Effective one-body dynamics in spin chains; Coherence, Interference and Decoherence

LaNAIS de RMS

Elena Rufeil Fiori

Dr. Horacio M. Pastawski, Dra. Patricia R. Levstein.

Facultad de Matemática, Astronomía y Física, Universidad Nacional de Córdoba, Córdoba, Argentina.

rufeil@famaf.unc.edu.ar; http://www.famaf.unc.edu.ar/~rufeil

Motivation

One-dimensional systems
One-body dynamics

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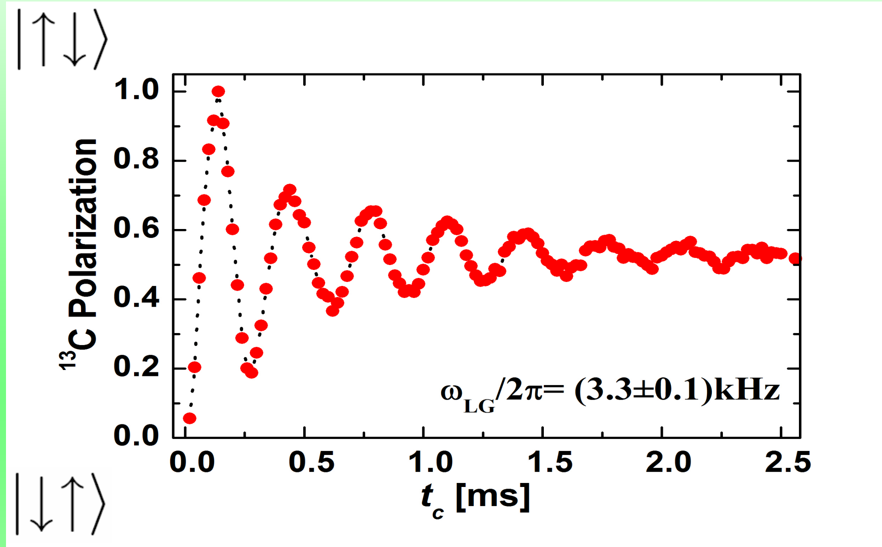
Quantum effects

Interference in time domain,
Coherence and Decoherence



Non-Markovian environment, many-body superposition states

How can we use NMR at room temperature as an effective one-body quantum system?

Mapping to non-interacting fermions

many-body ...

NMR in liquid state

$$H_{XY} = D_{i,i+1} \sum_{i=1}^{N} \left(I_i^+ I_{i+1}^- + I_i^- I_{i+1}^+ \right)$$

NMR in solid state

$$H_{DQ} = D_{i,i+1} \sum_{i=1}^{N} \left(I_i^+ I_{i+1}^+ + I_i^- I_{i+1}^- \right)$$

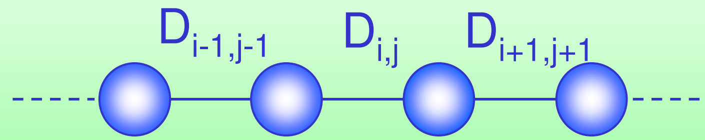
$$\left\langle I^z \right\rangle (t) = \sum J_M(t) \exp(-iM\phi)$$

$$P_{i,i}(t) = \left\langle I_i^z(t) I_i^z(0) \right\rangle$$

Jordan-Wigner

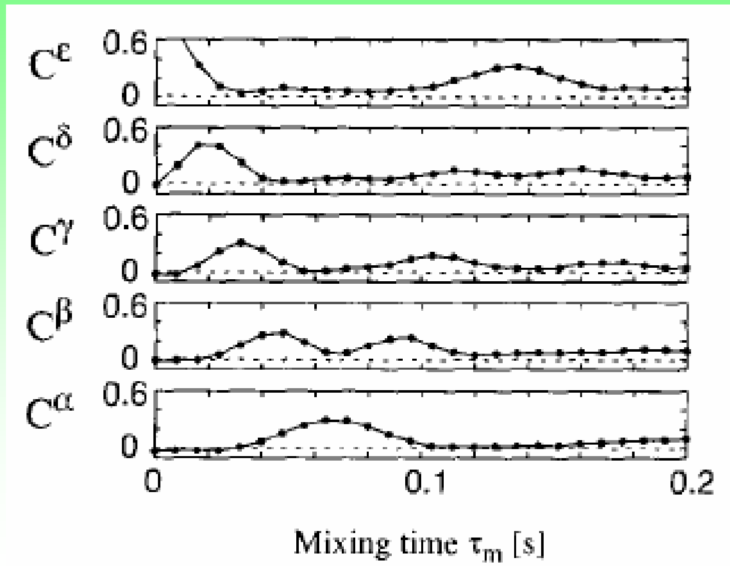
Feld´man et al.

one-body ...



Non-interacting fermions

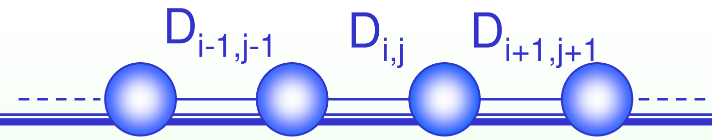
$$H_{TB} = D_{i,i+1} \sum_{i=1}^{N} \left(c_i^+ c_{i+1} + c_{i+1}^+ c_i \right)$$



Pair correlation function in a 5 spin chain, Liquid state NMR.

Z.L. Mádi et al. / Chemical Physics Letters 268 (1997) 300–305

Mapping to non-interacting fermions



many-body ...

NMR in liquid state

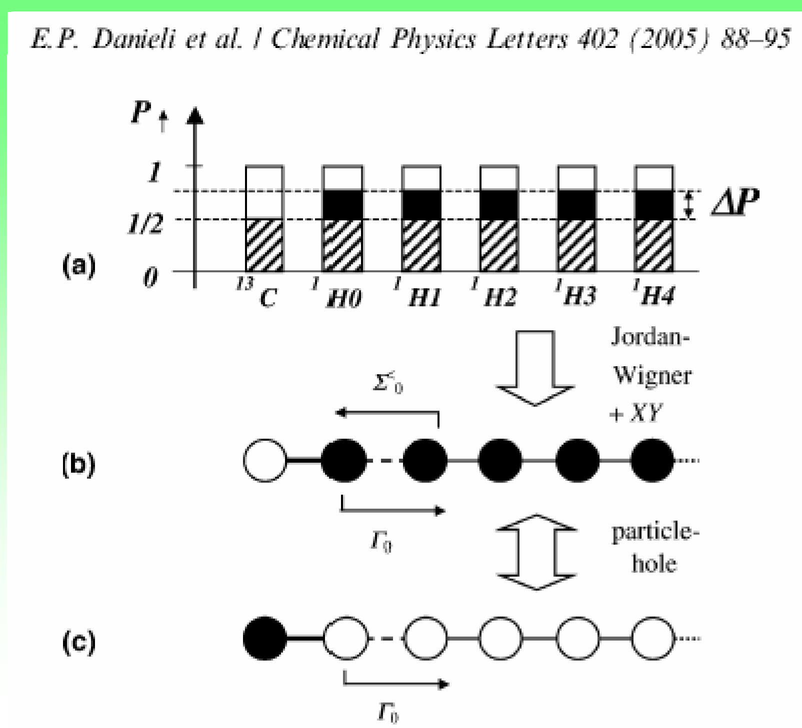
$$H_{XY} = D_{i,i+1} \sum_{i=1}^{N} \left(I_i^+ I_{i+1}^- + I_i^- I_{i+1}^+ \right)$$

Jordan-Wigner →

one-body ...

Non-interacting fermions

$$H_{TB} = D_{i,i+1} \sum_{i=1}^{N} \left(c_i^+ c_{i+1} + c_{i+1}^+ c_i \right)$$



Local Polarization, autocorrelation function

$$P_{i,i}(t) = \left\langle I_i^z(t) I_i^z(0) \right\rangle_{ens} \qquad T = \infty$$

Survival Probability

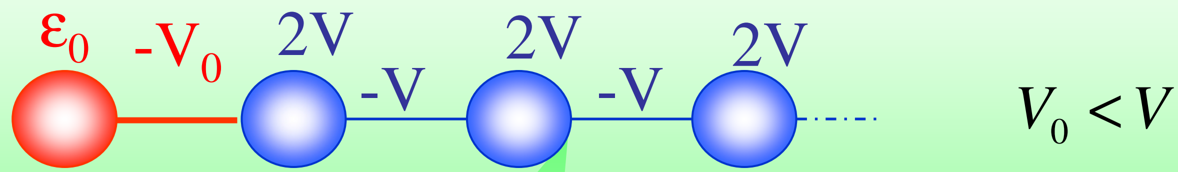
$$P_{i,i}(t) = \left| \left\langle i \right| \exp(-iHt) \left| i \right\rangle \right|^2 \qquad T = 0$$

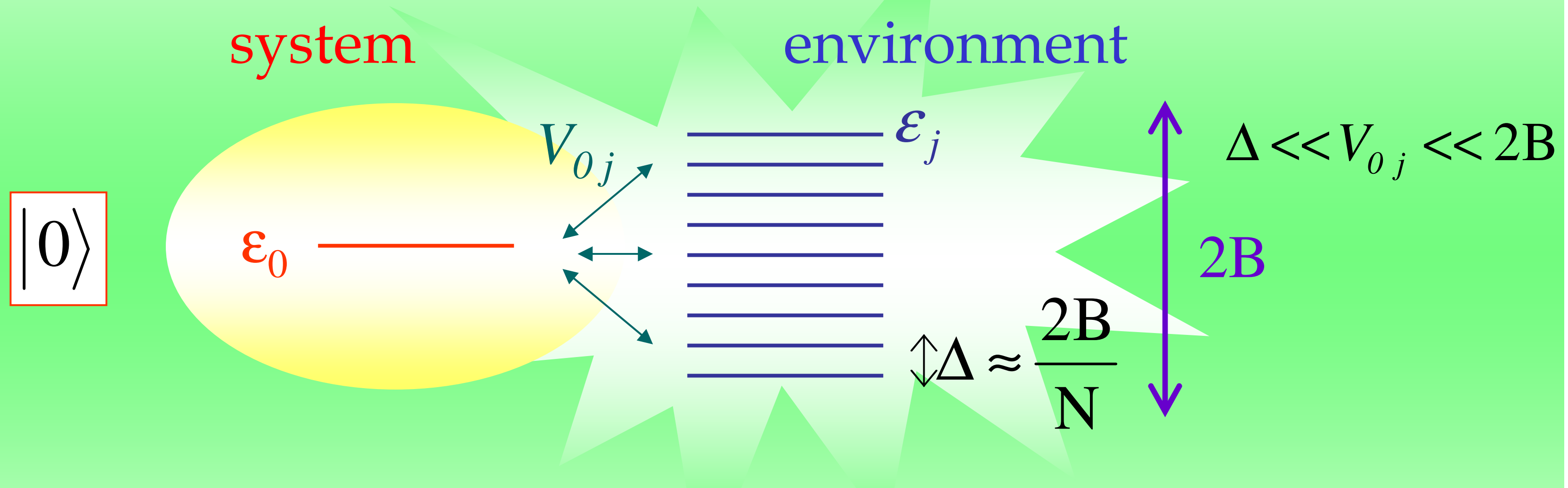
$\left| i \right\rangle$ **Single-particle state localized at site *i***

System-environment; Survival probability

$$P_{00}(t) = \left| \langle 0 | \exp(-iHt) | 0 \rangle \right|^2$$

Well-defined resonance





Wide band approx, Markovian approx

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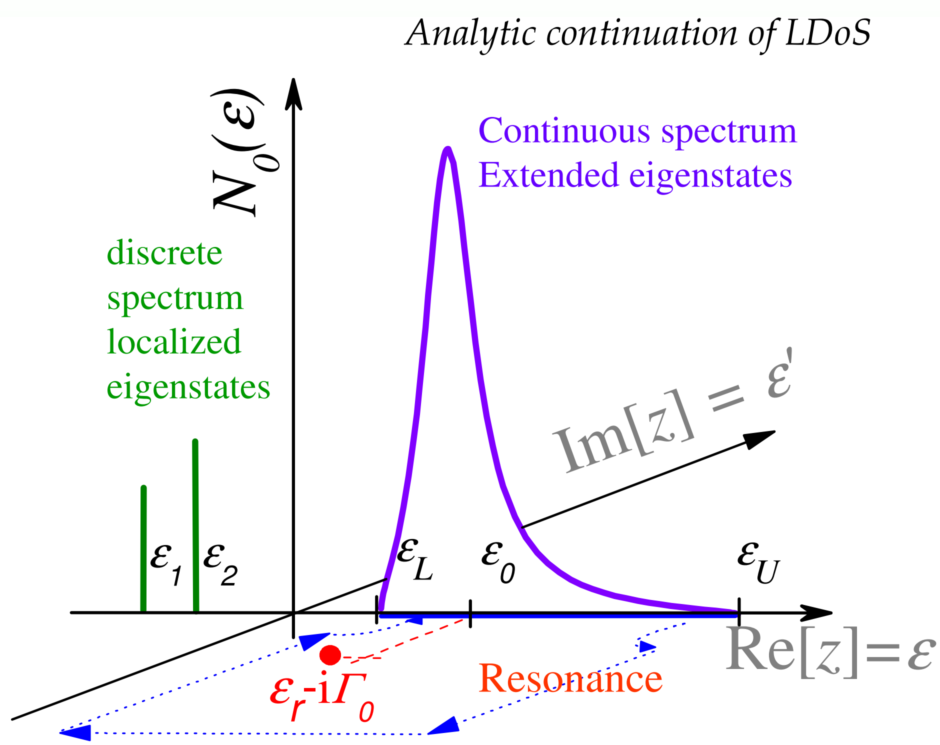
Exponential decay with a rate given by the Fermi Golden Rule (FGR) approx

FGR → 1st order approx in a perturbation theory, no returns from the environment, no memory effects... If one consider a non-Markovian environment...

Survival Probability and LDoS

$$P_{00}(t) = \left| \langle 0 | e^{-\frac{i}{\hbar} H t} | 0 \rangle \; \theta(t) \right|^2$$

$$P_{00}(t) = \left| \int_0^B d\varepsilon \, N_0(\varepsilon) \; e^{-\frac{i}{\hbar}\varepsilon t} \right|^2$$



residue theorem

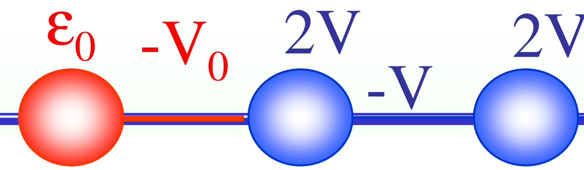
system without localized eigenstates

$$P_{00}(t) = \left| \; a \, e^{-(\Gamma_0 - i\varepsilon_r)t/\hbar} + \int_0^\infty d\varepsilon' e^{-\varepsilon' t/\hbar} \left[e^{-i\varepsilon_L t/\hbar} N_0(\varepsilon_L - i\varepsilon') - e^{-i\varepsilon_U t/\hbar} N_0(\varepsilon_U - i\varepsilon') \right] \right|^2$$

SC-FGR

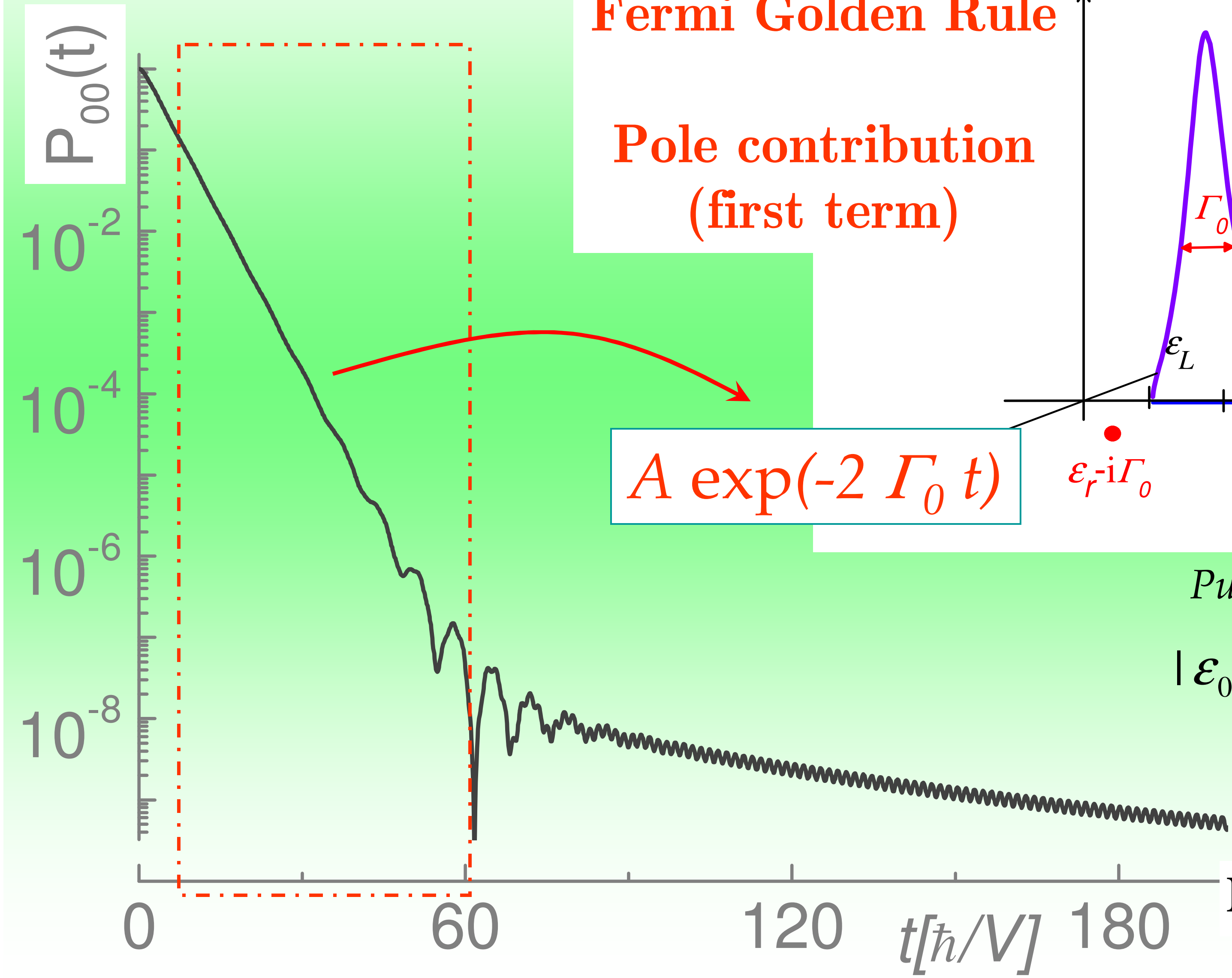
return correction from the environment

Survival Probability; Exponential Decay

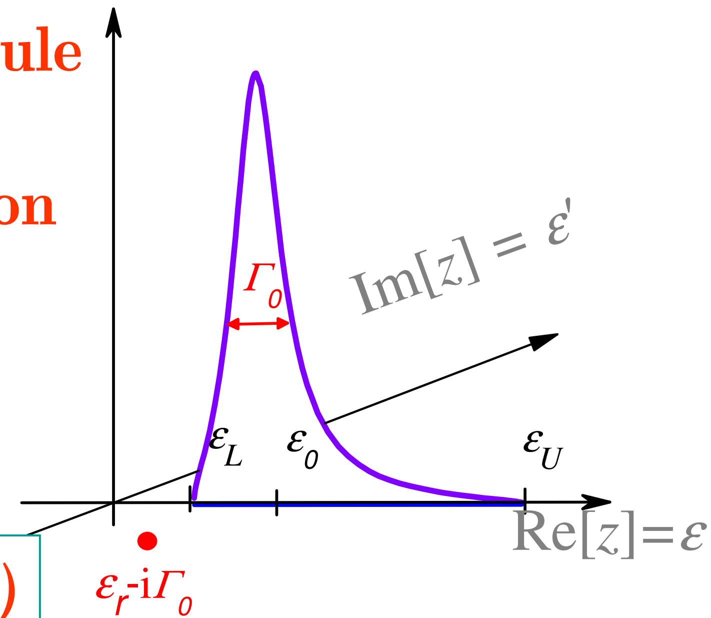


Self-Consistent Fermi Golden Rule

Pole contribution (first term)



$A \exp(-2\,\Gamma_0\,t)$



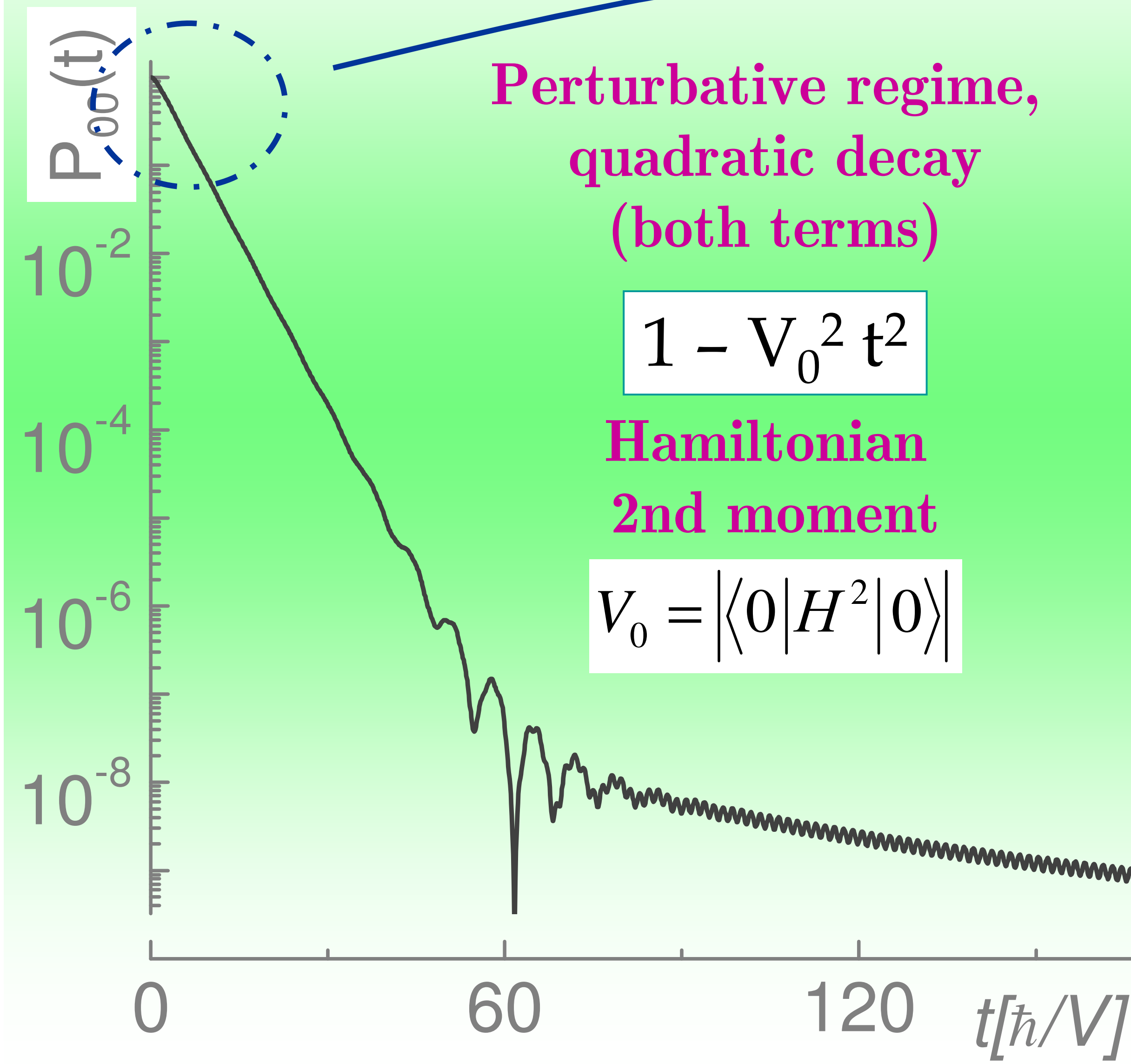
Pure continuous spectrum:

$$|\varepsilon_0 - 2V| < 2V - V_0^{\,2}/V$$

Well defined resonance at $\varepsilon_r - i\,\Gamma_0$:

$$\Gamma_0 << \varepsilon_r < B \equiv 4V$$

Survival Probability; Short time behaviour

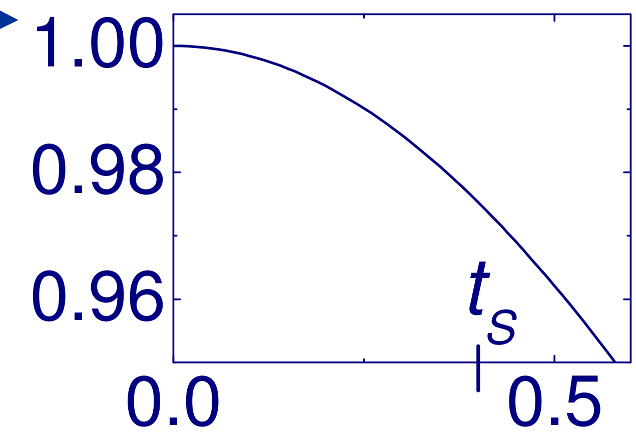


Perturbative regime, quadratic decay (both terms)

$$1 - V_0^2\, t^2$$

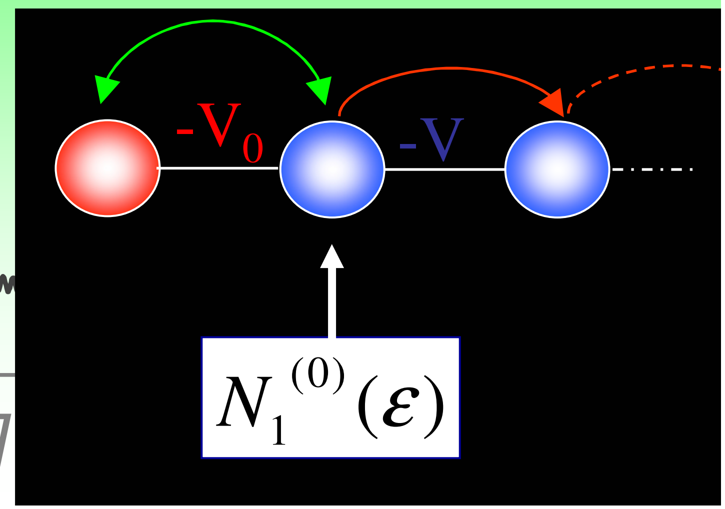
Hamiltonian 2nd moment

$$V_0 = \left|\langle 0 | H^2 | 0 \rangle\right|$$

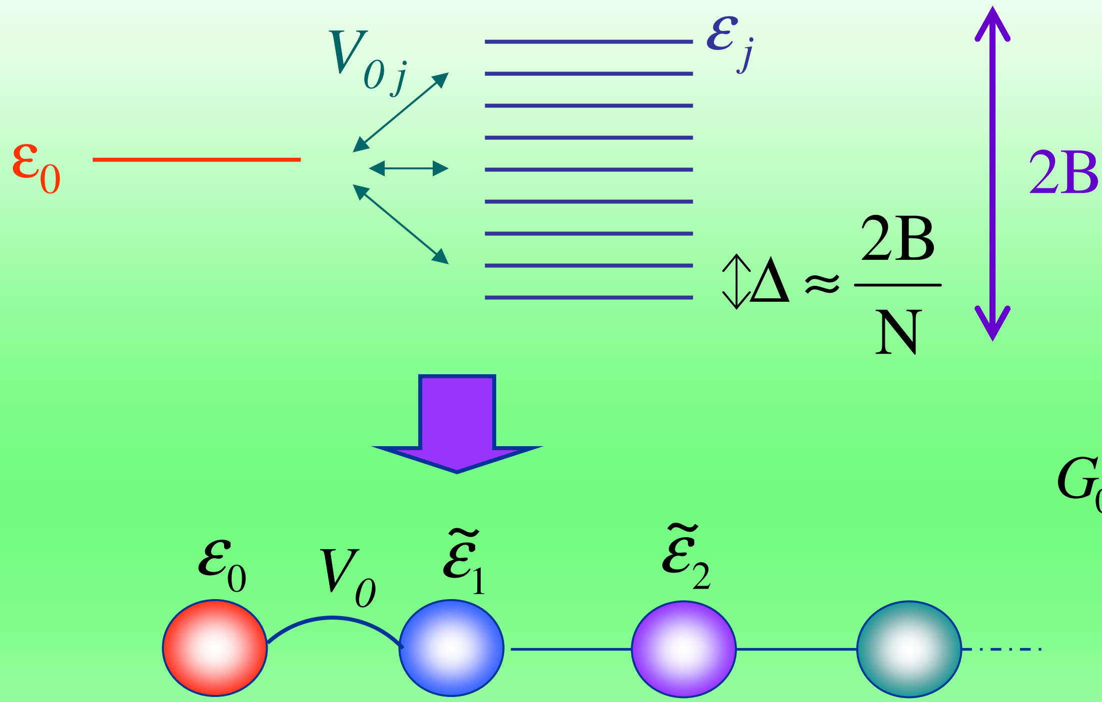


Last for a time t_S

$$t_S \approx \hbar \pi N_1^{(0)}(\varepsilon_r)$$



Short cross-over time and QZE



$$P_{00}(t) = 1 - V_0^2 (t/\hbar)^2 + \ldots$$

$$t_S \approx \hbar \Gamma_0 / V_0^2,$$

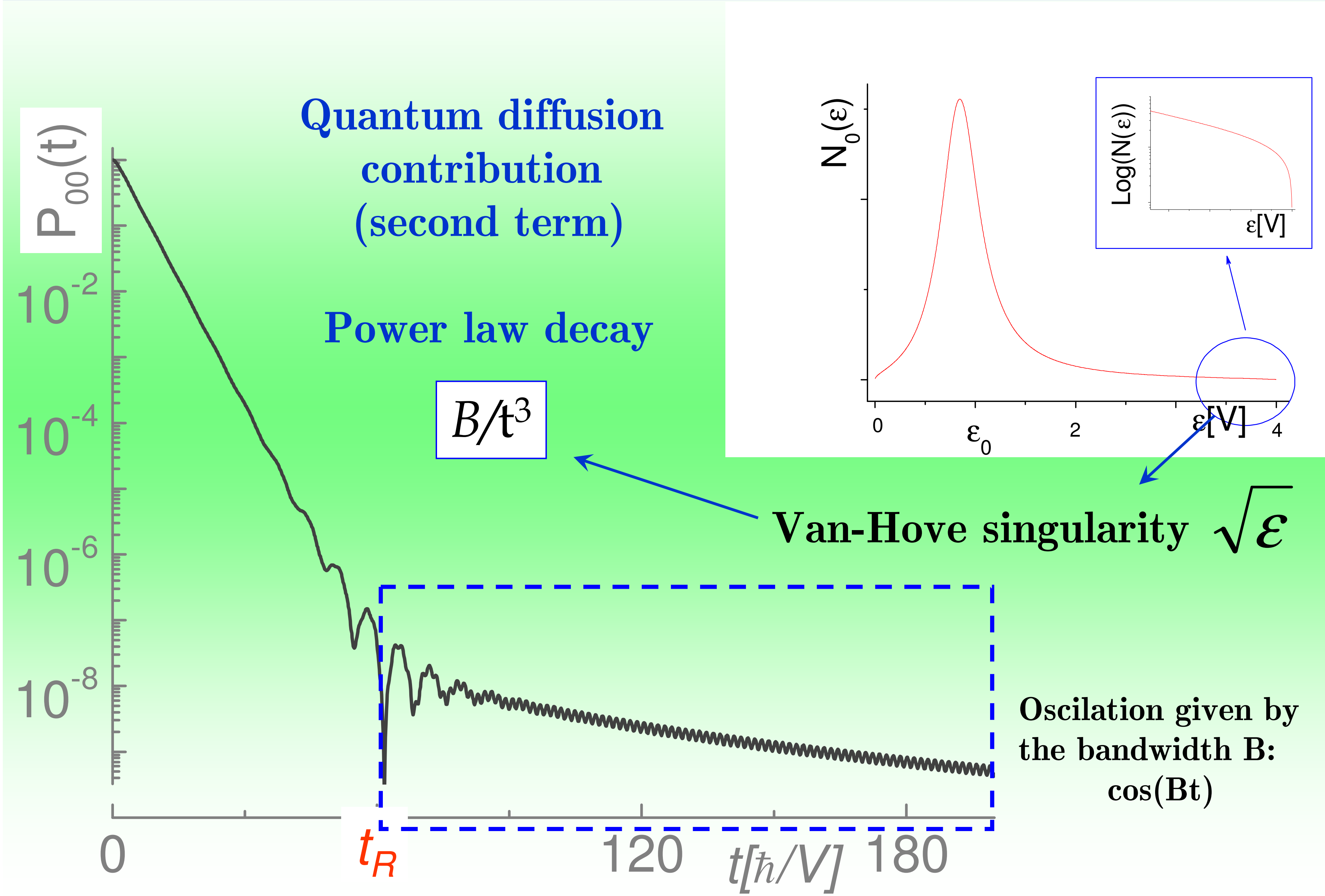
$$G_{00}(\varepsilon) = \frac{1}{\varepsilon - \varepsilon_0 - V_{01} G_{\tilde{1}\tilde{1}}^{(0)}(\varepsilon) V_{10}},$$

$$\left|\tilde{1}\right\rangle = \frac{1}{V_0} \sum_{j=1}^{N} V_{0\,j} \left|j\right\rangle; \quad V_0 = \sqrt{\sum_{j=1}^{N} \left|V_{0\,j}\right|^2}.$$

$$t_S \approx \hbar \pi N_{\tilde{1}}^{(0)}(\varepsilon_0)$$

In the range of quadratic decay a recursive projective measurement of state |0> at a time interval τφ would produce a deceleration of the decay, *Quantum Zeno effect.* Then, an upper bound for this time-scale is *τφ < tS.*

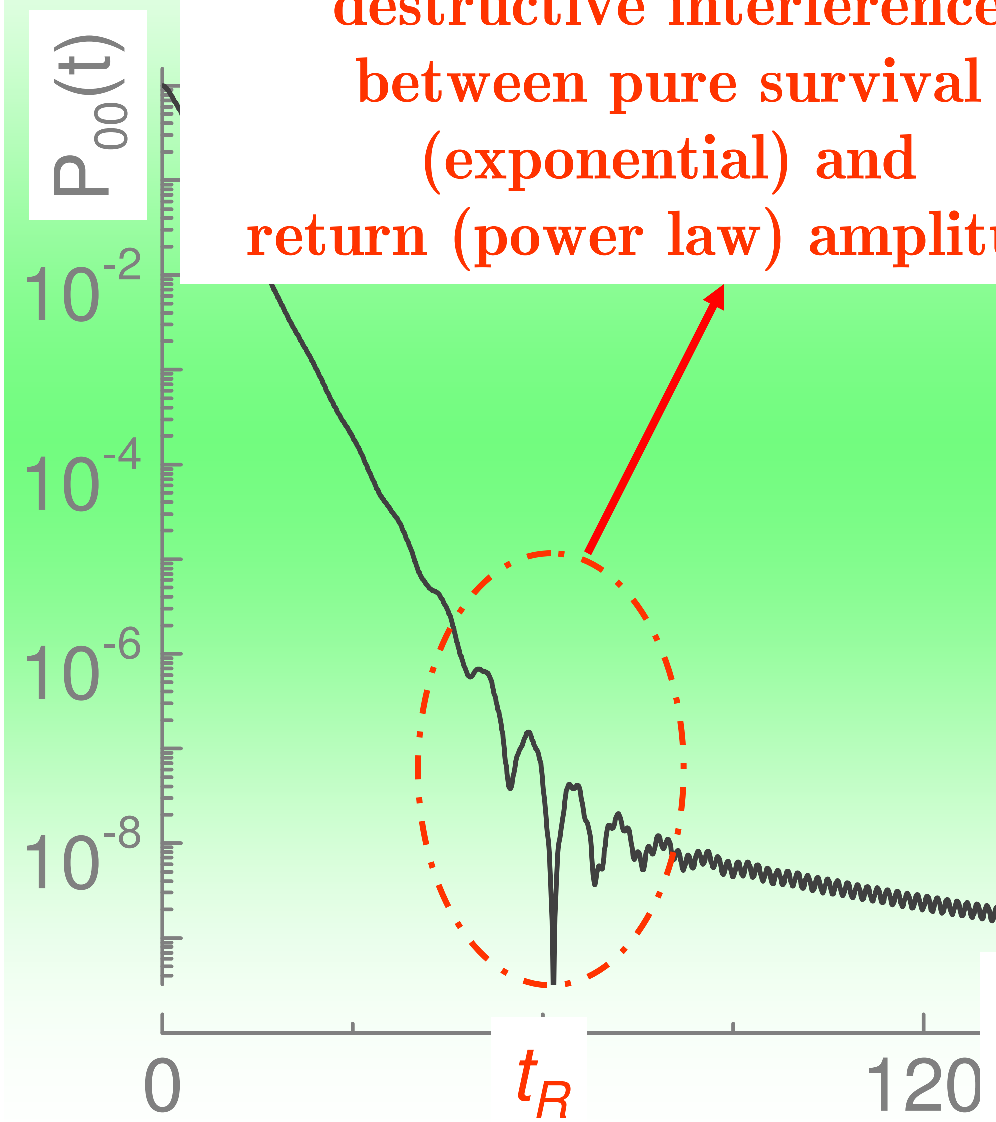
Survival Probability; Long time behaviour



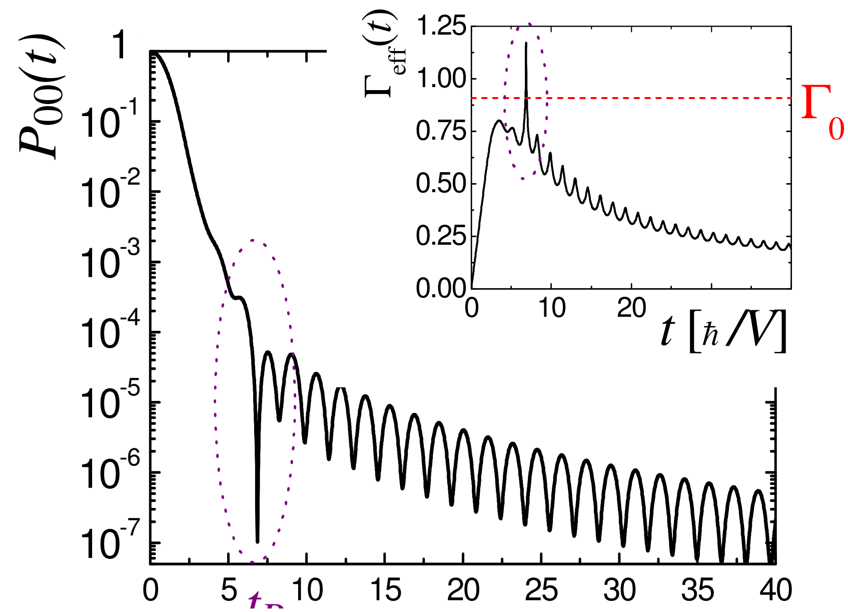
Long cross-over time and AZE

Survival collapse: destructive interference between pure survival (exponential) and return (power law) amplitude

$$t_R \approx \alpha \frac{\hbar}{\Gamma_0} \ln\left(\beta \frac{B}{4\Gamma_0} \right)$$

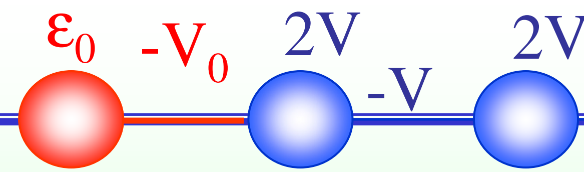


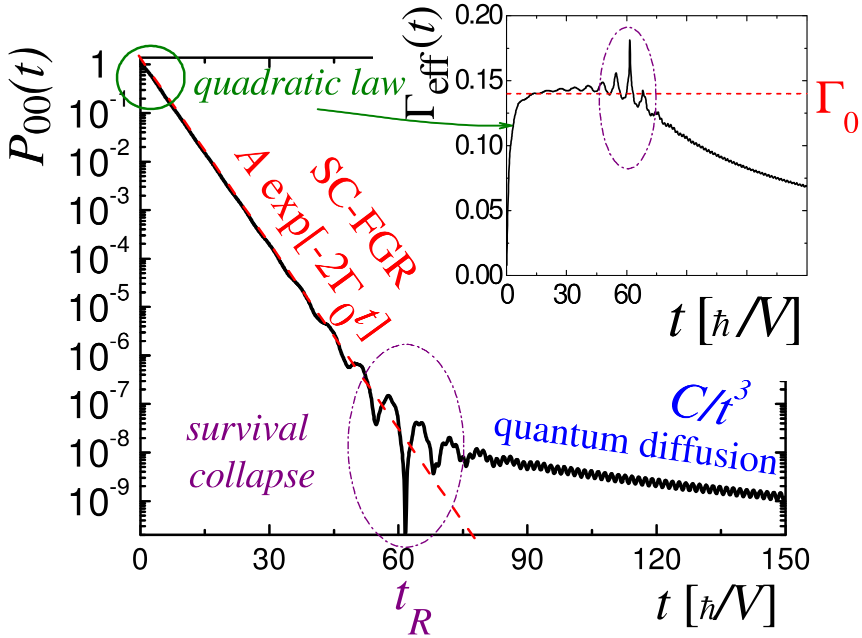
Strong coupling regime → Anti-Zeno



recursive projective measurement at a time interval $\tau_\varphi \approx t_R$ can produce acceleration of the decay

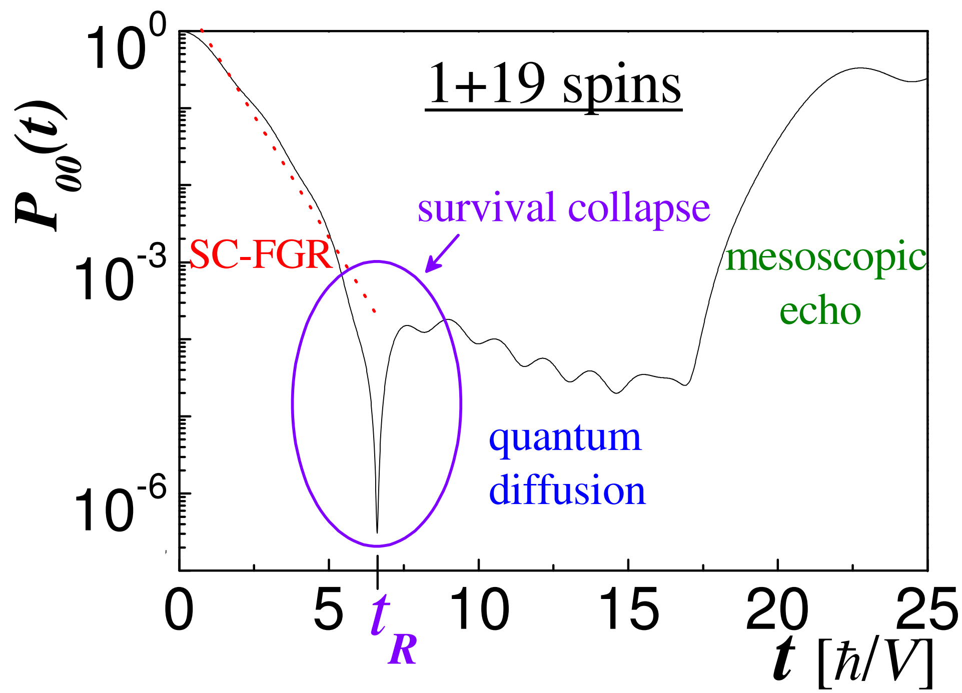
summary (of the first part...)





Characteristic times

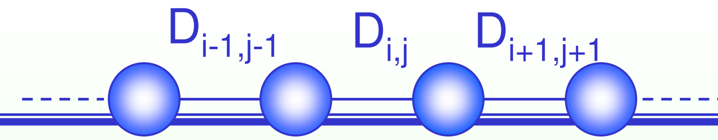
- t_S
- t_R



$P_{00}(t)$ Exact behaviour

- **Perturbative regime**
- **FGR regime**
- **Long time regime**

Mapping to non-interacting fermions



many-body ...

NMR in solid state

$$H_{DQ} = D_{i,i+1} \sum_{i=1}^{N} \left(I_i^+ I_{i+1}^+ + I_i^- I_{i+1}^- \right)$$

↓

do not conmute with thermal equilibrium state

$$\rho(0) = \frac{1}{Z} \left(\mathbf{1} - \alpha \sum_i I_i^z \right)$$

mixes subspaces with different spin projection (total magnetic quantum number) creating many-body superposition states: Multiple-Quantum Coherences →

one-body ...

$$\begin{array}{ccc} \rho(0) & \xrightarrow{\exp(-\mathrm{i}\, H_{DQ}\, t)} & \rho(t) \\ U \downarrow & & \uparrow U^{+} \\ \bar{\rho}(0) & \xrightarrow{\exp(-\mathrm{i}\, H_{XY}\, t)} & \bar{\rho}(t) \end{array}$$

↕

Non-interacting fermions

$$H_{TB} = D_{i,i+1} \sum_{i=1}^{N} \left(c_i^+ c_{i+1} + c_{i+1}^+ c_i \right)$$

↕

Effective one-body quantum dynamics manifested in the MQC orders

$$\langle I^z \rangle (t) = \sum J_M(t) \exp(-iM\phi)$$

Multiple-Quantum Coherence

Solid-state NMR N identical spins 1/2 → dipolar Hamiltonian:

$$H_{ZZ} = -\sum_{i,j} \frac{d_{ij}}{2}\left(2I_i^z I_j^z - \frac{I_i^+ I_j^- + I_i^- I_j^+}{2}\right),$$

→ total magnetic quantum number is a good quantum number:

$$I^z |s\rangle = m_s |s\rangle, \quad I^z = \sum_i I_i^z .$$

Off-diagonal elements of the density matrix, in the z-basis, the coherences

$$\rho_{rs} = \langle r|\rho(t)|s\rangle = \overline{c_r(t) c_s^*(t)}, \quad c_r(t)|r\rangle + c_s(t)|s\rangle.$$

Can be labeled by the difference of total magnetic quantum number between the states involved in the transition:

M-Quantum Coherence

$$M = m_r - m_s .$$

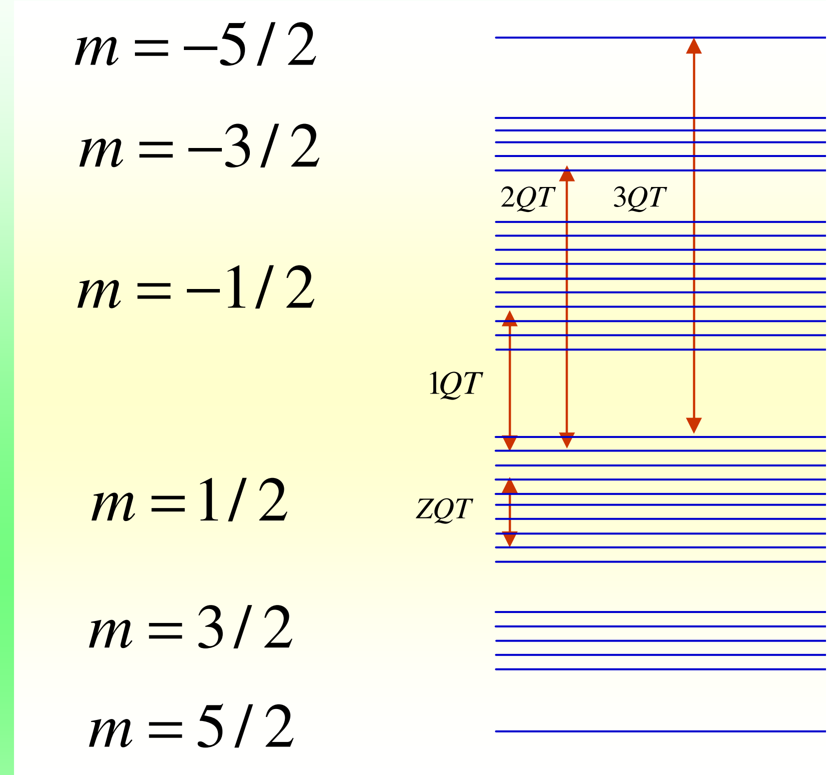
The intensities of the M-QC are:

$$J_M(t) = \sum\nolimits_{r,s}^{'} |\rho_{rs}(t)|^2$$

Multiple-Quantum Coherence

5 spins

$$M = m_r - m_s.$$



2 spins

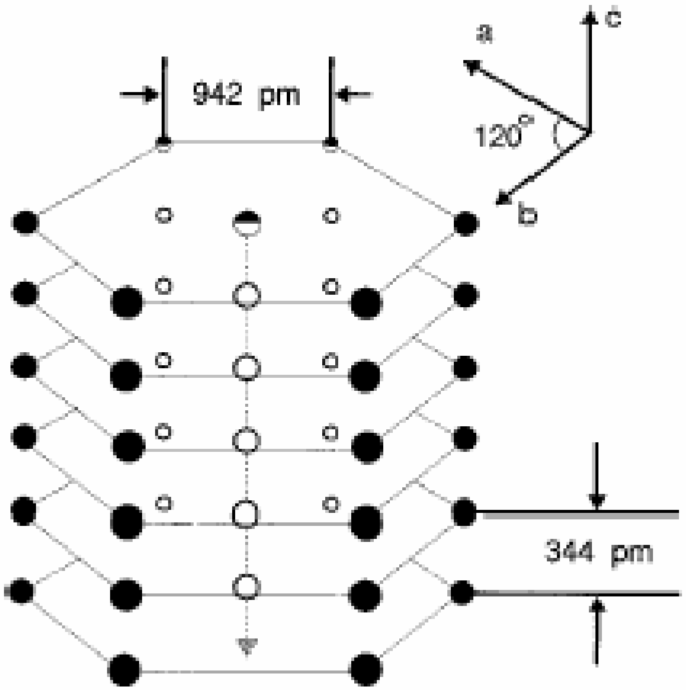
$$\rho(t) = \begin{array}{c} \\ \langle ++| \\ \langle +-| \\ \langle -+| \\ \langle --| \end{array} \begin{array}{cccc} |++\rangle & |+-\rangle & |-+\rangle & |--\rangle \\ \rho_{11} & \rho_{12} & \rho_{13} & \rho_{14} \\ \rho_{21} & \rho_{22} & \rho_{23} & \rho_{24} \\ \rho_{31} & \rho_{32} & \rho_{33} & \rho_{34} \\ \rho_{41} & \rho_{42} & \rho_{43} & \rho_{44} \end{array}$$

Zero Quantum Coherence and poblations ρ_{ii}

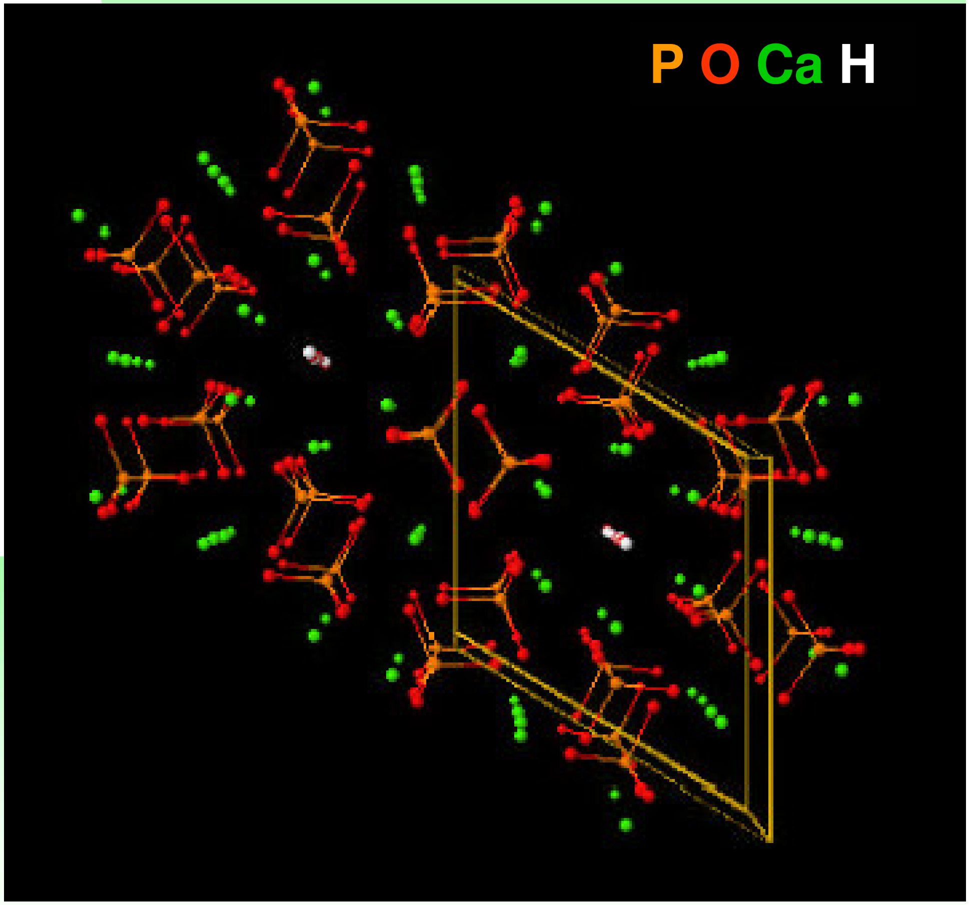
+/- 1 Quantum Coherence Transversal Magnetization

+/- 2 Quantum Coherence

Hydroxyapatite: a one-dimensional system



Hexagonal Hydroxyapat
$Ca_{10}(PO_4)_6(OH)_2$



$Ca_5(OH)(PO_4)_3$.

Arrangement of linear columns of protons in calcium hydroxyapatite.

Dynamical enhancement of the one-dimensionality

Solid state NMR -> dipolar interaction -> 1/r³
ratio between the intra and cross-chain interaction

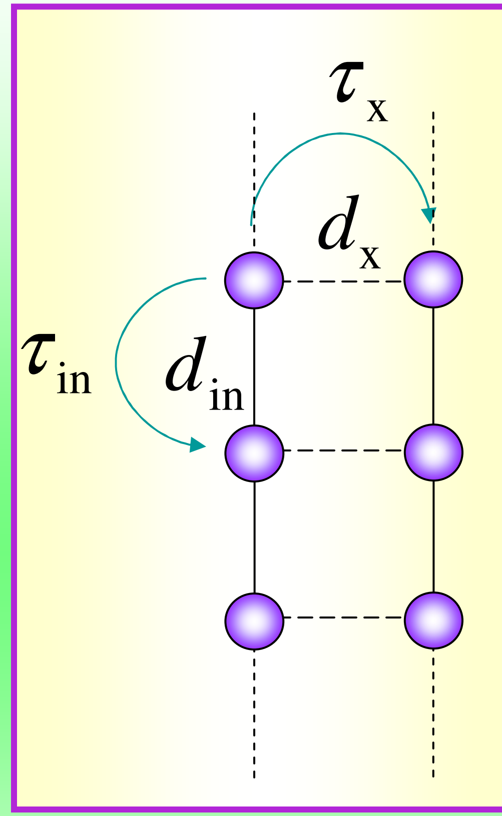
$$\frac{d_{in}}{d_x} = f(\theta_{max}) \text{ x } \left(\frac{r_x}{r_{in}}\right)^3 \approx 2 \text{ x } 20$$

Monocrystal (orientation that maximizes the intra-chain coupling)

ratio between a spin in a chain to a central spin surrounded by 6 neighbors 2nd moments

$$\sqrt{\left\langle \frac{M_{in}}{M_x} \right\rangle} = \left\langle f(\theta,\phi) \right\rangle \text{ x } \left(\frac{r_x}{r_{in}}\right)^3 \approx 1.5 \text{ x } 20$$

Polycrystal (average over solid angle)



Dynamical effect -> Quantum Zeno effect
ratio between characteristic time in the chain to cross-chain (FGR) dynamics

$$\tau_{in} \approx \frac{\hbar}{d_{in}}, \quad \frac{1}{\tau_x} \approx \frac{1}{\hbar} d_x{}^2 \frac{1}{d_{in}},$$

$$\Rightarrow \frac{\tau_{in}}{\tau_x} \approx \left(\frac{d_x}{d_{in}}\right)^2 \approx \left(\frac{r_{in}}{r_x}\right)^6 \approx \frac{1}{400}$$

Mapping to non-interacting fermions

many-body …

$$H_{DQ}, \rho_{eq}(0) \rightarrow all\ even\ M-QC$$

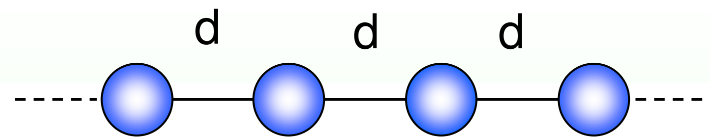
$$H_{DQ}, \rho_{eq}(0), nn \rightarrow only\ Z-QC, 2-QC$$

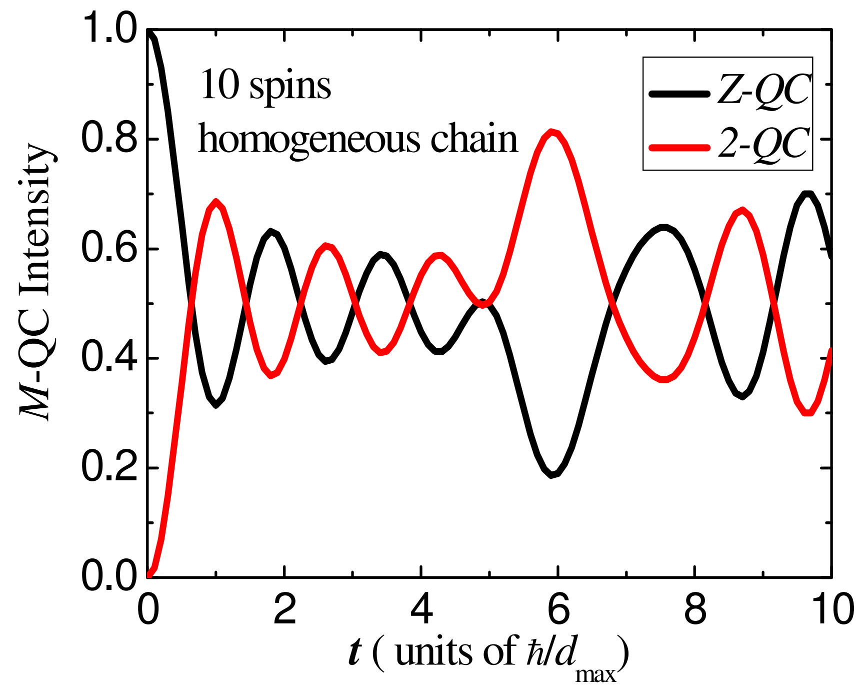
$$\begin{array}{ccc} \rho(0) & \xrightarrow{\exp(-i H_{DQ} t)} & \rho(t) \\ \downarrow U & & \uparrow U^{+} \\ \bar{\rho}(0) & \xrightarrow{\exp(-i H_{XY} t)} & \bar{\rho}(t) \end{array}$$

↓

only Zero- and 2-order coherences

… "one-body"

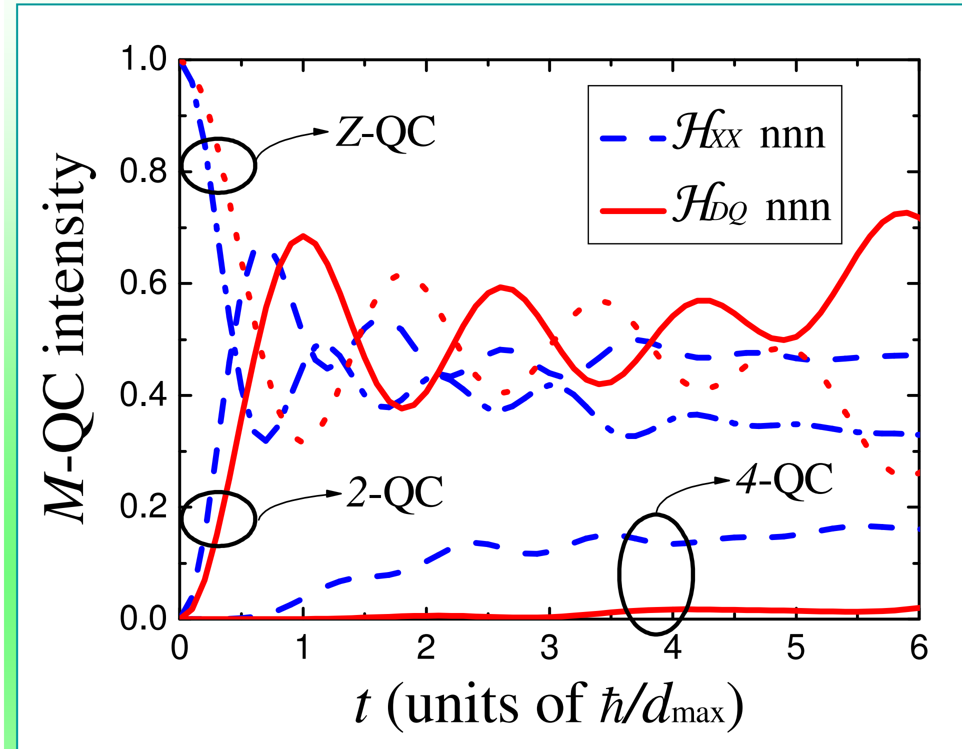




$$J_0(t) = \frac{1}{N} \sum_n \cos^2\left(4 d\, t \cos\left(\frac{\pi n}{N+1}\right)\right)$$

$$J_{\pm 2}(t) = \frac{1}{2N} \sum_n \cos^2\left(4 d\, t \sin\left(\frac{\pi n}{N+1}\right)\right)$$

Numerical Results: M-QC dynamics



M-QC dynamics under

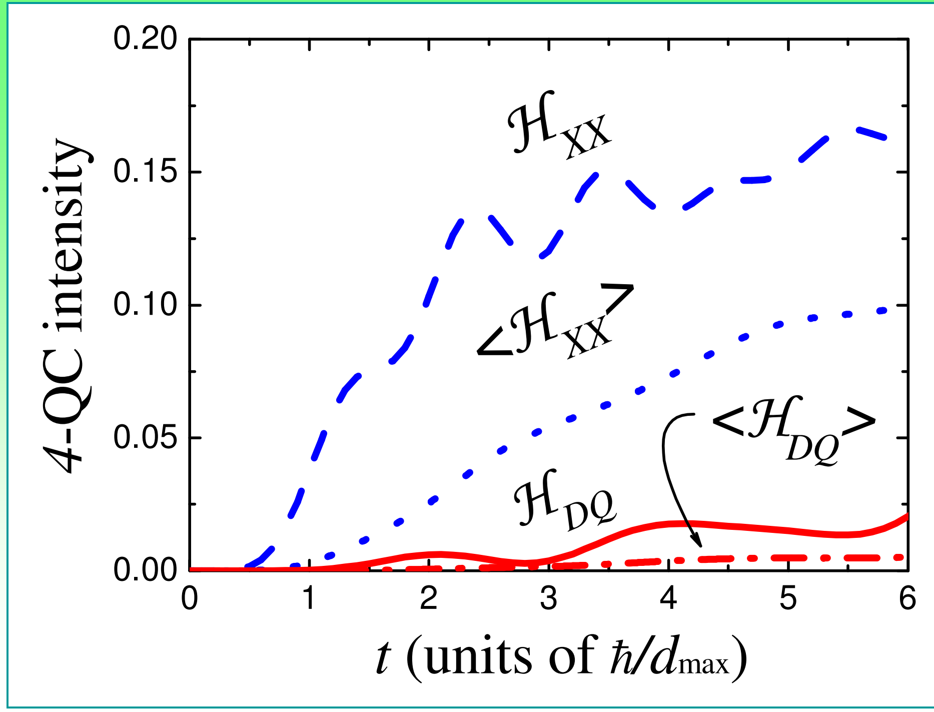
$$H_{DQ} \propto I_i^X I_j^X - I_i^Y I_j^Y,$$

contrasted with that of the many-body dynamics of the rotated dipolar Hamiltonian

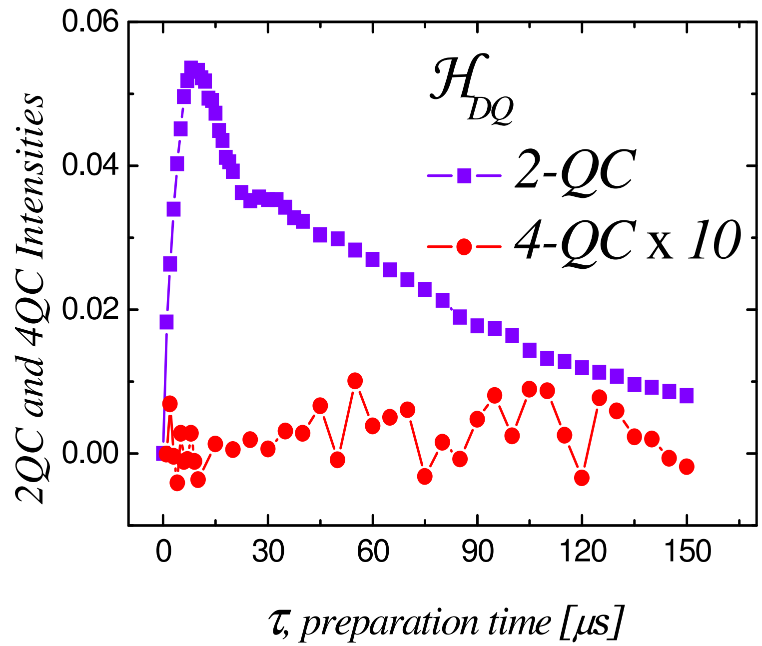
$$H_{XX} \propto 3 I_i^X I_j^X - I_i^Y I_j^Y - I_i^Z I_j^Z,$$

nnn: next nearest neighbor interaction breaks the "one-body" mapping

single orientation of the chain with respect to the external magnetic field and powder average < >

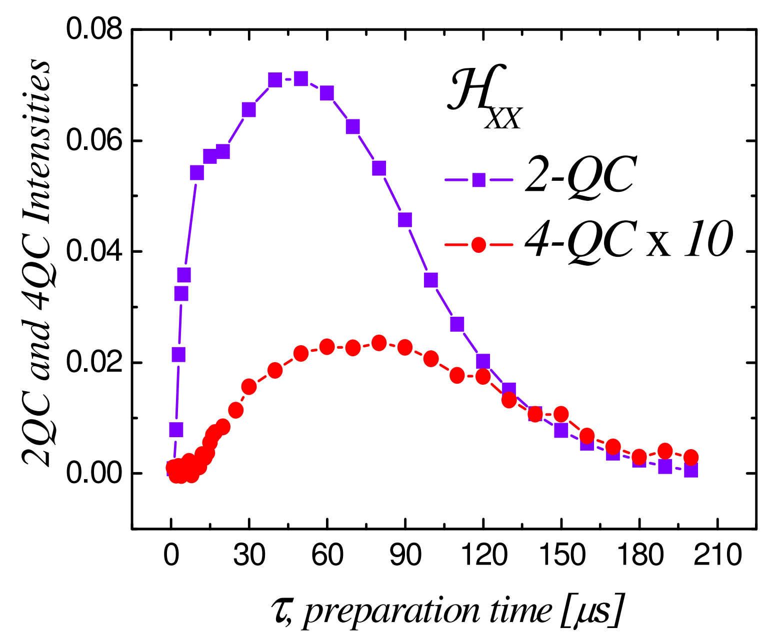


Experiental results: M-QC dynamics



H_{DQ} dynamics
2nd order quantum coherence,
4th order quantum coherence x 10.

ONLY 2-QC!!!



H_{XX} dynamics
2nd order quantum coherence,
4th order quantum coherence x 10.

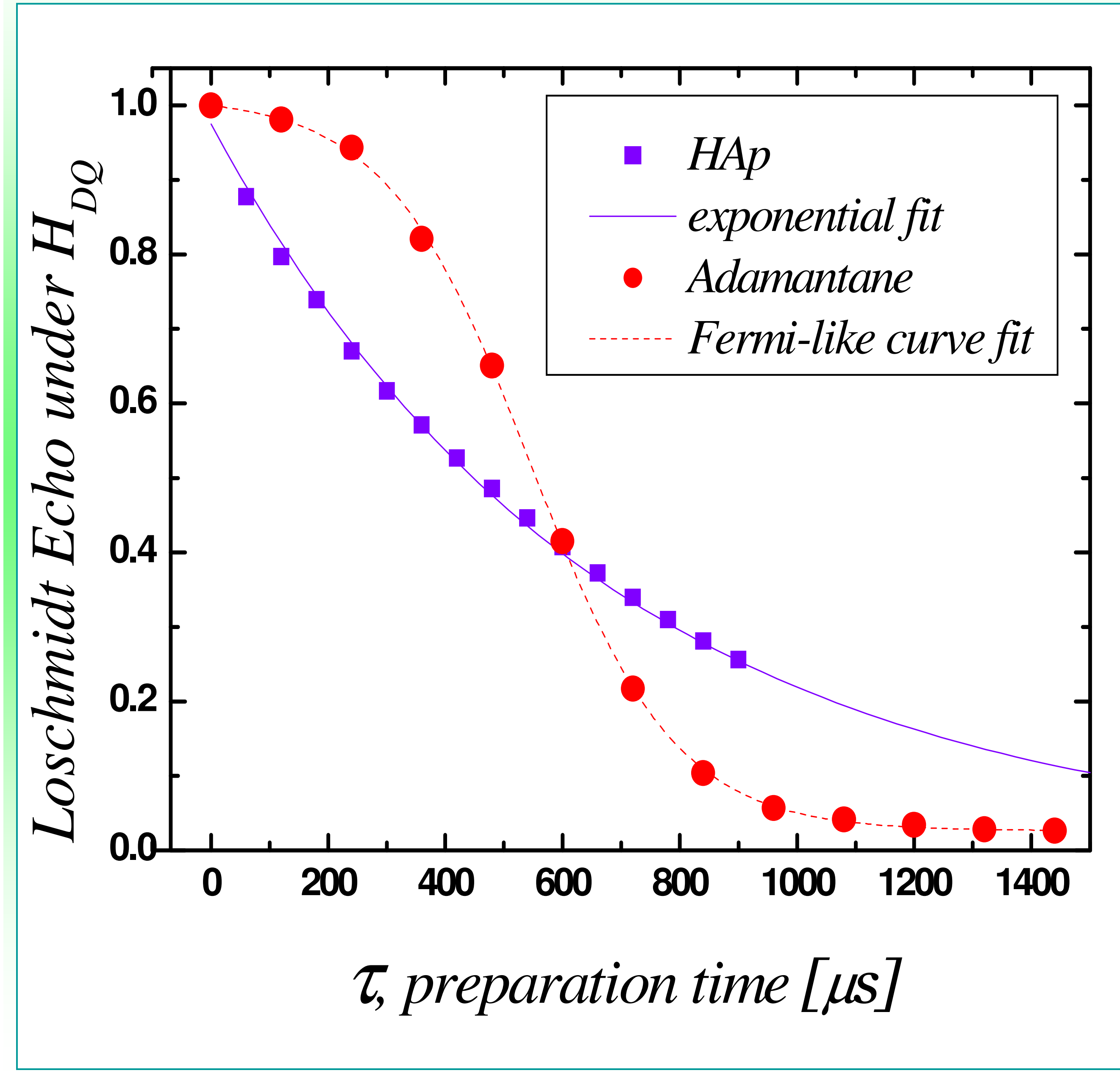
is not a limitation of signal to noise ratio

Summary (of the second part)

- **By using solid state nuclear magnetic resonance in a quasi 1d network of coupled spins, we built an effective one-body quantum dynamics and checked how it is manifested in the MQC orders. Results indicate that, in spite of the unavoidable residual nnn interactions, HAp can be used as a "quantum simulator" of non interacting fermion dynamics.**

- ***Decoherence* is tested through a form of Loschmidt echo experiment which reveals that in this 1-d system, the double-quantum dynamics presents an exponential decay, in contrast with results (Fermi-like decay) in 3-d systems.**

Experimental results: Loschmidt Echo under H_{DQ}



HAp
→ **1d system**
→ **exponential decay**

Adamantane
→ **3d system**
→ **Fermi-like curve:**

$$\frac{1}{1+\exp\left(\left(t-t_c\right)/\tau_\phi\right)}$$

$$HAp \rightarrow \tau_\phi = (770 \pm 50)\mu s$$

$$adam \rightarrow \begin{cases} t_c = (545 \pm 2)\mu s \\ \tau_\phi = (123 \pm 2)\mu s \end{cases}$$