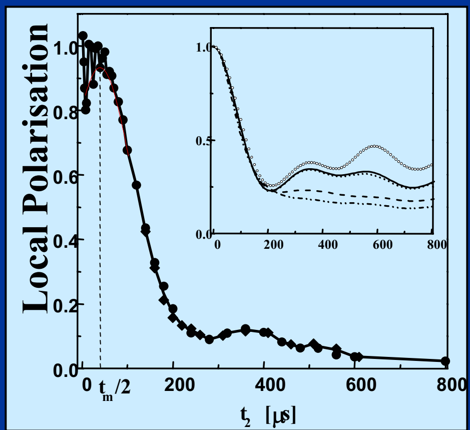
“spies”

the ^{1}H

spin



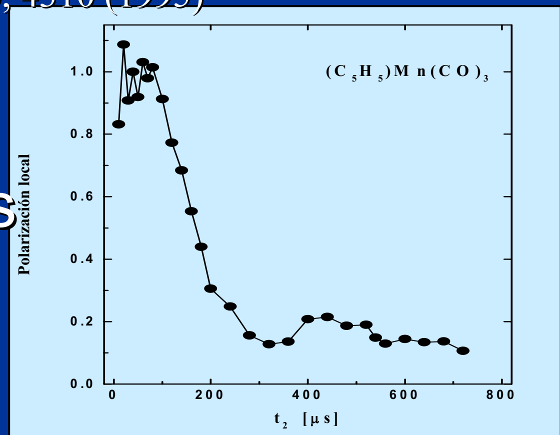
HMP, Levstein, Usaj, Phys.Rev.Lett. **75**, 4310 (1995)



finite ring size

→mesoscopic echoes

+…decoherence

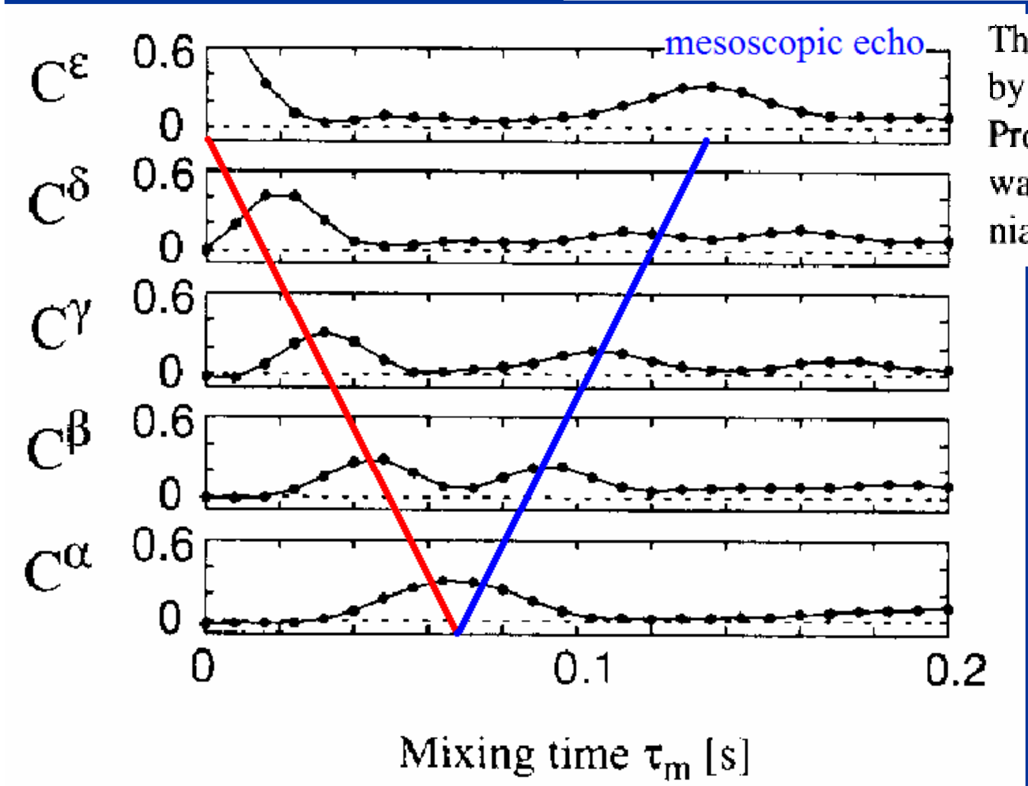


Mesoscopic Echoes: NMR experiments

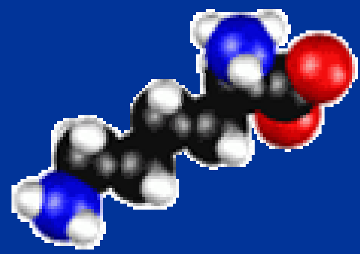
Time-resolved observation of spin waves in a linear chain of nuclear spins

Z.L. Mádi, B. Brutscher, T. Schulte-Herbrüggen, R. Brüschweiler, R.R. Ernst

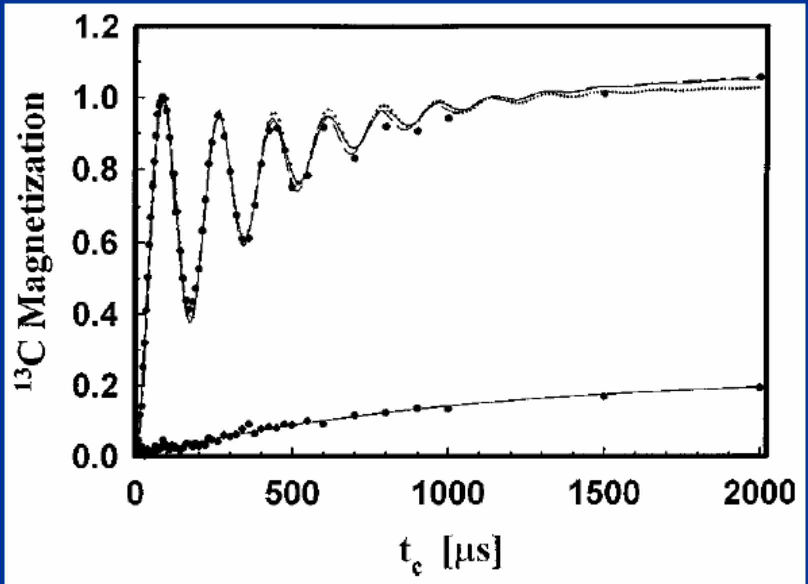
Laboratorium für Physikalische Chemie, ETH Zentrum, 8092 Zürich, Switzerland

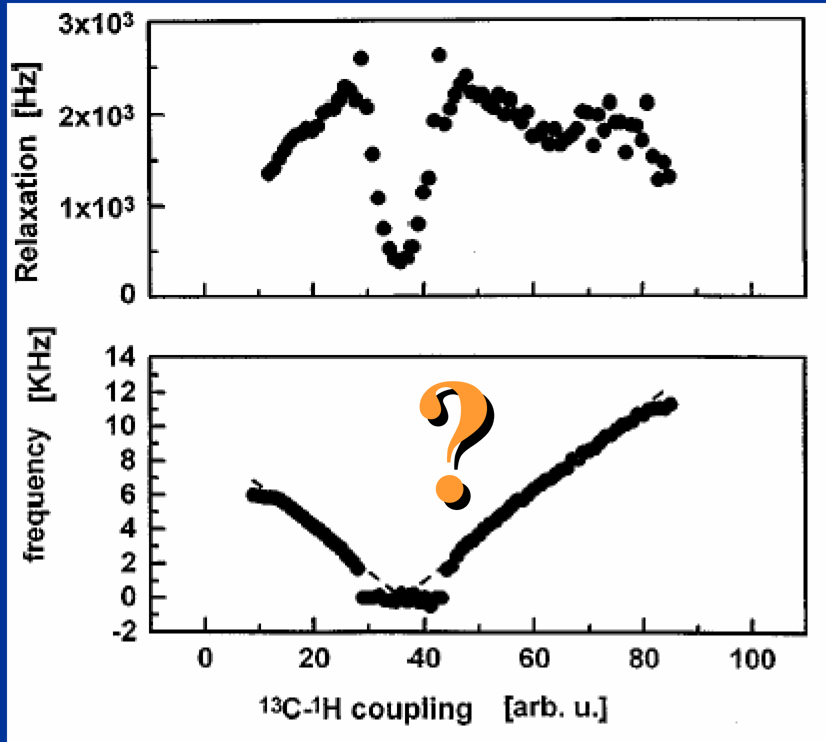


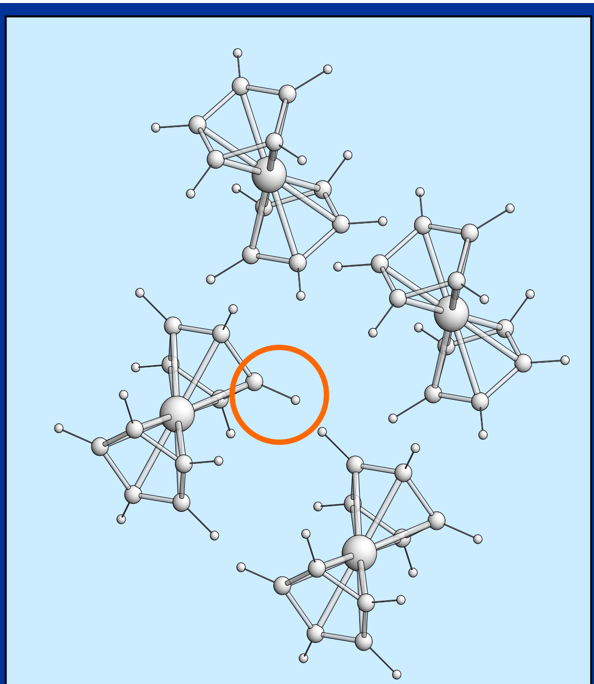
The study described in this letter has been inspired by discussions with Professor H.M. Pastawski and Professor P.R. Levstein who calculated nuclear spin wave evolution under a ‘planar’ or ‘XY’ Hamiltonian [3].



lysine







"ideal ^{13}C-^{1}H spin-swap gate"
evolves isolated

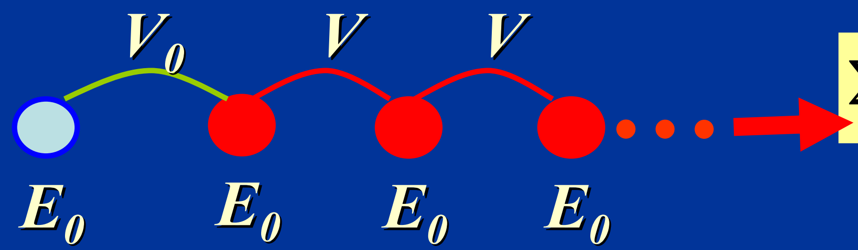
but… *^{1}H* spin bath interacts
with *^{13}C-^{1}H*

NMR Quantum Dynamics→ fermions

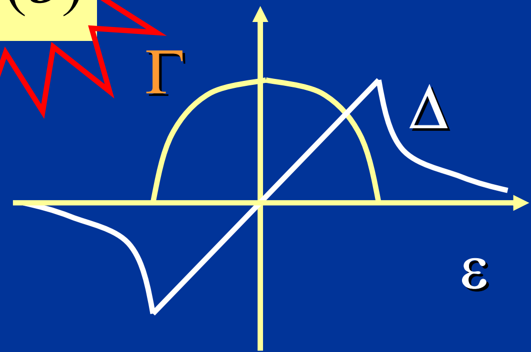
Effective Hamiltonian for OPEN Systems

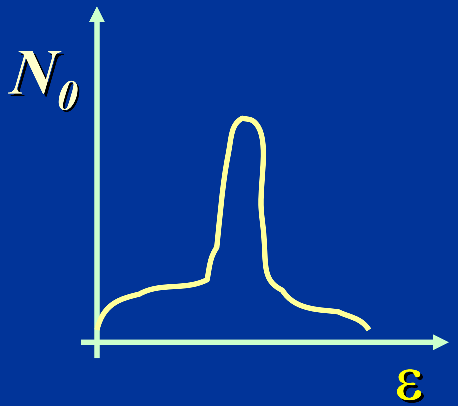
Ordered chain → Lead

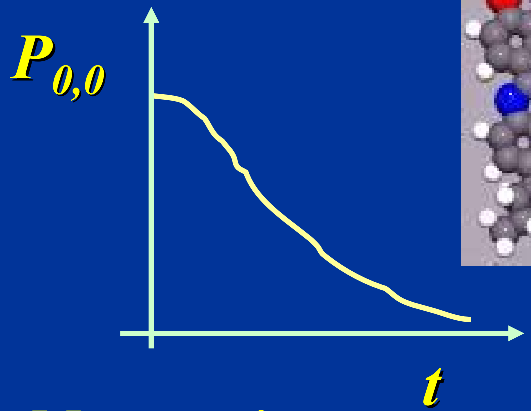
$$G^R_{0,0} = \frac{1}{\varepsilon - E_0 - \Sigma^R}$$

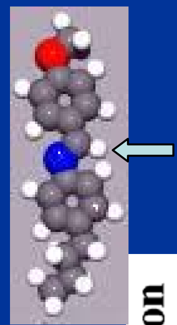


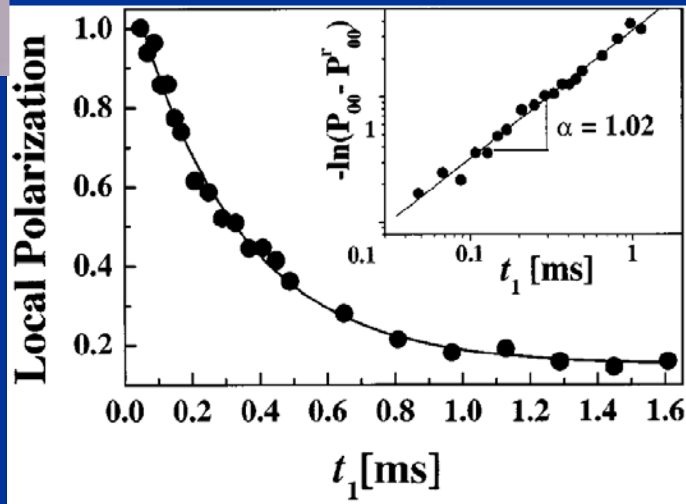
$$\Sigma^R = \Delta(\varepsilon) - \mathrm{i}\Gamma(\varepsilon)$$











X-tal→Continuum spectrum

Mesoscopic echo→∞

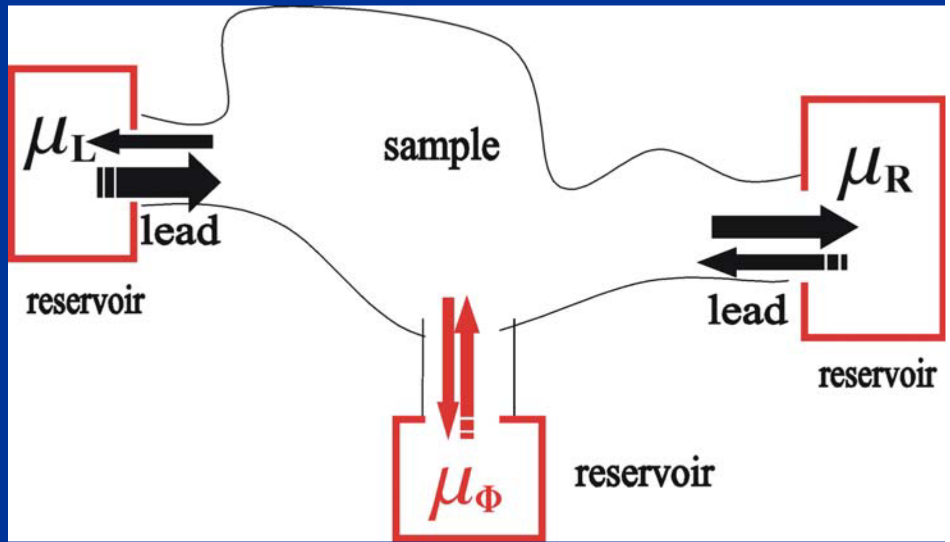
detailed dynamics Rufeil&HMP ChemPhysLett. 420,35 (2006)

⇨ but density is not conserved…! 1987

Levstein, Chattah, HMP, Raya&Hirschinger et al JCP 2004

Phenomenology of Decoherence

(Büttiker 1986)



$$I_\phi \equiv 0$$

voltmeter

$$0 = \frac{e}{h} T_{\phi,L}(\delta\mu_\phi - \delta\mu_L) + \frac{e}{h} T_{R,\phi}(\delta\mu_\phi - \delta\mu_R)$$

$$I_R = \frac{e}{h} \tilde{T}_{R,L}(\delta\mu_L - \delta\mu_R)$$

$$\tilde{T}_{R,L} = T_{R,L} + \frac{T_{R,\phi} T_{\phi,L}}{T_{R,\phi} + T_{\phi,L}}$$

coherent

incoherent

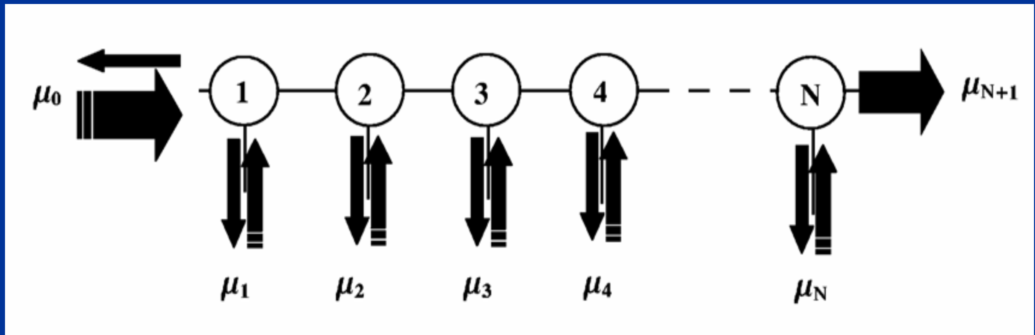
Decoherence and evolution: Keldysh=GLBE

$$T_{RL} = 2\Gamma_R \left| G^R_{RL} \right|^2 2\Gamma_L$$

Hamiltonian formulation D´Amato and HMP Phys. Rev. B **41**,7411 (1990); Datta JPCM **2**, 8023 (1990)

HMP Phys. Rev. 46 4053 (1992) review see HMP-Medina cond-matt 0103219

- Any **imaginary energy** Γ (as in the Fermi Golden Rule) requires a **thermodynamic limit** and involves "irreversible" decay to the environment
- Needs to add a charge conservation



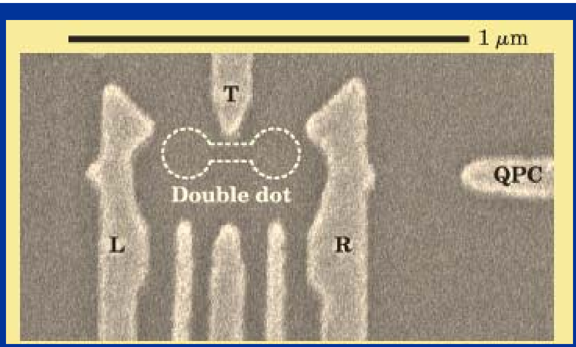
$$(1/g_i) = \sum_{j=0}^{N} T_{j,i}$$

$$I_i \equiv 0 = (1/g_i)\delta\mu_i - \sum_{j=0}^{N} T_{i,j}\,\delta\mu_j$$

$$\widetilde{T}_{R,L} = T_{R,L} + \sum_{i=1}^{N} T_{R,i} g_i T_{i,L} + \sum_{i=1}^{N}\sum_{j=1}^{N} T_{R,i} g_i T_{i,j} g_j T_{j,L} + \ldots$$

$$= T_{R,L} + \sum_{i=1}^{N} T_{R,i} g_i \widetilde{T}_{i,L}$$

↑ *last place where a dephasing collision occured*

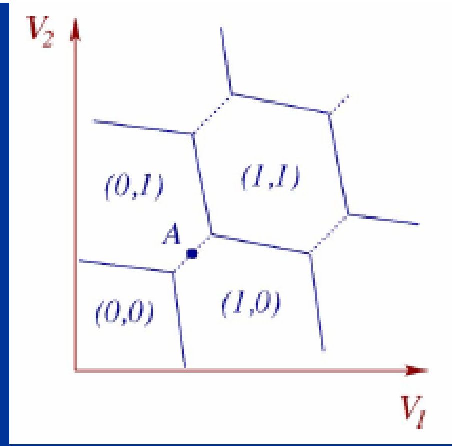


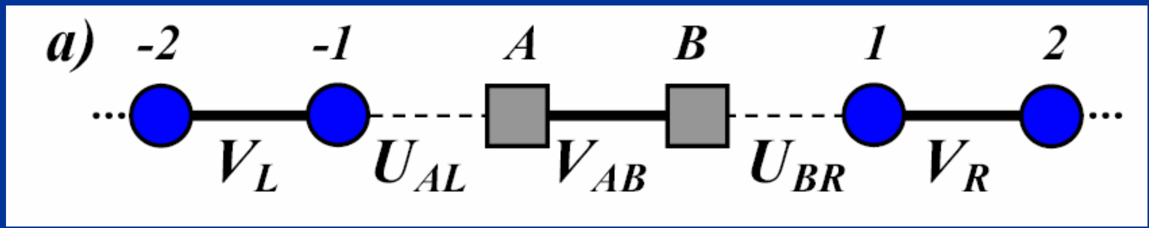
swap gate

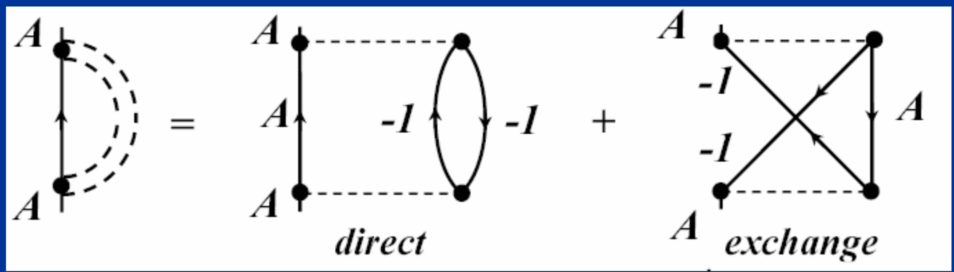
double dot charge q-bit

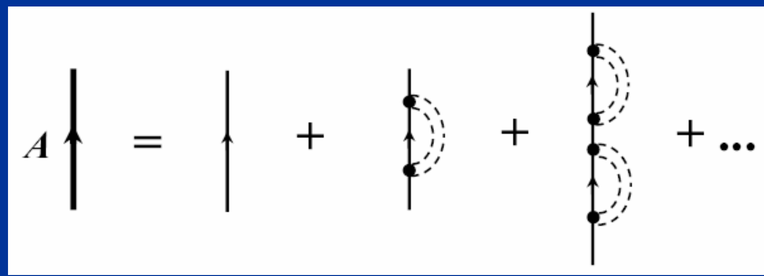
Fermions←→spins

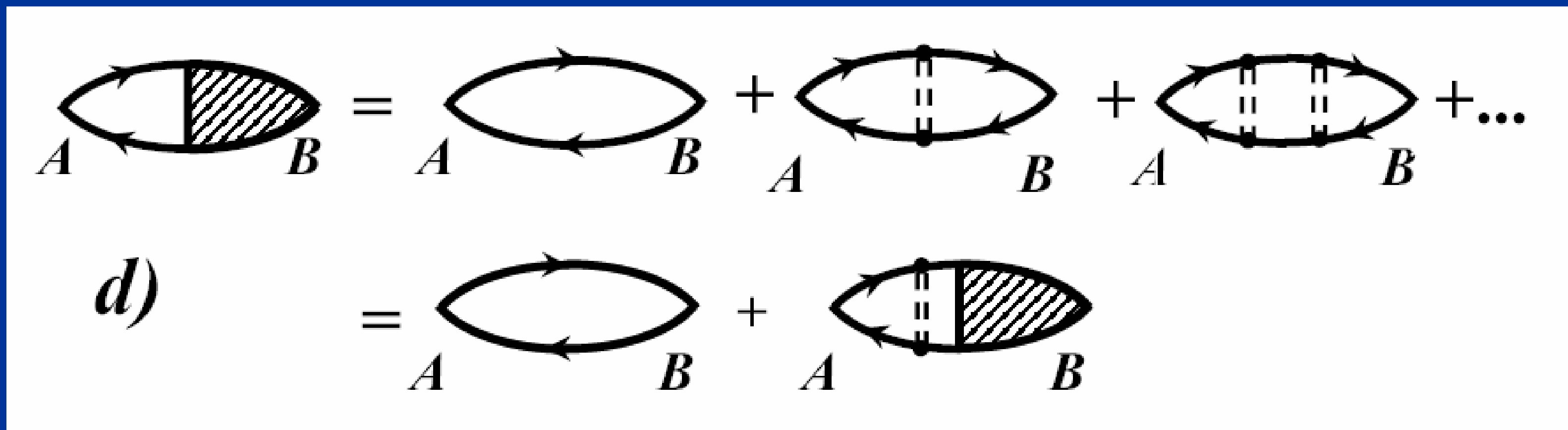
Coulomb←→Ising

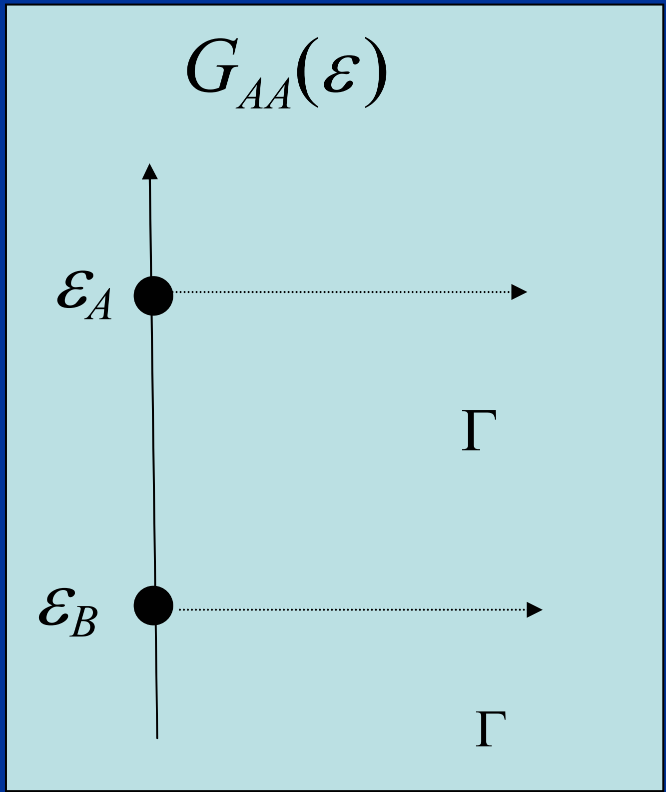


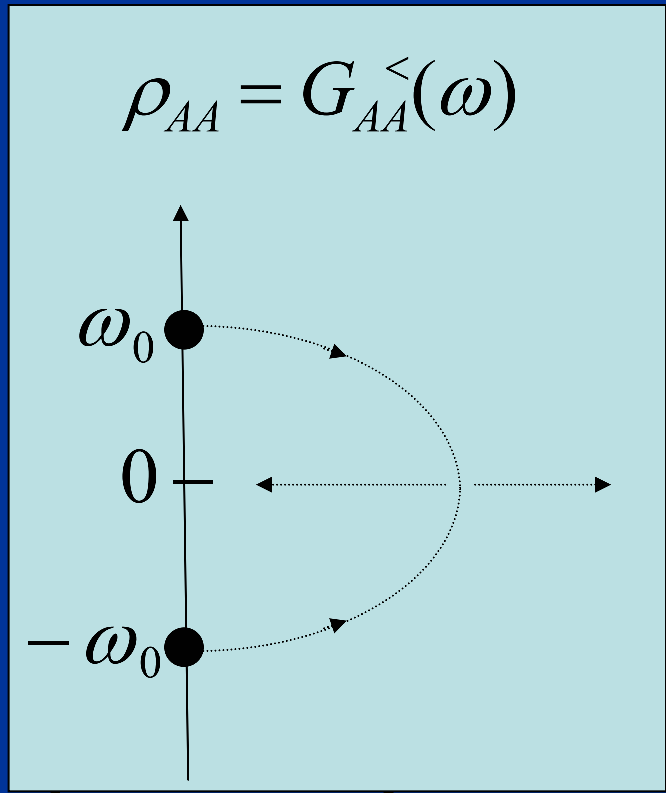


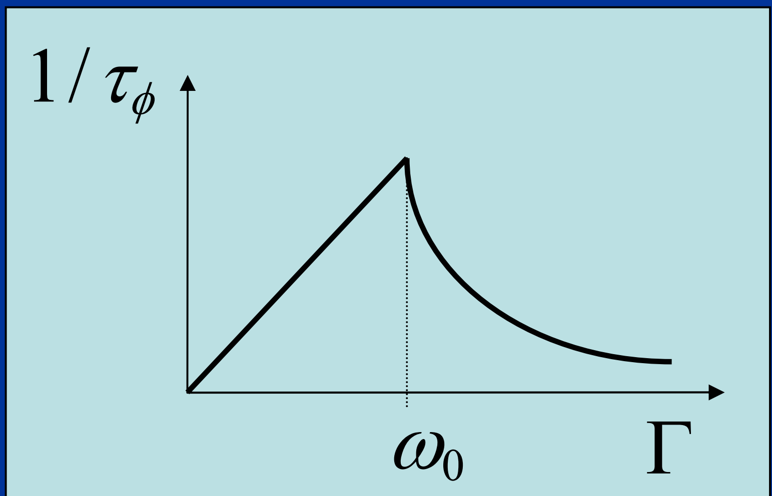






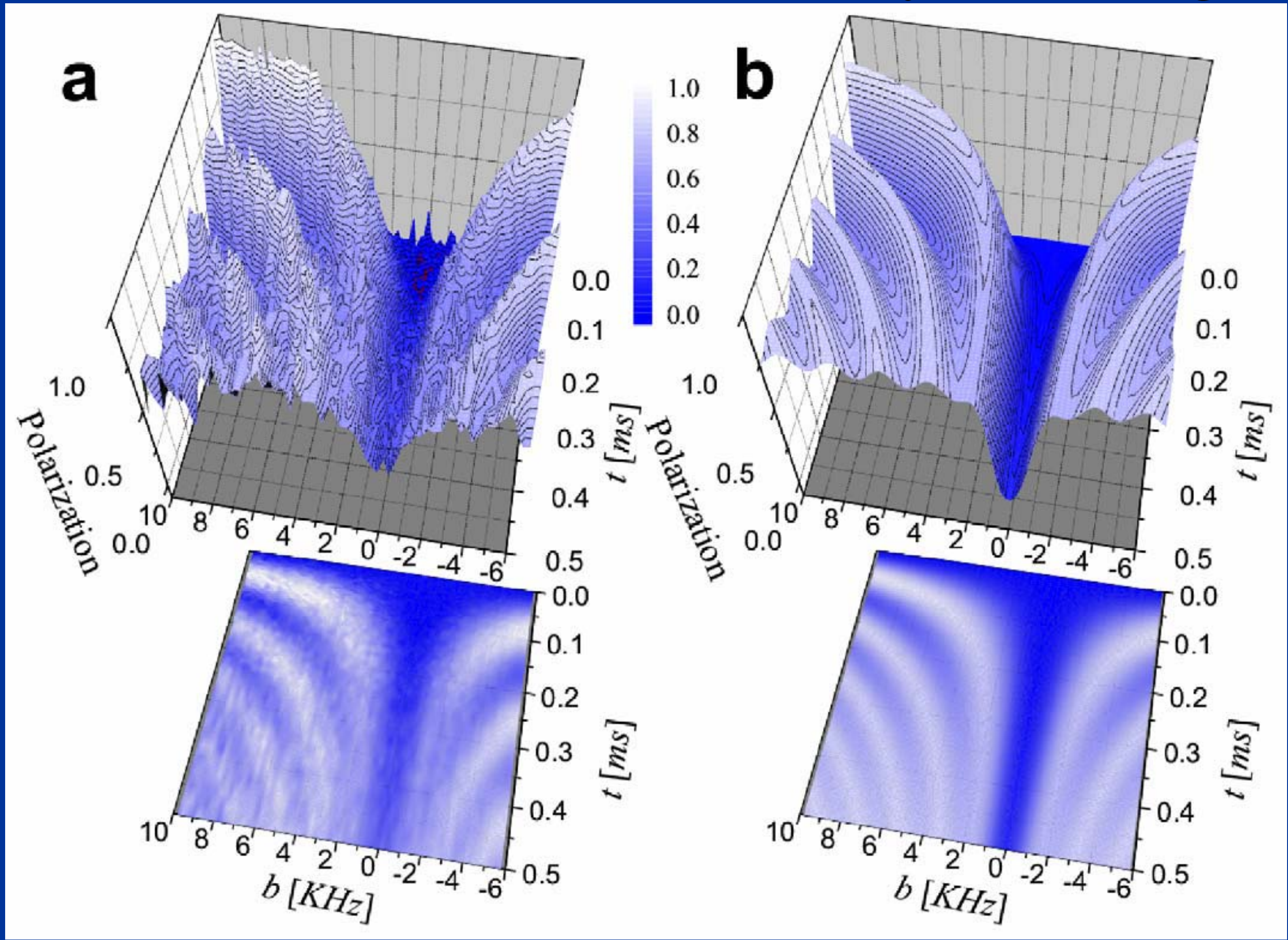






decoherence rate and **frequency**
are **non-analytic**
on the SE interaction strength

raw experimental data theory (no-fitting)



fermions + open systems+ time → Keldysh → GLBE (Landauer-Büttiker)

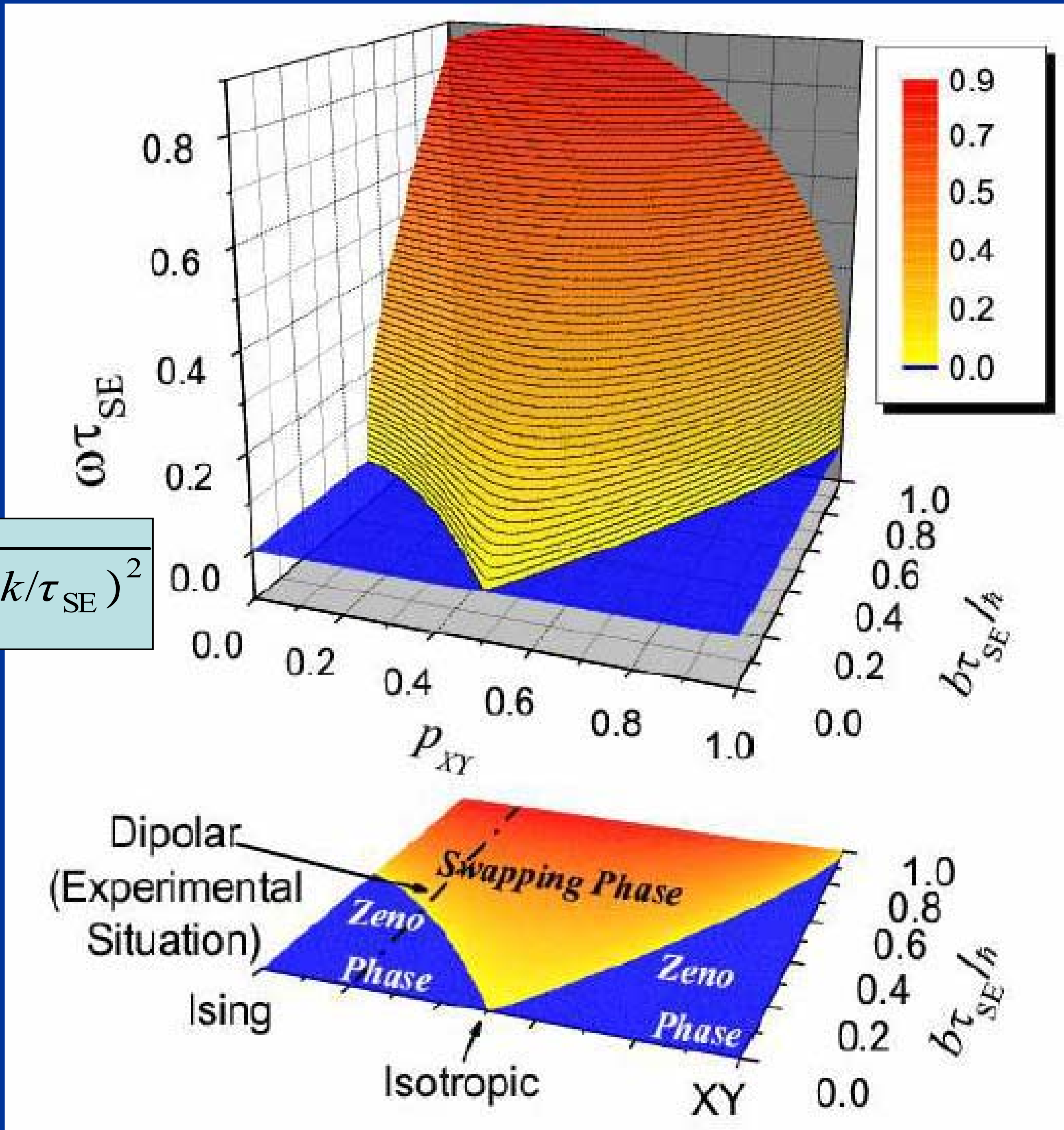
→quantum dynamical phase transition

condmat0504347 JCP06

quantum dynamical phase transition

$$\omega \propto \sqrt{(b/\hbar)^2 - (k/\tau_{SE})^2}$$

k=0 Heisenberg
k=1 XY



Summary

--We observed experimentally that the dynamics of swapping gate has a transition to a frozen regime…!
…consequence of the **"observation"** by the environment i.e. the **Quantum Zeno Effect.**

--Once more…as occurs with the Loschmidt Echo,

the **observables are non-analytic** on the Hamiltonian parameters… → **dynamical phase transition (bifurcation)**.

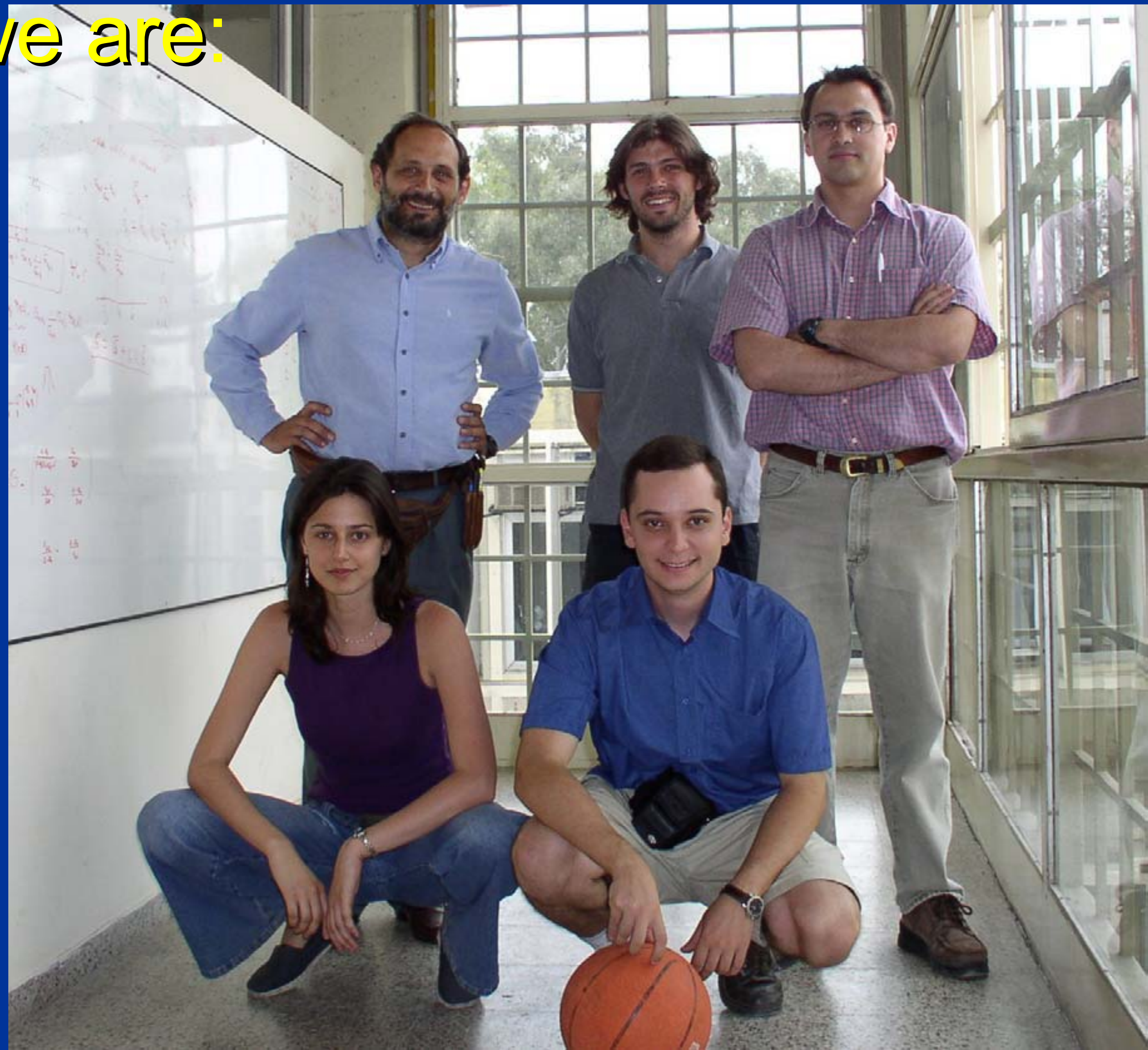
--SURPRISE: The isotropy in the spin-spin interaction can prevent the Quantum Zeno Effect

who we are:

François Vignon and Patricia Levstein

Patricia, Ernesto and Karina Chattah

Fernando Cucchietti and Gustavo Monti



Horacio, Ernesto Danieli, Gonzalo Usaj,

Elena Rufeil Fiori and Luis Foa Torres

Gonzalo Alvarez

Thank you Antorchas…!!

I'll answer your questions…!!

Keldysh in a Nutshell: GLBE Pastawski PhysRevB 92

quantum dynamics of open systems

$$\left[\overbrace{\Psi(X_2)\Psi^*(X_1)}^{\text{"detected general density"}}\right] = \hbar^2 \iint \underbrace{\mathrm{d}X_j\, G^R(X_2,X_j)}_{retarded}\,[\overbrace{\Psi(X_j)}^{\text{ret. inject.}}\ \underbrace{\overbrace{\Psi^*(X_k)}^{\text{adv. inject.}}]\,G^A(X_k,X_1)\ \overbrace{\mathrm{d}}^{init.coord.}X_k}_{advanced}$$

with $X_i = (r_i, t_i)$

Keldysh Density Function

➔Wigner's f.

= Density Matrix

$$G^<(X_2,X_1) = -\mathrm{i}\hbar\left[\overbrace{\Psi(X_2)\ \Psi^*(X_1)}^{\text{"detected general density"}}\right]$$

$$G^<(X_2,X_1) = \hbar^2 \iint \overbrace{\mathrm{d}\,r_j}^{init.coord.}\ G^R(X_2,r_j)\left[\overbrace{G^<(r_j,t_0;r_k,t_0)}^{\text{intial distrib.}}\right]\underbrace{G^A(r_k,X_1)\ \overbrace{\mathrm{d}\,r_k}^{init.coord}}_{advanced}$$

$$+\iint \underbrace{\overbrace{\mathrm{d}\,X_j}^{init.coord.}\ G^R(X_2,X_j)}_{retarded}\,[\overbrace{\Sigma^<(X_j,X_k)}^{\text{re-injects losses}}]\,\underbrace{G^A(X_k,X_1)\ \overbrace{\mathrm{d}\,X_k}^{init.coord.}}_{advanced}$$

$$G^<(r,r,t,\varepsilon) = \int G^<(r,t+\tfrac{1}{2}\delta t; r,t-\tfrac{1}{2}\delta t)\,\mathrm{e}^{\mathrm{i}\varepsilon\delta t/\hbar}\,\mathrm{d}\,\delta t \approx N_r(\varepsilon)\,\mathrm{f}_r(\varepsilon,t)$$

$$\Sigma^<(r,t) = {}^{\phi}\Gamma_r(\varepsilon)\,\mathrm{f}_r(r,\varepsilon,t)$$

$${}^{\phi}\Gamma(\varepsilon) = 2\pi V_\phi^2\,N(\varepsilon)$$

GLBE for spins (numerical implementation)

$$\frac{1}{\hbar^2}\mathbf{G}^{<}(t) = \mathbf{G}^{0\mathrm{R}}(t)\,\mathbf{G}^{<}(0)\,\mathbf{G}^{0\mathrm{A}}(t)\,(1-p)^{n} + \sum_{m=1}^{n}\mathbf{G}^{0\mathrm{R}}(t-t_m)\,\widetilde{\boldsymbol{\Sigma}}^{<}(t_m)\,\mathbf{G}^{0\mathrm{A}}(t-t_m)\,p\,(1-p)^{n-m}, \quad (4)$$

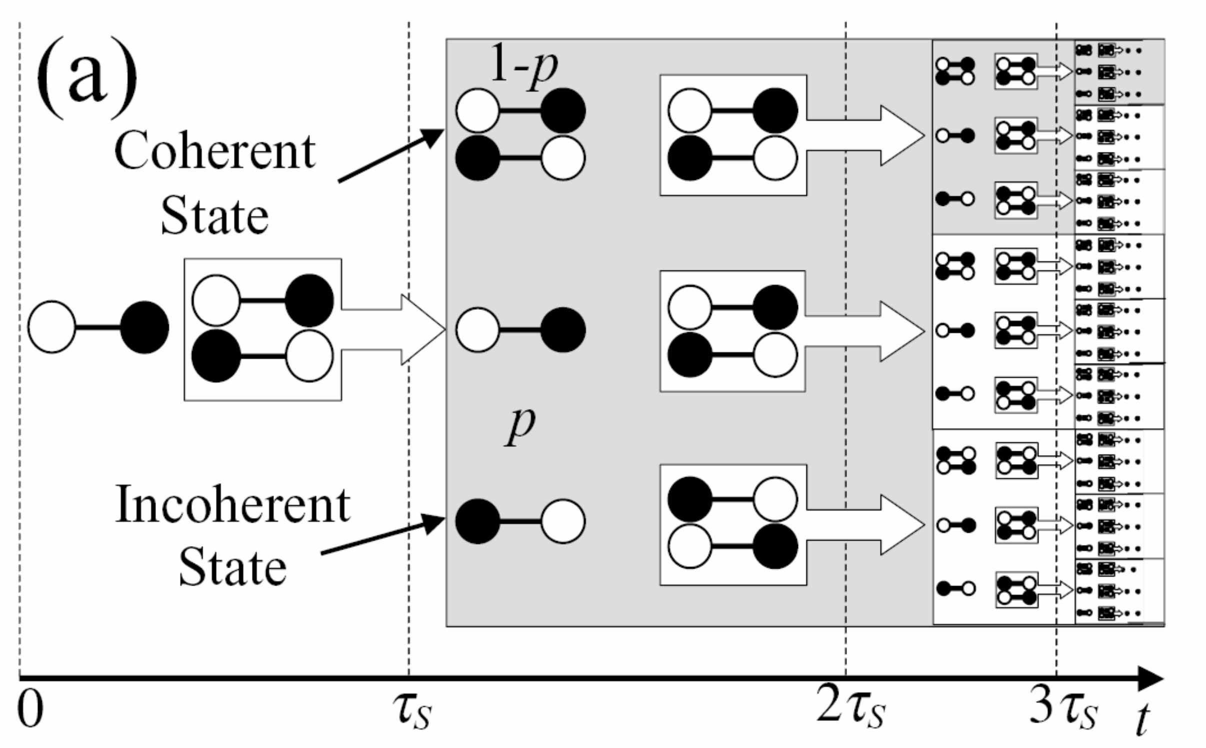
Danieli, Álvarez, HMP ChemPhysLett 2005;

Álvarez, Danieli, Levstein, HMP JChemPhys06

[cond-mat/0504347]

$$\boldsymbol{\Sigma}_{\mathrm{m}}^{<}(t) = \mathrm{i}\frac{\hbar}{\tau_{\mathrm{SE}}}\begin{pmatrix} \frac{\hbar}{\mathrm{i}}G_{11}^{<}(t) & 0 \\ 0 & \frac{\hbar}{\mathrm{i}}G_{22}^{<}(t) \end{pmatrix}$$

$$\boldsymbol{\Sigma}_{\mathrm{i}}^{<}(t) = 2\mathrm{i}\frac{\hbar\,p_{\mathrm{XY}}}{\tau_{\mathrm{SE}}}\begin{pmatrix} 0 & 0 \\ 0 & \left[1-\frac{\hbar}{\mathrm{i}}G_{22}^{<}(t)\right] \end{pmatrix}$$



Vacuum Rabi splitting (Nature Phys. 2006)

REVIEW ARTICLE

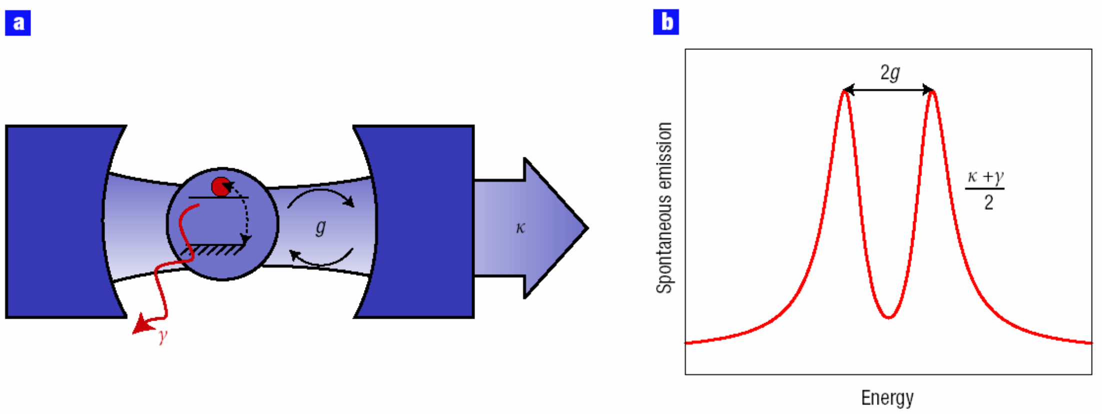
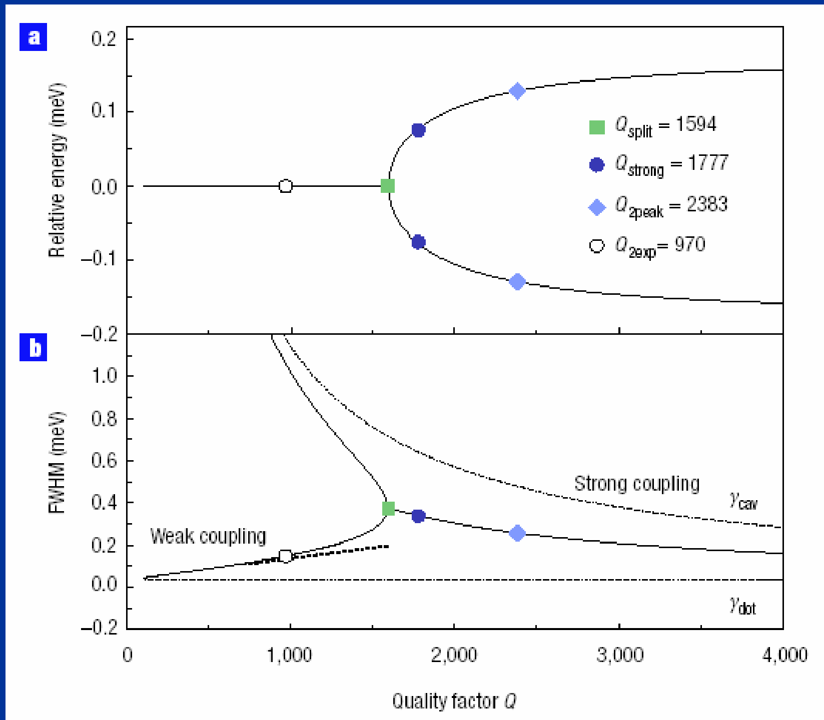
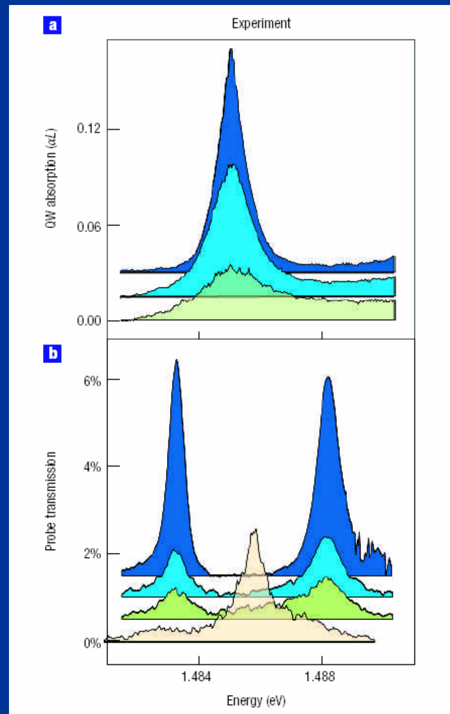


Figure 1 Vacuum Rabi splitting using an atom or dot in a small-volume cavity. **a**, Schematic of a single two-level atom with dephasing rate γ coupled to a cavity with photon loss rate κ by coupling strength g. **b**, VRS spectrum for zero atom-cavity detuning.

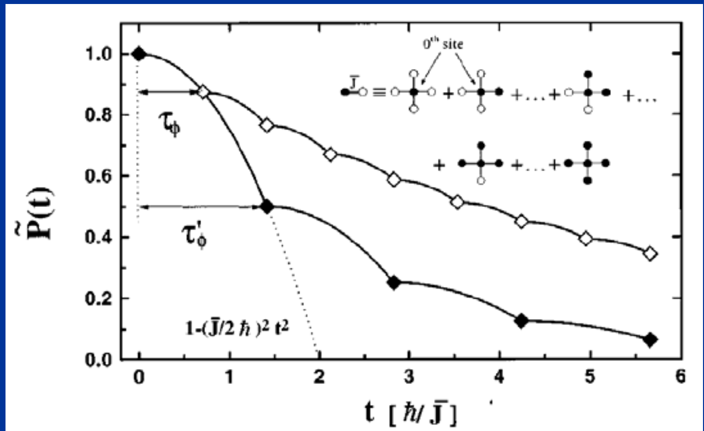


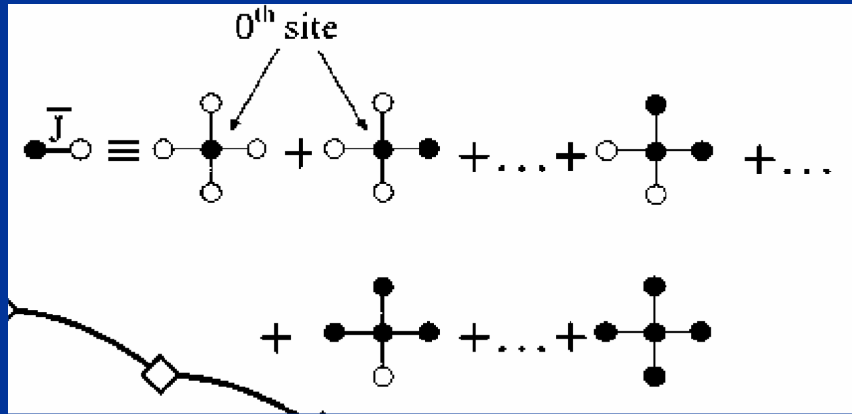


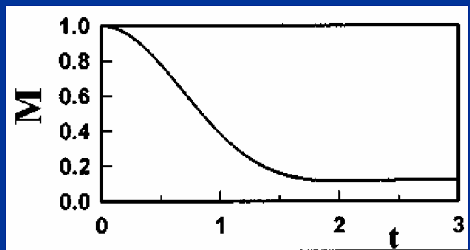
Quantum Zeno Effect

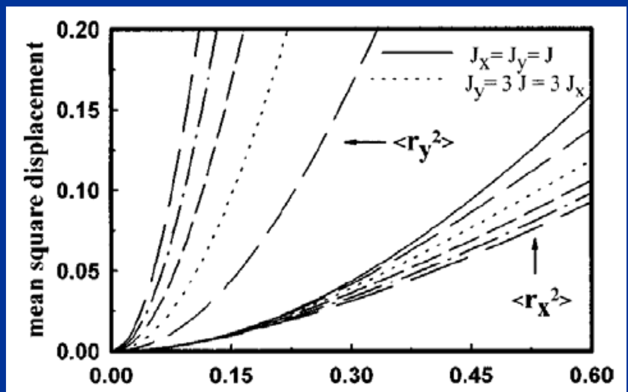
(many body environment=measurement)

Misra&Sudarsham J.Math.Phys.**18**,756 (1977); experiments→Levstein,HMP&Calvo J.Phys.Cond.Mat.**3**,1877(1991), theory→HMP&Usaj Phys.Rev.B **57**,5017 (1998)









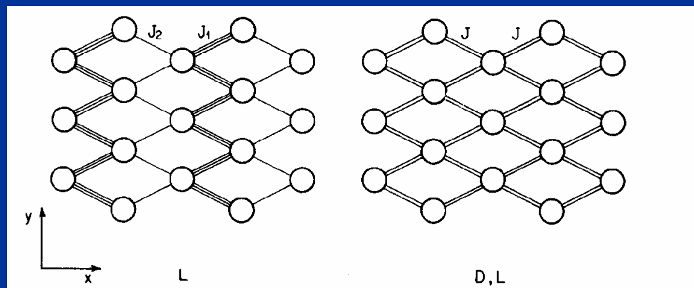
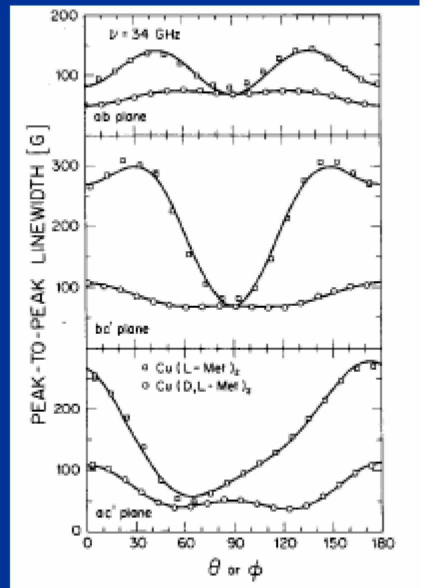
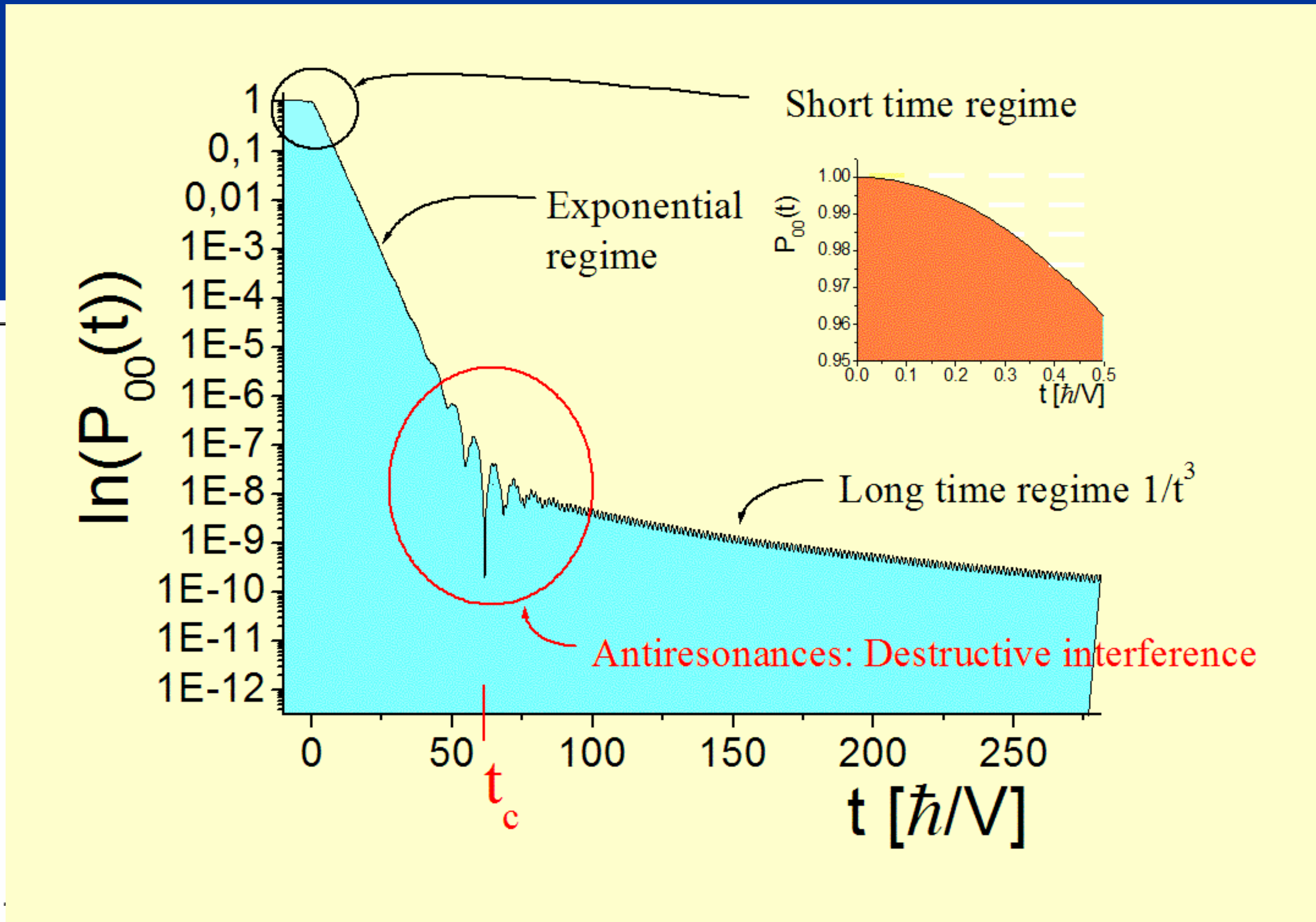


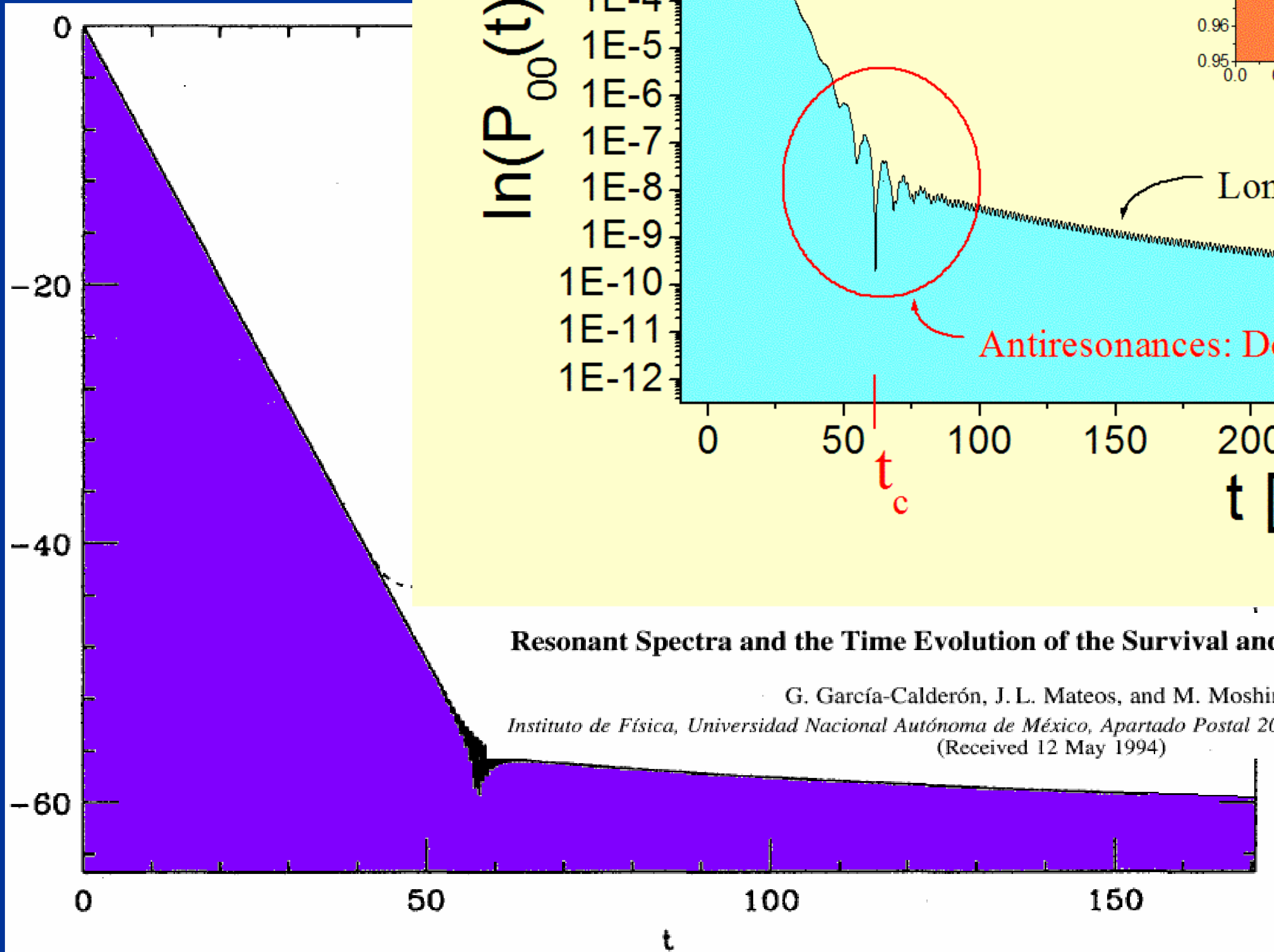
Figure 3. Schematic view of the exchange networks in L and DL systems.



dynamics beyond FGR...

E.Fiori&HMP, Chem.Phys.Lett. 2006





Resonant Spectra and the Time Evolution of the Survival and Nonescape Probabilities

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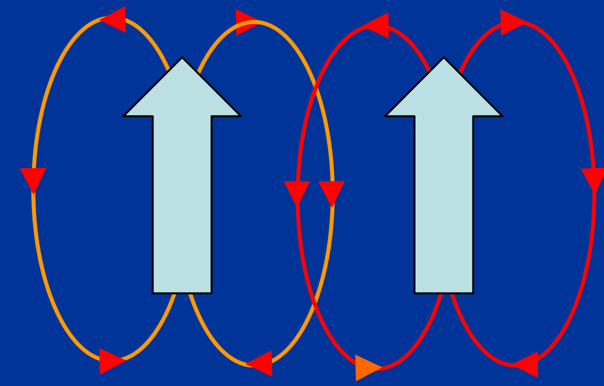
(Received 12 May 1994)

Interactions:
Zeeman, rf, dipolar (Ising + XY)

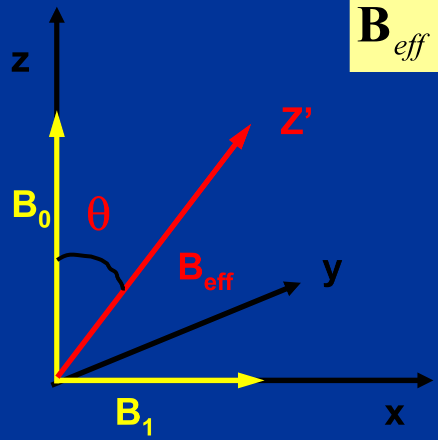
$$\mathcal{H} = -\sum_i \gamma\hbar\left[B_0 - \omega/\gamma\right] I^z - \gamma\hbar B_1 I^x + \sum_{i>j} d_{ij}\left[\underbrace{2I_i^z I_j^z}_{\text{Ising}} - \tfrac{1}{2}\underbrace{\left(I_i^+ I_j^- - I_i^- I_j^+\right)}_{XY}\right]$$

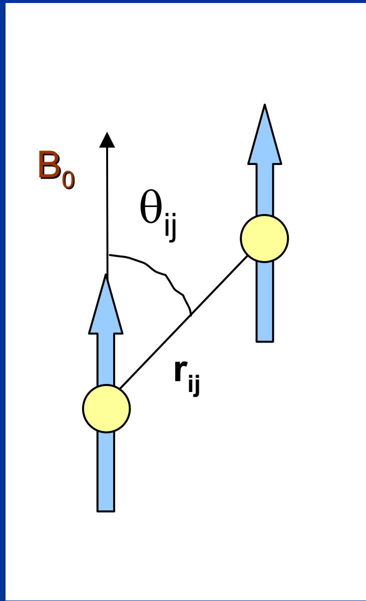


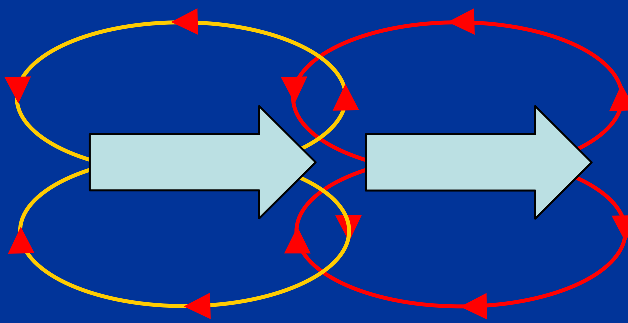
$$I^z = \sum_j I_j^z, \quad \text{etc.}$$

$$d_{ij} \equiv \frac{\gamma^2\hbar^2}{r_{ij}^3}\left(1 - 3\cos^2\theta_{ij}\right)$$

$$\mathbf{B}_{eff} = \breve{\mathbf{i}} B_1 + \breve{\mathbf{k}} B_0$$

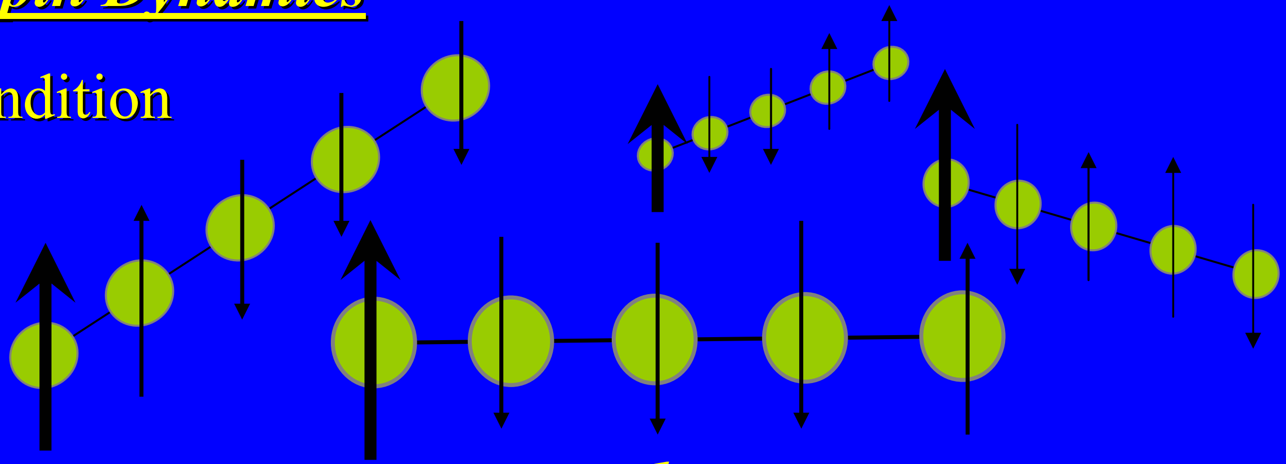


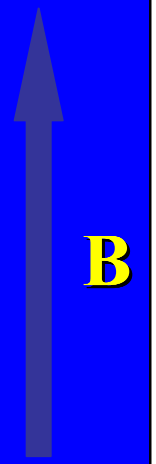




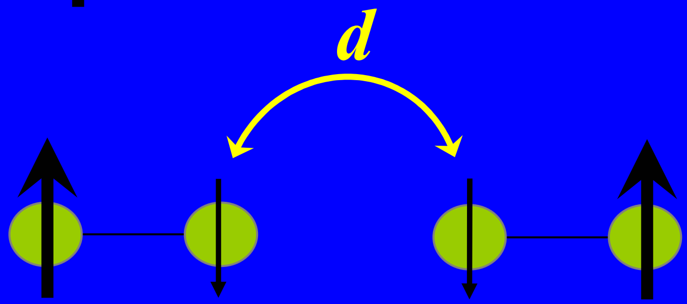
Quantum Spin Dynamics

- Initial Condition (liquid)

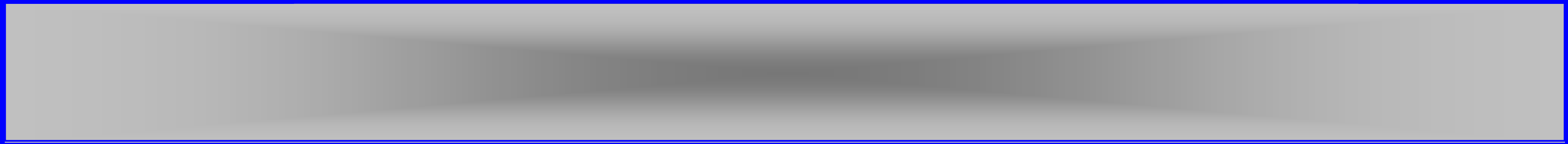




- source of dynamics



- ¿Spin Diffusion?

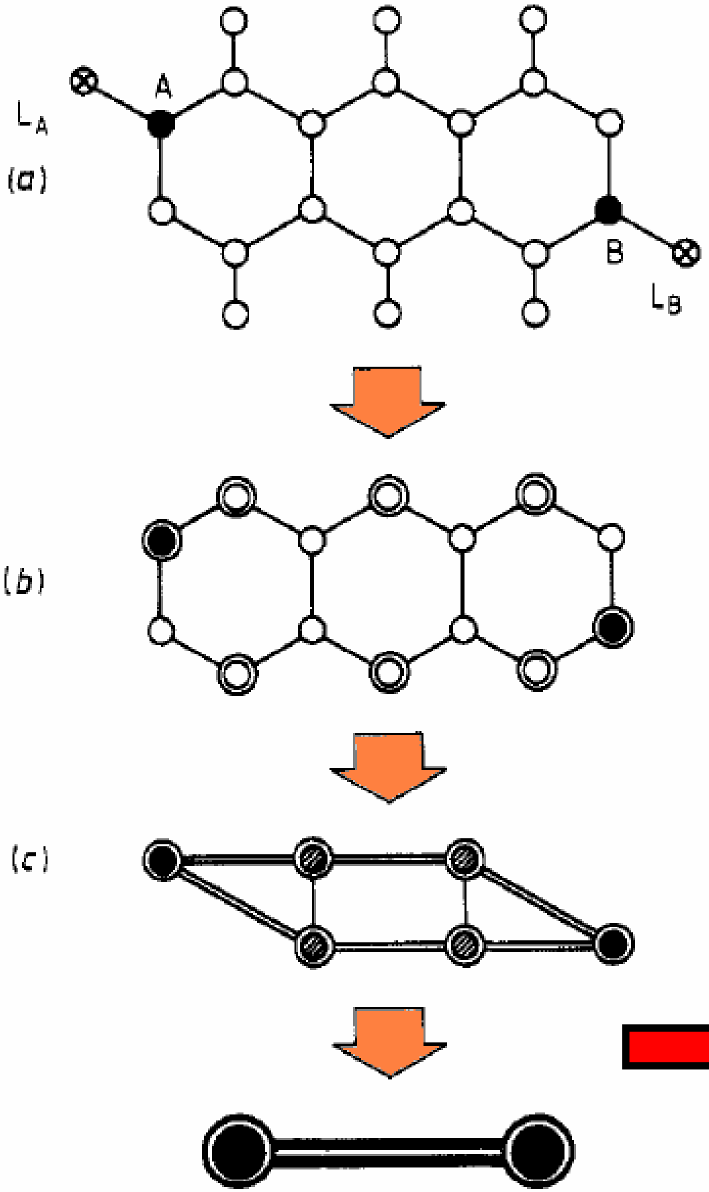


- No! → Quantum Dynamics:

local polarization ➔ *Mesoscopic Echoes*

HMP, Levstein, Usaj PRL 1995.

a related problem: electron transfer



Tuning the through-bond interaction in a two-centre problem J. Phys.: Condens. Matter **2** (1990) 1781–1794.

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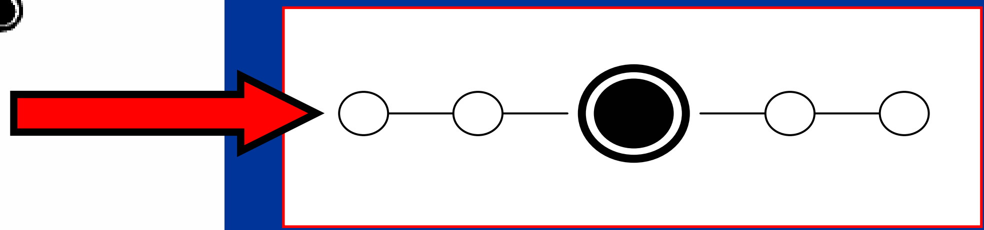
Received 16 May 1989, in final form 22 September 1989

Abstract. Two centres A and B connected by one or more sets of bridging states (pathways) define a graph in the space of states. The Hamiltonian is decimated in this space and the problem is reduced to that of two sites with corrected energies $\tilde{E}_A$ and $\tilde{E}_B$ and an effective interaction $\tilde{V}_{AB}$. The goal of the method is to make evident how the pathways should be modified in order to tune the resulting coupling. The condition for maximum coupling is $\tilde{E}_A = \tilde{E}_B$ (resonance) and is related to a generalised reflection–inversion symmetry while the coupling minimises if $\tilde{V}_{AB} = 0$ (anti-resonance). This is a non-trivial situation allowed by the topology of the system which occurs when two or more pathways interfere destructively. The effects of resonances and anti-resonances in electron transfer and other applications are discussed.



creating a “spy” in the atomic world:

the ^{1}H-^{13}C swapping gate in NMR

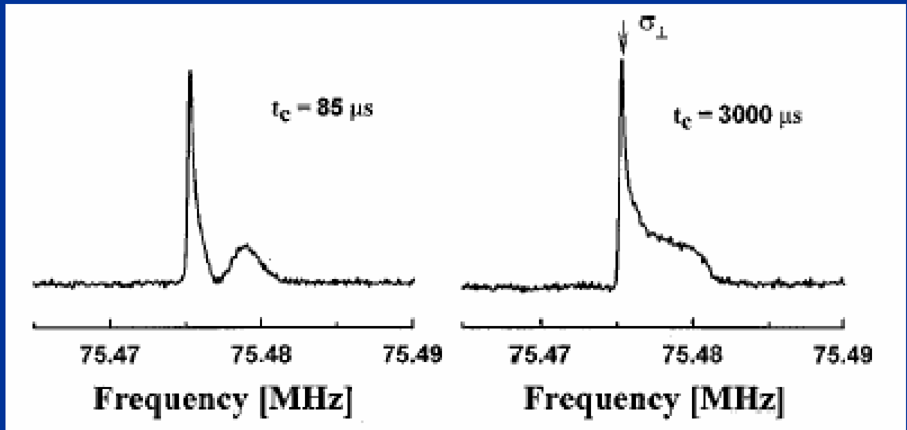
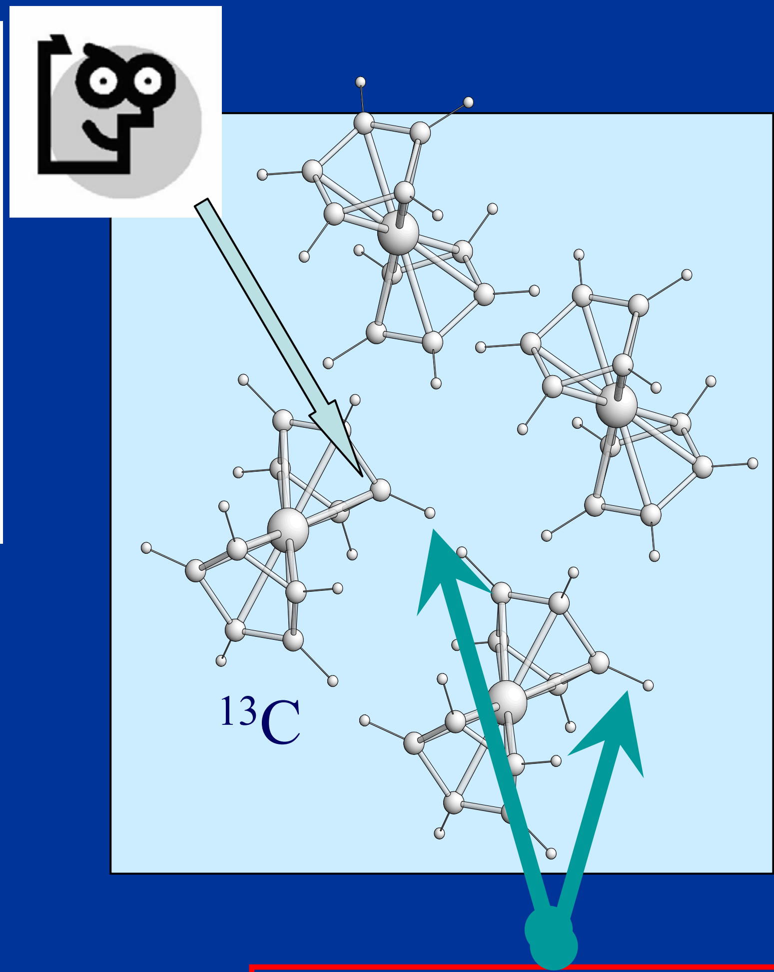


FIG. 3. ^{13}C-NMR spectra of polycrystalline ferrocene after a simple cross-polarization experiment with 85 μs and 3 ms contact times, respectively.



at room temperature
half of the spins are **up**
the other half is **down**

^{1}H-^{1}H Dipolar interaction

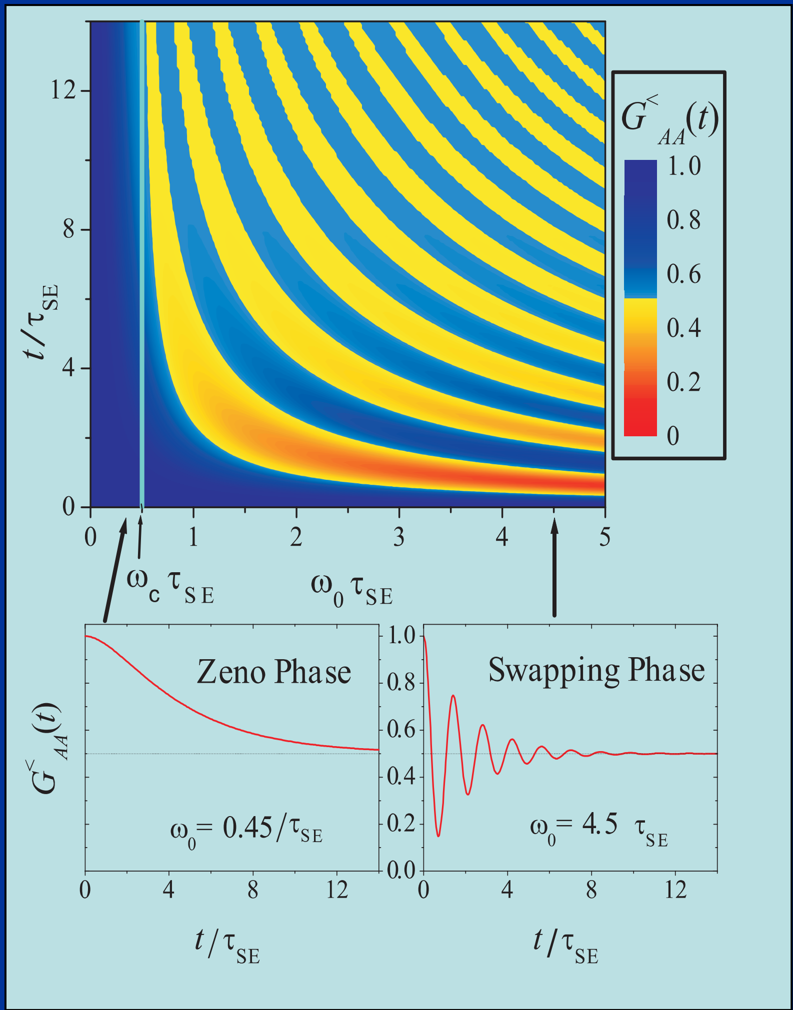
fermions

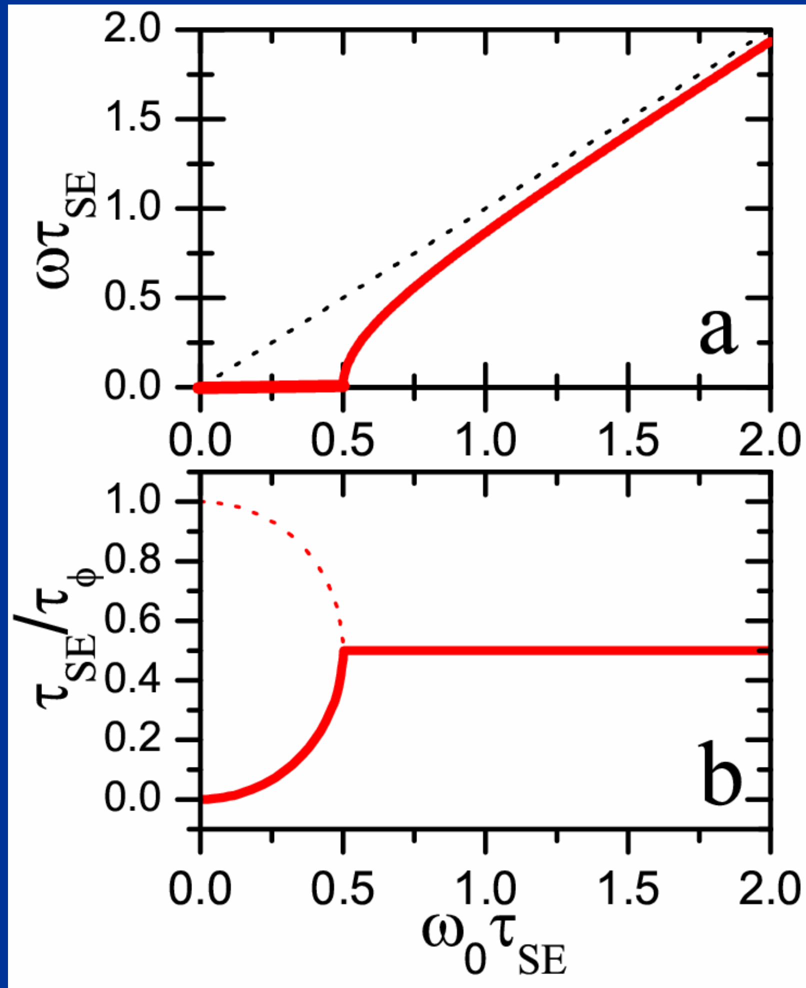
$$\omega = \begin{cases} \omega_0\sqrt{1-(2\omega_0\tau_{SE})^{-2}} & \omega_0 > \frac{1}{2\tau_{SE}} \\ 0 & \omega_0 \le \frac{1}{2\tau_{SE}} \end{cases}$$

$$\eta = \begin{cases} 0 & \omega_0 > \frac{1}{2\tau_{SE}} \\ \omega_0\sqrt{(2\omega_0\tau_{SE})^{-2}-1} & \omega_0 \le \frac{1}{2\tau_{SE}} \end{cases}$$

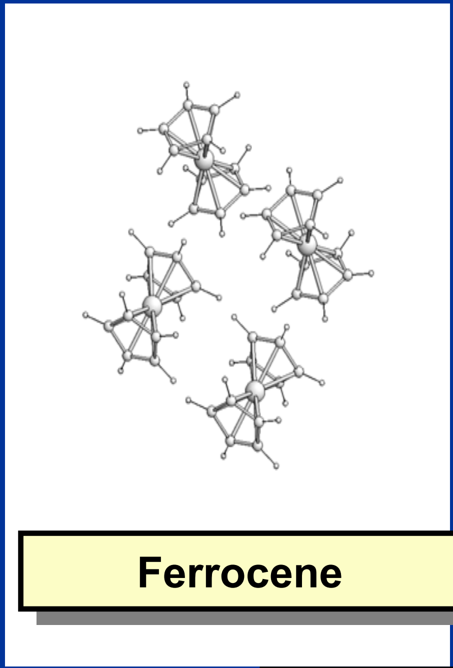
$$1/\tau_\phi = -\lim_{t\to\infty}\frac{1}{t}\ln[\tfrac{\hbar}{\mathrm{i}}G^<_{AA}(t,t)-\tfrac{1}{2}]$$
$$= 1/(2\tau_{SE}) \qquad \text{for} \quad \omega_0 \ge \frac{1}{2\tau_{SE}}$$

$$1/\tau_\phi = \frac{1}{2\tau_{SE}}\left[1-\sqrt{1-(2\omega_0\tau_{SE})^2}\right]$$
$$\simeq \omega_0^2\tau_{SE} \quad \text{for} \quad \omega_0 \ll \frac{1}{2\tau_{SE}}$$

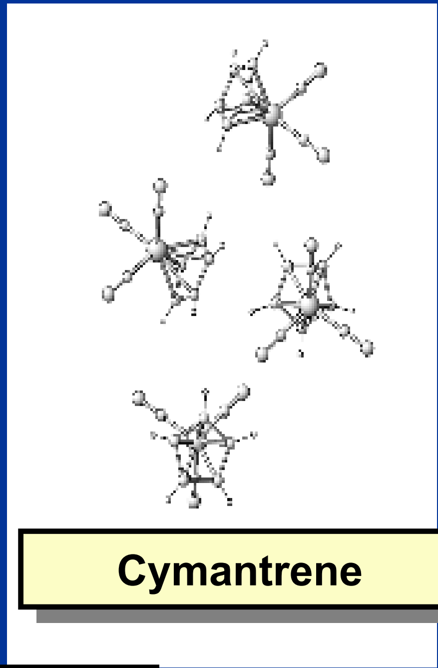




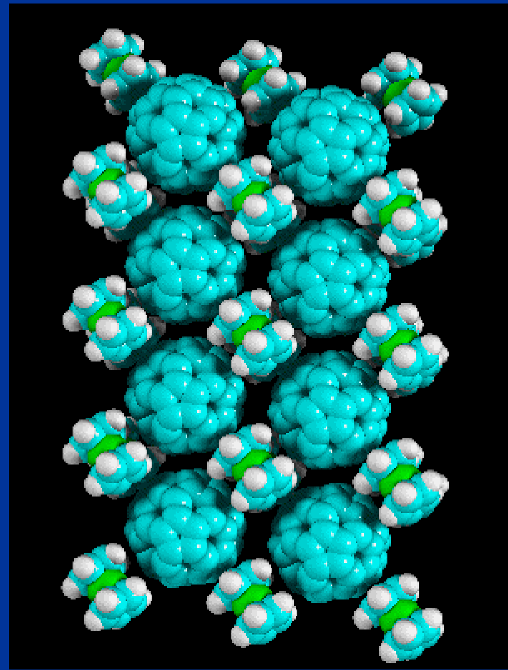
our experiments: finite and infinite networks of nuclear spins



Ferrocene

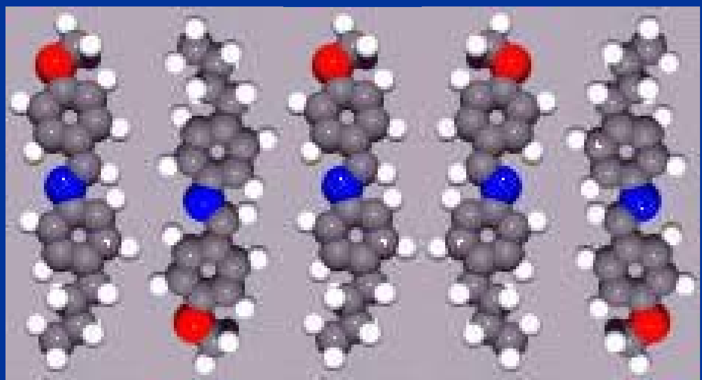


Cymantrene

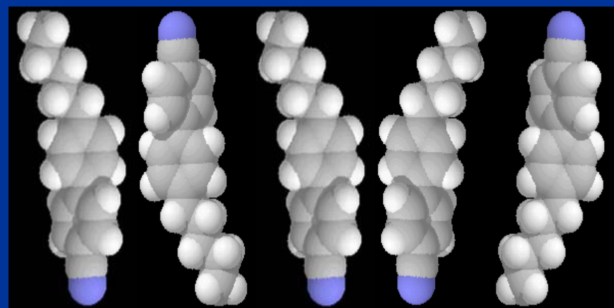


cobaltocene

$C_{60}(ferrocene)_2$



MBBA



5CB

8CB