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Can decoherence of a quantum system be suppressed by application of a strong electromagnetic field ?

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Abstract

The object of study here is a dissipative dynamics of a two-level system (TLS) coupled linearly to a set of harmonic oscillators (bath) and driven by a strong external electromagnetic field. This dynamics is represented by a multi-dimensional wave packet with up to 14 spatial degrees of freedom. The propagation is implementated within the multi-configuration time-dependent Hartree method (MCTDH). We investigate opportunities for suppression of dephasing in a damped TLS by means a strong external field.

Contents

1 Introduction

Many physical phenomena can be described by a model system consisting of only one or few variables in contact with an environment with many or even infinit number of degrees of freedom. The interaction between such open quantum system and the environment brings dissipation into the system. One of the most challenging tasks of quantum mechanics is to understand how to suppress dissipation in these open systems. The external control can be provided by application of a strong periodic laser field. The dynamics of the system can be changed from coherent to incoherent, and even decoherence can be completely suppressed. Moreover, this problem arises in many areas of physics as well as in chemistry, aimed at understanding the detailed dynamics of quantum systems that are exposed to a strong external field.

Currently, much attention is focused on the creation of quantum computers, i.e. devices for computation that make direct use of quantum mechanical phenomena. The controlling quantum decoherence represents a challenge for practical realization of quantum computers, since they are expected to rely heavily on the undisturbed evolution of quantum coherences. Simply speaking, they require that coherent states are preserved, in order to actually perform quantum computation.

For the description of a variety of phenomena the model of a two-level system (TLS) is widely used, i.e. of quantum system whose Hilbert space can be effectively restricted to a two-dimensional space. There are many examples such as electron transfer reactions, proton tunneling, macroscopic quantum coherence in Josephson solid-state devices. Such types of system are frequently in contact with an environment. Usually, the environment is modeled as a bath which consists of a large set of harmonic oscillators. In most applications the bath is linearly coupled to the TLS.

Without laser-field driving, such dissipative dynamics of a TLS coupled to a bath has been investigated since the late 1950s. In particular, Magilanskij pioneered the so-termed 'quantum Langevin equation' by starting from the full system-plus-bath Hamiltonian. On the other hand, *the driven isolated* TLS has also a long history, the first work must be attributed to Rabi for the linearly polarized field in so-called rotating-wave approximation (RWA). Physical phenomena occurring in the driven TLS coupled to the environment have been the object of strong interest until now [Wei08].

2 MCTDH

A quantum mechanical study can be done in the time-dependent picture by propagation of a wavepacket. The multiconfiguration time-dependent Hartree method (MCTDH) is an efficient algorithm for the solution of the time-dependent Schrodinger equation and for discription of multi-dimensional quantum dynamics. The MCTDH program has been created to perform quantum wavepacket propagations using this method. For a calculation the Hamiltonian operator and the input parameters must be defined. The variety of programs included in the MCTDH package serve to analyse the results of a calculation and compute observable quantities, which can be directly plotted with the help of external program.

As the program name indicates, a wave function with usually many degrees of freedom is written as a sum of a Hartree product basis set

$$\Psi(Q_1, ..., Q_a, t) = \sum_J A_J(t)\Phi_J(t) \quad , \quad J = (j_1, ..., j_a) \tag{1}$$

$$\Phi_J(t) = \prod_{k=1}^{a} \phi_{j_k}^{k}(Q_k, t) \tag{2}$$

where a is the number of degrees of freedom, $Q_1, ..., Q_a$ are the coordinates, the A_J denote the time-dependent expansion coefficients and the single particle functions ϕ_{j_k} form the time-dependent basis functions for degree of freedom k. They in turn are defined on a time-independent primitive grid. In general, a discrete variable representation (DVR) is used as primitive basis to present these single-particle functions. For large system, or even certain degrees of freedom are strongly coupled, it may be advantageous to combine degrees of freedom together and use multi-mode single-particle functions, due to it the number of the expansion coefficients A_J is significantly reduced that we made in our calculations.

Also for a quantum dynamical calculation, an initial wavefunction $\Psi(0)$ is required. Usually, $\Psi(0)$ is a simple Hartree product, i.e. a product of one-dimensional functions. Our choice for the one-dimensional initial functions are Gaussian functions corresponding to the ground states of the uncoupled system.

The set of analyzing programs of MCTDH can be used to obtain information from a calculation. For our investigations they allow to observe the evolution of the TLS and the bath. One of the analysis programs had to be modified to provide information about decoherence of our system.

3 The Hamiltonian

Because of the discreteness of the system, the dissipative dynamics of a TLS exposed to a strong field can be written in terms of 2×2 - Pauli matrices. In the presence of interaction with a bath and influence of the field, the Hamiltonian is

$$H(t) = \frac{1}{2}\varepsilon\sigma_z + \sum_a \frac{w_a}{2}(-\frac{\partial^2}{\partial Q_a^2} + Q_a^2)I + \sum_a \lambda_a Q_a \sigma_x + E(t)\sigma_x \qquad (3)$$

The first term $H_{TLS} = \frac{1}{2}\varepsilon\sigma_z$ describes the dynamics of the isolated TLS , where $\varepsilon = w_1 - w_2$ is the energy gap between two levels of this system. Here we restrict ourselves to a two-dimensional system but it is possible to generalize the formalism to higher-dimensional cases.

The second and third terms describe the environment as a set of harmonic oscillators linearly coupled in bath coordinates $Q_a = \sqrt{m_a w_a} x_a$ to the system via the interaction term $H_{int} = \sum_a \lambda_a Q_a \sigma_x$. Here w_a is the frequency of each harmonic oscillator of the bath and λ_a is the corresponding coupling parameter. Without the last term $H_{field} = E(t)\sigma_x$, the dissipative TLS is known as spin-boson model.

Finally, the last term describes the field and its coupling to the quantum system. In case of a periodic field we have

$$E(t) = A(t)\cos(w_f t + \varphi_0). \qquad (4)$$

The Pauli matrices are defined as

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad , \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

and I is the unit matrix .

The Hamiltonian (3) is written in atomic units ($\hbar = 1$).

We introduced the simplest model Hamiltonian which describes a TLS coupled linearly to a bath and driven by an external field. It is known that dissipative processes induce loss of coherence and our task is to outline methods of suppression of these quantum effects, in general.

From the solution of the time-dependent Schrodinger equation

$$i\frac{d\varphi(t)}{dt} = H\varphi(t) \qquad (5)$$

we can calculate the density matrix

$$\rho_{\sigma\sigma'}(t) = \int d\mathbf{Q_a}\, \varphi^*(\sigma, \mathbf{Q_a}, t)\, \varphi(\sigma', \mathbf{Q_a}, t). \qquad (6)$$

The appropriate density matrix $\rho_{\sigma\sigma'}$ is a 2×2 matrix elements where σ and σ' are 0 or 1. We denoted the diagonal matrix elements of the density matrix as ρ_{00} and ρ_{11}, the off-diagonal elements (so-called coherences terms) as ρ_{01} and ρ_{10}. The diagonal elements describe the population of the levels. It provides direct information about the evolution of the TLS. The off-diagonal elements give information about the order of decoherence in a quantum system. We consider the factor

$$c_{ij} = \frac{|\rho_{ij}|}{\sqrt{\rho_{ii}\rho_{jj}}} \quad i,j = 0,1 \quad i \neq j \ , \tag{7}$$

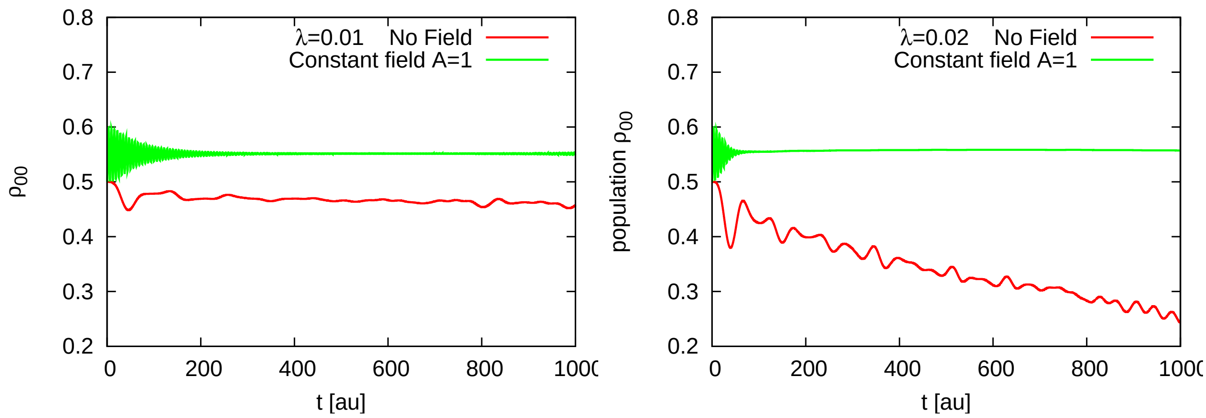
which indicates the level of coherence in the TLS. This factor varies in the range from 0 to 1 and reaches 1 for a completely coherent state of the system.

4 Results and Discussion

4.1 The coupling to a low-frequency bath

We start from the equally populated levels of the TLS $\rho_{00} = \rho_{11} = 0.5$ and consider the 12 bath frequencies w_{bath} in range from 0.005 to 0.06 with the step 0.005. In Figure 1 with the red curves we display the population ρ_{00} of the lower state of the TLS, induced by the bath only. The green curves present this population in case of interplay between an environment and a field. It is seen, that the higher the coupling parameter λ, the faster transition of the population between the two levels of the system. In the presence of constant field, the population is stabilized and it is faster (see (b)) for a strong coupling caused by the bath.

The degrees of coherence for three different coupling parameters are shown in Figure 2(a). It is obviously clear that the strong coupling (blue curve, (a)) tends to destroy coherence of the TLS. Comparing the cases (b), (c), (d) in Figure 2, we can conclude that the stronger the TLS interacts with the environment the more difficult to suppress decoherence (see (d)).



(a) (b)

Figure 1: The time evolution of the TLS (the population ρ_{00} of the lower state as a function of time t) for different coupling parameters: (a) $\lambda = 0.01$ and (b) $\lambda = 0.02$. The cases without field $E(t) = 0$ (red curves) and with constant field $E(t) = A = 1$ (green curves) are calculated with the following parameters: the energy gap of the TLS $\varepsilon = 0.1$, $w_{bath} \in [0.005\ ; 0.06]$.

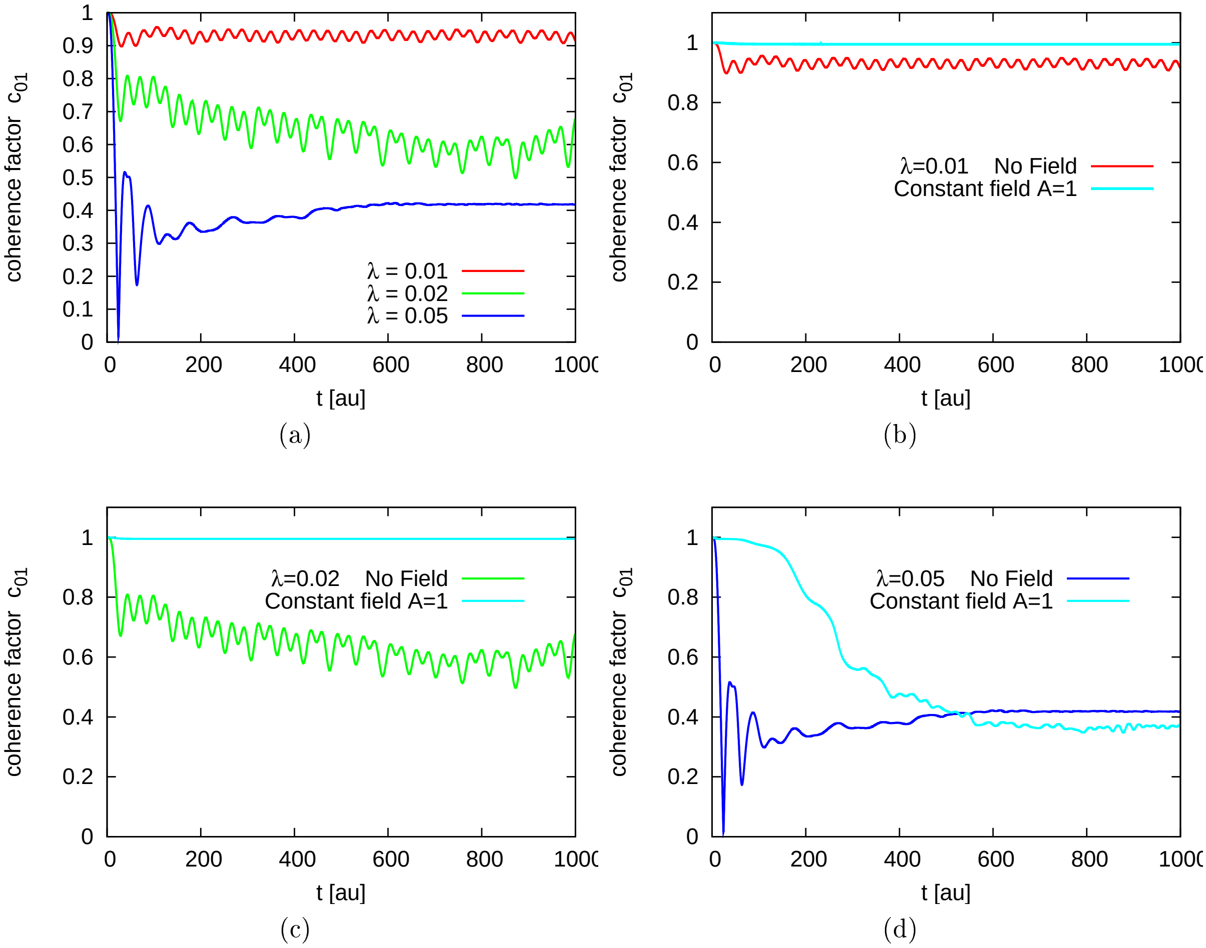


Figure 2: The degree of coherence of the TLS plotted as function of time t: (a) for different coupling parameters , $E(t) = 0$ and for each parameter separately (b) $\lambda = 0.01$, (c) $\lambda = 0.02$ and (d) $\lambda = 0.05$ under conditions of zero field and constant field $E(t) = A = 1$.

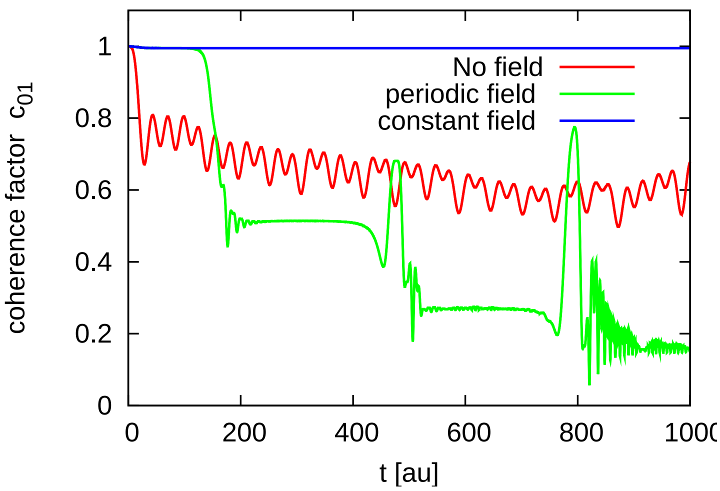


Figure 3: The degree of coherence of the TLS plotted as function of time t. The coupling parameter $\lambda = 0.02$. Red curve: $E(t) = 0$. Green curve: $E(t) = A\cos(w_f t)$, $A = 1$, $w_f = 0.01$. Blue curve: $E(t) = A = 1$

In the case of the periodic field, while the cosine vanishes every half-period we see only the effect of environment: in Figure 3 with the green curve we show the rapid losses of coherence in the TLS.

It is worth to consider separately an interesting case of resonance (Figure 4), i.e. the field frequency coincides with the TLS's one $\varepsilon = w_f = 0.1$. The system oscillates at the well known Rabi frequency, which depends only on the intensity of the field amplitude under these resonant conditions [Tan07]. By increasing the amplitude of the field it is possible to maintain or even enhance (see case at $A = 20$) a coherence of the TLS and thereby suppress the decoherence caused by the environment.

To understand the dynamics of this phenomenon we consider the time evolution of environment. The one-particle density matrix for each coordinate of bath gives us information about the bath evolution. We demonstrate observations which correspond to the frequency $w_{bath1} = 0.005$, so for bath coordinate Q_1 we have:

$$\rho(Q_1, t) = \sum_{\sigma=0,1} \int dQ_2 \ldots, dQ_{12}\, \varphi^*(\sigma, \mathbf{Q_a}, t)\, \varphi(\sigma, \mathbf{Q_a}, t)\, ,\; a = \overline{1, 12} \tag{8}$$

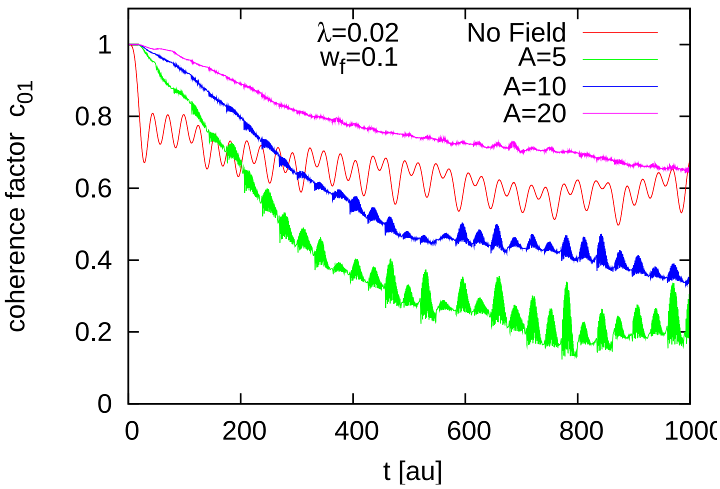


Figure 4: The degree of coherence of the TLS plotted as function of time t for different amplitudes of periodic field and in the absence of field. The resonance case : $\varepsilon = 0.1$, $w_f = 0.1$

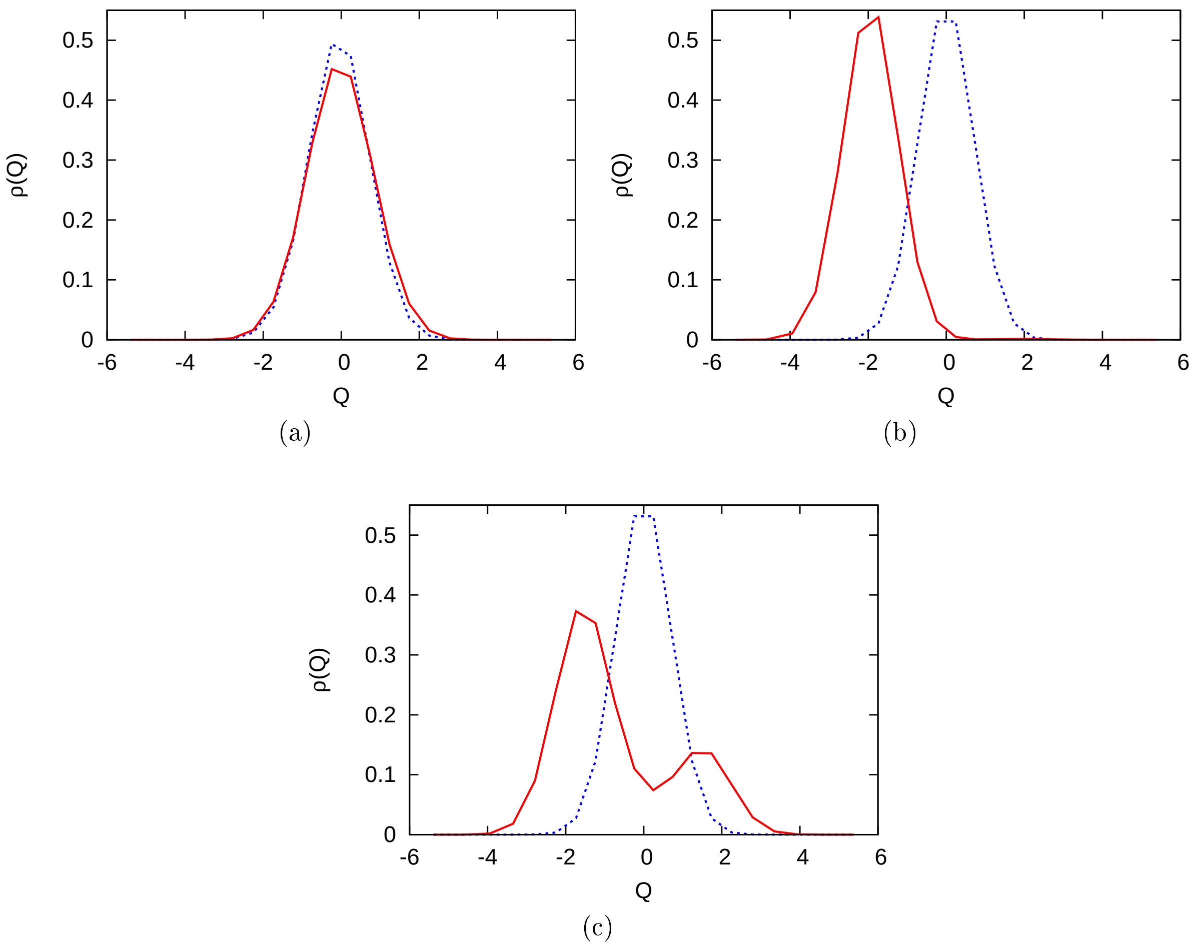


Figure 5: The one-particle density matrix plotted as function of bath coordinates for two random times ($t_1 = 140\,\text{au}$ - blue curve, $t_2 = 340\,\text{au}$ - red curve), the coupling parameter $\lambda = 0.02$. There are three different cases of the field :
(a)$E(t) = 0$ (b)$E(t) = A = 1$ (c) $E(t) = A\cos(w_f t)$, $A = 1$, $w_f = 0.01$

In Figure 5, the one-particle density matrix for two different times is presented in the absence of field (a), in the presence of constant field (b) and periodic field (c). Without field the bath only oscillates around an equilibrium position, takes energy from the TLS and gives it back. If the TLS is exposed by a constant field, then this acts on the bath through the TLS. That's why the bath mode moves (see (b)).

We also find the eigenvalues for the Hamiltonian (3) at one bath degree of freedom from the equation

$$\begin{pmatrix} \frac{\varepsilon}{2} + \frac{w_1 Q_1^2}{2} & \lambda_1 Q_1 + E(t) \\ \lambda_1 Q_1 + E(t) & -\frac{\varepsilon}{2} + \frac{w_1 Q_1^2}{2} \end{pmatrix} \tilde{\varphi} = \tilde{\varepsilon}\tilde{\varphi}\,. \tag{9}$$

The time-dependent eigenvalues of driven TLS coupled to one bath harmonic oscillator are

$$\tilde{\varepsilon}_{\pm} = \frac{1}{2}(w_1 Q_1^2) \pm \sqrt{\varepsilon^2 + 4(\lambda_1 Q_1 + E(t))^2} \tag{10}$$

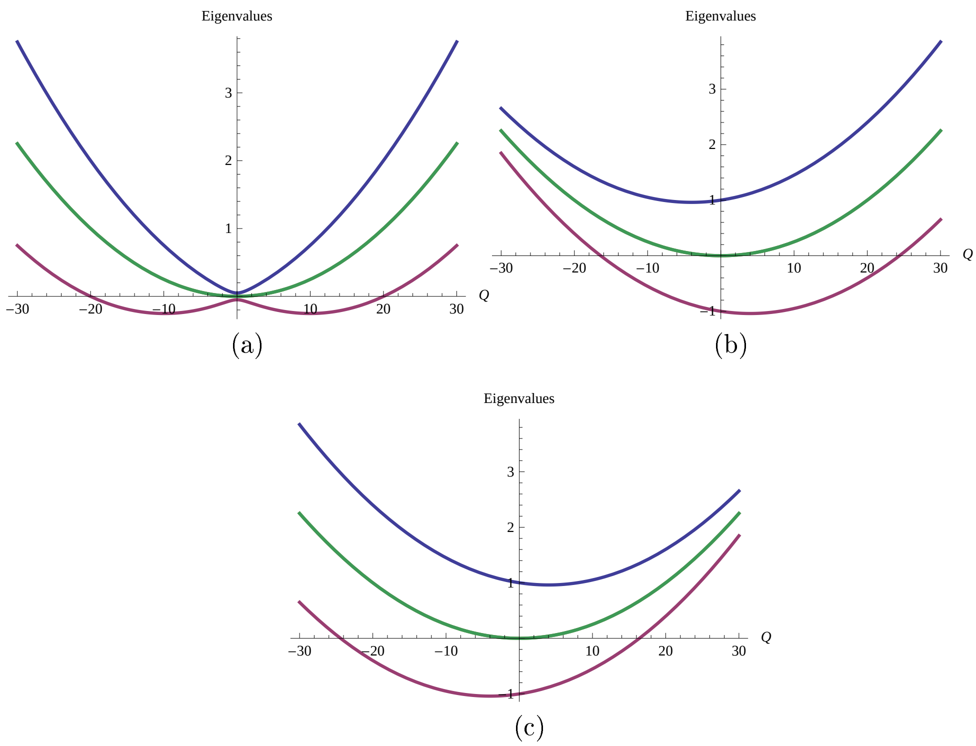


Figure 6: The eigenvalues of the TLS coupled to one harmonic oscillator plotted as functions of bath coordinates for the following cases: (a) $E(t) = 0$, (b) $E(t) = A = 1$ and (c) $E(t) = A = -1$. Blue curve shows the eigenvalue of the upper state, pink curve - the eigenvalue of the lower state, green one - the potential of bath harmonic oscillator.

In Figure 6, it is shown how the environment interacts with the TLS (see (a)) in absence of field, it changes the eigenvelues of the system's states. Also it is clear, the field provides the energy shift between the states of the TLS ((b), (c)). In the case of periodic field $E(t) = A\cos(w_f t)$, while the field changes sign we see the splitting in the one-particle density matrix (Figure 6, (c)).

4.2 The coupling to a high-frequency bath

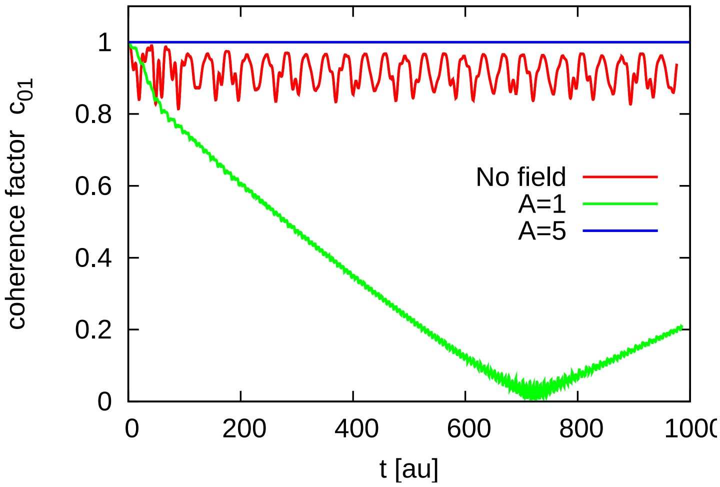


Figure 7: The degree of coherence of the TLS plotted as function of time t for different amplitudes of constant field and in the absence of field. The coupling parameter $\lambda = 0.1$

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Up to now, we have discussed the low-frequency (in comparison with the energy difference $\varepsilon = 0.1$ in the TLS) set of bath oscillators $w_f < \varepsilon$. The degree of coherence at the high-frequency range $w_{bath} \in [\,0.5\,; 0.555\,]$ is depicted in Figure 7.

We already understand that the constant field controls the energy difference ε between two states of the TLS. Changing the intensity of constant field we can make the energy gap closer to bath frequency range or farther from it. If the gap of the TLS has the same order as the bath energy we see a strong coupling, which increases a decoherence in the system. Otherwise, if the value of the gap ε is quite different from the bath modes, the system is weakly coupled to the environment, therefore the TLS becomes more coherent. These points that we have discussed are clearly presented in Figure 7. In case A = 1 (green curve), it is seen a strong influence of the bath, in consequence of that we have a sharp loss of coherence. For A = 5 (blue curve), a constant field increases the energy gap between states of the TLS more, makes it closer to the bath frequency range and thereby enhances a coherence in the system.

5 Summary

In general conclusion, we explored dissipative dynamics of a two-level system coupled linearly to a bath as a set of harmonic oscillators and driven by an external field. It is worth to point out the following:

- a constant field controls the energy gap of a TLS, which can be set in resonance or out of resonance with bath modes;

- for a periodic field, complete supression of decoherence has not been achieved with our model, even for quite large field amplitude. The oscillating nature of the field makes it possible that some decoherence occurs while the field changes sign.

6 Acknowledgments

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References

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