Harnessing a Quantum Dynamical Phase Transition in Experimental Systems.

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Autumn College on Non-Equilibrium Quantum Systems 2 - 13 May 2011 Buenos Aires, Argentina

held at University of Buenos Aires, Dept. of Physics, Mathematics and Computer Science Aula Magna of Pabellon I

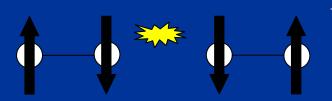
co-sponsored by:
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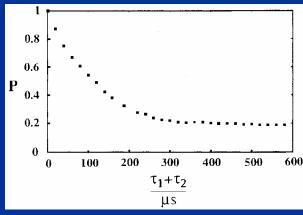
Wigner-Jordan: spins → fermions

flip-flop XY →hopping of electrons

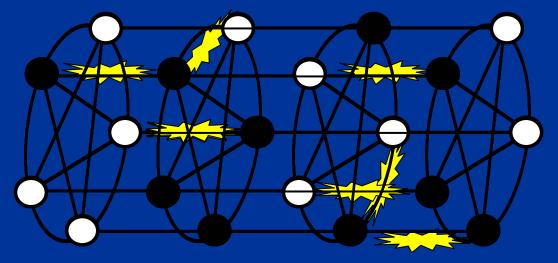
Ising → Hubbard







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

$$E_0$$
 E_1

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

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

Effective Hamiltonian



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

Green's function

$$G_{0,0}^{R} = \frac{1}{\varepsilon - \tilde{E}_{0}} = \frac{1}{\varepsilon - E_{0} - V_{0,1} \frac{1}{\varepsilon - E_{1}} V_{1,0}}$$

Self-energy

Series expansion: The Dyson Equation

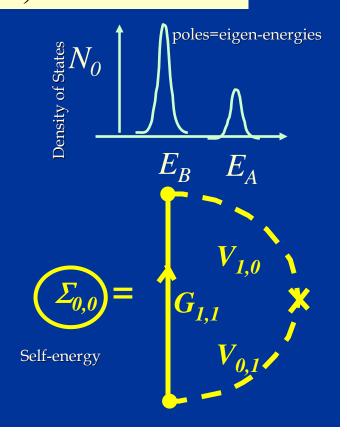
$$G_{0,0}^{R} = G_{00}^{(0)R} + G_{00}^{(0)R} V_{0,1} G_{1,1}^{(0)R} V_{1,0} G_{0,0}^{(0)R} + \dots$$

$$= G_{00}^{(0)R} + G_{00}^{(0)R} \sum_{0}^{R} G_{0,0}^{(0)R} + \dots$$

$$= G_{00}^{(0)R} + G_{00}^{(0)R} \sum_{0}^{R} G_{0,0}^{R}$$

Tuning the through-bond interaction in a two-center problem.

PR Levstein, HMP and JL D'Amato JPCM 2, 1781 (1990)

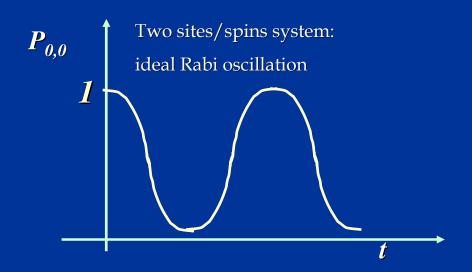


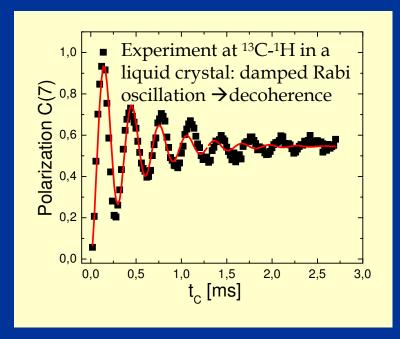
Simple Quantum Dynamics

$$\widetilde{\mathbf{H}}_{01} = \begin{pmatrix} \widetilde{E}_0 & \widetilde{V}_{0,1} \\ \widetilde{V}_{1,0} & \widetilde{E}_1 \end{pmatrix}$$

$$\mathbf{G}^R = \left[\varepsilon \mathbf{I} - \widetilde{\mathbf{H}}_{01} \right]^{-1}$$

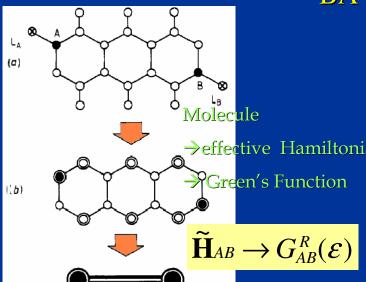
$$P_{0,0}(t) = \left| \int_{-\infty}^{\infty} \frac{\mathrm{d}\,\varepsilon}{2\pi\hbar} e^{-\mathrm{i}\varepsilon t/\hbar} G_{0,0}(\varepsilon) \right|^{2}$$





related problems

electron transfer k_{RA}



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

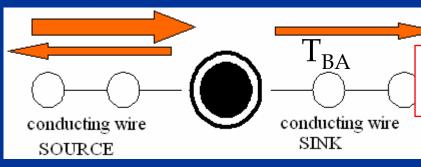
PR Levstein†, HM Pastawski‡ and JL D'Amato

Instituto de Desarrollo Tecnológico para la Industria Química, Güemes 3450, 3000 Santa Fe. Argentina

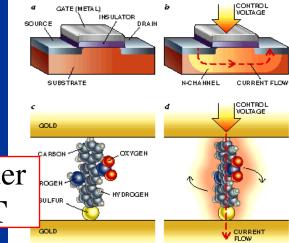
Received 16 May 1989, in final form 22 September 1989

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 $\tilde{E}_{\rm A}$ and $\tilde{E}_{\rm B}$ 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 $\hat{E}_A = \hat{E}_B$ (resonance) and is related to a generalised reflection-inversion symmetry while the coupling minimises if $V_{AB} = 0$ (anti-resonance). This is a non-trivial situation allowed by the reflective Hamiltonia repology 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.

molecular electronics



Rolf Landauer $1/R=e^2/h$ T

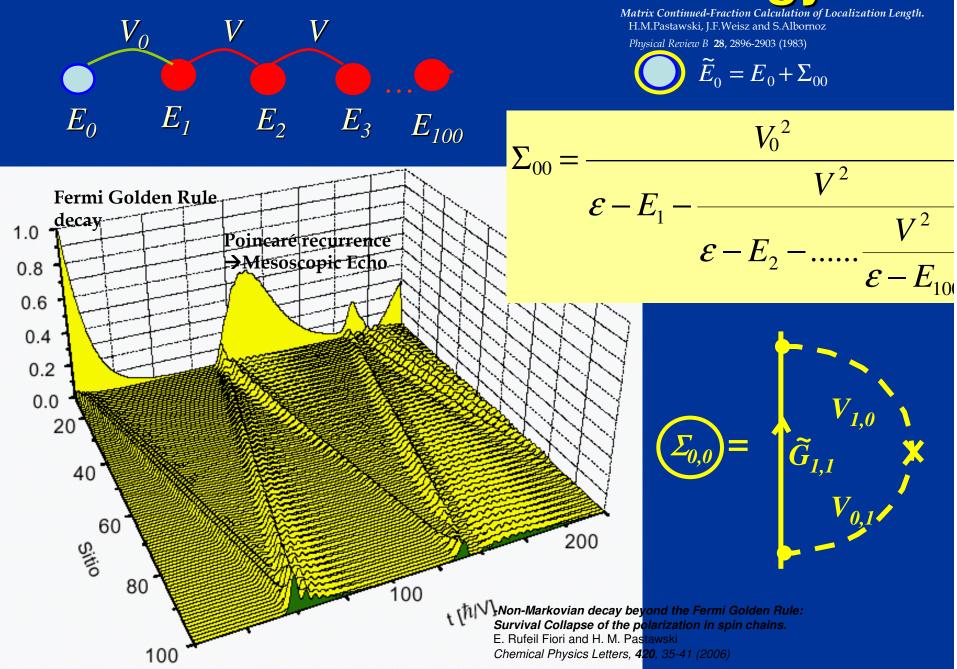


 $k_{BA} \propto T_{BA} \propto |G^R_{BA}(\mathcal{E})|^2$ Transmittance and kinetic constant are prop. Green's Function

Conductance is Transmittance

CONVENTIONAL MICROTRANSISTOR (a) has three terminals, known as the source, gate and drain. A positive voltage applied to the gate draws electrons to the insulator (b), enabling current to flow from the source to the drain. A molecule based on three benzene rings (c) was also used to switch an electric current. The center ring had asymmetric fragments, enabling it to be twisted by an electrical field (d). With a specific voltage applied, the electrical field twisted the molecule and permitted current to flow.

finite chain: real self-energy



spin -> fermion + Keldysh formalism

Danieli, HMP, Levstein Chem. Phys. Lett. 2003 and 2004

Polarization site at site f when injected at i:

$$P_{f,i}(t) = \frac{\left\langle \Psi_0 \left| \hat{S}_f^z(t) \hat{S}_i^z(0) \right| \Psi_0 \right\rangle}{\left\langle \Psi_0 \left| \hat{S}_i^z(0) \hat{S}_i^z(0) \right| \Psi_0 \right\rangle},$$

$$|\Psi_0\rangle = \sum_N a_N |\Psi_0^{(N)}\rangle$$

thermodynamical many-body equilibrium state constructed by adding states with different number N of spins up with appropriate statistical weights and random phases.

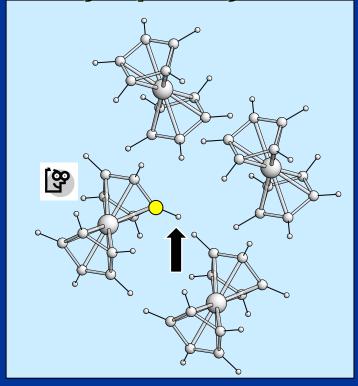
Jordan-Wigner,

$$\hat{S}_{n}^{z}(t) = \hat{c}_{n}^{+}(t)\hat{c}_{n}(t) - \frac{1}{2}$$

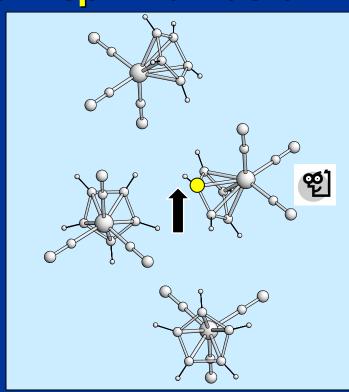
temperature
$$k_BT >> J$$
 $\hat{S}_n^z(t) = \hat{c}_n^+(t)\hat{c}_n(t) - \frac{1}{2}$ $G^{<}(X_2, X_1) = -i\hbar \sqrt{\psi(X_2)\psi^*(X_1)}$

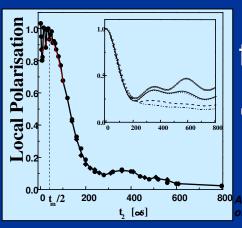
$$P_{f,i}(t) = \frac{\left\langle \Psi_0 \left| \hat{S}_f^z(t) \hat{S}_i^z(0) \right| \Psi_0 \right\rangle}{\left\langle \Psi_0 \left| \hat{S}_i^z(0) \hat{S}_i^z(0) \right| \Psi_0 \right\rangle} = -i\hbar 2G_{f,f}^{<}(t,t) - 1$$

many-spin dynamics >> quantum spin "diffusion"



a ¹³C "spies" the ¹H spin





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

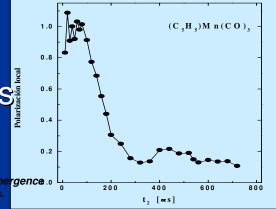
finite ring size

→ mesoscopic echoes

+...decoherence

Attenuation of polarization echoes in NMR: A test for the emergence.o of Dynamical Irreversibility in Many-Body Quantum Systems.

P.R. Levstein, G. Usaj, HMP J. Chem. Phys. **108**, 2718-2724 (1998)



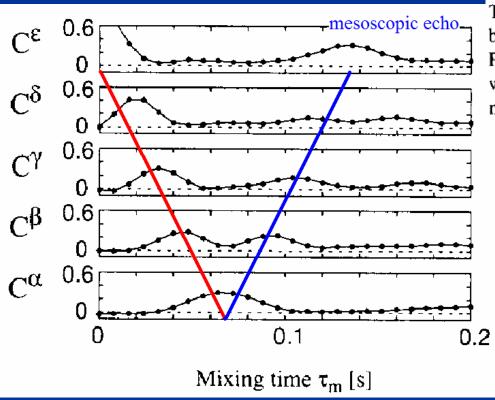
Mesoscopic Echoes: NMR experiments

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

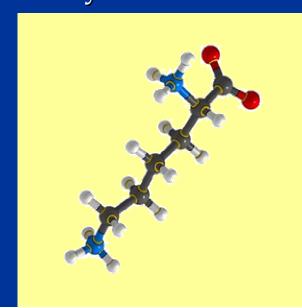
Laboratorium für Physikalische Chemie, ETH Zentrum, 8092 Zürich, Switzerland

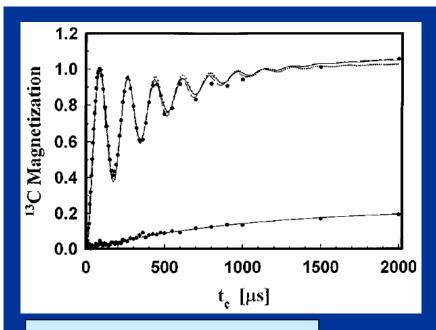


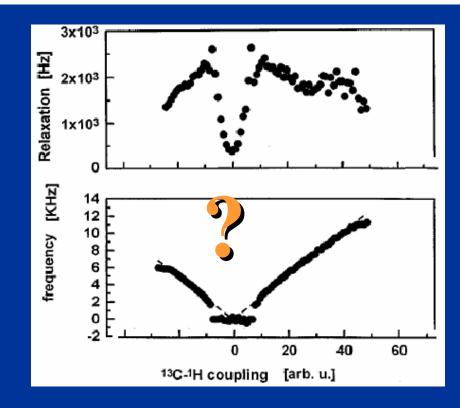


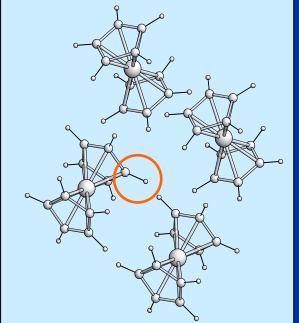
The study described in this letter has been inspired by discussions with Professor H.M. Pastawski and Professor P.R. Levstein who calculated nuclear spin wave evolution under a 'planar' or 'XY' Hamiltonian [3].

lysine









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

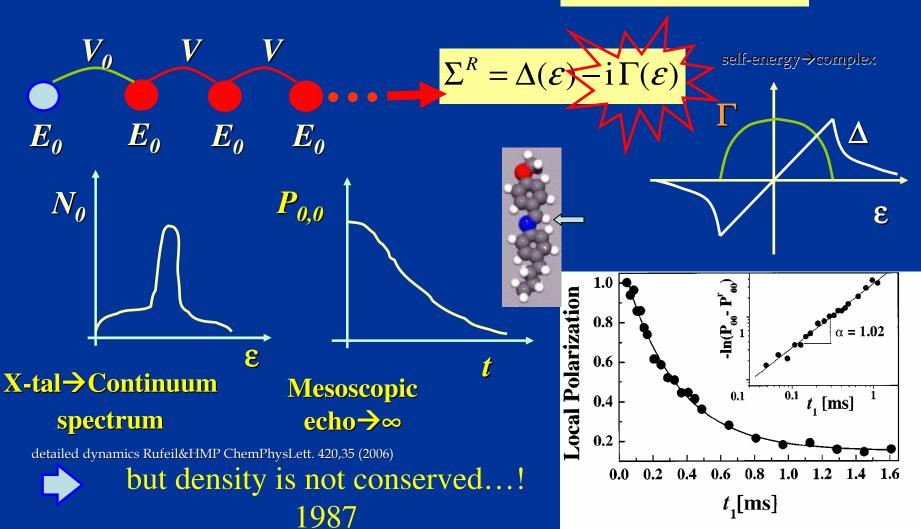
but... ${}^{13}C^{-1}H$ interacts with ${}^{1}H$ spin bath

NMR Quantum Dynamics -> fermions

Effective Hamiltonian for OPEN Systems

Ordered chain - Lead

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

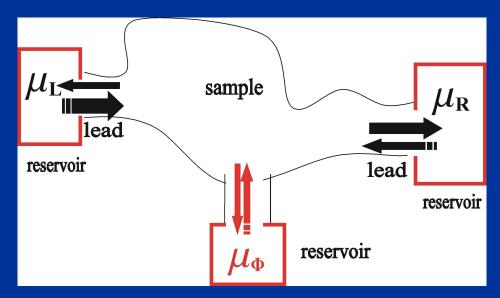


Phenomenology of Decoherence

(Büttiker 1986)

$$I_{\phi} \equiv 0$$

voltmeter



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

$$I_{R} = \frac{e}{h} \widetilde{T}_{R,L} (\delta \propto_{L} - \delta \propto_{R})$$

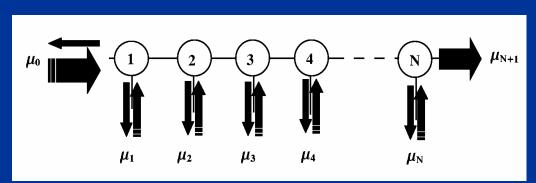
$$\begin{split} \widetilde{T}_{R,L} &= T_{R,L} + \frac{T_{R,\phi}T_{\phi,L}}{T_{R,\phi} + T_{\phi,L}} \\ &\text{coherent} \end{split}$$

Decoherence and evolution: Keldysh=GLBE

$$T_{RL} = 2\Gamma_{R} \left| G_{RL}^{R} \right|^{2} 2\Gamma_{L}$$

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 (Fermi Golden Rule)
 requires a thermodynamic limit and involves "irreversible" decay" to the environment
- charge conservation → Generalized Landauer Büttiker Equations=Keldysh



$$I_{i} \equiv 0 = (1/\mathcal{S}_{i})\delta \propto_{i} - \sum_{j=0}^{N} T_{i,j} \delta \propto_{j}$$

Charge is conserved at every point i

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

$$\begin{split} \widetilde{T}_{R,\,L} &= T_{R,\,L} + \sum_{i=1}^{N} \, T_{R,i} \, g_i T_{i,\,L} + \sum_{i=1}^{N} \sum_{j=1}^{N} \, T_{R,i} \, g_i T_{i,\,j} \, g_j \, T_{j,\,L} + \dots \\ &= T_{R,\,L} + \sum_{i=1}^{N} \, T_{R,i} \, g_i \, \widetilde{T}_{i,\,L} \end{split} \qquad \text{GLBE = Bethe-Salpeter}$$

Keldysh in a Nutshell: GLBE Pastawski PhysRevB 92

$$\begin{bmatrix}
\text{"detected general density"} \\
\Psi(X_2)\Psi^*(X_1)
\end{bmatrix} = \hbar^2 \iint dX_j G^R(X_2, X_j) \underbrace{\Psi(X_j)}_{retarded} \underbrace{\Psi^*(X_k)}_{advanced} \underbrace{G^R(X_k, X_1)}_{init.coord.} \underbrace{G^R(X_k, X_k)}_{advanced} \underbrace{G^R(X_k, X_k$$

quantum dynamics of open systems

Keldysh Density Function

- **→**Wigner function
- = Density Matrix

$$G^{<}(X_2, X_1) = -i \hbar \left[(Y(X_2) \Psi^*(X_1)) \right]$$

$$G^{<}(X_{2},X_{1}) = \hbar^{2} \iint_{C} dr_{j} G^{R}(X_{2},r_{j}) \underbrace{\begin{bmatrix} \text{intial distrib.} \\ G^{<}(r_{j},t_{0};r_{k},t_{0}) \end{bmatrix}}_{\text{init.coord.}} \underbrace{G^{A}(r_{k},X_{1}) dr_{k}}_{\text{advanced}}$$

$$+ \iint_{C} \underbrace{\frac{\text{init.coord.}}{dX_{j} G^{R}(X_{2},X_{j})}}_{\text{retarded}} \underbrace{\begin{bmatrix} \Sigma^{<}(X_{j},X_{k}) \end{bmatrix}}_{\text{coord.}} \underbrace{G^{A}(X_{k},X_{1}) dX_{k}}_{\text{advanced}}$$

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

$$\Sigma^{<}(r,t) = {}^{\phi}\Gamma_{r}(\mathcal{E}) f_{r}(r,\mathcal{E},t)$$

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

$$G_{k,l}^{<}(t_2,t_1) = \langle \Psi_{ne} \left| \hat{c}_k^{+}(t_1) \hat{c}_l(t_2) \right| \Psi_{ne} \rangle,$$

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

$$G_{k,l}^{R}(t_2,t_1) = -\frac{\mathrm{i}}{\hbar} \theta(t_2-t_1) \langle \Psi | \hat{c}_k(t_2) \hat{c}_l^{\dagger}(t_1) + \hat{c}_l(t_1) \hat{c}_k^{\dagger}(t_2) | \Psi \rangle.$$

$$\Sigma_0^R(\mathcal{E}) \approx -i\Gamma_0$$
 \leftarrow if $V_0 << V$

$$G_{n,m}^{<}(t_{2},t_{1}) = \hbar^{2} \sum_{l,k} G_{n,k}^{R}(t_{2},0) G_{k,l}^{<}(0,0) G_{l,m}^{A}(0,t_{1})$$

$$+ \sum_{k,l} \int_{t_{0}}^{t} \int_{t_{0}}^{t} G_{n,k}^{R}(t_{2},t_{k}) \Sigma_{k,l}^{<}(t_{k},t_{l}) G_{l,m}^{A}(t_{l},t_{1}) dt_{k} dt_{l}.$$

Non-equilibrium density at t=0 at site i-th

$$G_{k,l}^{<}(t=0,t=0) = \frac{i}{2\hbar} (\delta_{k,l} \delta_{i,l} + \delta_{k,l})$$

Occupation
probability

i-1 i i+1 Initial condition at t=0

sites

 $\sum_{0,0}^{<} (\varepsilon, t_k) = \int d \delta t \, e^{i \varepsilon \delta t / \hbar} \, \chi_0^* (t_k + \frac{1}{2} \delta t) \chi_0 (t_k - \frac{1}{2} \delta t)$

This term would collect incoherent or coherent reinjections given by,

$$\Sigma_{0,0}^{<}(\varepsilon,t_k) = i2\Gamma_0 f(\varepsilon,t_k) \delta_{k,0} \delta_{0,l}.$$

Two oscillators interacting through the environment:

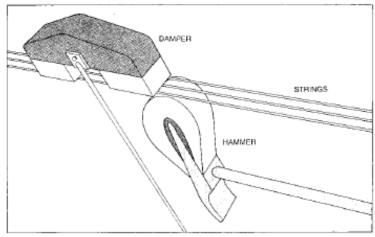
The Piano Lesson

Coupled piano strings

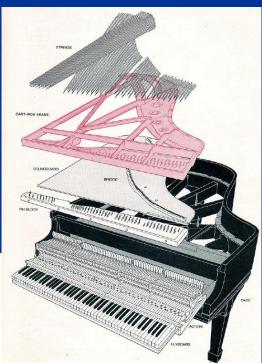
Gabriel Weinreich

1474

J. Acoust. Soc. Am., Vol. 62, No. 6, December 1977



HAMMER HITS THE STRINGS that correspond to one note with the same strength and at the same time. Because the hammer strikes the strings in the vertical direction, they move mostly in that direction. They also move, however, a little in the horizontal direction. This motion could be caused by small irregularities in the face of the hammer or the position of the strings.



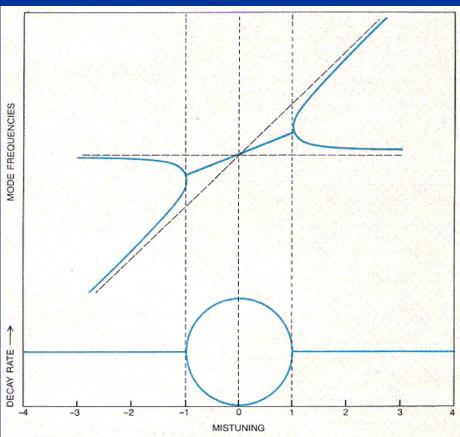
STRING DISPLACEMENT

STRING DISPLACEMENT

HAMMER IMPERFECTIONS can result in string amplitudes that are not absolutely equal. Here two strings are set in motion at the same time but with the colored string having a larger amplitude than the black one. The motions of the strings start to decay, and when the amplitude of the black string approaches zero, the bridge continues

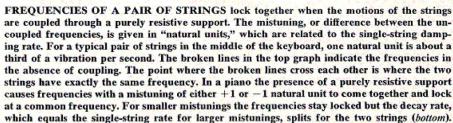
to move because it is still being forced to do so by the colored string. As a result the black string not only reaches zero amplitude but also goes "beyond" it, building up a vibration of the opposite phase by absorbing energy from the bridge. Ultimately the motions are exactly antisymmetric. Such antisymmetric motion gives rise to aftersound.

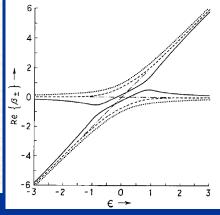
The piano lesson (cont.)



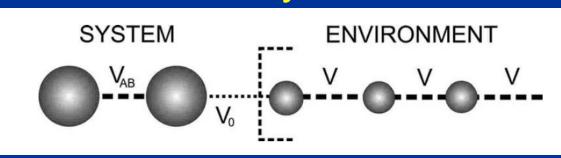
Because of the environment...

the two strings synchronize themselves...!





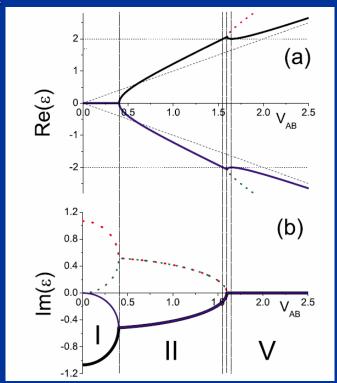
asymmetric environment



Infinite environment→FGR→Non-Hermitian effective Hamiltonian→ exceptional points in the spectrum→Quantum Dynamical Phase Transition

Ingrid Rotter 2009 *J. Phys. A: Math. Theor.* **42** 153001 **A non-Hermitian Hamilton operator and the physics of open uantum systems**

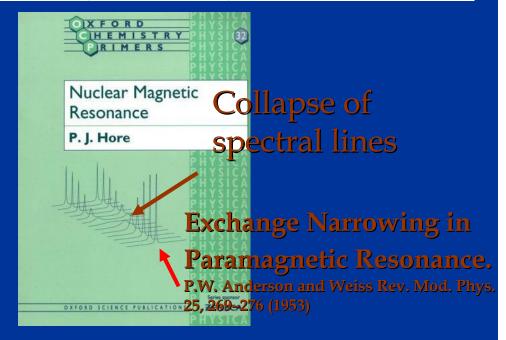
poles of the GF bifurcate



PHYSICAL REVIEW A 78, 062116 (2008)

Dynamical regimes of a quantum SWAP gate beyond the Fermi golden rule

Axel D. Dente, Raúl A. Bustos-Marún, 1,2 and Horacio M. Pastawski 1



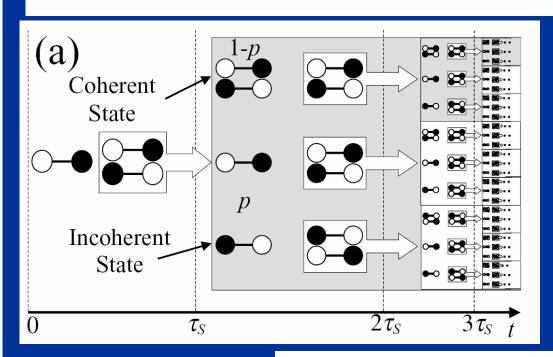
GLBE for spins: avoid memorize previous stories by using Trotter steps (Keldysh=Quantum Jumps).

$$\frac{1}{\hbar^2}\mathbf{G}^<\left(t\right) = \mathbf{G}^{0\mathrm{R}}\left(t\right)\mathbf{G}^<\left(0\right)\mathbf{G}^{0\mathrm{A}}\left(t\right)\left(1-p\right)^n + \quad \text{(4)} \qquad \qquad \text{HMP cond-mat/0504347}$$

$$\sum_{m=1}^{n}\mathbf{G}^{0\mathrm{R}}\left(t-t_m\right)\widetilde{\boldsymbol{\Sigma}}^<\left(t_m\right)\mathbf{G}^{0\mathrm{A}}\left(t-t_m\right)p\left(1-p\right)^{n-m}, \qquad \qquad \boldsymbol{\Sigma}^<_{\mathrm{m}}(t) = \mathrm{i}\frac{\hbar}{\tau_{\mathrm{SE}}}\begin{pmatrix}\frac{\hbar}{\mathrm{i}}G_{11}^<\left(t\right) & 0\\ 0 & \frac{\hbar}{\mathrm{i}}G_{22}^<\left(t\right)\end{pmatrix}$$

Danieli, Álvarez, HMP CPL05; Álvarez, Danieli, Levstein, HMP cond-mat/0504347

$$\Sigma_{\mathrm{m}}^{<}\left(t\right) = \mathrm{i}\frac{\hbar}{\tau_{\mathrm{SE}}} \left(\begin{array}{cc} \frac{\hbar}{\mathrm{i}} G_{11}^{<}\left(t\right) & 0\\ 0 & \frac{\hbar}{\mathrm{i}} G_{22}^{<}\left(t\right) \end{array}\right)$$



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

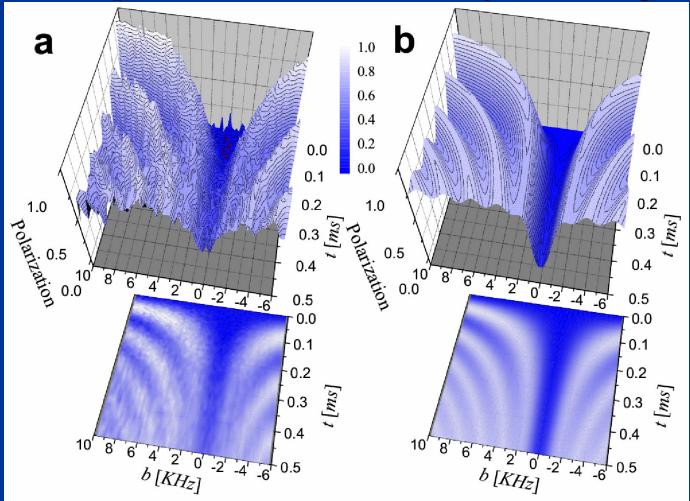
Integral GLBE-Keldysh →simpler Trotter evolution Carmichel's Quantum Jumps

PHYSICAL REVIEW A 75, 062116 (2007)

Decoherence under many-body system-environment interactions: A stroboscopic representation based on a fictitiously homogenized interaction rate

Gonzalo A. Álvarez, Ernesto P. Danieli, Patricia R. Levstein, and Horacio M. Pastawski*

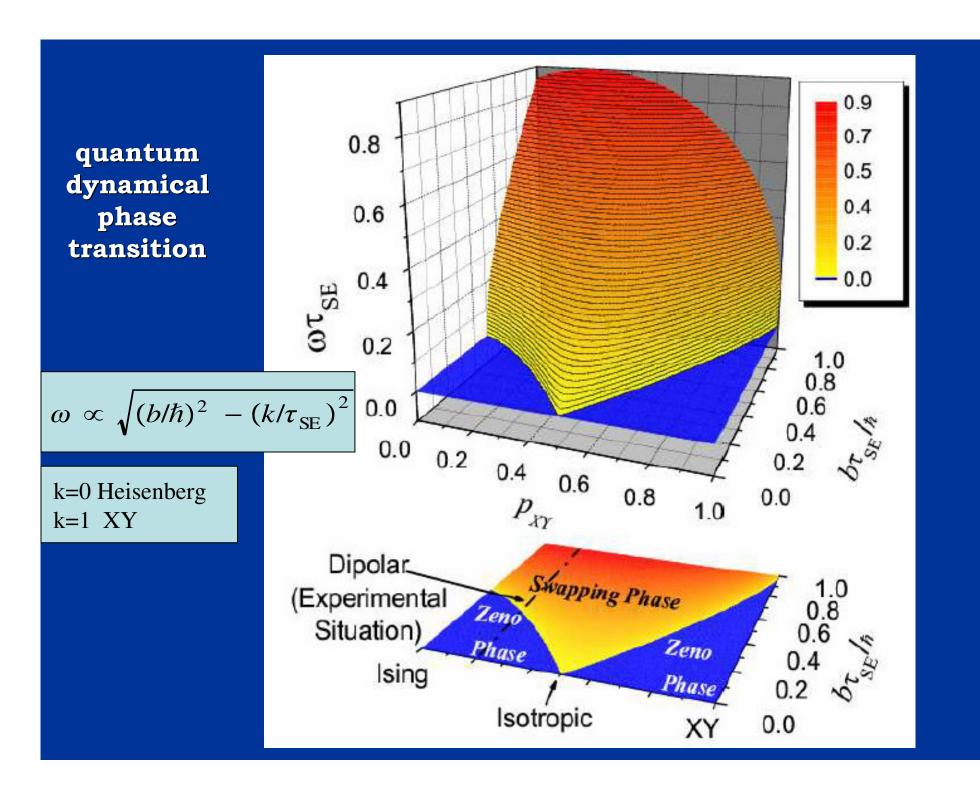
raw experimental data theory (no-fitting)



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

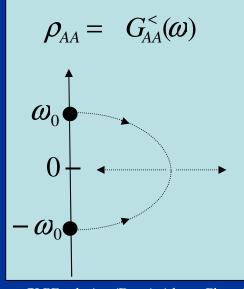
>quantum dynamical phase transition

Environmentally induced quantum dynamical phase transition in the spin swapping operation GA Álvarez, E P Danieli, PR Levstein, and HMP J. Chem. Phys. 124, 1 (2006)



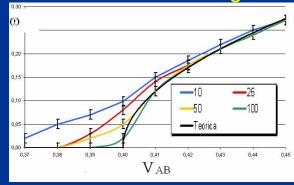
\mathcal{E}_{A} \mathcal{E}_{B} \mathcal{E}_{B} Γ

NO Phase Transition in the GF poles

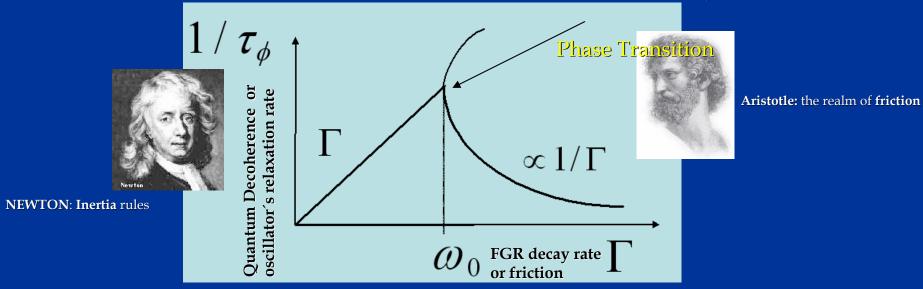


GLBE solution (Density) has a Phase Transition

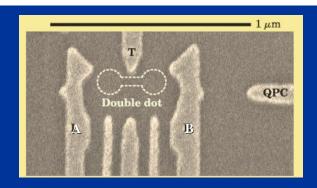
Ising interaction: decoherence rate and frequency are non-analytic on the SE interaction strength



NO finite system has a Phase Transition



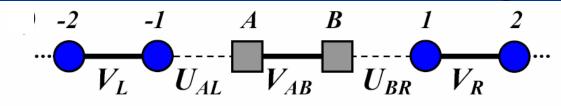
review on Quantum Dynamical Phase Transition and its philosophical implications: *Revisiting the Fermi Golden Rule: Quantum dynamical phase transition as a paradigm shift* HMP Physica B **398** (2007) 278

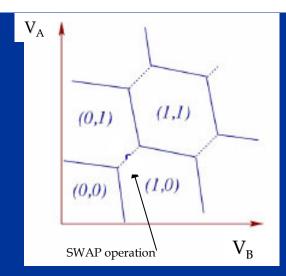


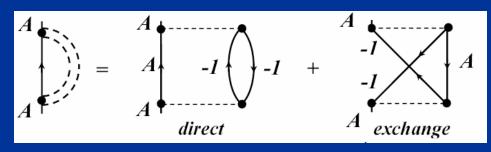
swap gate

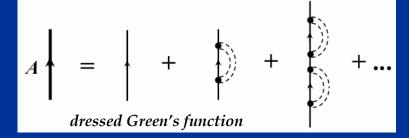
double dot charge q-bit

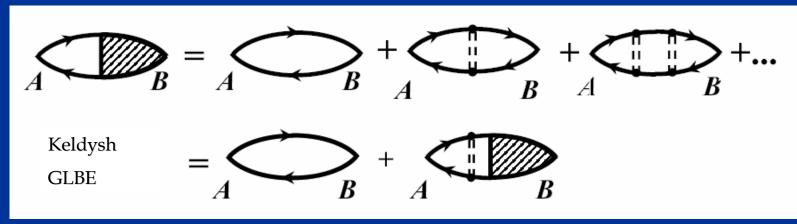
Fermions←→spins Coulomb←→Ising











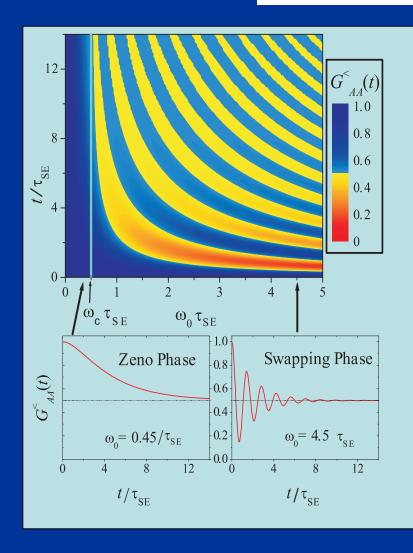
fermions

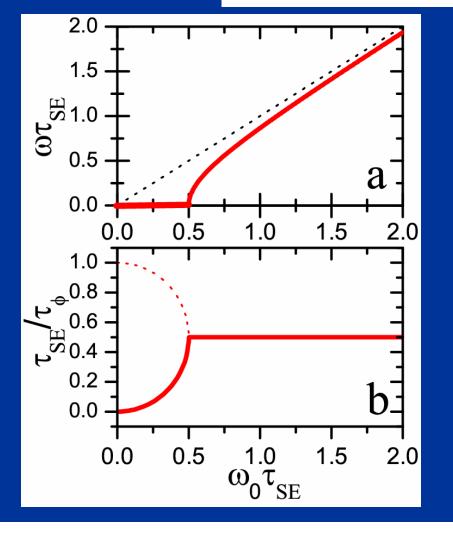
$$\omega = \begin{cases} \omega_0 \sqrt{1 - (2\omega_0 \tau_{SE})^{-2}} & \omega_0 > \frac{1}{2\tau_{SE}} \\ 0 & \omega_0 \le \frac{1}{2\tau_{SE}} \end{cases}$$

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

$$1/\tau_{\phi} = -\lim_{t \to \infty} \frac{1}{t} \ln\left[\frac{\hbar}{i} G_{AA}^{<}(t, t) - \frac{1}{2}\right]$$
$$= 1/\left(2\tau_{\text{SE}}\right) \quad \text{for} \quad \omega_{0} \ge \frac{1}{2\tau_{\text{SE}}}$$

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



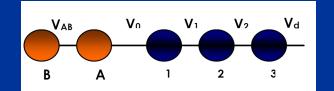


Why is Catalytic Molecular Disociación abrupt? a Quantum Dynamical Phase Transition...?

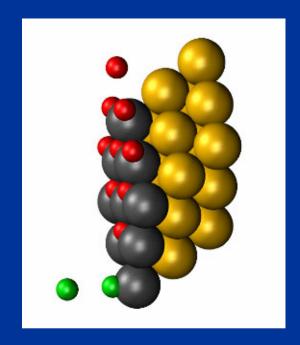
Axel Dente, Andrés Ruderman,

Raúl Bustos-Marún

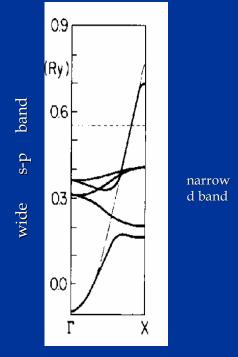
E. Santos, W.Schmickler





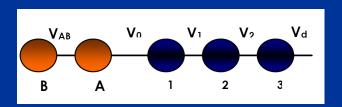


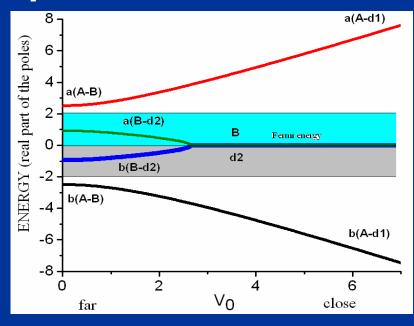
 $\begin{array}{c} \mbox{LDA mol. Dynamics:} \\ H_2 \ molecule \ on \\ top \ a \ Pt \ surface \end{array}$

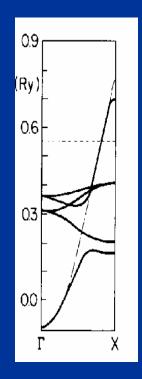


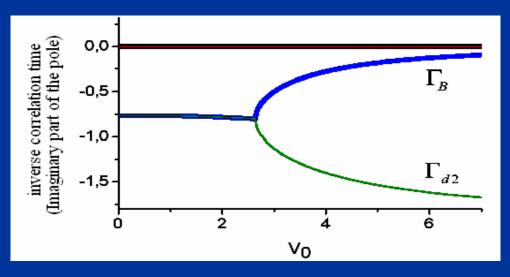
Pt band structure

Molecular Dissociation is a quantum dynamical phase transition









Summary

- --We observed experimentally that the dynamics of SWAP gate has a transition to a frozen regime...! ...it is 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...
- → quantum dynamical phase transition (bifurcation).
- **--SURPRISE:** The isotropy in the spin-spin interaction hinders the transition

original work on time dependent Keldysh Classical and Quantum Transport from Generalized Landauer-Büttiker Equations I and II: Time dependent tunneling. HMPPhys. Rev. B 44 6329(1991); Phys. Rev. B 46 4053 (1992)

review on Green's functions:

`Tight Binding' methods in quantum transport through molecules and small devices: From the coherent to the decoherent description. HMP and E. Medina Rev. Mex. Fisica 4 7s1, 1-23 (2001) cond-mat/0103219

review on FGR and Quantum Dynamical Phase Transition:

Revisiting the Fermi Golden Rule: Quantum dynamical phase transition as a paradigm shift

HMP Physica B **398** (2007) 278