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Signatures of a quantum dynamical phase transition in a three-spin system in presence of a spin environment

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Abstract

We have observed an environmentally induced quantum dynamical phase transition in the dynamics of a two-spin experimental swapping gate [G.A. Álvarez, E.P. Danieli, P.R. Levstein, H.M. Pastawski, J. Chem. Phys. 124 (2006) 194507]. There, the exchange of the coupled states $|\uparrow,\downarrow\rangle$ and $|\downarrow,\uparrow\rangle$ gives an oscillation with a Rabi frequency $b/\hbar$ (the spin-spin coupling). The interaction, $\hbar/\tau_{\mathrm{SE}}$ with a spin-bath degrades the oscillation with a characteristic decoherence time. We showed that the swapping regime is restricted only to $b\tau_{\mathrm{SE}} \gtrsim \hbar$. However, beyond a critical interaction with the environment the swapping freezes and the system enters to a Quantum Zeno dynamical phase where relaxation decreases as coupling with the environment increases. Here, we solve the quantum dynamics of a two-spin system coupled to a spin-bath within a Liouville–von Neumann quantum master equation and we compare the results with our previous work within the Keldysh formalism. Then, we extend the model to a three interacting spin system where only one is coupled to the environment. Beyond a critical interaction the two spins not coupled to the environment oscillate with the bare Rabi frequency and relax more slowly. This effect is more pronounced when the anisotropy of the system-environment (SE) interaction goes from a purely XY to an Ising interaction form.

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The control of quantum dynamics started to receive much attention because of its relevance to several applications ranging from quantum information processing [1] to nanotechnology [2]. Since the environment usually acts degrading the quantum dynamics of a system [3], its decoupling becomes a major challenge. Many techniques [2,4,5] are developed to avoid this loss of information that is characterized by a decoherence rate $1/\tau_\phi$. Spin systems are ideal candidates to test the procedures for QIP. Recently, we observed an environmentally induced quantum dynamical phase transition in the dynamics of a two-spin experimental swapping gate [6]. There, the exchange of the coupled states $|\uparrow,\downarrow\rangle$ and $|\downarrow,\uparrow\rangle$ gives an oscillation with a Rabi frequency $b/\hbar$ (i.e the spin-spin coupling). We showed that the swapping regime is restricted only to $b\tau_{\mathrm{SE}} \gtrsim \hbar$, where $\hbar/\tau_{\mathrm{SE}}$ is the system-environment (SE) interaction, and essentially within this regime $1/\tau_\phi \sim 1/\tau_{\mathrm{SE}}$. However, beyond a critical interaction with the environment, the swapping freezes and the system enters to a Quantum Zeno dynamical phase where the relaxation rate decreases as the coupling with the environment increases $1/\tau_\phi \sim b^2\tau_{\mathrm{SE}}$. Here, we will show how this criticality is useful to "isolate" a spin-pair.

Firstly, we solve the quantum evolution of a two-spin system coupled to a spin-bath within the Liouville–von Neumann quantum master equation [7,8], and compare the result with our previous one [6] using the Keldysh formalism [9]. Then, we extend the model to a three interacting spin system where only one is coupled to the environment. Beyond a critical interaction, the two spins not directly coupled to the environment oscillate with their bare frequency and relax more slowly. In a two-spin system there is always a critical point that depends on the anisotropy relation of the SE interaction quantified as the ratio between Ising and XY terms. However, in the

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three-spin system, the decoherence rate has a smooth cross-over from proportional to the SE interaction to inversely proportional to it. This cross-over approaches a critical transition as the anisotropy of the SE interaction goes from purely XY to Ising.

Experiments in Ref. [6] focus on two interacting spins 1/2 coupled to a spin-bath as modeled by the Hamiltonian $\mathscr{H} = \mathscr{H}_{\mathrm{S}} + \mathscr{H}_{\mathrm{SE}} + \mathscr{H}_{\mathrm{E}}$, with

$$\mathscr{H}_{\mathrm{S}} = \hbar\omega_z(I_1^z + I_2^z) + b(I_1^+ I_2^- + I_1^- I_2^+)/2, \tag{1}$$

$$\mathscr{H}_{\mathrm{SE}} = \alpha I_2^z F^z + \beta(I_2^+ F^- + I_2^- F^+)/2, \tag{2}$$

$$\mathscr{H}_{\mathrm{E}} = \hbar\omega_z \sum_{2<i} I_i^z + \sum_{2<i<j} b_{ij}[2I_i^z I_j^z - \tfrac{1}{2}(I_i^+ I_j^- + I_i^- I_j^+)], \tag{3}$$

where $\mathscr{H}_{\mathrm{S}}$ is the system Hamiltonian of the two coupled spins, $\mathscr{H}_{\mathrm{E}}$ is the spin-bath Hamiltonian with a truncated dipolar interaction and $\mathscr{H}_{\mathrm{SE}}$ is the SE interaction with $F^u = \sum_l b_{2l} I_l^u$, $u = x, y, z$ and $F^{\pm} = (F^x \pm \mathrm{i}F^y)$. $\mathscr{H}_{\mathrm{SE}}$ is an Ising interaction if $\beta/\alpha = 0$ and a XY, isotropic (Heisenberg) or the truncated dipolar interaction if $\alpha/\beta = 0, 1, -2$, respectively. We use the model proposed by Müller et al. [10] to calculate the spin dynamics in the experimental system of Ref. [6]. The model assumes that only one spin interact with the spin-bath which is described in a phenomenological way. In a quantum mechanical relaxation theory the terms F^u are bath operators while in the semi-classical theory [7,8] $F^u(t)$ represent classical stochastic forces. As the experimental conditions justify a high temperature approximation, the semiclassical theory coincides with a quantum treatment. By tracing on the bath variables the random SE interaction Hamiltonian is

$$\mathscr{H}_{\mathrm{SE}}(t) = \alpha F^z(t) I_2^z + \beta[F^-(t) I_2^+ + F^+(t) I_2^-]. \tag{4}$$

The time average of these random processes satisfy $\overline{F^u(t)} = 0$, where their correlation functions are $g^{(u,v)}(\tau) = \overline{F^u(t)F^{v*}(t+\tau)}$. Following the usual treatment to second order approximation, the dynamics of the reduced density operator is given by [7,8]

$$\frac{\mathrm{d}}{\mathrm{d}t}\sigma(t) = -\frac{\mathrm{i}}{\hbar}[\mathscr{H}_{\mathrm{S}}, \sigma(t)] - \widehat{\widehat{\Gamma}}\{\sigma(t) - \sigma_0\}, \tag{5}$$

where the relaxation superoperator $\widehat{\widehat{\Gamma}}$ contains the SE interaction. It accounts for the dissipative interactions between the reduced spin system and the spin-bath and imposes the relaxation of the density operator towards its equilibrium value σ_0. We assume that the correlation times of the fluctuations are extremely short compared with all the relevant transition rates between eigenstates of the Hamiltonian. In this extreme narrowing regime or fast fluctuation approximation we obtain

$$\widehat{\widehat{\Gamma}}\{\sigma\} = \frac{1}{2}\sum_{u,v} \xi_{u,v} \mathscr{J}^{(u,v)}(0)[I_2^u, [I_2^v, \sigma]], \tag{6}$$

where $\mathscr{J}^{(u,v)}(\omega) = \int_{-\infty}^{\infty} d\tau g^{(u,v)}(\tau)\exp\{-\mathrm{i}\omega\tau\}$ is the spectral density and $\xi_{u,v} = (\alpha\delta_{u,z} + \beta(\delta_{u,x} + \delta_{u,y}))$ $(\alpha\delta_{v,z} + \beta(\delta_{v,x} + \delta_{v,y}))$. The spatial directions are statistically independent, i.e. $g^{(u,v)}(\tau) = 0$ if $u \neq v$. Notice that the axial symmetry of $\mathscr{H}_{\mathrm{S}}$ around the z axis leads to the impossibility to evaluate separately $\mathscr{J}_x$ and $\mathscr{J}_y$, where $\mathscr{J}_u = \frac{1}{2}\mathscr{J}^{(u,u)}(0)$. Thus, they will appear only as the averaged value $\mathscr{J}_{xy} = (\mathscr{J}_x + \mathscr{J}_y)/2$. The superoperator now can be written as

$$\widehat{\widehat{\Gamma}}\{\sigma\} = \Gamma_{\mathrm{ZZ}}[I_2^z, [I_2^z, \sigma]] + \Gamma_{\mathrm{XY}}([I_2^x, [I_2^x, \sigma]] + [I_2^y, [I_2^y, \sigma]]), \tag{7}$$

where $\Gamma_{\mathrm{ZZ}} = \alpha^2 \mathscr{J}_z$ and $\Gamma_{\mathrm{XY}} = \beta^2 \mathscr{J}_{xy}$. Note that Γ_{ZZ} and Γ_{XY} contain the different sources of anisotropy. The usual approximation considers $\mathscr{J}_x = \mathscr{J}_y = \mathscr{J}_z$ (identical correlations in all the spatial directions) and $\alpha = \beta = 1$ (isotropic interaction Hamiltonian) [10]. A better approximation considers a dipolar interaction Hamiltonian, i.e. $\alpha = -2\beta = 2$ [6,11]. We consider the experimental initial local polarization on site 2, $\sigma(0) = [\mathbf{1} + \beta_{\mathrm{B}}\hbar\omega_{0I} I_2^z]/\mathrm{Tr}\{\mathbf{1}\}$ and the spin-bath polarized, where $\beta_{\mathrm{B}} = 1/(k_{\mathrm{B}}T)$. As the final state reaches the temperature of the spin-bath, $\sigma_0 = [\mathbf{1} + \beta_{\mathrm{B}}\hbar\omega_{0I}(I_1^z + I_2^z)]/\mathrm{Tr}\{\mathbf{1}\}$. Here, σ_0 commutes with $\mathscr{H}_{\mathrm{S}}$, not containing coherences with $\Delta M \geqslant 1$.

Following the standard formalism [7,8], we write the superoperator $\widehat{\widehat{\Gamma}}$ using the basis of eigenstates of the system Hamiltonian (1). After neglecting the rapidly oscillating non-secular terms with respect to the Hamiltonian, i.e. Γ_{ZZ}, $\Gamma_{\mathrm{XY}} \ll b$, we solve Eq. (5) and we calculate the magnetization of the spin 1 obtaining an extension of the result of Ref. [10]. Our essential contribution is that we specifically account for the anisotropy arising from the nature of SE interaction reflecting it in $\Gamma_{\mathrm{ZZ}} = \alpha^2 \mathscr{J}_z$ and $\Gamma_{\mathrm{XY}} = \beta^2 \mathscr{J}_{xy}$,

$$M_{I_1^z}(t) = \mathrm{Tr}\{I_1^z \sigma(t)\} = M_0[1 - \tfrac{1}{2}\mathrm{e}^{-\beta^2 \mathscr{J}_{xy} t} - \tfrac{1}{2}\cos(\omega_0 t)\,\mathrm{e}^{-(2\beta^2 \mathscr{J}_{xy} + \alpha^2 \mathscr{J}_z)t/2}], \tag{8}$$

where $\omega_0 = b/\hbar$ and $M_0 = \beta_{\mathrm{B}}\hbar\omega_{0I}/4$.

If we relax the condition Γ_{ZZ}, $\Gamma_{\mathrm{XY}} \ll b$, i.e. we do not neglect the non-secular terms for the superoperator $\widehat{\widehat{\Gamma}}$, the dynamics still occurs in the Liouville space of the populations and ZQT. We obtain exactly the same solution derived in Ref. [6] within the Keldysh formalism:

$$\frac{M_{I_1^z}(t)}{M_0} = (1 - a_0\mathrm{e}^{-R_0 t} - a_1\cos[(\omega + \mathrm{i}R_2)t + \phi_0]\mathrm{e}^{-R_1 t}), \tag{9}$$

where the real functions ω, R_0, R_1 and R_2 as well as a_0, a_1 and ϕ_0 depend exclusively on b, $1/\tau_{\mathrm{SE}} = \Gamma_{\mathrm{ZZ}} + \Gamma_{\mathrm{XY}}$ and $p_{\mathrm{XY}} = \Gamma_{\mathrm{XY}}/(\Gamma_{\mathrm{ZZ}} + \Gamma_{\mathrm{XY}})$. The complete analytical expression is given in Ref. [6]. There, we showed that if the SE interaction is *anisotropic* ($\Gamma_{\mathrm{XY}} \neq \Gamma_{\mathrm{ZZ}}$), the functional dependence of ω on τ_{SE} and b yields a critical value for their product, $b\tau_{\mathrm{SE}}/\hbar = k_{p_{\mathrm{XY}}}$, where the dynamical regime changes. We called this phenomenon a quantum dynamical phase transition [6,9] ensured by the condition $\omega R_2 \equiv 0$. This is evidenced by the functional change (non-analyticity) of the dependence of the observables (e.g. the swapping frequency ω) on the control parameter $b\tau_{\mathrm{SE}}/\hbar$. This non-analyticity is enabled by taking the thermodynamic limit of an infinite number of spins [12]. One identifies two parametric regimes: (1) The *swapping phase*, which is a form of sub-damped dynamics, when $b\tau_{\mathrm{SE}}/k_{p_{\mathrm{XY}}} > \hbar$ ($R_2 = 0$ in Eq. (9)). (2) A *Zeno phase*, with an over-damped dynamics for $b\tau_{\mathrm{SE}}/k_{p_{\mathrm{XY}}} < \hbar$ arising on the strong coupling with the environment (*zero frequency*, i.e. $\omega = 0$, in Eq. (9)). In the neighborhood of the critical point the swapping frequency takes the form:

$$\omega = \begin{cases} a_{p_{\mathrm{XY}}} \sqrt{(b/\hbar)^2 - k_{p_{\mathrm{XY}}}^2/\tau_{\mathrm{SE}}^2} & b\tau_{\mathrm{SE}}/k_{p_{\mathrm{XY}}} > \hbar, \\ 0 & b\tau_{\mathrm{SE}}/k_{p_{\mathrm{XY}}} \leqslant \hbar. \end{cases} \tag{10}$$

The parameters $a_{p_{\mathrm{XY}}}$ and $k_{p_{\mathrm{XY}}}$ only depend on p_{XY} which is determined by the anisotropy of the interaction Hamiltonian.

Three-spin system: The system Hamiltonian is

$$\mathscr{H}_{\mathrm{S}} = \hbar\omega_{\mathrm{L}}(I_0^z + I_1^z + I_2^z) + b(I_0^+ I_1^- + I_0^- I_1^+)/2 + b(I_1^+ I_2^- + I_1^- I_2^+)/2, \tag{11}$$

and the environment and SE Hamiltonian remains as before. Also, the environment is coupled to only one spin of the system. We solve Eq. (5) as before, without neglecting non-secular terms of the relaxation superoperator. Considering the initial condition $\sigma(0) = (\mathbf{1} + \beta\hbar\omega_{0I} I_0^z)/\mathrm{Tr}\{\mathbf{1}\}$ and a polarized spin-bath, the magnetization at site 0 is

$$M_{I_0^z}(t) = \mathrm{Tr}\{I_0^z \sigma(t)\} = M_0[1 - a_0 \mathrm{e}^{-R_0 t} - a_1 \mathrm{e}^{-R_1 t} + a_2 \sin(\omega_2 t + \phi_2)\mathrm{e}^{-R_2 t} + a_3 \sin(\omega_3 t + \phi_3)\mathrm{e}^{-R_3 t}]. \tag{12}$$

The coefficients a_i, R_i, ω_i and ϕ_i are real and they are functions of b, $1/\tau_{\mathrm{SE}}$ and p_{XY}. If $p_{\mathrm{XY}} \neq 0$ the final state has all the spins polarized because a net transfer of magnetization from the spin-bath is possible. However, for an Ising SE interaction, $p_{\mathrm{XY}} = 0$, we obtain that $R_0 = 0$ and $1 - a_0 = \frac{1}{3}$ (the asymptotic polarization) because the final state is the quasi-equilibrium of the three-spin system [11]. In Fig. 1 we show the frequencies ω_2 and ω_3 and the different relaxation rates as a function of $(b\tau_{\mathrm{SE}}/\hbar)^{-1}$ when the SE interaction is Ising ($p_{\mathrm{XY}} = 0$). Two changes, resembling the critical behavior of two-spin systems are observed. The same phenomenon occurs in Fig. 2(a) where the coefficients a_i are shown. The polarization evolution of an isolated three-spin system is $M_{I_0^z}(t) = (M_0/8)[3 + 4\cos(\omega_2^o t) + \cos(\omega_3^o t)]$ where $\omega_2^o = (\sqrt{2}/4)b/\hbar$ and $\omega_3^o = (\sqrt{2}/2)b/\hbar$ are the natural frequencies. When $(b\tau_{\mathrm{SE}}/\hbar)^{-1} \ll 1$, we observe that $\omega_2 \to \omega_2^o$, $\omega_3 \to \omega_3^o$, $a_1 \to \frac{1}{3} - \frac{3}{8}$, $a_2 \to \frac{1}{2}$ and $a_3 \to \frac{1}{8}$ as expected for an isolated three-spin dynamics. The dependence of ω_3 as a function of $(b\tau_{\mathrm{SE}}/\hbar)^{-1}$ is similar to that of the swapping frequency in Ref. [6]. However, instead of becoming zero when the SE interaction increases, it suddenly stabilizes at $\omega_0 = b/\hbar$, the bare two-spin Rabi

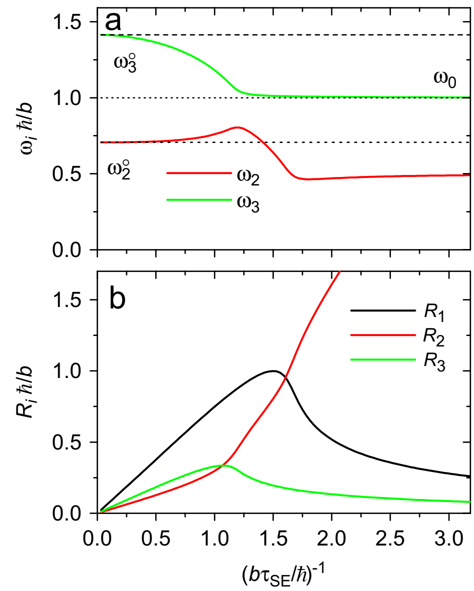

Fig. 1. (Color online) (a) Frequencies involved in the time evolution of the polarization in the three-spin system as a function of $(b\tau_{\mathrm{SE}}/\hbar)^{-1}$. Dashed lines represent the isolated system. Dot line corresponds to two spins decoupled from the environment. (b) Different relaxation rates of the polarization.

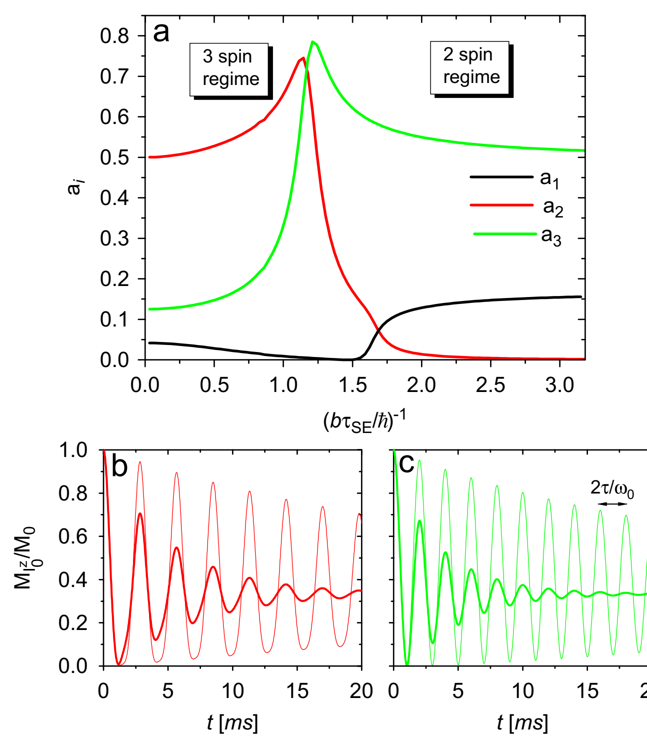

Fig. 2. (Color online) (a) Coefficients (weights) of the different terms of Eq. (12). At the critical region there is a switch between the two-spin and the three-spin regime. (b) and (c) Temporal evolutions of the polarization in the two-spin and three-spin regimes respectively for different τ_{SE}. In (b) $b/\hbar = 2\pi \times 1\,\mathrm{kHz}$ and $\tau_{\mathrm{SE}} = 1.43\,\mathrm{ms}$ for the thick line and $\tau_{\mathrm{SE}} = 10\,\mathrm{ms}$ for the thin line. In (c) $b/\hbar = 2\pi \times 1\,\mathrm{kHz}$ and $\tau_{\mathrm{SE}} = 0.1\,\mathrm{ms}$ for the thick line and $\tau_{\mathrm{SE}} = 0.01\,\mathrm{ms}$ for the thin line.

frequency. At the same point ω_2, R_2 and R_3 also have a sudden change. While R_2 and R_3 initially grow as $(b\tau_{SE}/\hbar)^{-1}$, there R_2 increases the growing speed while R_3 begins to decay as in the Zeno phase of Ref. [6]. Moreover, the coefficients a_2 and a_3 switch between them, a_2 suddenly goes down and a_3 goes up. These coefficients are the weights of the different frequency contributions in the time evolution. The changes on the decoherence rates and on the weight coefficients of the different oscillatory terms beyond the critical interaction (region) lead the system to oscillate with the bare Rabi frequency of two spins decoupled from the environment. If we keep increasing the control parameter $(b\tau_{SE}/\hbar)^{-1}$, this effect is enhanced by the next transition. After the second transition, R_1 begins to decrease as in the Zeno phase behavior of Ref. [6]. As the term of Eq. (12) that relaxes with R_1 leads the system to the three-spin quasi-equilibrium, when R_1 goes down, this final state is approached much slower. The effect is to avoid the interaction between the two-spins not coupled to the environment and I_2. After the second transition, the coefficient a_1 goes abruptly to zero leading to a more pronounced ‘‘isolation’’ of the two-spins. Thus, two dynamical regimes are observed: One characterized by the three-spin dynamics for $(b\tau_{SE}/\hbar)^{-1} \lesssim 1$ and a second one, for $(b\tau_{SE}/\hbar)^{-1} \gtrsim 1$, which has a two-spin behavior.

Fig. 2(b) and (c) show the temporal evolution of the magnetization of Eq. (12) on the three-spin and the two-spin regimes, respectively. While in Fig. 2(b) the two frequency contributions are evident, in Fig. 2(c) only the bare Rabi frequency is manifested. In each graph we show two curves with different SE interactions. In Fig. 2(b), we show that increasing the SE interaction the decoherence rates increase. However, in the two-spin regime (Fig.2(c)) when the SE interaction is increased, the decoherence rate decreases leading to a better ‘‘isolation’’. It is important to take into account that while the relaxation rates go to zero smoothly the swapping frequency acquire the bare value near the critical point. Another fact to remark is that this effect is more pronounced when the anisotropy of the SE interaction is close to a pure Ising SE interaction while an increase in the XY nature leads to a further smoothing of the transition. The reason is that, when $p_{XY} \neq 0$, there is a net transfer of magnetization to the system which is redistributed between the three spins, this redistribution begins to be slower at the second transition when R_3 goes down. In contrast, for a purely Ising interaction, there is no net polarization transfer and a purely decoherent process at site 3 freezes its dynamics but its fast energy fluctuations prevent the interaction with the other spins.

In summary, we found an analytical expression for the two-spin dynamics plus a spin-bath of the experimental swapping gate [6], showing that standard density matrix formalism leads to a quantum dynamical phase transition as does the Keldysh formalism [6,9]. Here, we extended the model to a three-spin system and showed that beyond a critical region the two spins become almost decoupled from the environment oscillating with the bare Rabi frequency and relaxing more slowly. While in the two-spin swapping gate the dynamical transition is critical, when we extend the system to three-spin the criticality is smoothed out. However, enough abruptness remains to give the possibility to use it to ‘‘isolate’’ a two-spin system with a finite SE interaction.

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