



## PAPER

## Activated and non-activated dephasing in a spin bath

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RECEIVED  
15 June 2016REVISED  
4 August 2016ACCEPTED FOR PUBLICATION  
8 August 2016PUBLISHED  
2 September 2016Original content from this  
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Keywords: decoherence, open quantum systems, dephasing

## Abstract

We analyze different decoherence processes in a system coupled to a bath. Apart from the well known standard dephasing mechanism which is temperature dependent an alternative mechanism is presented, the spin-swap dephasing which does not need initial bath activation and is temperature independent. We show that for dipole interaction in the weak coupling regime the separation of time scales between system and bath can not produce pure dephasing, the process being accompanied by dissipation. Activated and non-activated dephasing processes are analyzed in a diamond nitrogen-vacancy center.

## 1. Introduction

*Decoherence* is a fundamental process where a quantum system loses its wave properties enabling interference. As a result classical behavior emerges. Decoherence is a clear concept studied at least for 50 years [1] nevertheless, it is still ill defined, it cannot be associated with a unique observable [2–9]. New quantum technologies require control on the decoherence and knowledge on the transition from quantum to classical behavior [10–13]. In the implementation of possible future quantum technologies [14] and quantum information processing [15, 16] fast decoherence is destructive. A signature of decoherence is purity loss where purity is defined by  $\mathcal{P} = \text{tr} \{ \hat{\rho}^2 \}$ .

The origin of decoherence is the interaction of a system with its environment i.e., no quantum system is isolated. The general framework is of a mesoscopic or even macroscopic primary systems described by a Hamiltonian  $\hat{H}_S$  interacting through  $\hat{H}_{SB}$  with a background environment or a bath described by  $\hat{H}_B$

$$\hat{H} = \hat{H}_S + \hat{H}_B + \hat{H}_{SB}. \quad (1)$$

The interaction term generates quantum and classical correlation between the system and the environment. One outcome is energy transfer between the system and bath termed *dissipation*. In quantum mechanics this dissipation is always accompanied by decoherence. In addition, even when the energy exchange is negligible, decoherence is possible. This scenario is termed pure decoherence or simply *dephasing*. Pure dephasing can be defined as loss of quantum purity but maintaining the expectation of the energy projections. To quantify this loss one can employ the measure of coherence [9],  $\mathcal{C}_i(\hat{\rho}_S) = \sum_{i \neq j} |\hat{\rho}_{S,ij}|$ , where we sum over the off diagonal elements of the reduced density operator of the system  $\hat{\rho}_S = \text{tr}^{(B)} \hat{\rho}$  denoting  $\text{tr}^{(B)}$  the partial trace over the bath Hilbert space  $\mathcal{H}_B$ .

More than one scenario can generate pure dephasing. The obvious case is when the Hamiltonian  $\hat{H}_S$  describing the system commutes with  $\hat{H}_{SB}$ . In this scenario one can think of the environment as randomly modulating the system Hamiltonian generating a loss of phase during evolution. This scenario includes the case of a continuous monitoring of the system energy. Typically, this modulation is produced by single interactions between bath particles, higher order bath processes can also provide relaxation mechanisms [17].

Another scenario for pure dephasing, is the result of a separation of time scales between the system and bath. This will occur when there is an energy spectral gap between the system and the bath [18]. The process can be interpreted as the Bohr frequencies of the bath being out of range of the system. As a result energy exchanges are transients and suddenly energy is exchanged back and forth between the system and bath. The final outcome is no net energy change. As a result of this mechanism the system experiences dephasing.

Excitation of the bath can influence both mechanisms. Random modulation induced by the bath requires many of the bath modes to be excited. As a result this mechanism of dephasing is activated and subsequently, at low temperature it can be frozen out. The second mechanism of timescale separation is influenced by the bath excitation due to the possibility that the excitation modifies the spectrum, possibly changing pure dephasing to energy dissipation.

Noteworthy, only two basic types of environment have been studied, either a spin bath model [19] or a ‘spin-boson’ oscillator bath model [1]. Spin baths, composed of two level systems (TLS), are geared for the description of low energy dynamics of localized environmental modes. The difficulty in spin baths is the lack of a procedure to obtain the parameters defining the values experimentally. At low temperature a spin bath can be mapped into the spin-boson bath [19]. Spin-boson baths are used to model a central system weakly coupled to  $K$  environmental modes that are best adapted to delocalized modes with couplings  $\sim K^{-1/2}$ . However, at low energies, thermodynamical variables like entropy in almost any real physical system, are dominated by localized modes [20] relaxing very slowly at low temperature due to system–bath couplings independent of  $K$  [19].

The linear coupling to spin-boson baths is not a universal model of decoherence [18] and harmonic baths are not a generic quantum environment [21]. Nevertheless due to the similarity between classical and quantum harmonic baths they are easy to construct due to the fact that the system–bath parameters can be obtained from classical molecular dynamics [22]. For this reason harmonic baths are the starting point of many system–bath models [1, 23–25]. In contrast, a spin bath is universal and constitutes a universal quantum simulator. universal quantum gates can be built from 6 spins [26] manipulated to simulate the behavior of arbitrary quantum systems whose dynamics are determined by local interactions [27].

Historically, the main approach towards open system dynamics is to construct equations of motion for the primary system where the bath is treated implicitly. To this end, two different frameworks have been pursued: the weak coupling limit based on perturbation theory [28, 29], and the phenomenological dynamical semigroup formalism [30, 31]. The starting point for the perturbation theory is decomposition (1) of the total Hamiltonian and assumes weak coupling  $\hat{H}_{SB}$ . The small parameter is the system–bath coupling. Typically, using projecting operator techniques [29, 32] the equation of motion for the bath can be decoupled and solved assuming that the bath is maintained in equilibrium. The result is an equation of motion for the dynamics of the reduced density operator  $\hat{\rho}_S(t)$  of the primary system, the so called quantum master equation (QME) [33]. The construction leads to an integro-differential non-Markovian equation. The memory effects are the price to pay for a reduced description of the primary system. Further reduction, assuming the bath is fast (secular approximation), leads to a Markovian equation of motion [34].

The starting point of the dynamical semigroup formalism is the condition of complete positivity [35] and the Markovian assumption. The approach also provides an equation for the dynamics of the reduced density operator  $\hat{\rho}_S(t)$  of the primary system. In the so called Lindblad form [30, 31] the system is driven by its Hamiltonian  $\hat{H}_S$  and the interaction with the bath is modeling by Liouville super-operators [30], operators acting on operators. The weak coupling limit can lead to the Lindblad form [34], but the Lindblad form can be obtained in other limits such as the singular bath limit [36] or the scattering Poissonian model [37]. The Markovian assumption is equivalent to a tensor product structure of the system and bath at all times  $\hat{\rho} = \hat{\rho}_S \otimes \hat{\rho}_B$ .

Non-Markovian effects are abundant in many branches of physics. A correct treatment of the non-Markovian dynamics is necessary for the description of these systems in quantum technologies which require accurate control [38]. Approaches to reach beyond the Markovian approximation and possibly the weak coupling limit have been considered. Using perturbation theory it is possible to go beyond the second order terms like in the QME taking higher orders [39, 40]. For exponential decaying memory it is possible to embed the dynamics in a larger space leading to coupled Markovian equations [41]. Non-Hermitian projection operators have also been proposed [42] to include the memory effect in the bath. Non-Markovian quantum jumps [43] generalizing Monte Carlo wave function provide a correct identification between decay rates and jump probabilities. A hybrid stochastic hierarchy equations of motion approach allows a treatment of the low temperature behavior of non-Markovian open quantum systems [44]. Non-Markovian dynamical maps are used to accurately propagate a initial state of the system to arbitrarily long time scales [45]. Recently, the non-Markovianity of systems has been proposed to carry out quantum control tasks that could not be realized if the system is isolated [46].

The present paper studies pure dephasing processes based on an alternative approach which can deal with strong coupling avoiding the Markovian approximations. This paper is structured as follows. In section 2 we introduce an alternative approach, the surrogate Hamiltonian (SH) to analyze dephasing. In addition, we also present the spin swap process in the context of the SH. Section 3 describes a well known model of an harmonic oscillator coupled to a bath of spins to analyze the decoherence of the harmonic oscillator. Apart from energy dissipation and dephasing for commutativity of  $\hat{H}_S$  and  $\hat{H}_{SB}$  we introduce a new mechanism, spin swap, to

produce dephasing. This section also analyzes the effect of a finite bath energy spectrum in the dissipation and dephasing processes. In section 4 the different dephasing mechanisms are discussed in a more realistic scenario, a diamond nitrogen-vacancy (NV) center. Finally, we present conclusions and future outlooks.

## 2. The surrogate Hamiltonian

In the study of dephasing we use a complementary approach, the surrogate Hamiltonian (SH) [47]. The SH starts from a description of the total system and a representative bath, yielding a numerically feasible model whose validity is limited in time. The principal advantage of the method is that it goes beyond system–bath separability implied by the Markovian assumption. The starting point is equation (1) and again the bath degrees of freedom are treated implicitly by abstract, representative modes. The core idea of the SH is truncation of the infinite modes of the bath by selecting representative modes, the modes that interacts intimately with the system [47]. The truncation generates a new SH generating the dynamics of the surrogate wave function. In the limit where SH includes an infinite number of modes it coincides with the original Hamiltonian. The reduced dynamics of an open quantum system can be accurately computed by a finite effective Hamiltonian whose dimension can be *a priori* estimated [48]. More details about the construction of the SH can be found in [47, 53, 54].

The truncation leading to SH relies on the energy-time uncertainty principle. For a finite time  $t \ll \infty$  the system is only able to interact with a finite number of bath modes  $K \ll \infty$ , making it unnecessary to describe the full density of states of the bath. Two important observations are derived from this argument. First, the SH is a suitable approach for ultra-short processes, and secondly, the number of required modes in the bath increases with the interaction strength. Intermediate and strong couplings require a larger computational effort. Nevertheless, the approach does not rely on the weak coupling assumption.

The truncation and discretization of the bath made in the SH impose a bound in the information propagation time [48], once this time is overcome unphysical recurrences from the bath to the system appear. To extend the recurrence time, i.e. the convergence of the SH in the time domain, there are two routes: the obvious one is increasing simultaneously the number of spins and the computational cost. Invoking again the time-energy uncertainty relation, increasing the spectral density of bath modes the SH convergence time increases. In the examples below, the considered spectral density is linear in the number of bath modes, so the convergence time increases linearly with the number of bath modes.

An alternative route to extend the convergence time of the SH without increasing the number of modes is introducing a secondary bath that acts as a sink on the primary bath [49]. The secondary bath acts as a thermal boundary of the primary bath. The spin frequencies of both baths are identical and they interact by swapping spins randomly [50] at a rate faster than the recurrence time. As consequence the SH produces convergent results at long evolution times with a limited number of bath spins [49–51]. These swaps are generated by unitary operations on the bath Hilbert space, see section 2.2.

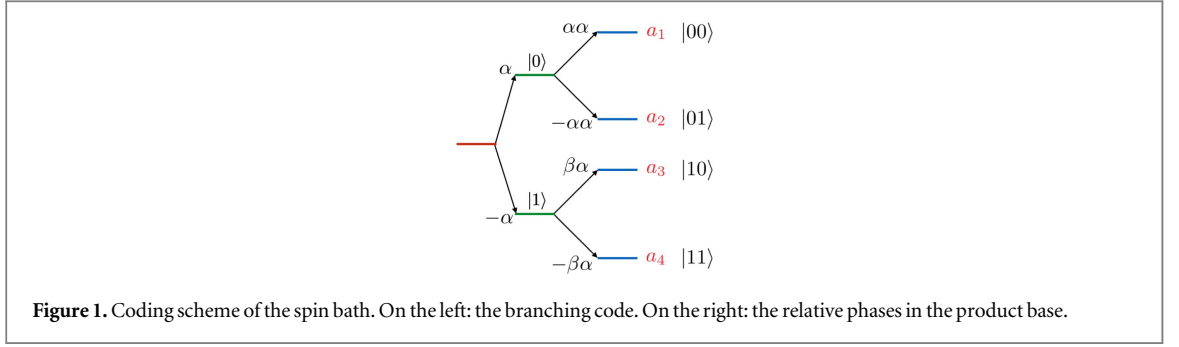
A collision model gives us a more physical insight of the process, and swaps can be interpreted as quasiparticles (phonons, excitons, magnons, plasmons, ...) stochastically colliding with the system and/or bath. The swap operation generates a tensor product state between the swapped spin and the remaining entangled wave function deteriorating the uncontrollable initial correlations of the spins that constitute the bath. As result, after a swap is produced, part of the system–bath entanglement is lost and new correlations are generating between the bath modes. By controlling the swap rate, the ratio between energy relaxation and dephasing can be determined.

The stochastic SH method allows to go beyond the Markovian and weak coupling regimes. Increasing the number of spins in bath and consequently the recurrence time, the required number of swap operations is reduced. In the limiting case of infinite bath modes in the SH no swaps are necessary. From a numerical point of view the spin swap operations produce faster convergence on local properties since swaps act as absorbent boundary conditions. The effect of a swap is to avoid reflections at the boundaries of the bath resetting the bound in the propagation time thus extending the convergence of the SH. If for example, the secondary bath is in thermal equilibrium, the SH leads the system to thermalization avoiding energy recurrences at long times [49]. This is the expected dynamics for almost any subsystem in interaction with a large enough bath [52].

### 2.1. The bit representation

The environment surrounding the primary system is considered to be a bath of TLS. The Hilbert space  $\mathcal{H}_B$  for the bath has dimension  $2^K$  resulting from the combination of a single TLS with the rest of  $K$  spins of the bath. To represent the single TLS space we choose the spin up  $|1\rangle$  (TLS excited) and spin down  $|0\rangle$  (TLS de-excited) base along the  $z$ -direction for the bit representation [47, 53] explained below.

The total Hilbert  $\mathcal{H}_S \otimes \mathcal{H}_B$  space has the product dimension of  $\mathcal{H}_S$  and  $2^K$ . To represent a total state of  $\hat{H}$  we need wave functions of dimension  $2^K N_g$  if the system is described by a grid of dimension  $N_g$ . For example, if



we consider a bath with  $K = 2$ , two spins, the wave function spinor is

$$\Psi^{K=2}(q) = \begin{pmatrix} \psi_0(q, \phi) \\ \psi_1(q, \phi) \\ \psi_2(q, \phi) \\ \psi_3(q, \phi) \end{pmatrix}, \quad (2)$$

where  $q$  represents the degrees of freedom of the system and  $\phi$  the bath degrees of freedom. The spinor is bit ordered, corresponding to a bit representation to each component of the spinor. In the example considered, the bit representation of each spinor components is  $0 \rightarrow |00\rangle$ ,  $1 \rightarrow |01\rangle$ ,  $2 \rightarrow |10\rangle$  and  $3 \rightarrow |11\rangle$ , starting the count of bits from the right. The zeroth component corresponds to no bath modes excited, the first and second component to the excitation of the first or second bath mode, and the third component to the simultaneous excitation of the first and second bath modes.

The bath operators are sums over operators acting on a single mode. In the bit representation the operator of mode  $k$  acts on the bit  $k$  in the  $2^K$  components of the spinor. Note the difference between bath mode and spinor components. There are  $K$  spin modes and  $2^K$  spinor components. For example, the  $k = 0$  mode that can be excited or de-excited should not be confused with the zeroth spinor component corresponding to all bath modes de-excited.

It is useful to note that any bath operator can be written in terms of creation and annihilation operators. The creation operator of the  $k$  mode is [53]

$$\hat{\sigma}_k^{\dagger K} = \prod_{i=1}^{K-k} \mathbb{I}_2 \otimes \hat{\sigma}^{\dagger} \otimes \prod_{i=1}^{k-1} \mathbb{I}_2, \quad (3)$$

where in the bit representation

$$\hat{\sigma}^{\dagger} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \quad (4)$$

The annihilation operator for the  $k$  mode is simply the conjugate expression of (3) built on  $\hat{\sigma}$ . The Pauli matrices for the  $k$  modes are given by

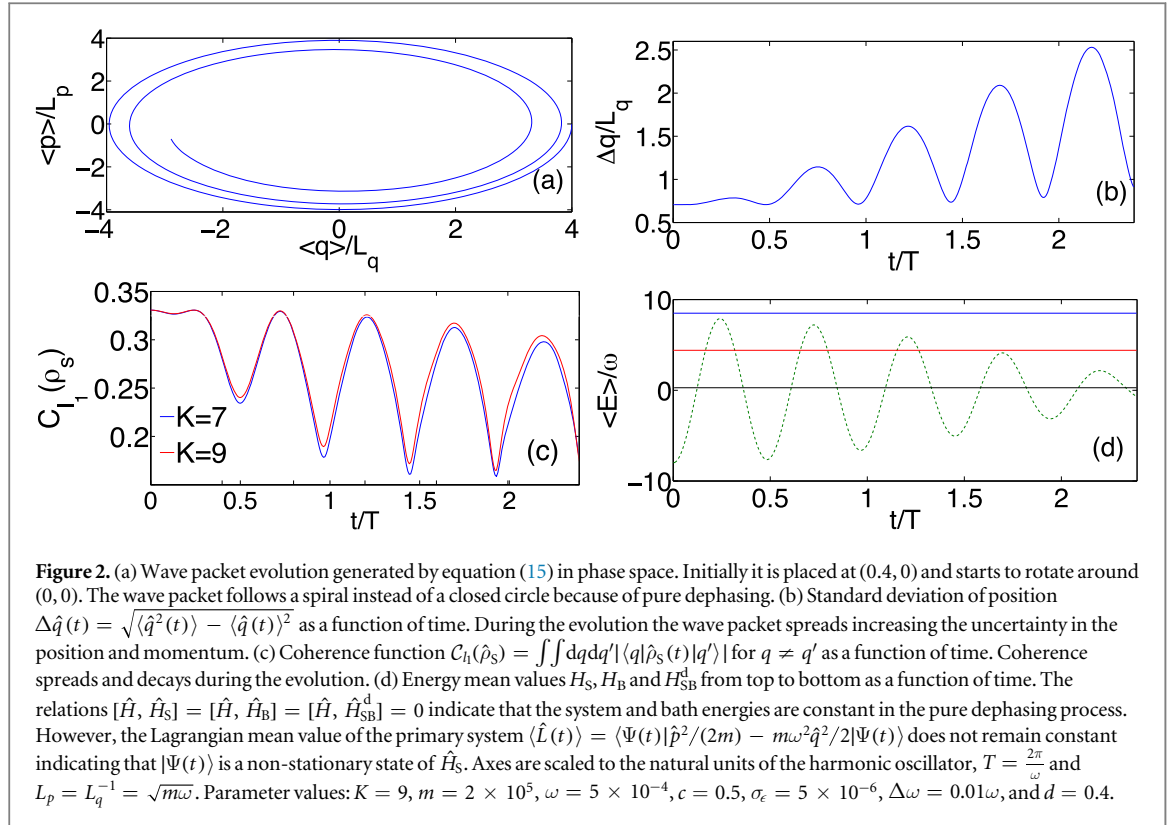
$$\hat{\sigma}_k^x = \frac{\hat{\sigma}_k^{\dagger} + \hat{\sigma}_k}{2}, \quad \hat{\sigma}_k^y = \frac{\hat{\sigma}_k^{\dagger} - \hat{\sigma}_k}{2i}, \quad \hat{\sigma}_k^z = \frac{\hat{\sigma}_k^{\dagger} \hat{\sigma}_k - \hat{\sigma}_k \hat{\sigma}_k^{\dagger}}{2}. \quad (5)$$

## 2.2. Spin swap

An important operation in the stochastic surrogate Hamiltonian is the swap of bath spins between the primary and secondary baths [50]. The challenge in generating the operation is to generate a tensor product between the swapped spin and the remainder of the wavefunction without affecting the entanglement of the un-swapped bath modes. The implementation is illustrated in the following example. The wave function of two spins can be represented as

$$\begin{aligned} |\phi\rangle &= \lambda_1|00\rangle + \lambda_2|01\rangle + \lambda_3|10\rangle + \lambda_4|11\rangle \\ &= \frac{1}{Z} (e^{a_1}|00\rangle + e^{a_2}|01\rangle + e^{a_3}|10\rangle + e^{a_4}|11\rangle), \end{aligned} \quad (6)$$

where  $\lambda_k$  and  $a_k \in \mathbb{C}$ , and  $Z^2 = \sum_k e^{a_k + a_k^*}$  being  $a_k^*$  the complex conjugate of  $a_k$ . The irrelevant global phase is chosen in such a way  $\sum_k a_k = 0$ . The relative phases of each  $a_k$  spinor can be related to the conditional amplitudes using a branching tree [50], as an example let's swap the right hand spin of the spinors, see figure 1



$$\begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} \alpha \\ \alpha\alpha \\ \beta\alpha \\ 0 \end{pmatrix}. \quad (7)$$

The inverse relation reads

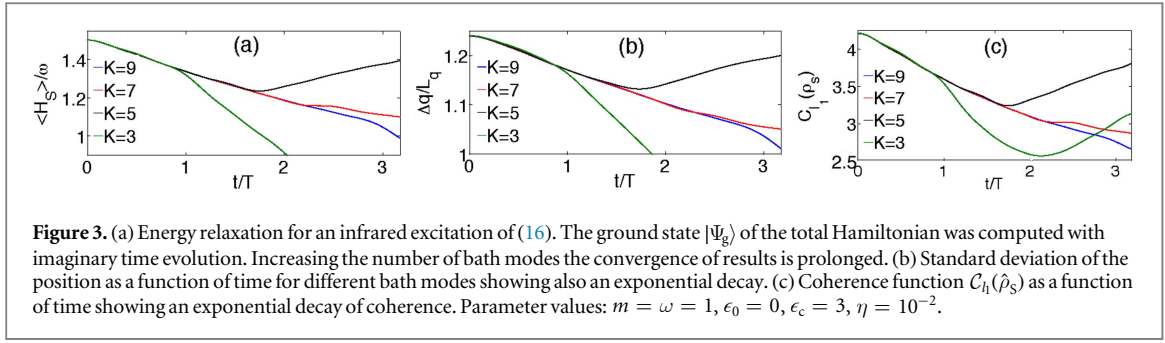
$$\begin{pmatrix} \alpha \\ \alpha\alpha \\ \beta\alpha \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & -1/2 & -1/2 \\ 1/2 & -1/2 & 0 & 0 \\ 0 & 0 & 1/2 & -1/2 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{pmatrix}. \quad (8)$$

In this example there are 4 spinors and each of them has 2 spins. The left-hand spin has a probability amplitude  $e^\alpha$  to be in  $|0\rangle$  and  $e^\beta$  to be in  $|1\rangle$ , as the total probability to be in  $|0\rangle$  or  $|1\rangle$  is constrained to be 1, only one parameter is necessary to describe the spin amplitude probability thus the phases  $\alpha$  and  $\beta$  can be re-shifted in such a way  $e^\alpha$  is the amplitude probability to be in  $|0\rangle$  and  $e^{-\alpha}$  to be in  $|1\rangle$ .

This argument is valid to characterize any branch in figure 1 since the branches are independent events. Once the left hand spin of the spinor is, for example, in  $|0\rangle$  with probability amplitude  $e^\alpha$  the amplitude probability to find also the right spin in  $|0\rangle$  is  $e^{\alpha+\alpha\alpha}$  and  $e^{\alpha-\alpha\alpha}$  to be in  $|1\rangle$ , where the symbol  $\alpha\alpha \neq \alpha^2$  represents the amplitude of the second spin once the first is in the  $|0\rangle$  state. Consequently, the amplitude of the spinor  $|00\rangle$  is  $e^{a_1} = e^{\alpha+\alpha\alpha}$  and so on. Similar coding schemes in figure 1 can be used to swap any other spin inside the spinors by reordering the amplitude on the branches. To realize the swap operation we proceed as follows:

- (1) Calculate the relative phases  $\{a_k\}$  from the computational coefficients  $\{\lambda_k\}$  using equation (6).
- (2) Using equation (8) compute the coefficients  $\alpha, \alpha\alpha$  and  $\beta\alpha$  from  $\{a_k\}$ .
- (3) Change  $\alpha\alpha = \beta\alpha = b$  to the value  $b$  of the new swapped spin.
- (4) Using equation (7) recalculate the set  $\{a'_k\}$  for the new branching coefficients  $\alpha, \alpha\alpha, \beta\alpha$ .
- (5) Calculate  $\{\lambda'_k\}$  using again equation (6).

Usually in step 1 when we compute  $\{a_k\}$  from  $\{\lambda_k\}$  the phases do not satisfy  $\sum_k a_k = 0$ , to solve it multiply and divide  $|\phi\rangle$  by  $e^c$  with  $c = -\frac{1}{2\pi} \sum_k [\log|\lambda_k| + i \arg(\lambda_k)]$  and define  $a_k = c + \log|\lambda_k| + i \arg(\lambda_k)$ . In step 3 we only modify the imaginary part of the  $\alpha, \alpha\alpha, \beta\alpha$  to avoid wave function renormalization.



The action of the swap operation is to generate a tensor product state between the swapped spin and the rest of the wavefunction keeping its entanglement. For example, after swapping the right-hand spin of the spinors we get

$$|\phi\rangle = (\lambda'_1|0\rangle + \lambda'_2|1\rangle) \otimes (\lambda'_3|0\rangle + \lambda'_4|1\rangle) \quad (9)$$

with  $\lambda'_3/\lambda'_4 = e^{2b}$ ,  $\lambda'_1 = e^\alpha/Z'$  and  $\lambda'_2 = e^{-\alpha}/Z'$  being  $Z'$  the new normalization constant.

For a simulation containing spin swap operations we make  $N_r$  realizations of the evolution to average the random swaps.

### 3. Dephasing and relaxation in the harmonic oscillator system

The generic example is the harmonic oscillator of mass  $m$  and a constant frequency  $\omega$  whose Hamiltonian is given by

$$\hat{H}_s = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2, \quad (10)$$

where  $\hat{p}$  and  $\hat{q}$  are the momentum and position quantum operators.

The bath is composed of  $K$  TLS with spins  $1/2$  governed by the Hamiltonian

$$\hat{H}_B = \sum_k^K \epsilon_k \hat{\sigma}_k^\dagger \hat{\sigma}_k, \quad (11)$$

where  $\epsilon_k$  is the energy, and  $\hat{\sigma}_k^\dagger$  and  $\hat{\sigma}_k$  are the creation and annihilation operators for the  $k$  mode. The bath has a spectrum of modes with energies in the interval  $\epsilon_k \in [\epsilon_0, \epsilon_c]$  with  $\epsilon_c$  the cutoff energy. For a bath containing  $K$  modes the interval is sampled selecting the discrete points  $\epsilon_0 < \epsilon_1 < \dots < \epsilon_{K-1}$ .

The interaction between system and bath depends on the decoherence problem to be analyzed. In addition to the classical decoherence, energy relaxation, quantum systems also show pure decoherence, phase relaxation. Energy relaxation is the exchange of energy between the primary system and the bath which will eventually lead to thermal equilibrium. The Hamiltonian describing the energy transfer of the bath modes and the system has a dipolar nature and is given by

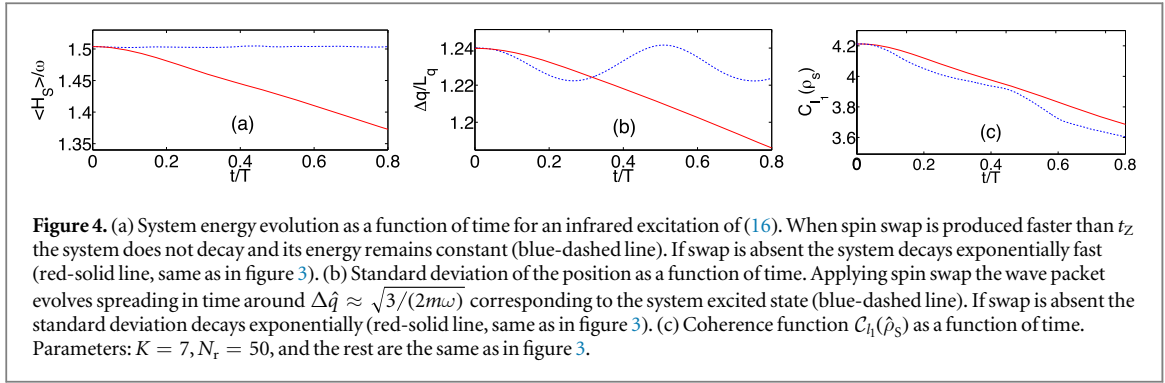
$$\hat{H}_{SB}^r = \hat{q} \otimes \sum_k^K d_k (\hat{\sigma}_k^\dagger + \hat{\sigma}_k), \quad (12)$$

where the coupling constants are given by  $d_k = \sqrt{J(\epsilon_k)/\rho(\epsilon_k)}$  with  $J(\epsilon_k)$  the spectral density and  $\rho(\epsilon_k)$  the density of states. For all the examples in this paper we consider a linear spectral density  $J(\epsilon_k) = \eta\epsilon_k$  being  $\eta$  a constant. The previous energy sampling specifies a density of states for the discrete bath  $\rho(\epsilon_k) \approx (\epsilon_{k+1} - \epsilon_k)^{-1}$ . The exchange energy process described by equation (12) can be understood as the subtraction of energy from the system and the creation of an excitation in a bath mode  $\hat{\sigma}_k^\dagger$  and the inverse process, a de-excitation of the bath mode  $\hat{\sigma}_k$  that injects energy into the primary system.

The phase relaxation, or simply dephasing, occurs due to inelastic interactions between the primary system and different bath modes, destroying the accumulated phase acquired by the system.

#### 3.1. Standard pure dephasing

The most studied process for pure dephasing is the result of commutativity between the system Hamiltonian  $\hat{H}_s$  and the interaction Hamiltonian  $\hat{H}_{SB}$ . In the SH it is governed by the interaction



$$\hat{H}_{SB}^d = \hat{H}_S \otimes \sum_{j < k}^K c_{jk} (\hat{\sigma}_j^\dagger \hat{\sigma}_k + \hat{\sigma}_k^\dagger \hat{\sigma}_j), \quad (13)$$

where the coupling constants  $c_{jk}$  are

$$c_{jk} = \frac{c}{K(K-1)} e^{\frac{(\epsilon_j - \epsilon_k)^2}{2\sigma_\epsilon^2}}, \quad (14)$$

being  $c$  the global dephasing parameter and  $\sigma_\epsilon$  the inelastic bias.

Equation (13) can be interpreted as a process where the excitation of a bath mode is generated at the expense of de-excitation of another mode and vice versa. To modulate the excitation of the primary system the bath spins have to be almost degenerate and their frequencies on-resonance with the system frequency. Due to the quasi-degeneracy of the bath frequencies the number of bath excitations is not changed  $[\hat{H}_{SB}^d, \hat{H}_B] = 0$ . Dephasing can occur only if the bath is initially *activated* i.e., initially excited. Note also that each of the parts  $\hat{H}_S$ ,  $\hat{H}_B$ , and  $\hat{H}_{SB}^d$  commute with the total Hamiltonian  $\hat{H}$ , therefore the system, bath and interaction energies remain constant during the process. To model pure dephasing processes in this system let us consider the model:

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 + \sum_k^K \epsilon_k \hat{\sigma}_k^\dagger \hat{\sigma}_k + \left( \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 \right) \otimes \sum_{j < k}^K c_{jk} (\hat{\sigma}_j^\dagger \hat{\sigma}_k + \hat{\sigma}_k^\dagger \hat{\sigma}_j), \quad (15)$$

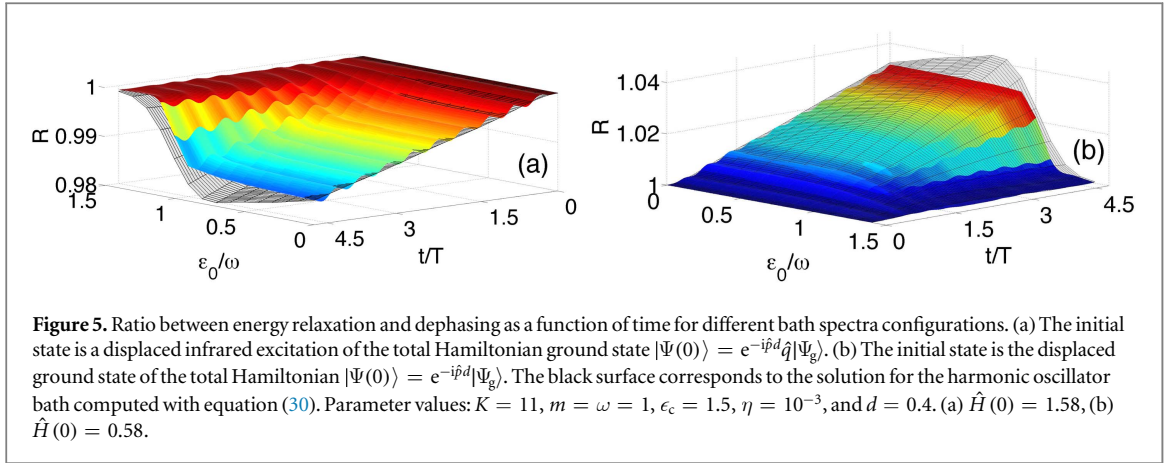
where the energy spectrum of the bath modes is in the interval  $\epsilon_k \in [\omega - \Delta\omega, \omega + \Delta\omega]$  ( $\Delta\omega \ll \omega$ ) to be on-resonance with the harmonic oscillator. The initial state  $|\Psi(0)\rangle$  was chosen such that the system is in its ground state and the bath is randomly excited. This state  $|\Psi(0)\rangle$  was displaced 0.4 a.u. and evolved in time. The state  $|\Psi(t)\rangle$  rotates around  $\langle \hat{q}(t) \rangle = \langle \Psi(t) | \hat{q} | \Psi(t) \rangle = 0$ ,  $\langle \hat{p}(t) \rangle = 0$  point in the phase space. Due to pure dephasing the wave packet also spreads during the revolution thus the wave packet does not complete a closed circle but a spiral one, see figure 2(a). Consequently the uncertainty of  $\Delta \hat{q}(t)$  and  $\Delta \hat{p}(t)$  increase in time destroying the coherence of the primary system. Figures 2(b) and (c) show how the initial state, displaced ground state of the harmonic oscillator  $\Delta \hat{q}(0) \approx \sqrt{1/(2m\omega)}$ , spatially spreads due to pure dephasing. The oscillation period of  $\Delta \hat{q}$  and  $C_l(\hat{\rho}_S)$  corresponds to the revolution of the wave packet in phase space, for example the maximums of the coherence function are  $\langle \hat{q}(t) \rangle = 0$  in figure 2(a) whereas the minimums  $\langle \hat{p}(t) \rangle = 0$ . As we stated before, the commutativity  $[\hat{H}_{SB}^d, \hat{H}_S] = [\hat{H}_{SB}^d, \hat{H}_B] = 0$  assures that pure dephasing does not change the energy of the system and bath, see figure 2(d). This fact does not mean that the state  $|\Psi(t)\rangle$  is an eigenvector of  $\hat{H}_S$ , for example if we compute the Lagrangian mean value  $\langle \hat{L}(t) \rangle$  it is not constant indicating that the wave packet is not stationary.

### 3.2. Spin swap dephasing

To study a second mechanism to produce pure dephasing, we consider the standard model used to analyze dissipative dynamics of the harmonic oscillator linearly coupled to a spin bath, the Hamiltonian is

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 + \sum_k^K \epsilon_k \hat{\sigma}_k^\dagger \hat{\sigma}_k + \hat{q} \otimes \sum_k^K d_k (\hat{\sigma}_k^\dagger + \hat{\sigma}_k), \quad (16)$$

where the bath has an energy spectrum  $\epsilon_k \in [0, 3\omega]$ . For an initial state  $|\Psi(0)\rangle = \hat{q}|\Psi_g\rangle$ , corresponding to an infrared excitation of the total ground state, it is well known that the energy system  $\langle \hat{H}_S(t) \rangle$  decays exponentially with a rate  $2\pi\eta\omega$  predicted analytically for weak coupling  $\eta$  [56], see figure 3. The coherence  $C_l(\hat{\rho}_S)$  and the spatial standard deviation  $\Delta \hat{q}(t)$  also show an exponential decay when the system decays from the excited  $\Delta \hat{q}(0) \approx \sqrt{3/(2m\omega)}$  to the ground state  $\Delta \hat{q} \approx \sqrt{1/(2m\omega)}$  of the harmonic oscillator.



This model can exhibit pure dephasing if the bath experiences spin swaps with a rate  $t_f$  faster than the Zeno time  $t_z$  of the system. The evolution of the initial state  $|\Psi(0)\rangle$  under (16) is governed by the evolution operator  $\hat{U}(t) = \exp(-i\hat{H}t)$ . The ‘survival probability’ at time  $t$  is  $P(t) = |\langle\Psi(0)|\Psi(t)\rangle|^2 = |\langle\Psi(0)|\hat{U}(t)|\Psi(0)\rangle|^2 = 1 - t^2/t_z^2$  with

$$t_z = 1/\Delta\hat{H} = (\langle\Psi(0)|\hat{H}^2|\Psi(0)\rangle - \langle\Psi(0)|\hat{H}|\Psi(0)\rangle^2)^{-1/2}. \quad (17)$$

The quantum Zeno effect [55] is the suppression of unitary time evolution by quantum decoherence produced not only by continuous measurements of the evolving state  $|\Psi(t)\rangle$  but also by interactions of the primary system with the bath, stochastic fields, etc. If we look at the effect from the frame that moves in such a way the unitary evolution is cancelled, the system, otherwise stationary, is guided by the decoherence processes. In our model, the initial infrared excitation of (16) is frozen due to the system–bath interactions performing spin swaps in the bath. The swaps suppress the exponential decay of the system keeping the system energy constant as in the pure dephasing process. The frozen state is not simply a stationary state of equation (16) as we infer from figure 4. Its spatial standard deviation spreads in time increasing the amplitude of the oscillations around  $\Delta\hat{q} \approx \sqrt{3}/(2m\omega)$ , corresponding to the excited state, showing a similar behavior as in the case of standard pure dephasing, figure 2(b). For this mechanism, initial activation of the bath is no necessary and pure dephasing can still produced when the temperature is reduced.

### 3.3. Off-resonance dephasing

As pointed out in the introduction a possible mechanism for pure dephasing is the separation of time scales between system and bath produced by an energy gap. In this section we analyze if the dipolar coupling (12) can produce pure dephasing through this mechanism in the weak coupling regime and the effect of a finite bath frequency spectrum in the energy relaxation and dephasing processes. To this end we employ again the same Hamiltonian as in the previous sections

$$\hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2}m\omega^2\hat{q}^2 + \sum_k^K \epsilon_k \hat{\sigma}_k^\dagger \hat{\sigma}_k + \hat{q} \otimes \sum_k^K d_k (\hat{\sigma}_k^\dagger + \hat{\sigma}_k), \quad (18)$$

where now different energy spectra of the bath modes  $\epsilon_k \in [\epsilon_0, \epsilon_c]$  are considered. We kept constant the cutoff frequency  $\epsilon_c = 1.5\omega$  and  $\epsilon_0$  takes values from 0 to  $1.4\omega$ . In contrast with the QME and the Lindblad formalisms that assume an infinite bath spectra and consequently there is always a bath frequency on resonance with the system, we can now study off-resonance processes and the finite effect of a bath spectrum. It is well known that in energy relaxation processes also dephasing occurs, however the inverse statement is not always true as we saw in sections 3.1 and 3.2, where in the pure dephasing processes system and bath do not exchange energy. To analyze the effect of the bath finite spectrum in the energy relaxation and dephasing processes we define the ratio

$$R(t) = \frac{\langle\hat{a}(0)\rangle \langle\hat{H}_S(t)\rangle}{\langle\hat{H}_S(0)\rangle \langle\hat{a}(t)\rangle}, \quad (19)$$

for  $R(t) < 1$  processes the energy exchange rate is faster than dephasing and vice versa. The results are presented in figure 5. To gain analytical insight and understand this figure let us modify our initial model constituted by a harmonic oscillator coupled to a spin bath and cast the environment by a bath constituted by harmonic oscillators instead. This is motivated by the equivalence between these two baths in the weak coupling regime [19]. First we define  $\epsilon_k := \omega_k$ ,  $\chi_k := d_k/\sqrt{2m\omega}$ ,  $\hat{a} = \sqrt{m\omega/2}[\hat{q} + i\hat{p}/(m\omega)]$ ,  $\hat{a}^\dagger = \sqrt{m\omega/2}[\hat{q} - i\hat{p}/(m\omega)]$ ,  $\hat{\sigma}_k^\dagger := \hat{b}_k^\dagger$ , and  $\hat{\sigma}_k := \hat{b}_k$ , where  $\hat{a}$ ,  $\hat{a}^\dagger$ ,  $\hat{b}_j$ ,  $\hat{b}_j^\dagger$ , are the boson annihilation and creation operators of the oscillator



and the  $j$ th bath mode. Replacing into equation (18) after assuming the rotating wave approximation ( $\hat{a}^\dagger \hat{\sigma}_k^\dagger + \hat{a} \hat{\sigma}_k \ll \hat{a}^\dagger \hat{\sigma}_k + \hat{a} \hat{\sigma}_k^\dagger$ ) we get

$$\hat{H} = \omega \left( \hat{a}^\dagger \hat{a} + \frac{1}{2} \right) + \sum_{k=1}^K \omega_k \hat{b}_k^\dagger \hat{b}_k + \sum_{k=1}^K \chi_k (\hat{b}_k \hat{a}^\dagger + \hat{b}_k^\dagger \hat{a}). \quad (20)$$

The advantage of this new Hamiltonian is that it can be completely solved analytically [57]. For convenience, we shift the zero energy point to cancel the  $\omega/2$  term and define  $\hat{c}_0 = \hat{a}$  and  $\hat{c}_k = \hat{b}_k$  to rewrite

$$\hat{H} = \mathbb{C}^\dagger \mathbb{H} \mathbb{C}, \quad (21)$$

where

$$\mathbb{H} = \begin{pmatrix} \omega & \chi_1 & \chi_2 & \cdots & \chi_K \\ \chi_1 & \omega_1 & 0 & \cdots & 0 \\ \chi_2 & 0 & \omega_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \chi_K & 0 & 0 & \cdots & \omega_K \end{pmatrix}, \quad \mathbb{C} = \begin{pmatrix} \hat{c}_0 \\ \hat{c}_1 \\ \vdots \\ \hat{c}_K \end{pmatrix}. \quad (22)$$

Let us assume that  $\mathbb{A}$  is the unitary transformation that diagonalizes  $\mathbb{H}$

$$\lambda = \mathbb{A}^\dagger \mathbb{H} \mathbb{A} = \begin{pmatrix} \lambda_0 & 0 & \cdots & 0 \\ 0 & \lambda_1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_K \end{pmatrix}. \quad (23)$$

The column vector  $\mathbb{C}$  transforms as  $\mathbb{B} = \mathbb{A}^\dagger \mathbb{C}$  and then the Hamiltonian equation (21) reads,  $\hat{H} = \mathbb{B}^\dagger \lambda \mathbb{B}$ . In this representation, the Heisenberg equations of motion for the  $\mathbb{B}$  operators are

$$i \frac{d\mathbb{B}}{dt} = [\mathbb{B}, \hat{H}] = \lambda \mathbb{B}, \quad (24)$$

whose solution is

$$\mathbb{B}(t) = e^{-i\lambda t} \mathbb{B}(0), \quad (25)$$

where the exponential of the diagonal matrix  $\lambda$  is defined by its series expansion. Inverting the transformation  $\mathbb{A}$  we find the evolution of the original operators

$$\mathbb{C}(t) = \mathbb{U}(t) \mathbb{C}(0), \quad (26)$$

where the evolution operator of our system is given by  $\mathbb{U}(t) = \mathbb{A} e^{-i\lambda t} \mathbb{A}^\dagger$ . In particular for the boson annihilation operator of the system we have

$$\hat{a}(t) = U_{00}(t) \hat{a}(0) + \hat{G}(t), \quad (27)$$

where

$$\hat{G}(t) = \sum_{j=1}^K U_{0j}(t) \hat{b}_j(0) \quad (28)$$

is a function expressed only in terms of the initial state of the bath. Taking the complex conjugate of expressions (27) and (28) we get a similar expression for the creation operator of the system. The system energy  $\hat{H}_S(t) = [\hat{a}^\dagger(t) \hat{a}(t) + 1/2] \omega$  can be expressed as

$$\hat{H}_S(t) = |U_{00}(t)|^2 \left( \hat{H}_S(0) - \frac{\omega}{2} \right) + \omega \left[ U_{00}^*(t) \hat{G}(t) \hat{a}^\dagger(0) + U_{00}(t) \hat{G}^\dagger(t) \hat{a}(0) + \frac{1}{2} \right]. \quad (29)$$

Once we have equations (27) and (29) an exact analytical expression for  $R(t)$  can be obtained, however due to the different essence of the spin and harmonic baths this exact expression does not reproduce exactly the oscillations of figure 5. However, we can get an expression that fits accurately the envelope of the figure setting  $\hat{G}(t) = \hat{G}(t)^\dagger = 0$

$$R(t) = |U_{00}(t)| - \frac{\omega}{2\hat{H}_S(0)} \left( |U_{00}(t)| - \frac{1}{|U_{00}(t)|} \right), \quad (30)$$

where the initial condition  $\hat{H}_S(0)$  is deduced from the spin bath model. For an explicit expression of  $|U_{00}(t)|$  in terms of the eigenvalues and eigenvectors see appendix. It is a positive function that at  $t = 0$  takes the maximum value  $|U_{00}(0)| = 1$  as a function of time. Figure 5 shows two different behaviors of  $R(t)$ . For initial system states with an energy  $\hat{H}_S(0) \gg \omega$  figure 5(a) shows  $R(t) < 1$ , energy relaxation rate is faster than the dephasing rate (decreasing slope of the figure as a function of  $t$ ). We observe that for  $\epsilon_0 < \omega$  the ratio is almost independent of  $\omega_0$ . In the weak coupling regime this region can be approximated by  $R(t) \approx 1 - \eta t/2$  [33], dissipation happens

twice faster than dephasing. In contrast, figure 5(b) shows for an initial system state with  $\hat{H}_S(0) \ll \omega$  that the dephasing rate is faster than the energy relaxation  $R(t) > 1$ . Also the ratio is independent of  $\omega_0$  for frequencies  $\epsilon_0 < \omega$ . In both cases, when all spin frequencies are off-resonance with respect to the harmonic oscillator  $\epsilon_0 > \omega$ , system and bath decouple freezing the dephasing  $\hat{a}(t) = \hat{a}(0)$  and the energy exchange  $\hat{H}_S(t) = \hat{H}_S(0)$ , consequently  $R(t) = 1$ .

We have numerical evidence that the dipole interaction given by equation (12) can not produce pure dephasing due to the separation of time scales between system and bath. Given the similarity between the spin and the oscillator baths in the weak coupling regime [19], it is also possible to theoretically demonstrate the inability of the interaction equation (12) to produce pure dephasing. A necessary condition for pure dephasing is that  $\langle \hat{H}_S(t) \rangle$  is constant. Neglecting  $\hat{G}(t)$  and  $\hat{G}^\dagger(t)$  in equation (29) we see that  $\langle \hat{H}_S(t) \rangle$  is proportional to  $|U_{00}(t)|^2$ . From equation (A.6) we find

$$|U_{00}(t)|^2 = \sum_{j=0}^K |y_0^{(j)}|^4 + \sum_{j=0}^{K-1} \sum_{i>j}^K 2 \cos[t(\lambda_j - \lambda_i)] |y_0^{(j)}|^2 |y_0^{(i)}|^2 \quad (31)$$

which remains constant if  $\lambda_i = \lambda_j \forall i$ . From equation (A.1) it occurs if  $\omega = \omega_i \forall i$ , all bath frequencies must be on-resonance with the system frequency. On the other hand, if all bath frequencies are equal, the coupling constants of the original system are  $d_i = \sqrt{J(\epsilon_i)/\rho(\epsilon_i)} \approx 0$  because  $\rho(\epsilon_i)^{-1} \approx (\epsilon_{i+1} - \epsilon_i) \approx 0$ . System and bath decouple due to the suppression of the interaction and no dephasing is produced.

#### 4. Dephasing in the NV center

Once we presented different dephasing processes in a generic harmonic oscillator coupled to a spin bath, let us now consider a more realistic system. We consider a single NV center in diamond surrounded by an environment of *P1* nitrogen centers where the system, bath, and interaction Hamiltonians are well studied, their parameters can be manipulated experimentally and dephasing can be controlled or even suppressed with dynamical decoupling techniques [58–60]. The primary system is the NV center immersed in a bath caused by the electron spins of the surrounding nitrogen atoms. The NV center is considered as a spin ( $S_0 = 1$ ) placed in a static magnetic field  $B$  along the  $z$ -axis. Its Hamiltonian is [3]

$$\hat{H}_S = D(\hat{S}_0^z)^2 + g_0 \mu_B B \hat{S}_0^z + A_0 \hat{S}_0^z \hat{I}_0^z + A_1 (\hat{S}_0^x \hat{I}_0^x + \hat{S}_0^y \hat{I}_0^y) - P_0 (\hat{I}_0^z)^2, \quad (32)$$

where  $D = 2.87$  GHz is the splitting between the levels  $|m_S = 0\rangle$  and  $|m_S = \pm 1\rangle$  at  $B = 0$ ,  $g_0 = 2$  is the Landé factor of the NV center,  $\mu_B$  is the Bohr's magneton,  $A_0 = 2.3$  MHz,  $A_1 = 2.1$  MHz, and  $P_0 = -5.1$  MHz. The first term of  $\hat{H}_S$  represents the single-axis anisotropy, the second represents the Zeeman term due to the interaction of the spin with the static magnetic field  $B$ , whereas the remaining terms take into account the hyperfine coupling at the NV site, they represent the coupling between the electron spin  $\hat{S}_0 = (\hat{S}_0^x, \hat{S}_0^y, \hat{S}_0^z)$  and the nuclear spin  $^{14}\text{N}$  ( $I_0 = 1$ ) of the NV center denoted by  $\hat{I}_0 = (\hat{I}_0^x, \hat{I}_0^y, \hat{I}_0^z)$ .

The bath is constituted by nitrogen atoms, *P1* centers, each surrounded by four carbons. The nitrogen atom shares an unpaired electron ( $S_k = 1/2$ ) with one of the neighboring carbons, consequently there are four different types of *P1* centers depending on the electron delocalization axis. The electron spin of each nitrogen interacts with the nuclear spin ( $I_k = 1$ ), with the external applied magnetic field, and with the remainder of the nitrogen atoms through dipole–dipole interactions [3]

$$\hat{H}_B = \sum_k^K \hat{H}_k^{\text{hf}} + \sum_{j<k} \hat{H}_{jk}^{\text{dip}}, \quad (33)$$

where  $K$  is the total number of spins in the bath. The hyperfine Hamiltonian for a single *P1* center is given by [3]

$$\hat{H}_k^{\text{hf}} = g_0 \mu_B B \hat{S}_k^z + A_Z \hat{S}_k^z \hat{I}_k^z + A_X (\hat{S}_k^x \hat{I}_k^x + \hat{S}_k^y \hat{I}_k^y) - P (\hat{I}_k^z)^2, \quad (34)$$

with  $g = 2$  the Landé factor of the nitrogens,  $A_Z = 114$  MHz,  $A_X = 81.3$  MHz,  $P = -4$  MHz,  $\hat{S}_k = (\hat{S}_k^x, \hat{S}_k^y, \hat{S}_k^z) = (\hat{\sigma}_k^x, \hat{\sigma}_k^y, \hat{\sigma}_k^z)/2$ , and  $\hat{I}_k = (\hat{I}_k^x, \hat{I}_k^y, \hat{I}_k^z)$  corresponds to the nuclear spin. We have added the Zeeman term because of the interaction of the  $\hat{S}_k$  spin with the external magnetic field  $B$ . Different *P1* centers interact with each other by dipole–dipole interactions

$$\hat{H}_{jk}^{\text{dip}} = \frac{\mu_0 \mu_B^2 g^2}{4\pi} \sum_{j<k}^K \frac{1}{r_{jk}^3} [\hat{S}_j \hat{S}_k - 3(\hat{S}_j \mathbf{n}_{jk})(\hat{S}_k \mathbf{n}_{jk})], \quad (35)$$

where  $\mu_0$  is the vacuum permeability and  $\mathbf{r}_{jk} = (r_{jk}^x, r_{jk}^y, r_{jk}^z)$  is the relative position between spins  $j$  and  $k$  ( $r_{jk} = |\mathbf{r}_{jk}|$  and  $\mathbf{n}_{jk} = \mathbf{r}_{jk}/r_{jk}$ ).

Finally the system–bath coupling is due to dipole–dipole interactions. Assuming that the NV center is placed at the origin [3]

$$\hat{H}_{\text{SB}} = \frac{\mu_0 \mu_{\text{B}}^2 g_0 g}{4\pi} \sum_k \frac{1}{r_k^3} [\hat{S}_0 \hat{S}_k - 3(\hat{S}_0 \mathbf{n}_k)(\hat{S}_k \mathbf{n}_k)], \quad (36)$$

where  $\mathbf{r}_k = (r_k^x, r_k^y, r_k^z)$  is the relative position of spin  $k$  with respect to the NV center ( $r_k = |\mathbf{r}_k|$  and  $\mathbf{n}_k = \mathbf{r}_k/r_k$ ).

The total Hamiltonian  $\hat{H} = \hat{H}_{\text{S}} + \hat{H}_{\text{B}} + \hat{H}_{\text{SB}}$  contains two different time scales, the anisotropy that produces the splitting between the  $|m_{\text{S}} = 0\rangle$  and  $|m_{\text{S}} = \pm 1\rangle$  levels set fast dynamics in the ns regime whereas, typically, the hyperfine and the dipole interaction strengths between electron spins  $\gamma_{jk} = \mu_0 \mu_{\text{B}}^2 g^2 / (4\pi r_{jk}^3)$  and  $\gamma_k = \mu_0 \mu_{\text{B}}^2 g g_0 / (4\pi r_k^3)$  are the order of MHz [3] which set a slower dynamics in the  $\mu\text{s}$  regime.

#### 4.1. Standard pure dephasing

Let us analyze the conditions where the total Hamiltonian  $\hat{H} = \hat{H}_{\text{S}} + \hat{H}_{\text{B}} + \hat{H}_{\text{SB}}$  given by equations (32), (35), and (36) produce standard pure dephasing. For a complete justification of the approximations made below in the strong magnetic field regime see [3], we summarize part of them. A strong magnetic field  $B$  can be applied splitting the degenerate  $|m_{\text{S}} = \pm 1\rangle$  levels. As a result, the central NV spin can be formally treated as a pseudo-spin  $\mathcal{S}_0 = 1/2$  connecting the  $|m_{\text{S}} = 0\rangle$  and  $|m_{\text{S}} = -1\rangle$  states. Projecting the Hamiltonian equation (32) onto the subspace spanned by  $|m_{\text{S}} = 0\rangle$  and  $|m_{\text{S}} = -1\rangle$  and excluding the non-secular terms the system Hamiltonian takes the form [3]

$$\hat{H}_{\text{S}} = A_0 \hat{\mathcal{S}}_0^z \hat{I}_0^z. \quad (37)$$

For the large magnetic field  $g\mu_{\text{B}}B \gg \gamma_k$  neither of the spins  $\hat{\mathcal{S}}_0$  or  $\hat{S}_k$  can be flipped due to dipole interactions because of the very large mismatch in energies between different states of  $\hat{\mathcal{S}}_0$  and  $\hat{S}_k$ . Applying the rotating wave approximation to equation (36) it simplifies to [3]

$$\hat{H}_{\text{SB}} = \sum_k \gamma_k [1 - 3(r_k^z)^2] (\hat{\mathcal{S}}_0^z - 1/2) \hat{S}_k^z. \quad (38)$$

If the strong magnetic field satisfies  $g\mu_{\text{B}}B \gg \gamma_{jk}$  as well, the bath Hamiltonian also simplifies. The single-spin flips are prohibited, they do not conserve energy. Even two-spin flip-flop processes are strongly suppressed [3]. As a result, at large magnetic fields spins are oriented along  $B$  and only a few spins can change their orientation. In addition, out of the strong magnetic field regime the spin flip-flops can be suppressed by tuning the value of spin anisotropy with radio frequency fields [61]. Applying the rotating wave to equation (35) and considering the hyperfine Hamiltonian equation (34) in the strong magnetic field regime the bath Hamiltonian reads [3]

$$\hat{H}_{\text{B}} = g\mu_{\text{B}}B \sum_k \hat{S}_k^z + A_1 \sum_k \hat{S}_k^z \hat{I}_k^z + \sum_{j<k} \gamma_{jk} [1 - 3(r_{jk}^z)^2] \hat{S}_j^z \hat{S}_k^z, \quad (39)$$

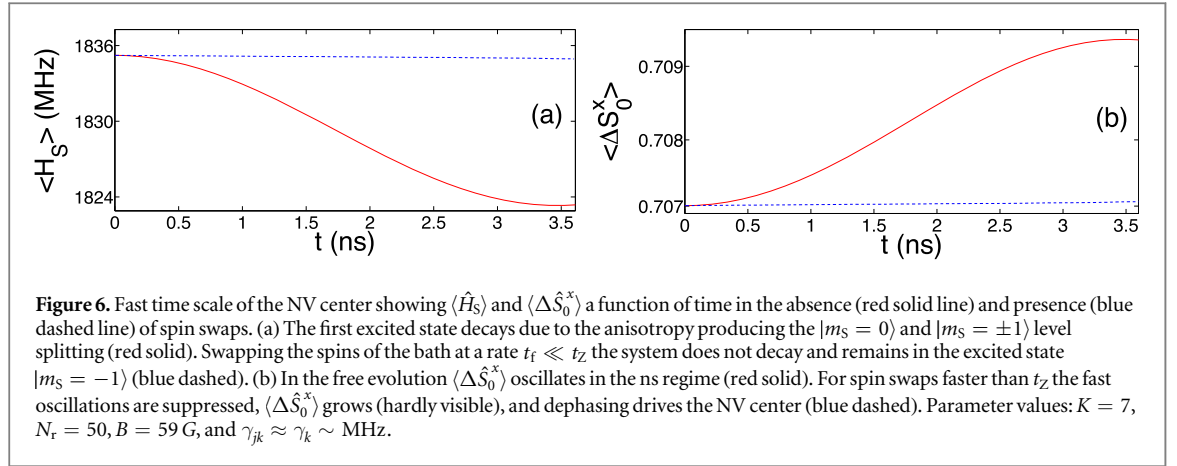
where  $A_1 = 114$  MHz or  $A_1 = 86$  MHz depending on the spin delocalization axis of the nitrogen atom.

Note that in the strong magnetic field regime  $[\hat{H}_{\text{SB}}, \hat{H}_{\text{S}}] = 0$ , thus no dissipation of the NV center takes place. Moreover as the total Hamiltonian  $\hat{H} = \hat{H}_{\text{S}} + \hat{H}_{\text{B}} + \hat{H}_{\text{SB}}$  commutes with the pseudo-spin operator  $[\hat{H}, \hat{\mathcal{S}}_0^z] = 0$  the populations of the  $|m_{\text{S}} = 0\rangle$  and  $|m_{\text{S}} = -1\rangle$  states do not evolve in time. The NV center loses its coherence due to pure dephasing mechanism without exchanging energy with the bath. Finally, note that  $[\hat{H}_{\text{SB}}, \hat{H}_{\text{B}}] = 0$  thus the interaction does not change the bath excitations and the NV center experiences dephasing if initially the bath is activated.

#### 4.2. Spin swap dephasing

To simulate the NV center dynamics we assume that the total Hamiltonian of the whole system is the sum of equations (32), (35) and (36), having  $\mathcal{H}$  a dimension  $2^K \times 2 \times 3^K \times 3$ , where the nitrogen atoms that represent the bath are randomly distributed. To solve the dynamics of this system the propagator associated with the full Hamiltonian has been expanded using Chebyshev polynomials [3, 62]. The initial state  $|\Psi(0)\rangle$  is prepared in such a way that the system, equation (32), is in the first excited state  $|m_{\text{S}} = -1\rangle$  and the bath is initially completely de-excited (in the bit representation only the first spinor component is non-zero). As in the case of the harmonic oscillator, we compute the dynamics of  $|\Psi(0)\rangle$  under the evolution of the total Hamiltonian in the presence of spin swaps faster than  $t_{\text{Z}}$  and in their absence, the results are plotted in figure 6. When no spin swaps are produced, system and bath exchange energy on a time scale of ns produced by the single-axis anisotropy as we infer from figure 6(a). The dipole–dipole interaction between system and bath makes the NV decay from the  $|m_{\text{S}} = -1\rangle$  excited state at a  $\mu\text{s}$  scale. Analyzing the decoherence through the standard deviation of the NV spin in the  $x$ -direction, we observe a similar result, red solid lines in figure 6(b).  $\langle \Delta \hat{S}_0^x \rangle$  shows fast oscillations with a period of ns eventually growing for a  $\mu\text{s}$  time evolution.

When spin swaps are performed in the bath with a rate faster than the Zeno time the situation changes drastically, dashed blue lines of figure 6. Looking at  $\langle \hat{H}_{\text{S}} \rangle$  we observe in figure 6(a) that the NV center does not



exchange energy with the bath remaining in the  $|m_S = -1\rangle$  state. The system remains excited but not stationary,  $\langle \Delta \hat{S}_0^x \rangle$  is not constant and evolve very slowly in time, figures 6(b). The unitary evolution is suppressed by the Zeno effect and dephasing guides the system. Note that for this mechanism no initial activation of the bath was necessary.

## 5. Discussion

We have analyzed decoherence processes in open quantum systems produced by the interaction between a primary system and the surrounding environment. In an initial generic model constituted by an harmonic oscillator coupled to a TLS bath we have presented a new pure dephasing mechanism which does not require initial activation of the bath and consequently is temperature independent. Spin swap dephasing can be present even at low temperatures. In contrast, standard dephasing occurs when initially the bath is excited. Reducing the temperature, the initial number of excited bath modes, this mechanism can be frozen out.

For weak coupling we show that the dipole interaction can not produce pure dephasing due to the separation of time scales between the system and the bath. However, dephasing can occur but it is accompanied by energy dissipation. The ratio between dissipation and dephasing depends on the initial state energy.

Activated and non-activated dephasing processes have been exemplified in a NV center where the primary system, interaction, and bath can be accurately modified applying a magnetic field and controlling the density of impurities.

We have presented here a new dephasing mechanism with the purpose of clarifying the relation between dephasing and the initial bath configuration. Nevertheless there are interesting other questions. For example, the study of the conditions for dephasing with higher order spin–spin interactions and nonlinear system–bath couplings.

## Acknowledgments

We thank D Gelman, A Levy, and C P Koch for fruitful discussions. We acknowledge funding by the Israel Science Foundation, the Basque Government (Grant No. IT472-10), Ministerio de Economía y Competitividad (FIS2015-67161-P), the program UFI 11/55 of UPV/EHU, and COST Action MP1209 ‘Thermodynamics in the quantum regime’. ET is supported by the Basque Government postdoctoral program.

## Appendix. Explicit expression for the evolution operator

It is possible to write the components of the evolution operator  $\mathbb{U}(t) = \mathbb{A}e^{-i\lambda t}\mathbb{A}^\dagger$  in terms of the eigenvalues and eigenvectors of the Hamiltonian equation (20). The characteristic equation  $\det(\mathbb{H} - \lambda\mathbb{I}) = 0$  can be rewritten as [57]

$$\omega - \lambda = \sum_{i=1}^K |\chi_i|^2 / (\omega_i - \lambda) \quad (\text{A.1})$$

which is the transcendental equation that defines the eigenvalues of (20). The eigenvectors are defined by

$$\mathbb{H}y^{(i)} = \lambda_i y^{(i)} \quad (i = 0, 1, \dots, K), \quad (\text{A.2})$$

with the aid of equation (21) the  $j$ th components of the  $i$ th eigenvector can be expressed in terms of the  $y_0^{(i)}$  component

$$y_j^{(i)} = -\frac{\chi_j y_0^{(i)}}{\omega_j - \lambda_i} \quad (i = 0, 1, \dots, K) \quad (j = 1, 2, \dots, K). \quad (\text{A.3})$$

Using the orthonormalization condition for the eigenvectors  $\sum_i |y^{(i)}|^2 = 1$  we find

$$|y_0^{(i)}|^2 = \left( 1 + \sum_{j=1}^K \frac{|\chi_j|^2}{(\omega_j - \lambda_i)^2} \right)^{-1} \quad (\text{A.4})$$

and finally the transformation  $\mathbb{A}$  that diagonalizes the Hamiltonian is explicitly written as

$$\mathbb{A} = (y^{(0)}, y^{(1)}, \dots, y^{(K)}) = \begin{pmatrix} y_0^{(0)} & y_0^{(1)} & \dots & y_0^{(K)} \\ \frac{y_0^{(0)} \chi_1}{\lambda_0 - \omega_1} & \frac{y_0^{(1)} \chi_1}{\lambda_1 - \omega_1} & \dots & \frac{y_0^{(K)} \chi_1}{\lambda_K - \omega_1} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{y_0^{(0)} \chi_K}{\lambda_0 - \omega_K} & \frac{y_0^{(1)} \chi_K}{\lambda_1 - \omega_K} & \dots & \frac{y_0^{(K)} \chi_K}{\lambda_K - \omega_K} \end{pmatrix}. \quad (\text{A.5})$$

The different components of the matrix corresponding to the evolution operator  $\mathbb{U}(t) = \mathbb{A}e^{-i\lambda t}\mathbb{A}^\dagger$  are

$$\begin{aligned} U_{00}(t) &= \sum_{j=0}^K |y_0^{(j)}|^2 e^{-i\lambda_j t} \\ U_{0k}(t) &= U_{k0}(t) = \sum_{j=0}^K |y_0^{(j)}|^2 \frac{\chi_k}{\lambda_j - \omega_k} e^{-i\lambda_j t} \quad (k \neq 0) \\ U_{jk}(t) &= \sum_{l=0}^K |y_0^{(l)}|^2 \frac{\chi_j \chi_k}{(\lambda_l - \omega_j)(\lambda_l - \omega_k)} e^{-i\lambda_l t} \quad (j, k \neq 0). \end{aligned} \quad (\text{A.6})$$

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