Phonon-induced relaxation and decoherence times of the hybrid qubit in silicon quantum dots

E. Ferraro,1∗ M. Fanciulli,1,2† and M. De Michielis1,
1CNR-IMM Agrate Unit, Via C. Olivetti 2, 20864 Agrate Brianza (MB), Italy
2Dipartimento di Scienza dei Materiali, University of Milano Bicocca, Via R. Cozzi, 55, 20126 Milano, Italy

We study theoretically the phonon-induced relaxation and decoherence processes in the hybrid qubit in silicon. Hybrid qubit behaves as a charge qubit when the detuning is close to zero and as spin qubit for large detuning values. It is realized starting from an electrostatically defined double quantum dot where three electrons are confined and manipulated through only electrical tuning. By employing a three-level effective model for the qubit and describing the environment bath as a series of harmonic oscillators in the thermal equilibrium states, we extract the relaxation and decoherence times as a function of the bath spectral density and of the bath temperature using the Bloch-Redfield theory. For Si quantum dots the energy dispersion is strongly affected by the physics of the valley, i.e. the conduction band minima, so we also included the contribution of the valley excitations in our analysis. Our results offer fundamental information on the system decoherence properties when the unavoidable interaction with the environment is included and temperature effects are considered.

I. INTRODUCTION

In solid state physics electrons or holes confined in 0-dimensional nanostructures, i.e. quantum dots (QDs), represent promising platforms for the realization of qubits, exploiting spin and/or charge, for quantum computing applications [1–6]. However qubits are inevitably coupled to the degrees of freedom of the surrounding environment causing a loss of coherence that deeply affects the qubit operations [7–8]. Depending on the nature of the host materials, a source of noise could be predominant with respect to the others. For example, materials belonging to group IV, such as Si and Ge, possess isotopes with zero nuclear spin that allow to reduce magnetic noise, while electrical noise remains an issue to be faced [9, 10]. Large progresses have also been done in studying semiconducting QDs in III-V compounds, such as GaAs [11, 12], that assure greater advantages in fabrication processes; however Si qubits attracted recently a lot of attention also due to the immediate integrability with the existing CMOS technology of the microelectronic industry [13, 14].

When Si QDs based qubits are considered, the six-fold degeneracy of the conduction band minima, that is due to the two-fold degeneracy of the ∆ valleys aligned along each one of the three main crystallographic directions, is an additional source of decoherence that may be overcome only if the typical qubit splitting energies are smaller with respect to the valley splittings [15, 16]. Otherwise, in order to have a complete picture, it becomes indispensable to include valley effects in the Hamiltonian model.

The hybrid qubit (HQ) is realized by the electrostatic confinement of three electron spins in a double quantum dot [17, 18]. We describe HQ with an effective three-level model adopting a basis whose logical states are encoded in the $S = 1/2$ and $S_z = −1/2$ subspace, where $S$ denotes the total angular momentum of the three electrons [19, 20]. Then, we model the environment with which the HQ unavoidably interacts, by a bath consisting of a series of harmonic oscillators with frequencies $\omega_j$. The effects of the bath temperature and of the bath spectral density on the qubit decoherence and relaxation times are studied.

In Ref. [21] the authors focus on ameliorating dominant sources of decoherence in order to increase the coherence time in a Si/SiGe HQ. They measure $dE_Q/d\epsilon$, where $E_Q$ is the qubit energy and $\epsilon$ is the detuning between the two QDs and demonstrate that HQ can be made resilient to charge noise by tuning appropriately the qubit parameters. More recently in Ref. [22] atomic scale disorder at the quantum well interface is put into direct connection with the dephasing of the HQ.

The study of the relaxation and decoherence processes is of fundamental as well as practical interest for quantum computation applications. For this reason, the aim of the present paper is to study theoretically the phonon-induced relaxation and decoherence times and how these times are affected by the HQ parameters as well as by the bath structure.

The paper is organized as follows. In Section II we present the theoretical model describing the Si HQ including valley degeneracy, the bath and their interaction; moreover the relaxation and decoherence times are derived following Bloch-Redfield theory. Section III is devoted to the analysis of the relaxation and decoherence processes when the effects of the bath are included and the space of the qubit parameters is explored. Finally concluding remarks are reported in Section IV.

II. THEORY

This Section is devoted to the description, through an effective Hamiltonian model, of the HQ interacting with a
bath of harmonic oscillators when temperature effects are included. The analytical expressions for the evaluation of relaxation and decoherence times are presented.

A. Model of the silicon hybrid qubit in a thermal bath

We describe effectively the HQ adopting a three-dimensional basis. The first state of the basis corresponds to a configuration with two electrons in the left dot and one in the other and consequently has a singlet charge form. The remaining basis states, on the contrary correspond to singlet and triplet charge configurations. The three-level matrix describing the qubit

\[
H_S = \begin{pmatrix}
\frac{\Delta_1}{2} & \Delta_2 & \Delta_1 \\
\Delta_2 & -\frac{\Delta_1}{2} & 0 \\
0 & 0 & -\frac{\epsilon}{2} + \Delta_R
\end{pmatrix},
\]

where \(\epsilon\) is the detuning between the two QDs, \(\Delta_1\) and \(\Delta_2\) refer to the tunnel couplings between different charge states from one dot to the other and \(\Delta_R\) corresponds to the low-energy splitting of the right dot, which could reflect a valley excitation, an orbital excitation or a combination. The estimation of such parameters is extractable from simulations adopting a tight-binding model as done in Ref. [22] for a strained Si quantum well sandwiched between strain-relaxed Si\(_{0.7}\)Ge\(_{0.3}\). An illustrative sketch of the theoretical model describing HQ is reported in Fig. 1.

![Figure 1](image.png)

Figure 1. A sketch of the HQ energy levels. The interdot tunnel couplings are \(\Delta_1\) and \(\Delta_2\), \(\epsilon\) is the detuning between the two QDs and \(\Delta_R\) corresponds to the low-energy splitting of the right dot.

We model the surrounding environment by a series of \(N\) harmonic oscillators with the Hamiltonian

\[
H_B = \sum_{j=1}^{N} \omega_j b_j^\dagger b_j,
\]

where \(b_j(b_j^\dagger)\) is the annihilation (creation) operator for the environment mode and \(\omega_j\) is the frequency associated to each mode \(j\).

The interaction Hamiltonian between HQ and the bath is written by [23]

\[
H_I = \sum_{j=1}^{N} \lambda_j (b_j^\dagger + b_j) \otimes \frac{1}{2} \hat{O}_S
\]

with \(\lambda_j\) representing the coupling qubit-bath and the system operator \(\hat{O}_S\) is equal to

\[
\hat{O}_S = \begin{pmatrix}
1 & 0 & 0 \\
0 & -1 & 0 \\
0 & 0 & -1
\end{pmatrix}.
\]

The total Hamiltonian given by the sum of the three contributions, i.e. \(H = H_S + H_B + H_I\), is transformed by adopting a unitary transformation \(U = [m_0, m_1, m_2]\). Each column of \(U\) contains the eigenvectors \(m_k\) of \(H_S\), in such a way that transforming \(H_S\) through \(U\), it results in a diagonal form. Explicating all the calculations for \(\tilde{H} = U^\dagger H U\), we finally obtain

\[
\tilde{H} = \begin{pmatrix}
E_0 & 0 & 0 \\
0 & E_1 & 0 \\
0 & 0 & E_2
\end{pmatrix} + \sum_{j=1}^{N} \lambda_j (b_j^\dagger + b_j) \otimes \frac{1}{2} \hat{O}_S + \tilde{H}_B,
\]

where \(E_i\) with \(i = 0, 1, 2\) are the eigenvalues of \(H_S\), \(\zeta = \sum_{j=1}^{N} \lambda_j (b_j^\dagger + b_j)\), \(\chi_{ij}\) are the transformed matrix elements of \(\hat{O}_S\) through \(U\) and \(\tilde{H}_B = H_B\).

B. Relaxation and decoherence times

We determine the explicit expressions for the relaxation and the decoherence times, firstly calculating the power spectrum \(S_\zeta(\omega)\) for a bath in thermal equilibrium at temperature \(T\). In the framework of the Lindblad master equation describing the HQ, we trace over the environmental bath degrees of freedom, obtaining

\[
S_\zeta(\omega) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \langle f(t) f(0) \rangle_\beta e^{i\omega t} dt.
\]

The correlator \(\langle f(t) f(0) \rangle_\beta\), where \(\beta \equiv (k_B T)^{-1}\), is evaluated analytically giving as a result

\[
\langle f(t) f(0) \rangle_\beta = \text{Tr}_B(e^{-\beta H_B} f(t) f(0)) = \\
= \text{Tr}_B(e^{-\beta H_B} e^{iH_B t} \zeta e^{-iH_B t} \zeta) = \\
= \sum_{j=1}^{N} \lambda_j^2 \left[ \cos (\omega_j t) \coth \left( \frac{\beta \omega_j}{2} \right) - i \sin (\omega_j t) \right],
\]

(7)
and the following relations have been exploited
\[
\langle b_j^\dagger b_j \rangle_\beta = \frac{1}{e^{\beta \omega} - 1} = \frac{1}{2} \coth \left( \frac{\beta \hbar \omega_j}{2} \right) - \frac{1}{2}, \\
\langle b_j b_j^\dagger \rangle_\beta = \langle b_j^\dagger b_j + 1 \rangle_\beta = \frac{1}{2} \coth \left( \frac{\beta \hbar \omega_j}{2} \right) + \frac{1}{2}. \tag{8}
\]
Inserting Eq. (7) into Eq. (6) we obtain
\[
S_\zeta(\omega) = \frac{\sum_{j=1}^{N} \chi_j^2}{2} \left\{ \delta(\omega + \omega_j) \left[ \coth \left( \frac{\beta \hbar \omega_j}{2} \right) - 1 \right] + \delta(\omega - \omega_j) \left[ \coth \left( \frac{\beta \hbar \omega_j}{2} \right) + 1 \right] \right\}.
\tag{9}
\]
In the hypothesis that \( N \) is large, the sum over \( j \) can be approximated by a frequency integral \( \sum_{j=1}^{N} \chi_j^2 \approx \int_{0}^{\infty} J(\omega) \ d\omega \). The parameter \( \zeta \) distinguishes among \( s=1 \) Ohmic, \( s>1 \) super-Ohmic and \( s<1 \) sub-Ohmic baths.

Following the theory \cite{24,25}, in which the Bloch-Redfield master equation has been used to describe the dynamics of the qubit interacting with the phonon bath, the relaxation time \( T_1 \), the pure dephasing time \( T_\phi \) and the decoherence time \( T_2 \) are directly linked to the power spectrum \( S_\zeta(\omega) \) by the following relations
\[
\frac{1}{T_1} = \frac{\pi}{2} \chi_0^2 \zeta_{0}(E_Q) \tag{12}
\]
\[
\frac{1}{T_\phi} = \frac{\pi}{4}(\chi_{11} - \chi_{00})^2 \zeta(0) \tag{13}
\]
\[
\frac{1}{T_2} = \frac{2}{T_1} + \frac{1}{T_\phi}, \tag{14}
\]
where \( E_Q \equiv E_1 - E_0 \) is the qubit energy.

\section*{III. RESULTS}

In this Section we report a detailed analysis on the relaxation and decoherence times when different experimental parameters related to the bath as well as to the HQ are varied.

In Fig. 2 the behaviour of the relaxation \( T_1 \) (red lines) and the decoherence \( T_2 \) (blue lines) times calculated through Eqs. \cite{12-14} is reported as a function of the bath temperature \( T \) for the three different regimes: \( s=1 \) Ohmic bath (solid lines), \( s=2 \) super-Ohmic bath (dot-dashed line) and \( s=1/2 \) sub-Ohmic bath (dashed line). The parameters of the HQ defined in Si/SiGe QDs as well as the bath parameters are taken from the literature \cite{23,26}. The relaxation time, as well as the decoherence one, increase when the bath passes from a sub-Ohmic to a super-Ohmic regime and decrease when the bath temperature grows.

Tuning appropriately the bath parameters and the electron-phonon coupling \( \eta \) and guided by experimental results in which the coherence times are estimated in the range of hundreds of ns \cite{21,22}, we choose to focus on the Ohmic regime. We analyse in Fig. 3 the relaxation \( T_1 \), the pure dephasing \( T_\phi \) and the decoherence \( T_2 \) times as a function of two significant qubit parameters that are the detuning \( \epsilon \) that is tunable from external control voltages and the low-energy splitting of the right dot \( \Delta_R \) that is linked to the qubit fabrication. We explore larger values of \( \Delta_R \) with respect to the Si/SiGe case in order to include the valley splitting achievable in Si-MOS HQs. For the 2D plots we select three significative temperatures for experimentalists, that are \( T=0.1 \) K, 0.3 K and 1.6 K.

As it is witnessed by Fig. 3 the relaxation time increases when the detuning is large and, in the region where \( \epsilon \) is smaller, the valley splitting \( \Delta_R \) has to be keep small in order to assures larger times. Looking at the pure dephasing time, it increases in the large bias region and presents also high values in a narrow section for high
\( \Delta_R \) where \((\chi_{11} - \chi_{00}) \simeq 0\) (see Eq. 13). When the relaxation time is combined to the pure dephasing time, it then gives a smaller contribution to the total decoherence time in the large bias region than at narrow section. The overall result is that the decoherence time in the large bias region rises above its values at the narrow section albeit the latter remains a local section of maximum for the coherence time. All the characteristic times generally reduce as the temperature is increased.

### A. Relaxation time

We focus now our attention on \(T_1\). In Fig. 3 we report how the two ingredients composing the \(T_1^{-1}\) behave against the detuning \(\epsilon\) and \(\Delta_R\): \(\chi_{10}^2\) is plotted in Fig. 4(a) whereas the power spectrum of the bath \(S_\zeta(E_Q)\) is presented in Fig. 4(b). Both the functions are calculated in the same range used in Fig. 3 and are marked in the plots with different symbols (circle, triangle, square and star). We also add two vertical lines highlighting the values of the detunings set to: \(\epsilon = 50\mu eV\) (cyan) and \(225\mu eV\) (green), that are the values chosen in Fig. 5(c)-(d) respectively. Fig. 5(c)-(d) show 2D plots in which \(T_1\), \(T_\varphi\) and \(T_2\) are reported as a function of \(\Delta_2\) and \(\Delta_R\) at the range boundaries explored in Fig. 4(c)-(d) and are marked in the plots with different symbols (circle, triangle, square and star). We also add two vertical lines highlighting the values of the detunings set to: \(\epsilon = 50\mu eV\) (cyan) and \(225\mu eV\) (green), that are the values chosen in Fig. 5(c)-(d) respectively. 

When the working point is set by choosing a value for \(\epsilon\), it is interesting to analyze how \(T_1\), \(T_\varphi\) and \(T_2\) are affected by the tunnel couplings, partially defined by the geometry of the HQ.

To show how this analysis is strictly connected to the HQ eigenvalues trend, we plot in Fig. 4(a) the eigenvalues of \(H_S\) and in Fig. 5(b) the qubit energy \(E_Q\) (solid black line) and its derivative with respect to \(\epsilon\), that is \(dE_Q/\partial \epsilon\) (dashed red line), both as a function of the detuning. All these quantities are calculated in correspondence to four different sets of \(\Delta_2\) and \(\Delta_R\) at the range boundaries explored in Fig. 4(c)-(d) and are marked in the plots with different symbols (circle, triangle, square and star). We also add two vertical lines highlighting the values of the detunings set to: \(\epsilon = 50\mu eV\) (cyan) and \(225\mu eV\) (green), that are the values chosen in Fig. 5(c)-(d) respectively.

### B. Pure dephasing and decoherence times

When the working point is set by choosing a value for \(\epsilon\), it is interesting to analyze how \(T_1\), \(T_\varphi\) and \(T_2\) are affected by the tunnel couplings, partially defined by the geometry of the HQ.

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Figure 5. (a) Eigenvalues of $H_S$ as a function of the detuning $\epsilon$ when $\Delta_2$ and $\Delta_R$ are set. The symbols at the corners of the subplots (circle, triangle, square and star) denote different qubit parameters (i.e. set of $(\Delta_2, \Delta_R)$ values) in correspondence to the range boundaries explored in (c) and (d). The colored vertical lines highlight the values of the detuning $\epsilon = 50 \mu eV$ (cyan) and $\epsilon = 225 \mu eV$ (green) chosen for the plots in (c) and (d) respectively. (b) Energy qubit $E_Q$ (solid black lines) and $dE_Q/d\epsilon$ (dashed red lines) as a function of $\epsilon$ for the same qubit parameter sets. (c) $T_1$ (top), $T_\phi$ (middle) and $T_2$ (bottom) as a function of $\Delta_2$ and $\Delta_R$ in correspondence to an Ohmic bath ($s = 1$) at $T=0.1$ K and $\epsilon = 50 \mu eV$. The other parameters are the same as in Fig. 2. (d) The same as (c) at $\epsilon = 225 \mu eV$.

To complete our analysis, we report in Fig. 6 the pure dephasing rate $T_\phi^{-1}$ as a function of $(dE_Q/d\epsilon)^2$ for the different temperatures studied.

As it can be seen, the pure dephasing rate of the qubit shows a linear dependence on $(dE_Q/d\epsilon)^2$ with higher temperatures leading to higher slopes. Note that the configurations where $\epsilon$ assumes high values (green symbols) assuring low $dE_Q/d\epsilon$, produce lower dephasing rates than the cases with high $dE_Q/d\epsilon$, when $\epsilon$ is low (cyan symbols).

IV. CONCLUSIONS

The phonon-induced relaxation and decoherence processes are studied in the hybrid qubit in silicon quantum dots. We extract the relaxation, pure dephasing and decoherence times as a function of the bath spectral density and of the bath temperature using the Bloch-Redfield theory. For Si quantum dots the energy dispersion is strongly affected by the physics of the valleys so the contribution of the valley excitations has been effectively included in our analysis. It is found that the characteristics of both the spectral density of the bath and the energy spectrum of the qubit play an essential role. Contribution of phonons to relaxation and pure dephasing effects is bias dependent, leading to the conclusion that the coherence time can be higher in the large bias region than at the small bias, due to stronger relaxation
and cyan symbols to $\epsilon$ (dotted line). The bath temperatures are: $T=1.6$ K (solid line), $T=0.3$ K (dashed line), $T=0.1$ K (dotted line).

Figure 6. Pure dephasing rate as a function of $(dE_Q/d\epsilon)^2$. The symbols correspond to different qubit parameters highlighted in Fig. 5 (green symbols correspond to $\epsilon = 50\mu$eV and cyan symbols to $\epsilon = 225\mu$eV). The bath temperatures are: $T=1.6$ K (solid line), $T=0.3$ K (dashed line), $T=0.1$ K (dotted line).

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