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# Decoherence dynamics of a qubit coupled to a quantum two-level system

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#### Abstract

We study the decoherence dynamics of a qubit coupled to a quantum two-level system (TLS) in addition to its weak coupling to a background environment. We analyze the different regimes of behaviour that arise as the values of the different parameters are varied. We classify those regimes as two weak-coupling regimes, which differ by the relation between the qubit and TLS decoherence times, and a strong-coupling one. We also find analytic expressions describing the decoherence rates in the weak-coupling regimes, and we verify numerically that those expressions have a rather wide range of validity. Along with obtaining the above-mentioned results, we address the questions of qubit–TLS entanglement and the additivity of multiple TLS contributions. We also discuss the transition from weak to strong-coupling as the parameters are varied, and we numerically determine the location of the boundary between the two regimes.

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### 1. Introduction

There have been remarkable advances in the quest to build a superconductor-based quantum information processor in recent years [1–14]. Coherent oscillations have been observed in systems of single qubits and two interacting qubits [2,4,5,8]. In order to achieve the desirable power of a functioning quantum computer, one would need to perform a large number of quantum gate operations of at least hundreds of qubits. One of the main obstacles to achieving that goal, however, are the relatively short decoherence times in these macroscopic systems (note that even a single superconductor-based qubit can be considered a macroscopic system). Therefore, there has been increasing experimental and theoretical activity aimed at understand-

\* Corresponding author. *E-mail address:* ashhab@riken.jp (S. Ashhab). ing the sources and mechanisms of decoherence of such systems in recent years [10-21].

The environment causing decoherence of the qubit is comprised of a large number of microscopic elements. There is a large wealth of theoretical work on the so-called spin-boson model [22], which models the environment as a large set of harmonic oscillators, to describe the environment of a solid-state system. However, recent experimental results suggest the existence of quantum two-level systems (TLSs) that are strongly coupled to the qubit [10,11,23]. Furthermore, it is well known that the qubit decoherence dynamics can depend on the exact nature of the noise causing that decoherence. For example, an environment composed of a large number of TLSs that are all weakly coupled to the qubit will generally cause non-Markovian decoherence dynamics in the qubit (see, e.g., [15]). Note that the mechanism of qubit-TLS coupling depends on the physical nature of the qubit and TLS. The exact mechanisms are presently unknown.

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The effect on the qubit of an environment consisting of weakly coupled TLSs with short decoherence times is rather well understood. As was presented in Ref. [18], one takes the correlation functions of the TLS dynamics in the frequency domain, multiplies each one with a factor describing the qubit-TLS coupling strength, and adds up the contributions of all the TLSs to obtain the effective noise that is felt by the qubit. We shall refer to that approach as the traditional weak-coupling approximation. In this paper, we shall study the more general case where no *a priori* assumptions are made about the TLS parameters. We shall identify the criteria under which the traditional weak-coupling approximation is valid. We shall also derive more general expressions that have a wider range of validity, as will be discussed below. Furthermore, we study the criteria under which our weak-coupling results break down, and the TLS cannot be easily factored out of the problem. It is worth noting here that we shall not attempt to theoretically reproduce the results of a given experiment. Although we find potentially measurable deviations from the predictions of previous work, we are mainly interested in answering some questions related to the currently incomplete understanding of the effects of a TLS, or environment of TLSs, on the qubit decoherence dynamics.

Since we shall consider in some detail the case of a weakly coupled TLS, and we shall use numerical calculations as part of our analysis, one may ask why we do not simulate the decoherence dynamics of a qubit coupled to a large number of such TLSs. Alternatively, one may ask why we separate one particular TLS from the rest of the environment. Focussing on one TLS has the advantage that we can obtain analytic results describing the contribution of that TLS to the qubit decoherence. That analysis can be more helpful in building an intuitive understanding of the effects of an environment composed of a large number of TLSs than a more sophisticated simulation of an environment composed of, say, twenty TLSs. The main purpose of using the numerical simulations in this work is to study the conditions of validity of our analytically obtained results.

The present paper is organized as follows: in Section 2 we introduce the model system and the Hamiltonian that describes it. In Section 3 we describe the theoretical approach that we shall use in our analysis. In Section 4 we use a perturbative calculation to derive analytic expressions for the relaxation and dephasing rates of the qubit in the weak-coupling regime and compare them with those of the traditional weak-coupling approximation. In Section 5 we numerically analyze the qubit decoherence dynamics in the different possible regimes. We also address a number of questions related to the intuitive understanding of the problem, including those of qubit-TLS entanglement and the case of two TLSs. In Section 6 we discuss the question of the boundary between the weak and strong-coupling regimes, and we perform numerical calculations to determine the location of that boundary. We finally conclude our discussion in Section 7.

#### 2. Model system

We consider a qubit that is coupled to a quantum TLS. We take the qubit and the TLS to be coupled to their own (uncorrelated) environments that would cause decoherence even if the qubit and TLS are not coupled to each other. We shall be interested in the corrections to the qubit decoherence dynamics induced by the TLS. The Hamiltonian of the system is given by

$$\widehat{H} = \widehat{H}_{q} + \widehat{H}_{\text{TLS}} + \widehat{H}_{I} + \widehat{H}_{\text{Env}}, \qquad (1)$$

where  $\hat{H}_q$  and  $\hat{H}_{TLS}$  are the qubit and TLS Hamiltonians, respectively,  $\hat{H}_I$  describes the coupling between the qubit and the TLS, and  $\hat{H}_{Env}$  describes all the degrees of freedom in the environment and their coupling to the qubit and the TLS. The qubit Hamiltonian is given by

$$\widehat{H}_{q} = -\frac{\varDelta_{q}}{2}\widehat{\sigma}_{x}^{(q)} - \frac{\epsilon_{q}}{2}\widehat{\sigma}_{z}^{(q)},\tag{2}$$

where  $\Delta_q$  and  $\epsilon_q$  are the adjustable control parameters of the qubit, and  $\hat{\sigma}_{\alpha}^{(q)}$  are the Pauli spin matrices of the qubit. For example, for the charge qubit in Ref. [2],  $\Delta_q$  and  $\epsilon_q$  are the energy scales associated with tunnelling and charging, respectively. Similarly, the TLS Hamiltonian is given by

$$\widehat{H}_{\text{TLS}} = -\frac{\Delta_{\text{TLS}}}{2}\widehat{\sigma}_x^{(\text{TLS})} - \frac{\epsilon_{\text{TLS}}}{2}\widehat{\sigma}_z^{(\text{TLS})}.$$
(3)

The energy splitting between the two quantum states of each system, in the absence of coupling between them, is then given by

$$E_{\alpha} = \sqrt{\varDelta_{\alpha}^2 + \epsilon_{\alpha}^2},\tag{4}$$

where the index  $\alpha$  refers to either qubit or TLS. For future purposes, let us also define the angles  $\theta_{\alpha}$  by the criterion

$$\tan \theta_{\alpha} \equiv \frac{\Delta_{\alpha}}{\epsilon_{\alpha}}.$$
 (5)

We take the interaction Hamiltonian between the qubit and the TLS to be of the form:

$$\widehat{H}_{\rm I} = -\frac{\lambda}{2} \widehat{\sigma}_z^{\rm (q)} \otimes \widehat{\sigma}_z^{\rm (TLS)},\tag{6}$$

where  $\lambda$  is the coupling strength between the qubit and the TLS. Note that the minus sign in  $\hat{H}_{I}$  is simply a matter of convention, since  $\lambda$  can be either positive or negative. It is worth mentioning here that the applicability of this form of interaction is not as limited as it might appear at first sight. Any interaction Hamiltonian that is a product of a qubit observable (i.e. any Hermitian  $2 \times 2$  matrix) and a TLS observable can be recast in the above form with a simple basis transformation.

We assume that all the terms in  $\hat{H}_{Env}$  are small enough that its effect on the dynamics of the qubit + TLS system can be treated within the framework of the Markovian Bloch–Redfield master equation approach. It is well known that the effect of certain types of environments cannot be described using that approach, e.g. those containing 1/f low-frequency noise. However, there remain a number of unanswered questions about the problem of a qubit experiencing 1/f noise. For example, it was shown in Ref. [16] that the decoherence dynamics can depend on the specific physical model used to describe the environment. Therefore, treating that case would make it more difficult to extract results that are directly related to the phenomenon we are studying, namely the effect of a single quantum TLS on the qubit decoherence dynamics. We therefore do not consider that case.

Depending on the physical nature of the system, the coupling of the qubit and the TLS to their environments is described by specific qubit and TLS operators. In principle one must use those particular operators in analyzing the problem at hand. However, since we shall present our results in terms of the background decoherence rates, which are defined as the relaxation and dephasing rates in the absence of qubit-TLS coupling, the choice of system-environment interaction operators should not affect any of our results. In fact, in our numerical calculations below we have used a number of different possibilities and verified that the results remain unchanged, provided that the background decoherence rates are kept constant. Furthermore, the background-noise power spectrum affects the results only through the background decoherence rates. Note that we shall not discuss explicitly the temperature dependence of the background decoherence rates. It should be kept in mind, however, that the background dephasing rates generally have a strong temperature dependence in current experiments on superconducting gubits.

It is worth noting that, since we are considering a quantum-mechanical TLS, the model and the intermediate algebra that we use are essentially identical to those used in some previous work studying two coupled qubits [24–26]. However, as opposed to being a second qubit, a TLS is an uncontrollable and inaccessible part of the system. Therefore, in interpreting the results, we only consider quantities related to the qubit dynamics.

#### 3. Theoretical analysis: master equation

As mentioned above, we take one particular element of the environment, namely the TLS, and do not make any *a priori* assumptions about its decoherence times or the strength of its coupling to the qubit. We assume that the coupling of the qubit to its own environment and that of the TLS to its own environment are weak enough that a Markovian master equation approach provides a good description of the dynamics. The combined qubit + TLS system has four quantum states. The quantity that we consider is therefore the  $4 \times 4$  density matrix describing that combined system. We follow the standard procedure to write the Bloch-Redfield master equation as (see e.g. Ref. [27]):

$$\dot{\rho}_{ab} = -i\omega_{ab}\rho_{ab} + \sum_{cd} R_{abcd}\rho_{cd},\tag{7}$$

where the dummy indices a, b, c and d run over the four quantum states,  $\omega_{ab} \equiv (E_a - E_b)/\hbar$ ,  $E_i$  is the energy of the quantum state labelled by i, and the coefficients  $R_{abcd}$  are given by

$$R_{abcd} = -\int_{0}^{\infty} dt \sum_{\alpha=q,TLS} \left\{ g_{\alpha}(t) \left[ \delta_{bd} \sum_{n} \langle a | \hat{\sigma}_{z}^{(\alpha)} | n \rangle \langle n | \hat{\sigma}_{z}^{(\alpha)} | c \rangle e^{i\omega_{cn}t} + \langle a | \hat{\sigma}_{z}^{(\alpha)} | c \rangle \langle d | \hat{\sigma}_{z}^{(\alpha)} | b \rangle e^{i\omega_{ca}t} \right] + g_{\alpha}(-t) \left[ \delta_{ac} \sum_{n} \langle d | \hat{\sigma}_{z}^{(\alpha)} | n \rangle \langle n | \hat{\sigma}_{z}^{(\alpha)} | b \rangle e^{i\omega_{nd}t} + \langle a | \hat{\sigma}_{z}^{(\alpha)} | c \rangle \langle d | \hat{\sigma}_{z}^{(\alpha)} | b \rangle e^{i\omega_{bd}t} \right] \right\}$$

$$(8)$$

$$g_{\alpha}(t) = \int_{-\infty}^{\infty} \mathrm{d}\omega S_{\alpha}(\omega) \mathrm{e}^{-\mathrm{i}\omega t}, \qquad (9)$$

where  $S_{\alpha}(\omega)$  is the background-noise power spectrum. In calculating  $R_{abcd}$  we neglect the imaginary parts, which renormalize the energy splittings of the qubit and TLS, and we assume that those corrections are already taken into account in our initial Hamiltonian. We do not use any secular approximation to simplify the tensor  $R_{abcd}$  any further. One of the main reasons for avoiding the secular approximation is that we shall consider cases where the coupling strength between the qubit and the TLS is very small, which results in almost degenerate quantum states, a situation that cannot be treated using, for example, the form of the secular approximation given in Ref. [27].

Once we solve Eq. (7) and find the dynamics of the combined system, we can trace out the TLS degree of freedom to find the dynamics of the reduced  $2 \times 2$  density matrix describing the qubit alone. From that dynamics we can infer the effect of the TLS on the qubit decoherence and, whenever the decay can be fit well by exponential functions, extract the qubit dephasing and relaxation rates.

### 4. Analytic results for the weak-coupling limit

We first consider a case that can be treated analytically, namely that of a strongly dissipative weakly coupled TLS. That is exactly the case where the traditional weak-coupling approximation is expected to work. Here, we perform a perturbative calculation on Eq. (7) where the coupling strength  $\lambda$  is treated as a small parameter in comparison with the decoherence times in the problem. We shall discuss the differences between the predictions of the two approaches in this section, and we shall show in Section 5 that our results have a wider range of validity than the traditional weak-coupling approximation.

In the first calculation of this section, we consider the zero-temperature case. If we take the limit  $\lambda \rightarrow 0$  and look for exponentially decaying solutions of Eq. (7) with rates that approach the unperturbed relaxation and dephasing rates  $\Gamma_1^{(q)}$  and  $\Gamma_2^{(q)}$ , we find the following approximate expressions for the leading-order corrections:

$$\begin{split} \delta \Gamma_{1}^{(q)} &\approx \frac{1}{2} \lambda^{2} \sin^{2} \theta_{q} \sin^{2} \theta_{TLS} \frac{\Gamma_{2}^{(TLS)} + \Gamma_{2}^{(q)} - \Gamma_{1}^{(q)}}{\left(\Gamma_{2}^{(TLS)} + \Gamma_{2}^{(q)} - \Gamma_{1}^{(q)}\right)^{2} + \left(E_{q} - E_{TLS}\right)^{2}} \\ \delta \Gamma_{2}^{(q)} &\approx \frac{1}{4} \lambda^{2} \sin^{2} \theta_{q} \sin^{2} \theta_{TLS} \frac{\Gamma_{2}^{(TLS)} - \Gamma_{2}^{(q)}}{\left(\Gamma_{2}^{(TLS)} - \Gamma_{2}^{(q)}\right)^{2} + \left(E_{q} - E_{TLS}\right)^{2}}, \end{split}$$
(10)

which are expected to apply very well when  $\Gamma_2^{(TLS)} + \Gamma_2^{(q)} \gg \Gamma_1^{(q)}$ . The above expressions can be compared with those given in Ref. [18]:

$$\delta\Gamma_{1}^{(q)} \approx \frac{1}{2}\lambda^{2}\sin^{2}\theta_{q}\sin^{2}\theta_{TLS}\frac{\Gamma_{2}^{(TLS)}}{\Gamma_{2}^{(TLS)^{2}} + (E_{q} - E_{TLS})^{2}}$$

$$\delta\Gamma_{2}^{(q)} \approx \frac{1}{2}\delta\Gamma_{1} + \frac{\lambda^{2}\cos^{2}\theta_{q}\cos^{2}\theta_{TLS}}{\Gamma_{1}^{(TLS)}}\operatorname{sech}^{2}\left(\frac{E_{TLS}}{2k_{B}T}\right).$$
(11)

The two approaches agree in the limit where they are both expected to apply very well, namely when the decoherence times of the TLS are much shorter than those of the qubit [note that we are taking T = 0 in Eq. (10)]. Our results can therefore be considered a generalization of those of the traditional weak-coupling approximation. We shall discuss the range of validity of our results in Section 5.3.1.

We now turn to the finite temperature case. In addition to treating  $\lambda$  as a small parameter, one can also perform a perturbative calculation to obtain the temperature dependence of the decoherence rates in the low temperature limit. In the general case where the qubit and TLS energy splittings are different and no assumption is made about the relation between qubit and TLS decoherence rates, the algebra is rather complicated, and the resulting expressions contain a large number of terms. Therefore we only present the results in the case where  $E_q = E_{TLS} \equiv E$ , which is the case that we shall focus on in Section 5. In that case we find the additional corrections to the relaxation and dephasing rates to be given by

$$\begin{split} \delta \Gamma_{1,T}^{(q)} &= 0\\ \delta \Gamma_{2,T}^{(q)} &= \lambda^2 e^{-E/k_{\rm B}T} \left( \frac{4\cos^2\theta_{\rm q}\cos^2\theta_{\rm TLS}}{\Gamma_1^{({\rm TLS})}}. \\ &- \frac{\sin^2\theta_{\rm q}\sin^2\theta_{\rm TLS}\Gamma_1^{(q)}}{\left(\Gamma_2^{({\rm TLS})} - \Gamma_2^{(q)}\right) \left(\Gamma_2^{({\rm TLS})} - \Gamma_2^{(q)} + \Gamma_1^{(q)}\right)} \right). \end{split} \tag{12}$$

Note that the first term inside the parentheses agrees with the expression given in Eq. (11) for the TLS contribution to the dephasing rate. If the decoherence times of the TLS are much shorter than those of the qubit, the second term is negligible. A similar situation occurs when  $E_q \neq E_{TLS}$ , i.e., all the terms can be neglected except for the one given in Eq. (11).

#### 5. Numerical solution of the master equation

We now turn to the task of numerically analyzing the effect of the TLS on the qubit with various choices of parameters. We analyze any given case by first solving Eq. (7) to find the density matrix of the combined

qubit + TLS system as a function of time. We then trace out the TLS degree of freedom to find the (time-dependent) density matrix of the qubit alone, which is perhaps most easily visualized as a curve in the Bloch sphere [28]. We then use the Hamiltonian of the qubit including the mean-field correction contributed by the TLS as a pole of reference in the Bloch sphere, from which we can extract the dephasing and relaxation dynamics of the qubit. In other words, we transform the qubit density matrix into the qubit energy eigenbasis, such that the diagonal matrix elements describe relaxation dynamics and the off-diagonal matrix elements describe dephasing dynamics. The relaxation rate is then defined as the rate of change of the diagonal matrix elements divided by their distance from the equilibrium value. The dephasing rate is defined similarly using the off-diagonal matrix elements [29].

Since our main goal is to analyze the different possible types of behaviour in the qubit dynamics, we have to identify the relevant parameters that determine the different behaviour regimes. As discussed in Section 2, the energy scales in the problem are the qubit and TLS energy splittings, their background decoherence rates (which are related to the environment noise power spectrum), the qubit-TLS coupling strength and temperature. Note that if the difference between the two energy splittings is substantially larger than the coupling strength, the effect of the TLS on the qubit dynamics diminishes rapidly. The above statement is particularly true regarding the relaxation dynamics. We therefore consider only the case where the two energy splittings are equal, i.e.  $E_q = E_{TLS}$ . In other words, we take the TLS to be on resonance with the qubit. Furthermore, we take the energy splitting, which is the largest energy scale in the problem, to be much larger than all other energy scales, such that its exact value does not affect any of our results. We take the temperature to be much smaller than  $E_{q}$ , so that environment-assisted excitation processes can be neglected. We are therefore left with the background decoherence rates and the coupling strength as free parameters that we can vary in order to study the different possible types of behaviour in the qubit dynamics.

## 5.1. Weak-coupling regimes

Although the discussion of the criterion that distinguishes between the weak and strong-coupling regimes is deferred to Section 6, we separate the results of this section according to that criterion. We start with the weak-coupling regimes. In Figs. 1 and 2, we show, respectively, the relaxation and dephasing rates of the qubit as functions of time for three different sets of parameters differing by the relation between the qubit and TLS decoherence rates, maintaining the relation  $\Gamma_2^{(\alpha)} = 2\Gamma_1^{(\alpha)}$ , where  $\Gamma_1^{(\alpha)}$  and  $\Gamma_2^{(\alpha)}$  are the background relaxation and dephasing rates, i.e. those obtained in the case  $\lambda = 0$ , and the index  $\alpha$  refers to qubit and TLS. The case  $\lambda = 0$  is trivial, and we only show it as a point of reference to demonstrate the changes that occur in the case



Fig. 1. Relative corrections to qubit relaxation rate as a function of scaled time in the case of (a) strongly, (b) moderately and (c) weakly dissipative TLS. The ratio  $\Gamma_1^{(TLS)}/\Gamma_1^{(q)}$  is 10 in (a), 1.5 in (b) and 0.1 in (c). The solid, dashed, dotted and dash-dotted lines correspond to  $\lambda/\Gamma_1^{(q)} = 0$ , 0.3, 0.6 and 0.9, respectively.  $\theta_a = \pi/3$  and  $\theta_{TLS} = 3\pi/8$ .



Fig. 2. Relative corrections to qubit averaged dephasing rate, i.e. after eliminating fast oscillations around the slowly varying function, as a function of scaled time in the case of (a) strongly, (b) moderately and (c) weakly dissipative TLS. The ratio  $\Gamma_1^{(\text{TLS})}/\Gamma_1^{(q)}$  is 10 in (a), 1.5 in (b) and 0.1 in (c). The solid, dashed, dotted and dash-dotted lines correspond to  $\lambda/\Gamma_1^{(q)} = 0$ , 0.3, 0.6 and 0.9, respectively.  $\theta_q = \pi/3$  and  $\theta_{\text{TLS}} = 3\pi/8$ .

 $\lambda \neq 0$ . All the curves shown in Figs. 1 and 2 agree very well with the formulae that will be given below.

#### 5.1.1. Relaxation dynamics

Characterizing the dynamics is most easily done by considering the relaxation dynamics. From Fig. 1 we can see that in the case  $\lambda \neq 0$ , there are several possible types of behaviour of the qubit depending on the choice of the different parameters in the problem. As a general simple rule, which is inspired by Fig. 1(a), we find that for small values of  $\lambda$  the relaxation rate starts at its background value and follows an exponential decay function with a characteristic time given by  $(\Gamma_2^{(\text{TLS})} + \Gamma_2^{(q)} - \Gamma_1^{(q)})^{-1}$ , after which it saturates at a steady-state value given by Eq. (10), with  $E_q = E_{\text{TLS}}$ :

$$\frac{dP_{\rm ex}(t)/dt}{P_{\rm ex}(t) - P_{\rm ex}(\infty)} \approx -\Gamma_1^{\rm (q)} - \frac{\lambda^2 \sin^2 \theta_{\rm q} \sin^2 \theta_{\rm TLS}}{2\left(\Gamma_2^{\rm (TLS)} + \Gamma_2^{\rm (q)} - \Gamma_1^{\rm (q)}\right)} \times \left(1 - \exp\left\{-\left(\Gamma_2^{\rm (TLS)} + \Gamma_2^{\rm (q)} - \Gamma_1^{\rm (q)}\right)t\right\}\right).$$
(13)

We can therefore say that the qubit relaxation starts with an exponential-times-Gaussian decay function for a certain period of time, after which it is well described by an exponential decay function with a rate that incorporates the effects of the TLS, namely that given in Eq. (10). Clearly the above picture is only valid when the expression for the transient time given above is much smaller than  $1/\Gamma_1^{(q)}$ . Furthermore, Eq. (13) is not well defined when  $\Gamma_2^{(\text{TLS})} + \Gamma_2^{(q)} - \Gamma_1^{(q)} = 0$ . However, even when the above condition about the short transient time is not satisfied, and even when the exponent in Eq. (13) becomes positive, we find that for times of the order of the qubit relaxation time, a very good approximation for the relaxation rate is still given by Eq. (13). The reason why that is the case can be seen from the expansion of Eq. (13) in powers of *t*:

$$\frac{dP_{\rm ex}(t)/dt}{P_{\rm ex}(t) - P_{\rm ex}(\infty)} \approx -\Gamma_1^{\rm (q)} - \frac{1}{2}\lambda^2 \sin^2\theta_{\rm q} \sin^2\theta_{\rm TLS} t, \qquad (14)$$

which can be integrated to give:

$$P_{\rm ex}(t) \approx \exp\{-\Gamma_1^{\rm (q)}t - \lambda^2 \sin^2 \theta_{\rm q} \sin^2 \theta_{\rm TLS} t^2/4\},\tag{15}$$

where we have assumed that  $P_{ex}(0) = 1$  and that  $P_{ex}(\infty)$  is negligibly small. Eq. (15) describes the initial decay for any ratio of qubit and TLS decoherence times. Whether that function holds for all relevant times or it turns into an exponential-decay function depends on the relation between  $\Gamma_1^{(q)}$  and  $\Gamma_2^{(TLS)} + \Gamma_2^{(q)}$ , as discussed above. In particular, in the case when the TLS decoherence rates are much smaller than those of the qubit, Eq. (15) holds at all relevant times, and the contribution of the TLS to the qubit relaxation dynamics is therefore a Gaussian decay function. We also note here that the relaxation rate shows small oscillations around the functions that we have given above. However, those oscillations have a negligible effect when the rate is integrated to find the function  $P_{ex}(t)$ .

#### 5.1.2. Dephasing dynamics

The dephasing dynamics was somewhat more difficult to analyze. The dephasing rate generally showed oscillations with frequency  $E_q$ , and the amplitude of the oscillations grew with time, making it difficult to extract the dynamics directly from the raw data for the dephasing rate. However, when we plotted the averaged dephasing rate over one or two oscillation periods, as was done in generating Fig. 2, the curves became much smoother, and we were able to fit those curves with the following simple analytic formula, which we obtained in an analogous manner to Eq. (13):

$$\frac{1}{\rho_{01}} \left( \frac{\mathrm{d}\rho_{01}}{\mathrm{d}t} \right) \approx -\Gamma_2^{(q)} - \frac{\lambda^2 \sin^2 \theta_{\mathrm{q}} \sin^2 \theta_{\mathrm{TLS}}}{4(\Gamma_2^{(\mathrm{TLS})} - \Gamma_2^{(q)})} \times \left( 1 - \exp\left\{ -\left(\Gamma_2^{(\mathrm{TLS})} - \Gamma_2^{(q)}\right) t \right\} \right).$$
(16)

Starting from this point, the analysis of the dephasing dynamics is similar to that of relaxation. When the decoherence rates of the TLS are much larger than those of the qubit, the dephasing rate starts from its background value but quickly reaches its steady-state value given by Eq. (10). In the opposite limit, where the TLS decoherence rates are much smaller than those of the qubit, a good approximation is obtained by expanding Eq. (16) to first order in t. In that case we find that:

$$\rho_{01}(t) \approx \rho_{01}(0) \exp\{-\Gamma_2^{(q)} t - \lambda^2 \sin^2 \theta_q \sin^2 \theta_{\text{TLS}} t^2/8\}.$$
 (17)

# 5.2. Strong-coupling regime

In the strong-coupling regime corresponding to large values of  $\lambda$ , the qubit relaxation and dephasing rates as plotted similarly to Figs. 1 and 2 show oscillations throughout the period where the qubit is far enough from its thermal equilibrium state. Therefore one cannot simply speak of a TLS contribution to qubit decoherence. Analytic expressions can be straightforwardly derived for the dynamics in the limit where the coupling strength is much larger than the decoherence rates. However, the algebra is quite cumbersome, and the results are rather uninspiring. Therefore, we shall not present such expressions here.

## 5.3. Further considerations

# 5.3.1. Comparison with traditional weak-coupling approximation

To demonstrate the differences between our results and those of the traditional weak-coupling approximation, we plot in Fig. 3 the relaxation rate (at the end of the transient time) as a function of the coupling strength  $\lambda$ . A similar figure can be obtained for the dephasing rate, but we do not include it here. Our numerical results agree with the perturbation calculation of Section 4 (Eq. (10)) up to the point



Fig. 3. The steady-state qubit relaxation rate as a function of the qubit– TLS coupling strength  $\lambda$ . The solid line represents the numerical results, the dashed line is the perturbation-calculation result of Section 4 and the dotted line is the result of the traditional weak-coupling approximation given by Eq. (11).  $\theta_q = 3\pi/20$ ,  $\theta_{TLS} = 2\pi/5$ ,  $\Gamma_1^{(q)}/\Gamma_1^{(TLS)} = 0.25$ ,  $\Gamma_2^{(q)}/\Gamma_1^{(TLS)} = 1$ , and  $\Gamma_2^{(TLS)}/\Gamma_1^{(TLS)}$ .

where the coupling can be classified as strong, as will be explained in Section 6. Therefore, we conclude that the results of our perturbation calculation have a much wider range of validity than those of the traditional weak-coupling approximation. The more non-negligible the TLS decoherence times are relative to those of the qubit, the larger the difference between the two approaches. Note that in our perturbation-theory calculation we took the limit where  $\lambda$  is much smaller than all the decoherence rates in the problem. It turns out, however, that the results of that calculation are valid as long as  $\lambda$  is substantially smaller than the TLS decoherence rates, assuming those are substantially larger than the qubit decoherence rates. No specific relation is required between  $\lambda$  and the qubit decoherence rates in that case.

For further demonstration of the differences between the predictions of the two approaches, we ran simulations of an experiment where one would sweep the qubit energy splitting and measure the relaxation and dephasing rates. We used a TLS with the parameters of Fig. 3(a) and  $\lambda$  ranging from 0.15 to 0.5. In such an experiment, one would see a peak in the relaxation and dephasing rates at the TLS energy splitting. According to the traditional weak-coupling approximation, the height of the dephasing peak should be half of that of the relaxation peak. In the numerical simulations with the above parameters, we see a deviation from that prediction by about 25%. The relation between the shapes of the two peaks agrees very well with the expressions in Eq. (10). That difference would, in principle, be measurable experimentally. Note, however, that since we are dealing with an uncontrollable environment, there is no guarantee that a TLS with the appropriate parameters will be found in the small number of qubit samples available at a given laboratory.

## 5.3.2. Two TLSs

In order to establish that our results are not particular to single quantum TLSs, we also considered the case of two TLSs that are both weakly coupled to the qubit. If we take the two TLS energy splittings to be larger than the widths of their frequency-domain correlation functions, we find that the relaxation dynamics is affected by at most one TLS, depending on the qubit energy splitting. The TLS contributions to pure dephasing dynamics, i.e. that unrelated to relaxation, are additive, since that rate depends on the zero-frequency noise. We then considered two TLSs with energy splittings equal to that of the qubit. We found that the TLS contributions to the qubit relaxation and dephasing dynamics are additive in both the large and small  $\Gamma^{(q)}/\Gamma^{(TLS)}$  limits. These results are in agreement with those found in Ref. [30], where a related problem was treated.

#### 5.3.3. Entanglement

It is worth taking a moment here to discuss the question of entanglement between the system and environment. It is commonly said that in a Markovian master equation approach the entanglement between a system and its surrounding environment is neglected, a statement that can be misinterpreted rather easily. In order to address that point, we consider the following situation: we take the parameters to be in the weak-coupling regime, where such a discussion is meaningful. We take the qubit to be initially in its excited state, with no entanglement between the qubit and the TLS. We find that the off-diagonal matrix elements of the combined system density matrix describing coherence between the states  $|\uparrow_q\downarrow_{TLS}\rangle$  and  $|\downarrow_q\uparrow_{TLS}\rangle$  start from zero at t = 0 and reach a steady state at the end of the transient time. Beyond that point in time, they decay with the same rate as the excited state population. We therefore conclude that the final relaxation rate that we obtain takes into account the effects of entanglement between qubit and TLS, even though the density matrix of the qubit alone exhibits exponential decay behaviour.

# 6. Criteria for strong-coupling between qubit and two-level system

There are a number of possible ways one can define the criteria distinguishing between the weak and strong-coupling regimes. For example, one can define a strongly coupled TLS as being one that contributes a decoherence rate substantially different from that given by some weak-coupling analytic expression. One could also define a strongly coupled TLS as being one that causes visible oscillations in the qubit dynamics, i.e. one that causes the relaxation and dephasing rates to change sign as time goes by. We shall use the criterion of visible deviations in the qubit dynamics from exponential decay as a measure of how strongly coupled a TLS is.

Even with the above-mentioned criterion of visible deviations in the qubit dynamics from exponential decay, one still has to specify what is meant by visible deviations, e.g. maximum single-point deviation or average value of deviation. One also has to decide whether to use relaxation or dephasing dynamics in that definition. We have used a number of different combinations of the above and found qualitatively similar results. Those results can essentially be summarized as follows: a given TLS can be considered to interact weakly with the qubit if the coupling strength  $\lambda$  is smaller than the largest (background) decoherence rate in the problem. The exact location of the boundary, however, varies by up to an order of magnitude depending on which part of the dynamics we consider and how large a deviation from exponential decay we require.

We have also checked the boundary beyond which our analytic expressions and numerical results disagree, and we found that the boundary is similar to the one given above. That result confirms the wide range of validity of our analytic expressions. Note in particular that even if the qubit–TLS coupling strength  $\lambda$  is larger than the decoherence rates of the qubit, that TLS can still be considered weakly coupled to the qubit, provided the TLS decoherence rates are larger than  $\lambda$ .

# 7. Conclusion

We have analyzed the problem of a qubit interacting with a quantum TLS in addition to its coupling to a background environment. We have characterized the effect of the TLS on the qubit decoherence dynamics for weak and strong-coupling, as well as weakly and strongly dissipative TLSs. We have found analytic expressions for the contribution of a single TLS to the total decoherence rates in the weak-coupling regimes, which is a much larger range than just the weak-coupling limits. We recover the results of the traditional weak-coupling approximation as a special case of our results, namely for a weakly coupled strongly dissipative TLS. We have found that weakly coupled weakly dissipative TLSs exhibit memory effects by contributing a non-exponential factor to the qubit decoherence dynamics. We have verified that the contributions of two TLSs to the qubit relaxation and dephasing rates are additive in the weak-coupling limit. We have discussed the transition from weak to strong-coupling and numerically found that the transition occurs when the qubit-TLS coupling strength exceeds all the decoherence rates in the problem.

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