

Non-Markovian decay beyond the Fermi Golden Rule: Survival collapse of the polarization in spin chains

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Abstract

The decay of a local spin excitation in an inhomogeneous spin chain is evaluated exactly: (i) It starts quadratically up to a spreading time t_S . (ii) It follows an exponential behavior governed by a *self-consistent Fermi Golden Rule*. (iii) At longer times, the exponential is overrun by an inverse power law describing return processes governed by quantum diffusion. At this last transition time t_R a *survival collapse* becomes possible, bringing the polarization down by several orders of magnitude. We identify this strongly destructive interference as an antiresonance in the time domain. These general phenomena are suitable for observation through an NMR experiment.

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1. Introduction

A typical quantum exponential decay [1,2] involves a finite set of states in presence of an ‘environment’, i.e., weakly coupled to a set of states whose spectrum is dense. The decay of these states is usually described with the Fermi Golden Rule (FGR). However, this description contains approximations [3] that leave aside some intrinsically quantum behaviors. Various works on models for nuclei, composite particles [4–6], excited atoms in a free electromagnetic field [7] and in photonic lattices [8], and models for decoherence [9], showed that the exponential decay has superimposed beats and does not hold for very short and very long times, compared with the lifetime of the system. The short time regime has received recent attention in connection to the Quantum Zeno Effect [10,11,7,12] and has been observed in trapped atoms [13]. In contrast, although different models predict some form of power law for long times [14–16], the cross-over to this long time behavior has not been neither experimentally observed nor physically interpreted.

In this Letter, we present a model describing the evolution of a local excitation in the otherwise homogeneous polarization of a system of interacting spins. This situation has two desirable properties: (1) the full dynamics can be solved analytically and interpreted; (2) an actual nuclear magnetic resonance (NMR) experiment can be tailored to observe this dynamics. Specifically, our model describes a linear chain of nuclear spins interacting under an XY (planar) interaction. In this situation, the evolution of a local spin excitation reduces to the dynamics of a localized density excitation in a system of non-interacting fermions [17–19]. This excitation decays into a well resolved wave packet propagating along the spin chain. Such decay could be observed with NMR because it also describes the dynamics of a multiple quantum coherence experiment [20] in a chain of spins with dipolar interactions in the solid state [21]. Furthermore, a full experimental dynamics of an effective XY Hamiltonian is achieved using NMR pulse sequences in liquid samples where the spin wave dynamics has been observed [22].

Based on our model, we are able to quantify the quantum nature of the deviations from the Fermi Golden Rule. We identify three well defined time regimes: (1) For short times the decay is quadratic ($1 - [tV_0/\hbar]^2$), as is expected when the coupling V_0 of the local state with the continuum

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is treated perturbatively. This lasts for a time $t_S \approx \hbar\pi\bar{N}_1(\varepsilon_r)$, where $\bar{N}_1(\varepsilon_r)$ is the spectral density of the final states at the resonance energy ε_r . (2) An intermediate regime characterized by an exponential behavior, the *self-consistent Fermi Golden Rule* (SC-FGR) where the rate, the pre-exponential factor and the resonance energy are found self-consistently. (3) A long-time regime in which the exponential law is overrun by an inverse power law which is identified with the quantum diffusion in the chain. At this last cross-over, the oscillations could lead to a dip of several orders of magnitude in the local polarization. This *survival collapse* is identified with a destructive interference between the *pure survival amplitude*, i.e., the SC-FGR component, and the *return amplitude*, associated with higher orders in a perturbation theory. This striking quantum phenomenon can be seen as a dynamical version of the antiresonance that has been described for steady-state observables [23–25]. Now, the destructive interference is also due to the splitting of the wave among two different families of pathways in space. However, the interference is now restricted to the narrow time window when the amplitudes are comparable and the phases are opposite.

2. Dynamics in a nuclear spins chain

We use the known mapping between spins and fermions [26] together with a new formulation for spin dynamics based on the non-equilibrium Keldysh formalism [27] developed in Refs. [19,28].

The two spin correlation function in a system with M spins $1/2$ evolving under a Hamiltonian \hat{H} ,

$$P_{f,i}(t) = \frac{\langle \Psi_{\text{eq}} | \hat{S}_f^z(t) \hat{S}_i^z(t_0) | \Psi_{\text{eq}} \rangle}{\langle \Psi_{\text{eq}} | \hat{S}_i^z(t_0) \hat{S}_i^z(t_0) | \Psi_{\text{eq}} \rangle}, \quad (1)$$

gives the amount of the z component of the local polarization on the site f th at time t , provided that the system was, at time $t_0 \leq t$, in its equilibrium state with a spin ‘up’ added at the i th site. Here, $\hat{S}_f^z(t) = e^{i\hat{H}t} \hat{S}_f^z e^{-i\hat{H}t}$ is the spin operation the Heisenberg representation and $|\Psi_{\text{eq}}\rangle = \sum_N s_N |\Psi_{\text{eq}}^{(N)}\rangle$ is the many-body equilibrium mixed state constructed by adding states with different number N of spins up with the appropriate statistical weights and random phases. We will assume the high temperature limit, that leads to equal statistical weights $|s_N|^2 = \frac{1}{2^M} \binom{M}{N}$. We consider a linear chain of M spins in an external magnetic field. They interact with their nearest neighbors at distance a_0 through an XY coupling

$$\hat{H} = \sum_{n=0}^{M-1} \hbar\Omega_n \hat{S}_n^z - \sum_{n=0}^{M-2} \frac{1}{2} J_{n+1,n} [\hat{S}_{n+1}^x \hat{S}_n^x + \hat{S}_{n+1}^y \hat{S}_n^y], \quad (2)$$

where \hat{S}_n^u ($u = x, y, z$) represents the Cartesian spin operator. The first term of this Hamiltonian is the Zeeman energy, where Ω_n is the chemical shift precession frequency; the second term, \hat{H}_{XY} contains the $J_{n+1,n}$ coupling between sites n and $n+1$. It gives the flip-flop interaction

$\hat{S}_{n+1}^+ \hat{S}_n^- + \hat{S}_{n+1}^- \hat{S}_n^+$ in terms of the rising and lowering spin operator $\hat{S}_n^\pm = \hat{S}_n^x \pm i\hat{S}_n^y$.

The Jordan–Wigner (J–W) transformation [26] establishes the relation between spin and fermion operators at each site n . When \hat{H} commutes with the number operator, the different subspaces N are decoupled. Further simplification is obtained for Hamiltonians which are quadratic in the fermionic operator, as the case of \hat{H}_{XY} , as they can be reduced to non-interacting fermions. Due to the short range interaction, after a J–W transformation, the only non-zero coupling terms are proportional to $\hat{c}_{n+1}^+ \hat{c}_n = \hat{S}_{n+1}^+ \hat{S}_n^-$, where \hat{c}_n^+ and \hat{c}_n are the creation and destruction operators for fermions. The Hamiltonian become

$$\hat{H} = \sum_{n=0}^{M-1} \varepsilon_n \left[\hat{c}_n^+ \hat{c}_n - \frac{1}{2} \right] - \sum_{n=0}^{M-2} V_{n+1,n} [\hat{c}_{n+1}^+ \hat{c}_n + \text{c.c.}], \quad (3)$$

where $\varepsilon_n \equiv \hbar\Omega_n$ are the site energies and $V_{n+1,n} \equiv \frac{1}{2} J_{n+1,n}$ are the hoppings. Each subspace has N non-interacting fermions. The eigenfunctions $|\Psi_\gamma^{(N)}\rangle$ are expressed as a single Slater determinant built-up upon the single particle wave functions ψ_k describing a particle of energy ε_k in a chain. Under this condition and defining $|i\rangle \equiv \hat{c}_i^+ |\emptyset\rangle$, with $|\emptyset\rangle$ the fermion vacuum, Eq. (1) reduces to

$$P_{f,i}(t) = |\langle f | \exp[-i\hat{H}t/\hbar] | i \rangle \theta(t)|^2, \quad (4)$$

$$\equiv \hbar^2 |G_{f,i}^R(t)|^2, \quad (5)$$

where $G_{f,i}^R(t)$ is the retarded Green’s function for a single fermion.

Therefore, for systems represented by a 1- d chain of spins with nearest neighbors XY interaction, at high temperature, the dynamics of a *local polarization amplitude* corresponds exactly to the *wave function of single particle* evolving according to a tight-binding Hamiltonian.

3. Local excitation: the exponential decay and beyond

Let us describe the evolution of a local excitation $|0\rangle \equiv \hat{c}_0^+ |\emptyset\rangle$ in a Hamiltonian whose spectrum has a finite support. This is the case of most excitations in a lattice. The autocorrelation function is Eq. (4) with $|i\rangle = |f\rangle = |0\rangle$. Expanding the initial condition in the eigenstates $|\psi_k\rangle$ obtains [3,4]

$$\begin{aligned} P_{00}(t) &= \left| \theta(t) \sum_{k=1}^M |\langle \psi_k | 0 \rangle|^2 \exp[-i\varepsilon_k t/\hbar] \right|^2 \\ &= \left| \theta(t) \int_{-\infty}^{\infty} d\varepsilon \left[\sum_{k=1}^M |\langle \psi_k | 0 \rangle|^2 \delta(\varepsilon - \varepsilon_k) \right] \exp[-i\varepsilon t/\hbar] \right|^2. \end{aligned} \quad (6)$$

The term in brackets is the Local Density of States (LDoS) $N_0(\varepsilon)$ at site 0th. It can be evaluated using the retarded Green’s function,

$$N_0(\varepsilon) = -\frac{1}{\pi} \text{Im} \int dt G_{00}^R(t) e^{i\varepsilon t} = -\frac{1}{\pi} \text{Im} G_{00}^R(\varepsilon).$$

Then, we can express the autocorrelation function as the Fourier transform of the LDoS

$$P_{00}(t) = \left| \theta(t) \int_{-\infty}^{\infty} d\varepsilon N_0(\varepsilon) \exp[-i\varepsilon t/\hbar] \right|^2. \quad (7)$$

This expression has numerical and analytical advantages because the Green's function can be accurately calculated in the energy representation, and the integral is limited to the spectral support. Besides, a clear identification of quantum interferences will be obtained by analyzing the argument under the modulus operator.

Alternatively, the autocorrelation function can be written as

$$P_{00}(t) = \theta(t) \int_{-\infty}^{\infty} d\omega \mathcal{J}_0(\omega) \exp[-i\omega t], \quad (8)$$

where the spectral density of the particle excitations at site 0th

$$\mathcal{J}_0(\omega) = \hbar \int_{-\infty}^{\infty} d\varepsilon N_0(\varepsilon) N_0(\varepsilon + \hbar\omega) \quad (9)$$

has a direct physical interpretation and can be easily computed [29].

All the previous equations remain valid when the size of the system, and hence the dimension of the Hilbert space, becomes unbounded ($M \rightarrow \infty$). In this case, either part or the whole of the discrete (pure point) spectrum, may become a *continuous energy band* of delocalized (extended) states in the finite range $[\varepsilon_L, \varepsilon_U]$. If the system does not present localized eigenstates [30], $N_0(\varepsilon)$ vanishes outside the band (Fig. 1). On the other hand, if the initial state $|0\rangle$ has a finite weight over one or more localized states its evolution cannot fully decay. Here, we consider cases that exclude such situation. Hence, if $|0\rangle$ requires an expansion in an infinite number of eigenstates, its evolution becomes an irreversible decay. In particular, the unperturbed state of energy $\varepsilon_0 = \langle 0|\hat{H}|0\rangle$ becomes a well defined resonance if $|0\rangle$ is expanded in terms of the eigenstates within a small breath Γ_0 around an energy $\varepsilon_r = \varepsilon_0 + \Delta_0$, where Δ_0 is a small shift due to the interaction. Furthermore, the validity

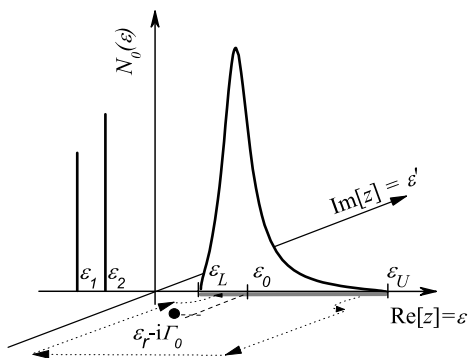


Fig. 1. Local spectrum (LDoS) in the complex plane $z = \varepsilon + i\varepsilon'$. ε_L and ε_U are the lower and upper band-edges, respectively. ε_1 and ε_2 localized states. The resonance energy is $\varepsilon_r = \varepsilon_0 - \Delta_0$ and the pole appears in $\varepsilon_r - i\Gamma_0$. The integration path is shown with dotted lines; consist of four straight lines and two arcs, that avoid the band-edges singularities.

of the Fermi Golden Rule for $P_{00}(t)$ requires [31] that the state $|0\rangle$ is similarly coupled to each of the unperturbed states $|\phi_k^0\rangle$ with energies ε_k^0 in a continuum spectrum.

In order to evaluate the local dynamics, we perform the integral in Eq. (7) using the residue theorem and following the path shown in Fig. 1. In the analytical continuation $N_0(z) \equiv N_0(\varepsilon + i\varepsilon')$, resonances appear like poles in the complex plane. We will consider Hamiltonians where an initially localized state with energy ε_0 interacting with a continuum gives rise to a single resonance, i.e., the LDoS presents poles at $\varepsilon_r \pm i\Gamma_0$. The van Hove singularities on the contour are excluded with circle arcs with radii R . Their contribution to the integral vanish when $R \rightarrow 0$, because the band edges are of the form $(\varepsilon - \varepsilon_L)^{\nu}$ with $\nu > -1$. Also, the integral over the contour $z = \varepsilon - iL$; $\varepsilon \in [\varepsilon_L, \varepsilon_U]$, vanish when $L \rightarrow \infty$. Then, we obtain

$$P_{00}(t) = \left| \underbrace{a e^{-(\Gamma_0 + i\varepsilon_r)t/\hbar}}_{\text{SC-FGR}} + \underbrace{\int_0^{\infty} d\varepsilon' e^{-\varepsilon' t/\hbar} [e^{-i\varepsilon_L t/\hbar} N_0(\varepsilon_L - i\varepsilon') - e^{i\varepsilon_U t/\hbar} N_0(\varepsilon_U - i\varepsilon')]}_{\text{return correction from quantum diffusion}} \right|^2, \quad (10)$$

where $a = \lim_{z \rightarrow \varepsilon_r - i\Gamma_0} [2\pi i (z - \varepsilon_r + i\Gamma_0) N_0(z)]$ and $t \geq 0$. If we approximate the LDoS by a Lorentzian function that jumps to zero outside the band, we can see that

$$A \equiv |a|^2 \simeq 1 + \delta, \quad (11)$$

where

$$0 < \delta = \frac{2}{\pi} \frac{\Gamma_0}{(\varepsilon_r - \varepsilon_L)} \frac{(\varepsilon_U - \varepsilon_L)}{(\varepsilon_U - \varepsilon_r)} \ll 1. \quad (12)$$

The first term of Eq. (10) already supersedes the usual Fermi Golden Rule approximation since it has a pre-exponential factor ($A \gtrsim 1$) and the exact rate of decay Γ_0 . This result is the *self-consistent Fermi Golden Rule* (SC-FGR). By analogy with a classical Markov chain, this exponential term is identified with a *'pure survival' amplitude*. Within the same analogy, the second term will be called *'return' amplitude*, as it is fed upon the initial decay. The first is the dominant one for a wide range of times, while the diffusive decay of the second, dominates for long times and brings out the details of the spectral structure of the system. In the quantum case, the second term is also fundamental for the normalization at very short times where the most excited energy states of the whole system can be virtually explored. Both terms combine to provide the initial quadratic decay (Quantum Zeno regime) required by the perturbation theory:

$$P_{00}(t) = 1 - \frac{t^2}{\hbar^2} \langle (\varepsilon - \varepsilon_r)^2 \rangle_{N_0} + \dots \quad (13)$$

$$= 1 - \frac{t^2}{2!} \langle \omega^2 \rangle_{J_0} + \dots \quad (14)$$

Here $\langle(\varepsilon - \varepsilon_r)^2\rangle_{N_0}$ and $\langle\omega^2\rangle_{J_0}$ are the energy and frequency second moments of the densities $N_0(\varepsilon)$ and $J_0(\omega)$, respectively. This expansion holds for a time shorter than the spreading time t_S of the wave packet formed by the decay. In other systems, the divergence of the second moment leads to different short time decays [32].

For long times, the behavior of $P_{00}(t)$ is governed by the slowly decaying second term in Eq. (10). Only small values of ε' contribute to the integral. In turn this restricts the integration of the LDoS to a range near the band-edges.

Then, one can go back to Eq. (7) and retain only the van Hove singularities of the Local Density of States at these edges (e.g., $N_0(\varepsilon) \propto \theta(\varepsilon - \varepsilon_L)(\varepsilon - \varepsilon_L)^v$ which implies [29] $J_0(\omega) \propto \theta(\omega)\omega^{2v+1}$). Each singularity would contribute to the slow decay at long times ($P_{00}(t) \propto |t|^{-2(v+1)}$). The relative participation of the energy states at each edge of the LDoS is given by the relative weight of the Lorentzian tails at these edges

$$\beta = \frac{(\varepsilon_r - \varepsilon_L)^2 + \Gamma_0^2}{(\varepsilon_U - \varepsilon_r)^2 + \Gamma_0^2}. \quad (15)$$

Then, the polarization for long times is

$$P_{00}(t) \sim \left[1 + \beta^2 - 2\beta \cos(Bt/\hbar)\right] \left| \int d\varepsilon' e^{-\varepsilon't/\hbar} N_0(\varepsilon_L - i\varepsilon') \right|^2, \quad (16)$$

where $B = \varepsilon_U - \varepsilon_L$. This means that the long time behavior is just the power law decay of the integral multiplied by a factor having a modulation with frequency B/\hbar .

4. Survival collapse

In steady-state transport [23] as well as in dynamical electron transfer [25] there are situations when a particle can reach the final state following two alternative pathways. Since each of them collects a different phase, this allows a destructive interference blocking the final state. This phenomenon has been dubbed antiresonance [23,25]. It extends the Fano resonances describing the anomalous ionization cross-section [24]. In the present case, the survival of the local excitation also recognizes two alternative pathways: the *pure survival* amplitude which is typically described by the Fermi Golden Rule, and the paths where the excitation has decayed, explored the environment, and then returns. These two alternatives can interfere. We rewrite Eq. (10) to emphasize that the local polarization $P_{00}(t)$ is the result of *two* different contributions:

$$P_{00}(t) = |\Psi_S + \Psi_R|^2, \quad (17)$$

$$= |\Psi_S|^2 + |\Psi_R|^2 + 2\text{Re}[\Psi_S^* \Psi_R], \quad (18)$$

where the phase in Ψ_R arise from the exponentials with ε_L and ε_U (the LDoS is real for any argument). Hence,

$$\Psi_S(t) = |a| e^{-i\phi_a} e^{-\Gamma_0 t/\hbar} e^{-i(\varepsilon_r - \varepsilon_L)t/\hbar}, \quad (19)$$

$$\Psi_R(t) = |\Psi_R(t)| e^{i\phi(t)}; \quad (20)$$

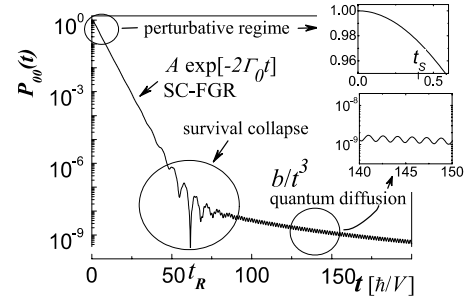


Fig. 2. Local polarization, in a semilogarithmic scale, as a function of time. We consider an unperturbed energy of $\varepsilon_0/V = 1$ and interaction strength $V_0/V = 0.4$ that leads to a resonance energy $\varepsilon_r/V = 0.9$ and an exponential rate $\Gamma_0/V = 0.14$. This is the case that we consider in Fig. 1. The decay exhibits: (1) The quadratic perturbative regime, which is shown amplified in the upper inset. (2) The exponential behavior as described by the self-consistent Fermi Golden Rule. (3) An asymptotic cubic power law decay, where $b = C/\Gamma(\varepsilon_r)^3$ (Eq. (34)). The lower inset shows the oscillation that modulates this decay. The cross-over time t_R when the survival collapse takes place is indicated.

$$\phi(t) = \arctan \left(\frac{\beta \sin(Bt/\hbar)}{1 - \beta \cos(Bt/\hbar)} \right), \quad (21)$$

where Eq. (21) results using the long time limit of Eq. (16).

While the interference term in $P_{00}(t)$ is present along the whole exponential regime, it becomes important when both, the *pure survival* amplitude and the *return* contribution, are of the same order. This occurs at the cross-over time t_R between the exponential regime and the power law. The interference term can produce a *survival collapse*, i.e., a pronounced dip that takes $P_{00}(t)$ close to zero (see Fig. 2). In order to obtain a full collapse, two simultaneous conditions are needed:

$$|\Psi_S(t_R)| = |\Psi_R(t_R)| \quad \text{and} \quad (22)$$

$$(\varepsilon_r - \varepsilon_L)t_R/\hbar - \phi(t_R) = (\pi - \phi_a) + 2\pi n, \quad n \text{ integer}, \quad (23)$$

which are satisfied with a fair precision because

$$|(\varepsilon_r - \varepsilon_L)/\hbar| \gg \Gamma_0/\hbar > 2\pi/t_R \geq |\phi(t_R)|/t_R, \quad (24)$$

i.e., while the return amplitude has a phase with a slow variation, the pure survival term oscillates rapidly. When both amplitudes are of the same order, the destructive interference will be noticeable.

5. Decay in a semi-infinite chain

Now we focus on a specific case of Eq. (7) that can be achieved experimentally and has simple analytical properties. We consider the Hamiltonian of Eq. (3) with the 0th site (spin) in the chain different from the others sites in both site energy (chemical shift) and hopping (J -coupling), i.e., $\varepsilon_0 \neq \varepsilon_n \equiv 2V$ and $V_{0,1} = V_0 < V_{n,n+1} \equiv V$ for $n > 0$. This defines a continuous spectrum in the range $[0, B \equiv 4V]$ which, in the lower edge, describes a particle of mass m in the continuum with $V = \hbar^2/(2ma_0^2)$. Our model presents a resonance provided that the site energy is not to close to

the band edge, i.e., $|\varepsilon_0 - 2V| < 2V - V_0^2/V$. Otherwise, $|0\rangle$ would give rise to a localized state [33]. The LDoS for this problem is evaluated using the Dyson equation

$$\left[\overline{G}_{0,0}^R(\varepsilon)\right]^{-1} = \left[\overline{G}_{0,0}^R(\varepsilon)\right]^{-1} + V_{0,1}\overline{G}_{1,1}^R(\varepsilon)V_{1,0}, \quad (25)$$

following the general continued fraction procedure described in Ref. [33]:

$$N_0(\varepsilon) = \frac{1}{2\pi} \times \frac{\theta(\varepsilon)\theta(4V - \varepsilon)\left(\frac{V_0}{V}\right)^2 \sqrt{\varepsilon}\sqrt{4V - \varepsilon}}{\left[\varepsilon - \varepsilon_0 - \left(\frac{V_0}{V}\right)^2 \left(\frac{\varepsilon - 2V}{2}\right)^2\right]^2 + \left(\frac{V_0}{V}\right)^4 \left[V^2 + \left(\frac{\varepsilon - 2V}{2}\right)^2\right]}. \quad (26)$$

Note that, because of surface effects in the semi-infinite d -dimensional space, the LDoS has van Hove singularities of the form $\overline{N}_1^{(d)}(\varepsilon) \propto \varepsilon^{d/2}$, which differ from those in the bulk $N^{(d)}(\varepsilon) \propto \varepsilon^{(d-2)/2}$. Fig. 1 shows $N_0(\varepsilon)$ for $V_0/V = 0.4$ and $\varepsilon_0/V = 1$. The resonant state (the poles of the LDoS) appears in $\varepsilon_r \pm i\Gamma_0$, where

$$\varepsilon_r = \varepsilon_0 + A_0; \quad A_0 = \frac{V_0^2}{V^2 - V_0^2} \frac{\varepsilon_0 - 2V}{2}, \quad (27)$$

$$\Gamma_0 = \frac{V_0^2}{V^2 - V_0^2} \Gamma_c; \quad \Gamma_c = \sqrt{V^2 - V_0^2 - \left(\frac{\varepsilon_0 - 2V}{2}\right)^2}. \quad (28)$$

Identifying the local density of states at the first site in absence of interactions with the 0-site as

$$\begin{aligned} \overline{N}_1(\varepsilon) &= -\frac{1}{\pi} \text{Im} \overline{G}_{1,1}^R(\varepsilon) \\ &= \frac{16}{\pi} \frac{1}{B^2} \left(\frac{1}{2} \sqrt{\varepsilon} \sqrt{B - \varepsilon}\right) \theta(\varepsilon) \theta(B - \varepsilon) \\ &= \frac{16}{\pi} \frac{1}{B^2} \Gamma(\varepsilon). \end{aligned} \quad (29)$$

Note that $a_0\Gamma(\varepsilon)/\hbar$ is the group velocity of a wave packet with energy ε and $\Gamma_c \approx \Gamma(\varepsilon_0)$. One realizes that the expression (26) factorizes as a pure Lorentzian and $\overline{N}_1(\varepsilon)$

$$N_0(\varepsilon) = \frac{V^2}{2\Gamma_c} \frac{\Gamma_0}{(\varepsilon_r - \varepsilon)^2 + \Gamma_0^2} \overline{N}_1(\varepsilon). \quad (30)$$

Then, applying the convolution theorem to Eq. (7) we get a convolution integral of two functions in the time domain with well characterized time dependence

$$G_{00}^R(t) = \frac{-i}{\hbar} \frac{V^2}{2\Gamma_c} \theta(t) \int_{-\infty}^{\infty} e^{-\Gamma_0|t'|/\hbar} e^{-i\varepsilon_r t'/\hbar} g(t - t') dt'. \quad (31)$$

The first factor inside the integral is the renormalized survival amplitude as described by the SC-FGR. The second factor is the return amplitude to site 1 in a semi-infinite chain where site 0 is missing. It is expressed in term of the Bessel function of the first kind as $g(t) = 2e^{-i2Vt/\hbar} J_1(2Vt/\hbar)/(2Vt/\hbar)$, which shows fast oscillations and decays with the power law $t^{-3/2}$. This describes the quantum diffusion in the chain [34,28]. It appears convoluted with an

exponential kernel whose oscillation and decay have a longer time scale. For positive times $g(t)$ coincides with the response function. This knowledge allows us to solve the integral in the different time regimes (short, exponential and long time). After some algebra we get:

$$P_{00}(t) \approx \begin{cases} 1 - (V_0 t/\hbar)^2, & t < t_S, \\ A \exp(-2\Gamma_0 t/\hbar), & t_S < t < t_R, \\ C \left[1 - \frac{2\beta}{1+\beta^2} \sin(Bt/\hbar)\right] \left(\frac{\hbar}{\Gamma(\varepsilon_r)t}\right)^3, & t_R < t, \end{cases} \quad (32)$$

where t_S is the cross-over time from the short time regime to the exponential SC-FGR, and time t_R separates the SC-FGR and the power law regime. Also,

$$A = \frac{1}{4\Gamma_c^2} \sqrt{\varepsilon_r^2 + \Gamma_0^2} \sqrt{(B - \varepsilon_r)^2 + \Gamma_0^2} \gtrsim 1, \quad (33)$$

$$\begin{aligned} C &= \frac{\Gamma(\varepsilon_r)^3 V}{4\pi\Gamma_c^2} \frac{\Gamma_0^2}{(\Gamma_0^2 + \varepsilon_r^2)^2} [1 + \beta^2] \\ &\simeq \frac{1}{4\pi} \left(\frac{V_0}{\varepsilon_0}\right)^2 \left(\frac{\Gamma_0}{\varepsilon_r}\right) \end{aligned} \quad (34)$$

and β was defined in Eq. (15). Here, we used $V_0 \ll V$ and $\varepsilon_0 \simeq \varepsilon_r + \mathcal{O}(V_0^2/V)$ in Eq. (28) to obtain $\Gamma_0 \simeq \pi V_0^2 \overline{N}_1(\varepsilon_r)$ which coincides with the SC-FGR. Near the band edge $\Gamma_0 \simeq 8V_0^2/B\sqrt{\varepsilon_r/B}$, and $\Gamma(\varepsilon_r) \simeq \Gamma_c \simeq \sqrt{V\varepsilon_r}$. For long times, and averaging in a period, one gets

$$P_{00}(t) \simeq \left(\frac{V_0}{\varepsilon_0}\right)^2 \left(\frac{1}{4\pi} \frac{\Gamma_0}{\varepsilon_r}\right) \left(\frac{\hbar}{\Gamma(\varepsilon_r)t}\right)^3. \quad (35)$$

At long times, the probability of finding the particle at site 0 is proportional to the probability of finding it at site 1, i.e., $P_{00}(t) \simeq (V_0/\varepsilon_0)^2 P_{01}(t)$. Hence, the factor gives the probability of tunneling back to $|0\rangle$. It measures how the component of the band edge (that determine the long time behavior) over the surface state $|1\rangle$ mixes with state $|0\rangle$. The assignation of a time scale to the return probability in the last term is arbitrary. We choose $\Gamma(\varepsilon_r)$, the dominant group velocity of propagating wave packet of energy ε_r . Hence, the second factor becomes the inverse of the number of cycles within the main decay.

It is important to note that the cubic power law decay obtained for long times is a consequence of the $\sqrt{\varepsilon}$ dependence of the LDoS, i.e., this power law is consistent with Eq. (16) taken together with Eq. (26). Notice also that the short time scale, \hbar/V_0 , can also be obtained from the local second moment of the Hamiltonian.

From the analytical result given in Eq. (32), we get the characteristic times t_S and t_R . A good estimate of t_S is obtained from the minimal distance between the short time decay and the exponential

$$\frac{d}{dt} [1 - (V_0 t/\hbar)^2 - A \exp(-2\Gamma_0 t/\hbar)]|_{t=t_S} = 0. \quad (36)$$

Expanding the exponential in its Taylor series, we get:

$$t_s = \frac{\hbar\Gamma_0 A}{V_0^2 + 2\Gamma_0^2 A}, \quad (37)$$

$$\simeq \hbar\pi\bar{N}_1(\varepsilon_r) \simeq \frac{8\hbar}{B} \sqrt{\frac{\varepsilon_r}{B}} \quad \text{for } \varepsilon_r \ll 2V. \quad (38)$$

Here, we see that in this parametric regime the short time cross-over is only determined by $\bar{N}_1(\varepsilon_r)$, the local density of states at the first site of the chain.

We may invoke the optical theorem [33], to interpret $\bar{N}_1(\varepsilon_r)$ as the time scale at which a wave packet with energy ε_r escapes from the 1st site region, i.e., the excitation build from the decay, preventing the return to the original 0th site [33,35].

The time t_R is obtained from the cross-over between the exponential regime and the power law decay

$$A \exp(-2\Gamma_0 t_R/\hbar) = C \left(\frac{\hbar}{\Gamma(\varepsilon_r) t_R} \right)^3. \quad (39)$$

We can use $\sqrt{A/C} \simeq 2\sqrt{\pi}\varepsilon_0/V_0\sqrt{\varepsilon_r/\Gamma_0}$ and solve iteratively the transcendental equation, i.e.,

$$t_R^{(0)} = \frac{\hbar}{\Gamma_0} \ln \left(2\sqrt{\pi} \frac{\varepsilon_0}{V_0} \sqrt{\frac{\varepsilon_r}{\Gamma_0}} \right), \quad (40)$$

$$t_R^{(n+1)} = \frac{\hbar}{\Gamma_0} \ln \left(2\sqrt{\pi} \frac{\varepsilon_0}{V_0} \sqrt{\frac{\varepsilon_r}{\Gamma_0}} \right) + \frac{3\hbar}{2\Gamma_0} \ln \left[\frac{\Gamma(\varepsilon_r)}{\hbar} t_R^{(n)} \right].$$

Already in the third order we get a very good agreement with the cross-over observed in the exact dynamics.

6. Numerical verification

We verify the above results following two independent procedures. Since one has a closed analytical expression for $N_0(\varepsilon)$, the numerical Fourier transform is straightforward. Alternatively, we find the dynamics from the numerical eigenvalues and eigenvectors of the finite system with M sites. Both of them coincide as long as M is big enough so that the finite system effects become negligible. This requires that the mesoscopic echo [18], arising at a time $t_{ME} \approx \hbar M/B$, appears well beyond the cross-over time t_R . Both procedures provide perfect agreement with the analytical results. In Fig. 2 we show $P_{00}(t)$ in a semilogarithmic scale. The exact decay confirms the time dependences exhibited by the analytical approximation of Eq. (32). The initial quadratic decay is amplified in the upper inset. Then, the curve is followed by the exponential SC-FGR. Finally, it presents a cross-over at t_R to the asymptotic power law decay. This time-scale is easily identified through the survival collapse shown as a dip in the survival probability. There, the polarization suddenly decreases from its average by almost three orders of magnitude. The inset on the bottom shows the small oscillation that modulates the power law.

Since the model solved in the previous section could be applied to spins in a molecule or excitations in a designed nanostructure, both of which have finite size, it is interesting to verify that the main features discussed also could be

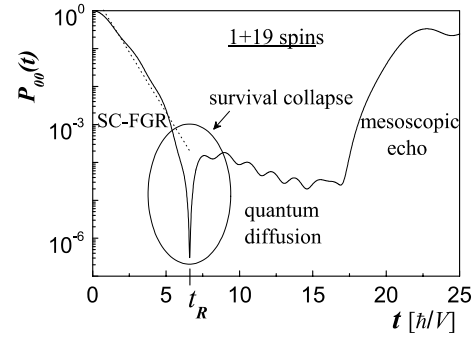


Fig. 3. Local polarization, in a semilogarithmic scale, as a function of time, in units of \hbar/V , for $\varepsilon_0/V = 1.3$, $V_0/V = 0.75$, that leads to a resonance energy $\varepsilon_r/V = 0.85$ and a SC-FGR exponential, shown with a dotted line, with rate $\Gamma_0/V = 0.72$ and pre-exponential factor $A = 2.86$. The ‘environment’ has $M - 1 = 19$ spins. The decay exhibits a noticeable survival collapse followed by a cubic power law modulated with a well defined frequency. At later times, the mesoscopic echo shows up.

observed in such situations. In Fig. 3, we show the dynamics of one spin in presence of an ‘environment’ consisting on a chain of 19 identical 1/2 spins. The three regimes just discussed are clearly manifested. Later on, it appears a mesoscopic echo at $tV/\hbar \geq 20$. Note that already at $t_R \approx 6\hbar/V$ the magnetization decreases in seven orders of magnitude. For a brief period around t_R coherent interference ensure an almost complete depolarization of the surface site that could not be achieved through decoherent decay.

7. Conclusions

In the present work we have discussed the exact dynamics of a local excitation that decays through the interaction with a continuum spectrum with finite support that acts as an ‘environment’. Our approach goes beyond the usual Markovian approximation that uses the Fermi Golden Rule to describe these environmental interactions. Within a simple, yet realistic model of a linear chain of nuclear spins with XY interaction, we found the exact behavior of the autocorrelation function for all times. The evolution starts with the expected quadratic decay. Then, it follows the usual exponential FGR regime, but with a corrected rate and a pre-exponential factor, i.e., the SC-FGR. Finally, we get the long time regime, that consists of a cubic power law decay modulated by oscillations whose frequency is determined by the bandwidth. This power law decay is a consequence of the $\sqrt{\varepsilon}$ behavior of the LDoS in the band-edge (Eq. (16)). A similar result is obtained in models for unstable nuclei [4–6], an atomic excitation in the free space [7], and interacting with a photonic band [8]. In those cases, the decay law is the regular van Hove singularity of the free space. Here, the surface modifies the singularity and hence, the time decay. Also, we found the analytical expressions for the cross-over times t_s and t_R of Eq. (32) enabling us to assert the range of validity of each regime.

Finally, we find and quantify the survival collapse. This effect, hinted but not explained in previous works, is visualized as the destructive interference between the pure survival amplitude and the return amplitude that arises from pathways that have already explored the rest of the system. This non-Markovian result fully considers the memory effects to infinite order.

In summary, through the exhaustive solution of a particular model, we made a conceptual analysis of a general quantum decay process applicable to the great variety of systems where a quantum exponential decay is observed. Besides this generality, what gives a particular interest to our model is its suitability for an experimental test. This would imply the same procedure devised [22] to test the mesoscopic echoes [17,18]. In order to tailor an XY Hamiltonian in an NMR experiment, it uses a radio frequency pulse sequence that produces the truncation of the natural Heisenberg (J -coupling) Hamiltonian. Alternatively, using the relationship between the dynamics described by an XY Hamiltonian and multiple quantum dynamics [21], the dynamics of our model could be observed with multiple-quantum experiments in solid state NMR [20]. The application of one of the above procedures to relatively small linear molecules would enable the observation of the survival collapse. One could freeze the dynamics at this time obtaining an almost null survival of the local excitation. Since the survival collapse depends critically on the cooperative coherence, of the whole system it, would be quite sensitive to decoherent processes and hence it could be applied to evaluate them.

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