Pure dephasing of two charge qubits in vertically coupled quantum dots

W. Ben Chouikha\textsuperscript{a}, S. Jaziri\textsuperscript{b,\textsuperscript{*}}, R. Bennaceur\textsuperscript{a}

\textsuperscript{a}Laboratoire de Physique de la Matière Condensée, Faculté des Sciences de Tunis, Tunisia
\textsuperscript{b}Département de Physique, Faculté des Sciences de Bizerte, Jarzouna 7021 Bizerte, Tunisia

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Abstract

Pure dephasing of two electrons in vertically coupled quantum dots due to the interaction with acoustic and optical phonons is calculated. We study the effect of pure dephasing on the entanglement of the two-level subsystems. Our results show the role of the size and the distance between the two quantum dots on the pure dephasing rates.

1. Introduction

Semiconductor quantum dots (QDs) are often considered as candidate devices for a solid-state implementation of quantum information processing \cite{1–3}. A QD molecule might in principle provide the minimal system of two-coupled qubits required for the implementation of quantum gates \cite{2,3}.

The implementation of charge states in QD systems, recently supported by an experimental demonstration \cite{4}, has driven a lot of investigations on coherence properties of these systems. In contrast to spin qubits, charge qubits in semiconductors have the substantial advantage of being easy to manipulate and to measure since the experimental techniques for measuring single electron charges in semiconductors are extremely well-developed (the direct controllability via external voltage sources). Coherent oscillations in double quantum—dot qubit are observed \cite{5}. Robustness against decoherence in QDs is usually expected as a result of quantum confinement, implying discrete energy levels below the semiconductor band gap with a very restricted phase space available for various scattering mechanisms.

It has been demonstrated that scattering by phonons can significantly influence electron transport through double dot system \cite{6} and qubit dynamics during measurement \cite{7}.

Relaxation is not the only way that the charge can be decohered. The decoherence can due to the pure dephasing \cite{8–11}.

Entanglement is one of the fundamental constituent of quantum theory \cite{12,13}. In ideal situations, entangled states would not decohere during processing and transmission of quantum information. However, real quantum system will inevitably be influenced by surrounding environments. The entanglement, as a non-local property of a composed quantum system, should be very fragile under the influence of the environment. This fragility is a main obstacle for the realization of practical quantum computers. The pure dephasing mechanism can affect entangled states. Stavrou and Hu \cite{9} have studied the pure dephasing of one charge qubit due to electron–phonon interactions.

In this work, we analyze the pure dephasing of two electrons in double quantum-dot (DQD) due to both acoustic and optical phonons as a function of the parameters of the double dot structure. The resulting qubit is supposed to evolve in the basis spanned by the states $|0\rangle$ and $|1\rangle$ which describe the electron localized in the left and right dot, respectively.
We assume that the temperature is low enough such that the effect of electrons transitions to the higher energy levels can be neglected.

The present paper is organized as follows: in Section 2 we introduce the model system and the Hamiltonian that describes it. The DQD electrons states are described within the effective mass scheme. In Section 3, we evaluate the dephasing rates for double dot trapping two electrons due to electron–phonon interaction. We discuss the results as function of our system parameters. Section 4 is devoted to the conclusion.

2. Model system

The QD molecule consists of two vertically coupled QDs at mutual distance $2d$. We assume throughout this work that the two QDs have identical shape and size. Electrons states are described within effective mass approximation. The system Hamiltonian is thus [14–16]:

$$
H_0 = \sum_{i=1,2} \left( \frac{\hbar^2}{2m^*} \left( \frac{\partial^2}{\partial \vec{r}_i^2} \right)^2 + \frac{m^* \omega^2}{2} \left( \frac{x^2}{a_i^2} + \frac{y^2}{b_i^2} + \frac{z^2}{c_i^2} \right)^2 \right)
+ \frac{\epsilon_0^2}{|\epsilon| \left| \vec{r}_1 - \vec{r}_2 \right|} \sum_{i=1,2} h_i(\vec{r}_i, \vec{P}_i) + H_{\text{Coul}},
$$

(1)

where $\alpha$ is the anisotropy parameter which determines the strength of the vertical confinement relative to the lateral one. The last term in Eq. (1) represents the Coulomb interaction. We take as material parameters for GaAs, $m^* = 0.067m_0$ for the electron effective mass and $\epsilon_r = 13.1$ for the dielectric constant.

We consider $\alpha = 0.5$. The four lowest eigenstates of $H_0$, are given as $H_0 |\psi_n\rangle = E_n |\psi_n\rangle$ where $E_n = E_{s1}$, $E_T$, $E_{s2}$, $E_{s3}$ and $|\psi_n\rangle = |\psi_{s1}\rangle, |\psi_T\rangle, |\psi_{s2}\rangle, |\psi_{s3}\rangle$. We use the linear combination of atomic orbitals (LCAO) [17] in order to construct the one particle molecular orbital states. The single electron wave function $|\phi_{s}\rangle$ is given by a superposition of the single dot wavefunctions $|\phi_{s}\rangle = \beta_{\pm}((0 \pm 1))$, where $\beta_{\pm}$ are the normalisation coefficient which dependent of the parameters of the system.

The eigenenergies are given as

$$
E_{s1} = (\epsilon_+ + \epsilon_-) + \frac{J_+ + J_-}{2}
- \sqrt{\left( \epsilon_+ - \epsilon_- \right) + \left( \frac{J_+ + J_-}{2} \right)^2 + X^2},
$$

$$
E_{s3} = (\epsilon_+ + \epsilon_-) + \frac{J_+ + J_-}{2}
+ \sqrt{\left( \epsilon_+ - \epsilon_- \right) + \left( \frac{J_+ + J_-}{2} \right)^2 + X^2},
$$

$$
E_T = \epsilon_+ + \epsilon_- + V_-, \text{ and }
$$

$$
E_{s2} = \epsilon_+ \epsilon_- + V_+ \text{ where }
$$

$$
\epsilon_{\pm} = \langle \phi_{\pm}(\vec{r}_1)|\phi_{\pm}(\vec{r}_2)|h_1|\phi_{\pm}(\vec{r}_1)|\phi_{\pm}(\vec{r}_2)\rangle,
$$

$$
J_{\pm} = \langle \phi_{\pm}(\vec{r}_1)|\phi_{\pm}(\vec{r}_2)|H_{\text{Coul}}|\phi_{\pm}(\vec{r}_1)|\phi_{\pm}(\vec{r}_2)\rangle,
$$

$$
V_{\pm} = \langle \phi_{+}(\vec{r}_1)|\phi_{-}(\vec{r}_2) \pm \phi_{-}(\vec{r}_1)|\phi_{+}(\vec{r}_2)|H_{\text{Coul}}|\phi_{+}(\vec{r}_1)|\phi_{-}(\vec{r}_2) \pm \phi_{-}(\vec{r}_1)|\phi_{+}(\vec{r}_2)\rangle,
$$

$$
X = \langle \phi_{+}(\vec{r}_1)|\phi_{+}(\vec{r}_2)|H_{\text{Coul}}|\phi_{-}(\vec{r}_1)|\phi_{-}(\vec{r}_2)\rangle.
$$

The corresponding eigenstates are given as $\psi_{s1} = \gamma_1 \phi_{+}(\vec{r}) \phi_{+}(\vec{r}) - \delta_1 \phi_{-}(\vec{r}) \phi_{-}(\vec{r})$, $\psi_T = \frac{1}{\sqrt{2}} (\phi_{+}(\vec{r}) \phi_{-}(\vec{r}) - \phi_{-}(\vec{r}) \phi_{+}(\vec{r}))$, $\psi_{s2} = \frac{1}{\sqrt{2}} (\phi_{+}(\vec{r}) \phi_{-}(\vec{r}) + \phi_{-}(\vec{r}) \phi_{+}(\vec{r}))$, $\psi_{s3} = \delta_1 \phi_{+}(\vec{r}) \phi_{+}(\vec{r}) - \gamma_1 \phi_{-}(\vec{r}) \phi_{-}(\vec{r})$.

The coefficients $\delta_1$ and $\gamma_1$ depend on the half interdot distance $d$ for a given double QDs.

In a polar semiconductor like GaAs, electrons couple to all types of phonons. More specifically, in GaAs electrons couple to longitudinal acoustic phonons through a deformation potential, to longitudinal and transverse acoustic phonons through piezoelectric interaction, and to the optical phonons through the polar interaction. The electron–phonon Hamiltonian is given by the following expression [18]:

$$
H_{\text{int}} = \sum_{i=1,2} \sum_k \left( M_k \epsilon e^{-ik\vec{r}} a_k^+ + M_k \epsilon e^{ik\vec{r}} a_k \right),
$$

(3)

where $a_k^+$ and $a_k$ are the creation and annihilation operators of the phonons with the wave vector $k$, and $M_k$ is the bulk matrix element, which depends on the type of the interaction.

We have used in the calculations an isotropic linear phonon dispersion $\omega_k = c_s k$ for acoustic phonons and $\omega_k = \omega_{\text{LO}}$ for longitudinal optical phonons.

The bulk matrix element for the deformation potential coupling is given by

$$
M_k^{\text{def}} = \left( \frac{\hbar k}{2V\sigma c_s} \right)^{1/2} D_c,
$$

(4)

where $c_s$ is the phonon sound velocity, $\sigma$ the crystal density of GaAs, $V$ the normalisation volume and $D_c$ the deformation potential coupling constant. For our calculations, we consider $D_c = 8.6$ meV, $\sigma = 5.3$ g/cm$^3$ and $c_s = 37 \times 10^4$ cm/s.
The bulk matrix element for the piezoelectric potential is given by
\[ M_{\text{B}}^k = \frac{e\alpha_d}{\eta_0\kappa} \left( \frac{h}{2\pi\sigma_c|k|} \right)^{1/2}, \]  
where \( e\alpha_d = 0.16 \text{ C/m}^2 \) is the piezoelectric constant [19].

We use the standard Fröhlich coupling for electron–LO phonon interaction \( M_{\text{F}}^k = (A/V^{1/2}) \), where

\[ A^2 = 2\pi e^2\hbar\omega_{\text{LO}} \left( \frac{1}{\varepsilon_{\infty}} - \frac{1}{\varepsilon_r} \right), \]

where \( \varepsilon_{\infty} \) is the high frequency dielectric constant. For numerical calculations, we take \( \hbar\omega_{\text{LO}} = 36.25 \text{ meV} \) and \( \varepsilon_\infty = 10.89 \).

Now that we have identified all the electron–phonon interaction involved in our system, we are ready to evaluate the dephasing rates for two electrons in a vertically coupled QDs due to its interaction with the phonons.

3. Dephasing rates

Electron–phonon interaction causes not only relaxation between qubit states, but also dephasing between them if the electron is in a superposition state. If the energy difference between the two charge states fluctuates, phase information will get lost and decoherence occurs, such as pure dephasing due to bosonic bath. In our case we have four states for two charge qubits. We are interested in studying the dephasing for two charges qubits.

For a charge qubit, previous work used [8,9,20,21] the general analytical expression for the density operator of one electron in the bosonic bath to evaluate the dephasing rate. Here we calculate the dephasing between two charge qubits states. We have four states, so we find six dephasing rates.

For two charge qubits we introduce the density operator of two electrons in a bosonic bath written in the eigenbasis states as

\[ \rho_{ \alpha_1 \beta_1 } (0) e^{-B_{ \alpha_1 \beta_1 } (\Delta t) + i\alpha_1 \Delta t / h} \]

where \( \alpha_y = E_j - E_i \) and \( \rho_{ \alpha_y } (0) \) are the elements of the electrons density matrix written in the eigenbasis states (Eq. 2).

The exponent function \( B_{ \text{nm} } (t) \) and the factor \( I_{ \text{nm} } (k) \) are defined by

\[ B_{ \text{nm} } (t) = \frac{V}{h \pi^2} \int d^3k \frac{|M_{\text{F}}^k|^2}{\omega_k^2} |I_{ \text{nm} } (k)|^2 \sin^2 \left( \frac{\omega_k T}{2} \right) \coth \left( \frac{\hbar \omega_k}{2k_B T} \right), \]

\[ I_{ \text{nm} } (k) = \frac{1}{2} \left( \langle \psi_n | e^{ik\vec{r}_1} + e^{ik\vec{r}_2} | \psi_m \rangle - \langle \psi_m | e^{ik\vec{r}_1} + e^{ik\vec{r}_2} | \psi_n \rangle \right). \]

The last factor represents the dephasing matrix element for two charge qubits.

\[ B_{ \text{nm} } \] represents the dephasing rate due to the dephasing between the states \( \psi_n \) and \( \psi_m \).

We show that pure dephasing causes a decay in the off-diagonal element of the density matrix.

According to Eq. (2) we find that \( B_{s1s2}^2 = B_{s1sT}^2 = B_{s2s3}^2 = B_{T1s3}^2 = B_{T2s2}^2 = 0 \)

For a discussion of the qualitative behaviour of the pure dephasing rate, we first analyze the factor \( I_{ \text{nm} } (k) \).

In our calculation we find that

\[ I_{s1sT} (k) = \frac{1 - 2\delta_1^2}{2} \left( \langle \phi_{+} | e^{ik\vec{r}} | \phi_{+} \rangle - \langle \phi_{-} | e^{ik\vec{r}} | \phi_{-} \rangle \right) (1 - 2\delta_1^2) \mathcal{I} (k), \]

\[ I_{s1s3} (k) = (1 - 2\delta_1^2) \left( \langle \phi_{+} | e^{ik\vec{r}} | \phi_{+} \rangle - \langle \phi_{-} | e^{ik\vec{r}} | \phi_{-} \rangle \right) = 2 I_{s1sT} (k), \]

where \( \mathcal{I} (k) \) is the dephasing matrix element for one charge qubit (one electron in the double dot) [9]. We note that

\[ \langle \phi_{\pm} | e^{ik\vec{r}} | \phi_{\mp} \rangle = 2\beta_{\pm}^2 \exp(-k^2a^2/4) \exp(-K^2a^2/4a^2) \]

\[ \times \left( \cos(akz) - \exp(-d^2/a^2) \right), \]

where \( k = k_\perp + k_z \) (\( k_\perp \) is the in-plane component of \( k \)) and \( a \) is the characteristic dot radius \( a = \sqrt{\hbar / me\omega_z} \).

At small interdot distance \( \delta_1 \approx 1 \), we find \( I_{s1sT} (k) = \mathcal{I} (k) \); the dephasing matrix element for two charge qubits and one charge qubit are the same. At large interdot distance, we have \( 1 - 2\delta_1^2 \approx 0 \), which indicates that the pure dephasing rate decreases to zero for large distance. According to Eq. (11), the pure dephasing rate \( B_{s1s3}^2 \) should be more greater than the rate \( B_{s1sT}^2 \). The evolution of the pure dephasing rate of \( B_{s1sT}^2 \) is shown in Fig. 1. We consider \( T = 77 \text{ K}, \hbar\omega_z = 16 \text{ meV} \) and \( d = 100 \text{ Å} \). We observe that the weight of the contribution of deformation potential and piezoelectric interaction are comparable. The curves rapidly increase for the first 10 ps, after this time the dephasing rate saturates. The very fast initial dephasing is due to the interaction between the two electrons and the acoustic phonons. According to Eq. (8), we observe that the fast time dependence of dephasing is
due to the trigonometric dependence on phonon frequencies and time \( \sin^2(\omega_o t/2) \). After 10 ps, the pure dephasing rate is constant, it means that the dephasing will not produce a decaying signal in terms of, for example, oscillations in electrons. Instead, it simply reduces the contrast in charge oscillations.

Fig. 2 shows the evolution of the total rates of \( B_{s1T}^2 \) and \( B_{s1s3}^2 \) at the same parameters that in Fig. 1. It is worth to note that the dephasing rates have the same time dependence, except that the rate \( B_{s1s3}^2 \) is greater than the rate \( B_{s1T}^2 \). This can be seen from Eq. (11).

The effect of optical phonons is given by the rate:

\[
B_{mn}^2(t) = \frac{A^2}{\Pi^2(\hbar\omega_{LO})^2} \sin^2\left(\frac{\omega_{LO} t}{2}\right) \coth\left(\frac{\hbar\omega_{LO}}{2k_B T}\right)
\times \int d^2k \left| \frac{I_{mn}(\mathbf{k})}{k^2} \right|^2.
\]  

The time dependence is given by the trigonometric function \( \sin^2(\omega_o t/2) \).

The parameters of two dots on which depends the interaction with phonons are the dots size and the interdot distance. The time \( t \) is chosen to be 40 ps. The pure dephasing rate decreases to zero when the half interdot distance increases (Fig. 3(a) and (b))). The dependence on interdot distance appears in Eqs. (11) and (12). As we have already noted, for large interdot distance we have \( 1 - 2\delta_i^2 \approx 0 \). For \( d = 30 \text{ Å} \), we find \( \delta_1 = 0.996 \) and for \( d = 250 \text{ Å} \), we find \( \delta_1 = 0.708 \) \( (\delta_i^2 = 0.502) \).

We should stress on the fact that the pure dephasing rate due to acoustic phonons is much more intense than that due to optical phonons. Moreover, for large interdot distance all types of phonons do not contribute as source of dephasing (Fig. 3). The dependence of the pure dephasing rates on dot size is shown in Fig. 4. The latter shows that all curves decrease to zero as a function of the dot size. In the case of strong confinement, the pure dephasing is...
we note that for small dots the term \(\exp(-2d^2/a^2)\) goes to zero.

The effects of dephasing on two charges qubits is limited by the choice of the parameters of the system. The contribution of optical phonons in the pure dephasing is much more smaller than that of acoustic phonons.

### 4. Conclusion

In summary, we evaluated the pure dephasing rates of two charge qubits. The pure dephasing is due to the dephasing between two states of two electrons confined in vertically coupled QDs (no relaxation). Our results show that the pure dephasing rates depend on the interdot distance and the size of dots. The pure dephasing of two charge qubits is dominated by acoustic phonons.

### References