Phonon-induced entanglement dynamics of two donor-based charge quantum bits

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Received 12 September 2011, in final form 7 November 2011
Published 15 December 2011
Online at stacks.iop.org/JPhysB/45/015503

Abstract
The entanglement dynamics of a pair of donor-based charge qubits is obtained in an analytical form. The disentanglement is induced by off-resonant scattering of acoustical phonons in the semiconductor host. According to our results, a rather unusual recovery of entanglement occurs that depends on the geometrical configuration of the qubits. In addition, for large times a non-vanishing stationary entanglement is predicted. For the cases of one and two initial excitations, a simple kinetic interpretation allows for an adequate analysis of the observed dynamics. Our results also reveal a direct relation between the disentanglement rate and the inter-donor decoherence rates.

1. Introduction
Quantum information processing promises highly efficient solutions to cryptographic problems and exhaustive database searches that outperform the best known algorithms with classical computers [1]. Such quantum algorithms rely on the capability of processing correlations among quantum subsystems. The quantum part of these correlations is denoted as entanglement. Most commonly, the subsystems are identified as two-level systems, representing a quantum counterpart of classical bits, called quantum bits (qubits). Among the well-known applications of quantum information are quantum teleportation [2], superdense coding [3] and secure distribution of cryptographic keys [4].

Entanglement, being the key ingredient of such applications, at the same time is highly fragile and can be easily deteriorated during state preparation, addressing and controlling of individual qubits, and final readout. Hence, it is necessary to encode quantum information in physical systems, where entanglement is protected or can be preserved in a robust way from ambient effects. Prominent examples of physical implementations are trapped ions [5], nuclear magnetic resonance [6], atoms in cavities [7], quantum dots [8], semiconductor impurities [9], superconducting qubits [10] and impurities in diamond [11].

Among the solid-state implementations [12–14], impurities embedded in a semiconductor substrate offer the advantage of comparably easy scaling and production due to highly developed fabrication techniques. The encoding of qubits in the charge degrees of freedom of pairs of donor sites allows for the addressing of individual qubits by metallic gates [15, 16]. Tunnelling of the electron between donor sites together with Coulomb repulsion of electrons bound in neighbouring qubits has been shown to allow for the realization of a CNOT gate [15, 17]. Such a gate is the elemental building block of any quantum algorithm. Typical coherence times of such systems are limited by phonon scattering to the order of 1 ps [18–20]. Therefore, the state-preparation process must be faster and one may expect that entanglement is rapidly lost on this timescale.

In this work, we have shown that to a large extent the entanglement survives beyond this timescale, and therefore suffers further degradation only from other sources of decoherence, i.e. charge fluctuations on the control electrodes. The disentanglement dynamics is obtained in an analytical form showing non-Markovian features, similar to the decoherence dynamics of a single qubit [19–21].
Furthermore, it is shown that the disentanglement rate is directly related to inter-donor decoherence rates for the cases of one and two initial excitations. The structure of this rate can be explained by a simple kinetic interpretation that allows for the determination of the disentanglement rate from the geometry of the constituent donor sites.

The paper is organized as follows. In section 2 the dynamics of a general N-qubit system subject to off-resonant scattering of acoustical phonons is derived. Using these results the dynamics of entanglement between two qubits is analytically obtained in section 3 for the cases of one and two excitations. Finally, in section 4 we present a summary and conclusions.

2. Phonon-induced dephasing dynamics of qubits

In this section, we deduce the dynamics of the reduced density operator of the qubit system, which is induced by off-resonant scattering of acoustical phonons within the semiconductor material. It is assumed here that 2N donor sites are present to form N qubits, see figure 1. The results will later be specialized to the case of N = 2 qubits. The dynamics of a single qubit formed by two donor sites has been derived recently by us [19]. The present work goes beyond the case of two donors, which implies a more complex dynamics together with the possibility of studying the entanglement between pairs of qubits.

We consider the situation where a single electron is confined to each pair of donors, conforming the N qubits being centred at the positions \( \mathbf{r}_b \), where \( b = 1, \ldots, N \) labels the qubit under consideration. In addition, we assume that the distances between these qubits are much larger than the inter-donor vectors \( \mathbf{d}_b \) within the qubits, i.e.

\[
|\mathbf{r}_b - \mathbf{r}_{b'}| \gg |\mathbf{d}_b|, \quad \forall b, b', b''.
\]

Under these circumstances the tunnelling of electrons between different qubits can be safely neglected. Considering the interaction of the qubit charges with acoustical phonons in the semiconductor substrate at room temperature or below, off-resonant phonon scattering is the main source of decoherence in the electron dynamics [19]. This type of electron–phonon interaction is accurately described by the spin-boson Hamiltonian

\[
\hat{H} = \hbar \sum_{b} (\omega_b \hat{S}_{b,z} + \Delta_b \hat{S}_{b,x}) + \sum_{k} \hbar v_k \hat{\alpha}_k^\dagger \hat{\alpha}_k
\]

\[
+ \hbar \sum_{b} (\hat{S}_{b,z} \sum_{k} (g_{b,k} \hat{\alpha}_k^\dagger + g_{b,k}^* \hat{\alpha}_k)),
\]

where the individual interaction rate of qubit \( b \) reads

\[
g_{b,k} = \frac{D}{\hbar} \sqrt{\frac{2\hbar v_k}{M_0}} \frac{m_b}{m_{b,k}} \frac{e^{-i k (r_b + m_{b,k} d_b)}}{\left[1 + \left(\frac{m_{b,k}}{2}ight)^2\right]}. \tag{3}
\]

Here, \( \hat{\alpha}_k \) are the annihilation operators of a longitudinal acoustic phonon with the dispersion relation \( \nu_k = sk \), with \( s \) being the sound speed. Moreover, \( M_0 \) is the mass within the unit cell and \( D \) is the deformation constant of the semiconductor. Each donor site is described by a s-wave ground state with the Bohr radius \( a_0, m_0 \), and the electronic transition of each qubit \( b \) is generated by the pseudo-spin-1/2 operator \( \hat{S}_{b,x} \), where

\[
\hat{S}_{b,z} = \frac{1}{2} \left( \left| r_b + \frac{d_b}{2} \right| - \left| r_b - \frac{d_b}{2} \right| \right), \tag{4}
\]

with \( |r_b \pm d_b/2| \) being the states with the electron being localized at the corresponding donor site. In what follows, we assume that during the free evolution of the system, tunnelling is inhibited by either an applied potential barrier between the donor sites, or due to a strong bias between the qubit levels, \( |\omega_b| \gg |\Delta_b| \), which can be provided for by the application of a dc electric field.

Following the same steps as in our previous work [19], the Hamiltonian (2) can be diagonalized to obtain the complete set of eigenstates as displaced number states

\[
|E_{(s)}, (N_k) \rangle = |(m_b) \rangle \otimes \hat{D}\left(\{\alpha_{(s)}, k\}\right)|\{N_k\}\rangle. \tag{5}
\]

with eigenenergies

\[
E_{(s)}, (N_k) = \hbar \sum_{b} (\omega_b m_b + \hbar v_k N_k) \tag{6}
\]

Here the multi-mode displacement operator reads

\[
\hat{D}(\{\alpha_k\}) = \exp \left( \sum_{k} (\alpha_k \hat{\alpha}_k^\dagger - \alpha_k^* \hat{\alpha}_k) \right) \tag{7}
\]

and \( |\{N_k\}\rangle = \prod_k |N_k\rangle \) are multi-mode number states of the acoustic phonons, and the displacement amplitude reads

\[
\alpha_{(s), k} = \sum_b m_b \alpha_{b,k}. \tag{8}
\]
where $a_{\theta b} = g_{\theta b}/\nu_k$. Furthermore, the quantum state of the qubits is encoded in the register state

$$|{m}_b\rangle = |{m}_1\rangle \otimes |{m}_2\rangle \otimes \cdots \otimes |{m}_N\rangle,$$

(9)

where each of the qubits can be in states $|{m}_b\rangle = \pm \frac{1}{2}$ ($b = 1, \ldots, N$).

Given the eigenstates (5) and eigenenergies (6), the general solution of the reduced density operator of the qubits, i.e. traced over the phonons, reads

$$\hat{\rho}(t) = \sum_{|{m}_b\rangle} \langle {m}_b| \langle{E}|_{|{m}_b\rangle} \langle{E}|_{|{m}_b\rangle} |{m}_b\rangle.$$

(10)

Here the matrix elements of the initial density operator of the complete electron–phonon system in the basis of the energy eigenstates (5) are

$$\hat{\rho}(t) = \sum_{|{m}_b\rangle} \langle E_{|{m}_b\rangle} |{m}_b\rangle \langle E_{|{m}_b\rangle} |{m}_b\rangle.$$

(11)

These density matrix elements are determined by the state-preparation process that is utilized to set up the initial entanglement between the qubits. A generic state-preparation process can be described as follows.

We assume that initially the system is at low enough temperature, $k_B T \ll h\nu_k$, such that it has relaxed completely into a state where all the qubits are in their lowest energy states, $|{m}_b\rangle = -1/2$ ($b = 1, \ldots, N$) and coexist in thermal equilibrium with the phonons in the substrate. Starting from this state, the system undergoes a state-preparation process in which the qubits can be coherently transferred into a superposition of ground and excited states, without affecting the quantum state of the phonons. The probability amplitudes to transfer from the initial qubit state $\frac{-1}{2}, -\frac{1}{2}, \ldots, -\frac{1}{2}$ to the qubit states $|{m}_b\rangle$ shall be denoted by $\hat{\psi}_{|{m}_b\rangle}$. The corresponding transition can be generated by the application of the operator

$$\hat{S}_{+}|{m}_b\rangle = \Pi_0 \left[ \delta_{m_0, \frac{1}{2}} \right] \hat{S}_{+} + \left( 1 - \delta_{m_0, \frac{1}{2}} \right) \hat{S}_{-}.$$

(12)

where $\hat{S}_{\pm}$ is the identity operator in the Hilbert space of qubit $b$. Thus, the matrix elements of the prepared initial state (11) become

$$\hat{\rho}_{|{m}_b\rangle} = \hat{\psi}_{|{m}_b\rangle} \hat{S}_{+} = \hat{\psi}_{|{m}_b\rangle} \hat{S}_{+} |{m}_b\rangle \langle{E}|_{|{m}_b\rangle} \langle{E}|_{|{m}_b\rangle} |{m}_b\rangle.$$

(13)

where

$$\hat{\psi}_{|{m}_b\rangle} = \sum_{|{m}_b\rangle} P_{|{m}_b\rangle} |{m}_b\rangle \langle{E}|_{|{m}_b\rangle} \langle{E}|_{|{m}_b\rangle} |{m}_b\rangle.$$

(14)

is the initial thermal state with the phonon statistics

$$P_{|{m}_b\rangle} = Z^{-1} \exp \left( -\sum_k g_{kk} N_k \right).$$

(15)

with $Z$ satisfying $\sum_{|{m}_b\rangle} P_{|{m}_b\rangle} = 1$, and $g_{kk} = \hbar \nu_k / k_B T$.

We note that the corresponding prepared initial reduced density operator of the qubits is pure, i.e. is of the form $|\psi(0)\rangle\langle\psi(0)|$, with the qubit state being the sought superposition

$$|\psi(0)\rangle = \sum_{|{m}_b\rangle} \psi_{|{m}_b\rangle} |{m}_b\rangle.$$

(16)

Thus, the presence of the phonons does not prevent a coherent preparation of the initial qubit state.

The generic state preparation, as described above, can be implemented for example by switching the gate voltages so that the on-site energies within a qubit cross each other inducing Landau–Zener transitions. At the end of the process, the system will be in a coherent superposition of all possible states of the system depending on how fast its two-level components were driven across the level crossing. Alternatively, it may be implemented by time-controlled tunnelling and employing the Coulomb repulsion between neighbouring qubits to generate entangled qubit states, as proposed for implementing CNOT gates [15, 17]. Furthermore, it could also be implemented by THz Raman transitions between the donor sites [22].

We note that the matrix elements of the initial reduced electronic density operator are obtained from equation (10) as

$$\langle{E}|_{|{m}_b\rangle} \langle{E}|_{|{m}_b\rangle} |{m}_b\rangle.$$

(17)

with the non-diagonal elements containing the Franck–Condon-type transition amplitudes:

$$\chi_{|{m}_b\rangle} = \langle{E}|_{|{m}_b\rangle} \langle{E}|_{|{m}_b\rangle} |{m}_b\rangle.$$

(18)

These factors are overlap integrals of two displaced phonon number states with displacements $\alpha_{|{m}_b\rangle}$ and $\alpha_{|{m}_b\rangle}$, respectively. Their presence is due to the fact that the initial density matrix of the complete electron–phonon system (11) is in the basis of the energy eigenstates (5), whereas the matrix elements of equation (17) are in the basis of the product states $|{m}_b\rangle \otimes |{m}_b\rangle$ that differ by the displacement of the phonons.

Consistent with a dephasing model, the diagonal elements follow from equation (10) as invariants:

$$|{m}_b\rangle \langle{E}|_{|{m}_b\rangle} \langle{E}|_{|{m}_b\rangle} |{m}_b\rangle.$$

(19)

However, this dephasing—being induced by off-resonant scattering of acoustical phonons—modifies the time evolution of the off-diagonal density matrix elements as

$$\langle{E}|_{|{m}_b\rangle} \langle{E}|_{|{m}_b\rangle} |{m}_b\rangle.$$

(20)

It can be observed in equation (20) that apart from the free oscillation with angular frequencies $\omega_{b\nu_k}$, a dephasing is induced by differing phonon numbers in combination with the presence of the Franck–Condon factor.

To further evaluate the dephasing of the off-diagonal density matrix elements of the $N$ qubits, we insert the initial
complete density matrix elements (11) together with equation (14) into equation (20). From this we obtain
\[
\langl|m_b\rangle|\hat{\xi}(t)|\langle n_b\rangle\rangle = \psi^{*}_{|m_b\rangle}\psi_{|n_b\rangle} e^{-i\sum_{m_b \rightarrow n_b}\omega_{m_b}t} \\
\times \sum_{|M_b\rangle} P_{|M_b\rangle} \sum_{N_b,N_b'} e^{-i\sum_{m_b \rightarrow n_b}v_{N_b} N_b' + 1} \\
\times f_{|n_b\rangle}\{N_b'|{-\frac{1}{2}},...,-\frac{1}{2}\} f_{|n_b\rangle}\{N_b|{-\frac{1}{2}},...,-\frac{1}{2}\} \\
\times f_{|n_b\rangle}\{N_b'|{-\frac{1}{2}},...,-\frac{1}{2}\} f_{|n_b\rangle}\{N_b|{-\frac{1}{2}},...,-\frac{1}{2}\}. \\
\] (21)

Employing the thermal phonon statistics (15), the sum over the phonon numbers in equation (21) can be rewritten as a trace, which leaves us with
\[
\langl|m_b\rangle|\hat{\xi}(t)|\langle n_b\rangle\rangle = \psi^{*}_{|m_b\rangle}\psi_{|n_b\rangle} e^{-i\sum_{m_b \rightarrow n_b}v_{N_b} N_b' + 1} \\
\times \text{Tr}\{\hat{D}(\{\alpha_{|m_b\rangle},t\})\hat{D}(\{\alpha_{|n_b\rangle},t\})\} \\
\times \hat{D}(\{\alpha_{|m_b\rangle},t\})\hat{D}(\{\alpha_{|n_b\rangle},t\}) \\
\times e^{-\sum_{N_b} v_{N_b} N_b'}.
\] (22)

where we defined the time-dependent phonon displacement amplitude \(\alpha_{|m_b\rangle}(t) = \alpha_{|m_b\rangle} \exp(-iv_{N_b}t)\). The displacement operators in equation (22) can be combined to obtain
\[
\langl|m_b\rangle|\hat{\xi}(t)|\langle n_b\rangle\rangle = \psi^{*}_{|m_b\rangle}\psi_{|n_b\rangle} e^{-i\sum_{m_b \rightarrow n_b}v_{N_b} N_b' + 1} \\
\times e^{-2i(h\omega_{m_b} + 1)} e^{-\sum_{N_b} v_{N_b} N_b'}.
\] (23)

with the time-dependent phase being
\[
\Delta_{|m_b\rangle,|n_b\rangle}(t) = \sum_{k} \alpha_{|n_b\rangle},|k\rangle \alpha^{*}_{|m_b\rangle},|k\rangle (e^{iv_{N_b}t} - 1).
\] (24)

Here we have defined sum and difference displacements:
\[
\alpha_{|m_b\rangle,|n_b\rangle} = \alpha_{|m_b\rangle} + \alpha_{|n_b\rangle} - 2\alpha_{|\frac{1}{2},...,-\frac{1}{2}\rangle},
\] (25)
\[
\delta_{|m_b\rangle,|n_b\rangle} = \alpha_{|m_b\rangle} - \alpha_{|n_b\rangle}.
\] (26)

The trace in equation (23) represents a thermal average that can be evaluated in phase space to obtain
\[
\langl|m_b\rangle|\hat{\xi}(t)|\langle n_b\rangle\rangle = \psi^{*}_{|m_b\rangle}\psi_{|n_b\rangle} e^{-i\sum_{m_b \rightarrow n_b}v_{N_b} N_b' + 1} \\
\times \text{exp}\left\{ - \int_{0}^{t} dt' \Gamma_{|m_b\rangle,|n_b\rangle}(t') \right\},
\] (27)

where the decoherence rate of the qubit state is defined as
\[
\Gamma_{|m_b\rangle,|n_b\rangle}(t) = \sum_{b,b'} (m_b - s_b)(m_{b'} - s_{b'})\gamma_{b,b'}(t).
\] (28)

Whereas this rate depends on the quantum numbers of the density matrix element under consideration, the relation of pairs of bits is governed by the inter-bit decorrelation rate, given by
\[
\gamma_{b,b'}(t) = 4 \sum_{m_{b'}} m_{b'} s_{b'} \gamma_{|b\rangle,|b\rangle,|m_{b'}\rangle,|s_{b'}\rangle,|b,|b',|b'\rangle,|s_{b'}\rangle}. (29)

This rate in turn depends via the inter-donor decoherence rate \(\gamma(t; a, a', l)\) on the Bohr radius of the four donor sites of the two qubits and on the six possible distances between these four donors,
\[
l_{b,m_{b'},s_{b'}} = |r_{b} + m_{b}\mathbf{d}_{b} - (r_{b'} + s_{b}\mathbf{d}_{b'})|.
\] (30)

Moreover, the inter-donor decoherence rate is obtained from equations (23)–(30) as
\[
\gamma(t; a, a', l) = \Gamma_{B} \left( \frac{4a_{B}a_{B}a_{B}a_{B}}{(2\pi)^{4}} \right)^{2} \sum_{\sigma = \pm 1} \sigma \left( \frac{l - \sigma s t}{a_{B}} \right)^{2} \\
+ \frac{2}{a_{B}^{2}} \left( \frac{5a_{B}a_{B}a_{B}a_{B}}{(2\pi)^{4}} \right)^{2} e^{-2|l - \sigma s t|/a_{B} + (a \leftrightarrow a')} \right). (31)
\]

In this expression the temperature-dependent rate reads \(\Gamma_{B} = \omega_{B}(T/T_{B})\), where the convenient temperature scale is chosen as
\[
k_{B}T_{B} = N_{B} a_{B}^{2} \left( \frac{\hbar a_{B}}{D} \right)^{2}.
\] (32)

Here, \(\omega_{B} = 2\pi s/a_{B}\), with \(a_{B}\) being the average Bohr radius of all donor sites, and \(N_{B}\) is the number of unit cells within the average Bohr volume \(a_{B}^{3}\).

In the limit of identical donor sites, \(a_{B,m_{b}} \rightarrow a_{B} (b = 1, \ldots, N)\), the inter-donor decoherence rate (31) approaches the form \(\gamma(t; a, a', l) \rightarrow \gamma(t; l)\) with
\[
\gamma(t; l) = \Gamma_{B} \frac{a_{B}a_{B}}{l} \sum_{\sigma = \pm 1} \sigma \left( \frac{l - \sigma s t}{a_{B}} \right)^{2} \\
+ \frac{5}{a_{B}^{2}} \left( \frac{5a_{B}a_{B}a_{B}}{(2\pi)^{4}} \right)^{2} e^{-2|l - \sigma s t|/a_{B}}.
\] (33)

We note that in the limit of the vanishing distance between the donor sites, \(l \rightarrow 0\), this function becomes
\[
\gamma(t; 0) = \Gamma_{B} \left( \frac{2}{3} \left( \frac{s t}{a_{B}} \right)^{3} + \left( \frac{s t}{a_{B}} \right)^{2} + \frac{2}{a_{B}^{2}} \left( \frac{s t}{a_{B}} \right) \right) e^{-2st/a_{B}}.
\] (34)

This is a function peaked at \(t \sim a_{B}/s\), i.e. at the time a phonon needs to travel the distance of 1 Bohr radius, see figure 2 (red curve). Different from this special case \((l \rightarrow 0)\) for \(l > 0\), the inter-donor decoherence rate is peaked at the time \(t \sim l/s\) that is required for a phonon to travel the distance \(l\), see figure 2 (green and blue curves).
3. Dynamics of entanglement between two qubits

In the following, we will discuss the special case of two qubits being present in the semiconductor system, i.e. \( N = 2 \). In this case, the state of the qubits \(|m_2\rangle\), with \( b = 1, 2 \) lives in a four-dimensional Hilbert space and the entanglement of this bipartite system can be described by the concurrence \( C \)[23]. This quantity is a measure of entanglement bounded in the range between 0 and 1, with the maximum entanglement corresponding to unit concurrence. On the other hand, for separable states, lacking any entanglement, the concurrence is zero.

Furthermore, due to the pure dephasing effect of the phonon scattering, no transitions of the qubits are induced. Therefore, the phonon scattering will transform an initial general superposition state

\[
|\psi(0)\rangle = \sum_{m_1, m_2} \psi_{m_1 m_2} |m_1, m_2\rangle,
\]

into a non-pure statistical mixture of only those states that initially already existed. Thus, during the time evolution the density operator stays within the Hilbert subspace defined by the initial state. This feature allows us to separately treat the two prominent cases of having initially one or two ‘excitations’, respectively.

3.1. The case of one excitation

Assume the initial state of the two qubits to be of the form

\[
|\psi(0)\rangle = \psi_{\{1, -\frac{1}{2}\}} |\frac{1}{2}, \frac{1}{2}\rangle + \psi_{\{-\frac{1}{2}, \frac{1}{2}\}} |\frac{1}{2}, -\frac{1}{2}\rangle.
\]

Since only one of the qubits is in its ‘excited’ state, this superposition is usually denoted as the ‘one-excitation’ case. Choosing the basis vectors of the bipartite system as \(|\{\frac{1}{2}, \frac{1}{2}\}\rangle, |\{\frac{1}{2}, -\frac{1}{2}\}\rangle, |\{-\frac{1}{2}, \frac{1}{2}\}\rangle, |\{-\frac{1}{2}, -\frac{1}{2}\}\rangle\rangle\), following equation (27), the time-dependent density matrix can be written as

\[
\rho(t) = \begin{pmatrix}
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{pmatrix}.
\]

For this particular form of the density matrix, the concurrence simplifies to

\[
C(t) = 2|\psi_{\{\frac{1}{2}, -\frac{1}{2}\}}|\psi_{\{-\frac{1}{2}, \frac{1}{2}\}}|t|.
\]

Inserting the corresponding density matrix element from equation (27) into equation (38), the concurrence results as

\[
C(t) = 2\sqrt{p(1-p)} \exp\left[-\int_0^t dt' \Gamma_{\{\frac{1}{2}, -\frac{1}{2}\}}|\psi_{\{-\frac{1}{2}, \frac{1}{2}\}}|t'\right],
\]

where \( p = |\psi_{\{\frac{1}{2}, -\frac{1}{2}\}}|^2 \) is the initial probability for the two qubits being in state \(|\{\frac{1}{2}, -\frac{1}{2}\}\rangle\rangle\rangle\). The maximum initial concurrence is of course obtained for equal weights, \( p = 1/2 \), of the two constituent states.

From equation (39) it becomes apparent that the decoherence rate of the state of the qubits acts as a disentanglement rate. This rate is shown in figure 3 for qubits with \( d_1 = d_2 = 10a_0 \), an inter-qubit distance of \( 20a_0 \) and a relative angle of \( 45^\circ \), see the inset of figure 3. It shows a series of alternating maxima and minima at increasing times. The principal positive maximum at the beginning occurs at \( t \approx a_0/\tau \), which is the time needed by the phonon to travel within a donor site. This is the main source of disentanglement. The times of the subsequent extrema can be identified as the travel times between pairs of donor sites, as indicated in the inset of figure 3. Whereas the positive maxima destroy, the negative minima restore the entanglement between the qubits. The mapping of the phonon path between the donor sites leads to positive or negative extrema in the disentanglement rate, which can be established as follows.

The concurrence is given by the modulus of the density matrix element \( \psi_{\{\frac{1}{2}, -\frac{1}{2}\}}|\psi_{\{-\frac{1}{2}, \frac{1}{2}\}}|t\rangle\rangle\rangle\) that describes the time-dependent correlation between states \(|\{-\frac{1}{2}, \frac{1}{2}\}\rangle\rangle\rangle\) and \(|\{\frac{1}{2}, -\frac{1}{2}\}\rangle\rangle\rangle\). Correlations between these states can only be created when a phonon travels between a donor site occupied by one state to another donor site that is occupied by the other state. The corresponding site occupations of each of the states involved are indicated in the inset of figure 3 by black and white, respectively. The sites of each qubit are marked by blue for \( m_b = -\frac{1}{2} \) and red for \( m_b = +\frac{1}{2} \). With this colour scheme, the creation of correlations mediated by sound waves is produced via phonon travels between a black and a white donor site.

These phonon travels are: the passage within the individual qubits for the distance \( 10a_0 \), that produces in figure 3 the negative minimum 1, and the passages between blue and red sites at distances \( 16.5a_0 \) and \( 23.6a_0 \) that produce the minima 2 and 4. All of the other phonon passages produce decorrelation and destroy the entanglement at distances \( 18.6a_0 \) and \( 25.0a_0 \), which generate the positive maxima 3 and 5 in figure 3.

We note that diminishing the \( 45^\circ \) angle between the qubit axes results in lengths 2 and 4, and lengths 3 and 5, respectively, becoming progressively comparable. In the limiting case of...
two collinear qubits, i.e. 0° angle, these pairs of lengths are identical so that as a consequence the disentanglement rate shows only two positive and two negative peaks, as shown in figure 4(a). On the other hand, as one approaches the limiting angle of 90°, i.e. the CNOT configuration [15, 17], the extrema first sparse and finally peaks 2 and 4 cancel peaks 3 and 5, respectively. As a result, the disentanglement rate shows only the principal positive peak at \( t \approx a_B/s \), see figure 4(b).

The evolution of the concurrence for the case of 45° between the qubit axes is shown in figure 5. It can be seen that a stationary and non-vanishing value of the concurrence is reached for large times. Moreover, the temperature dependence indicates only a minor loss of entanglement at temperatures \( T/T_B < 0.01 \). Given that for P impurities embedded in a Si substrate the characteristic temperature is of the order of \( T_B \approx 300 \text{ K} \), this case corresponds to liquid He temperatures.

Note that in order to enhance the separation and visibility of individual peaks, we have chosen, for the case shown above, rather closely spaced qubits with a distance only twice as large as the distance between donor sites within the qubits. Strictly speaking, the validity of our model requires ratios

\[
\begin{align*}
\rho(t) & = \begin{pmatrix}
\varrho_{1\frac{1}{2}, 1\frac{1}{2}}(t) & 0 & 0 & \varrho_{1\frac{1}{2}, 1\frac{1}{2}}(-\frac{1}{2}, -\frac{1}{2})(t) \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
\varrho_{1\frac{1}{2}, -1\frac{1}{2}}(t) & 0 & 0 & \varrho_{1\frac{1}{2}, -1\frac{1}{2}}(-\frac{1}{2}, -\frac{1}{2})(t)
\end{pmatrix},
\end{align*}
\]

Also for this case the concurrence simplifies to a simple expression, given by

\[
C(t) = 2\left| \varrho_{1\frac{1}{2}, -1\frac{1}{2}, -1\frac{1}{2}, -1\frac{1}{2}}(t) \right|,
\]

which, after insertion of equation (27), becomes

\[
C(t) = 2\sqrt{p(1-p)} \exp \left[ -\int_{0}^{t} dt' \Gamma_{1\frac{1}{2}, 1\frac{1}{2}, -1\frac{1}{2}, -1\frac{1}{2}}(t') \right].
\]
of the cases of one and two excitations, respectively. The offset shows the geometrical configuration of the donor sites: \( d_1 = d_2 = 10a_B, \) \( |r_1 - r_2| = 20a_B, \) 45° angle between the qubit axes. The rounded lengths of the inter-donor distances in units of \( a_B \) are as follows: \( l/a_B = 10 \) (1), 16.53 (2), 18.6 (3), 23.6 (4), 25.0 (5).

3.3. The case of a general X-shaped density matrix

In fact, the above analysis can be extended to the more general case of an initial X-shaped density matrix,

\[
\rho(t) = \begin{pmatrix}
\rho_{11}^{(2,1)} & \rho_{12}^{(2,1)} & \rho_{13}^{(2,1)} & \rho_{14}^{(2,1)} \\
\rho_{21}^{(2,1)} & \rho_{22}^{(2,1)} & \rho_{23}^{(2,1)} & \rho_{24}^{(2,1)} \\
\rho_{31}^{(2,1)} & \rho_{32}^{(2,1)} & \rho_{33}^{(2,1)} & \rho_{34}^{(2,1)} \\
\rho_{41}^{(2,1)} & \rho_{42}^{(2,1)} & \rho_{43}^{(2,1)} & \rho_{44}^{(2,1)}
\end{pmatrix}
\]

In general, a state of this form is a statistical mixture. Only the special cases of one and two excitations, as discussed above, correspond to pure states.

As before, the concurrence can be obtained in an analytic form, and reads

\[
C(t) = 2 \max \{0, f_1(t), f_2(t)\},
\]

where we defined

\[
f_1(t) = \frac{\rho_{12}^{(2,1)}(t) - \rho_{34}^{(2,1)}(t)}{\sqrt{\rho_{12}^{(2,1)}(0)\rho_{34}^{(2,1)}(0)}}, \quad f_2(t) = \frac{\rho_{13}^{(2,1)}(t) - \rho_{24}^{(2,1)}(t)}{\sqrt{\rho_{13}^{(2,1)}(0)\rho_{24}^{(2,1)}(0)}}.
\]

In [24] a spin-boson Hamiltonian with generic coupling constants was studied, and it was shown that the initial state could be classified as robust or fragile. Whereas robust states maintain a non-vanishing concurrence at large times, fragile states suffer from a complete decay of their concurrence. In our case, choosing an initial mixture of maximally entangled one- and two-excitation states, the classification between robust and fragile states depends both on the weights of the initial statistically mixed state and on temperature. Robust states are transformed into fragile ones, either by increasing the temperature or by approaching the equally weighted statistical mixture.

4. Summary and outlook

In this paper, we considered the time evolution of entanglement in donor-based charge qubits that is induced by off-resonant scattering with acoustical phonons. We showed that this system can be solved analytically and that a non-Markovian behaviour emerges with negative disentanglement rates, leading to non-monotonic disentanglement in time. Moreover, for the cases of one and two initial excitations the disentanglement rate is proportional to the decoherence rate of the two-qubit state. In both cases, the concurrence attains a stationary and non-vanishing value at large times, which means that phonon scattering does not completely destroy the entanglement of the initially prepared two-qubit state. For a more general case of a density matrix in X shape, the behaviour of the case of either one or two excitations is recovered with an additional negative offset that may lead to entanglement sudden death and birth.

The choice of the geometry of the donor sites determines the features of the concurrence as a time-dependent function. These features can be understood by a simple kinetic
interpretation of phonon travels among the donor sites. In this work, we focused on the cases of initially one and two excitations, and general X-shaped density matrices, where analytic expressions for the concurrence could be found. However, we believe that this framework could also be useful for more general states beyond the limitation of being X-shaped. Furthermore, our model already includes the case of \( N > 2 \) qubits, where a trace over \( N - 2 \) qubits would be required to obtain the entanglement between a selected pair of qubits. This will be the subject of future work.

Acknowledgments

SW thanks J H Eberly for valuable discussions. FL and SW acknowledge support by grant FONDECYT 1095214. FL acknowledges support from Financiamiento Basal project no 0807. SW acknowledges support by grants NSF PHY-0855701 and ARO W911NF0910385.

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