Decoherence of charge states in double quantum dots due to cotunneling

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Abstract

Solid state quantum bits are a promising candidate for the realization of a *scalable* quantum computer, however, they are usually strongly limited by decoherence. We consider a double quantum dot charge qubit, whose basis states are defined by the position of an additional electron in the system of two laterally coupled quantum dots. The coupling of these two states can be controlled externally by a quantum point contact between the two dots. We discuss the decoherence through coupling to the electronic leads due to cotunneling processes. We focus on a simple Gedanken experiment, where the system is initially brought into a superposition and then the inter-dot coupling is removed nonadiabatically. We treat the system by invoking the Schrieffer-Wolff transformation in order to obtain a transformed Hamiltonian describing the cotunneling, and then obtain the dynamics of the density matrix using the Bloch-Redfield theory. As a main result, we show that there is energy relaxation even in the absence of inter-dot coupling. This is in contrast to what would be expected from the Spin-Boson model and is due to the fact that a quantum dot is coupled to *two* distinct baths.

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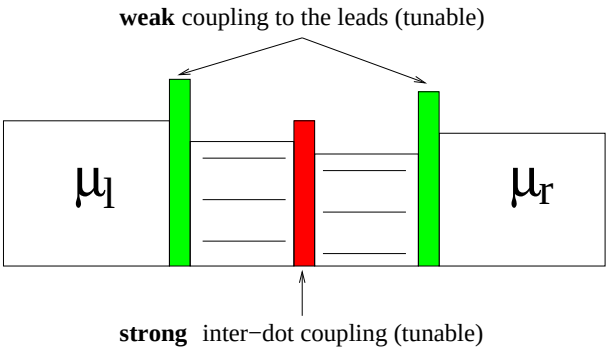

FIG. 1: Sketch of the double dot system. The coupling of the double dot to the leads is assumed to be weak, whereas the coupling between the dots can be strong. The leads are biased such that sequential tunneling is supressed.

Quantum dots ("artificial atoms") are prototype systems for studying the properties of discrete levels embedded in a solid-state environment [1]. In particular, various schemes for realizing quantum bits, fully controlled quantum coherent two-state systems, using quantum dots have been brought forward. Next to using optically excited charge states in quantum dots [2] and electronic quantum dots used for spin manipulation [3], it has been proposed [4] to use the charge states of a double quantum dot as a computational basis. The proposed setup is sketched in Figure 1. In order to minimize the inevitable decoherence through coupling to the electronic leads, the system can be brought into the Coulomb blockade regime where sequential tunneling is supressed. We are going to discuss in this article, how the inevitable cotunneling still decoheres the system in this regime. The calculation is carried out for one specific Gedanken experiment which should capture the most generic features, the decay of a superposition state when the coupling between the dots is switched off. A more complete treatment of this setup is in preparation [5].

We restrict our analysis on spin-polarized electrons. The relevant Hilbert space is characterized by four basis states, written as $|i,j\rangle$, which denotes i additional electrons on the left dot, j additional electrons on the right dot. The two states $|1,0\rangle$ and $|0,1\rangle$ define the computational basis [6]. In order to describe cotunneling, we use the closest energetically forbidden states as virtual intermediate states. These are $|v_0\rangle = |0,0\rangle$ and $|v_2\rangle = |1,1\rangle$. Zero- and two electron states with internal polarization are energetically even less favorable due to the high charging energy of the individual dots.

The Hamiltonian of this system can be written as

$$
\begin{aligned}
H &= H_0 + H_1 && (1)\\
H_0 &= \epsilon_{\mathrm{as}}(\hat{n}_l - \hat{n}_r) - \epsilon_\alpha \hat{n}_{v_0} + \epsilon_\beta \hat{n}_{v_2} \\
&\quad + \gamma \sum_n (a_n^{L\dagger} a_n^R + a_n^{R\dagger} a_n^L) + \sum_{\vec{k}} \epsilon_{\vec{k}}^L b_{\vec{k}}^{L\dagger} b_{\vec{k}}^L + \sum_{\vec{k\prime}} \epsilon_{\vec{k\prime}}^R b_{\vec{k\prime}}^{R\dagger} b_{\vec{k\prime}}^R && (2)\\
H_1 &= t_c \sum_{\vec{k},n} (a_n^{L\dagger} b_{\vec{k}}^L + a_n^L b_{\vec{k}}^{L\dagger}) + t_c \sum_{\vec{k\prime},m} (a_m^{R\dagger} b_{\vec{k\prime}}^R + a_m^R b_{\vec{k\prime}}^{R\dagger}) && (3)
\end{aligned}
$$

Note, that the sum over dot states only runs over the restricted Hilbert space described above. H_0 describes the energy spectrum of the uncoupled system, whereas the tunneling part H_1 describes the coupling of each dot to its lead and will be treated as a perturbation. $\hat{n}_{l/r}$ are the number operators for the additional electrons on either dot. The asymmetry energy ϵ_{as} describes the difference between the energy level for the additional electron in left dot and the corresponding energy level in the right dot. It can be tuned through via the gate voltages which are applied at each dot. ϵ_β and ϵ_α are the energy differences towards the higher level $|v_2\rangle$ and the lower level $|v_0\rangle$ respectively. γ is the tunable inter-dot coupling. The $a^{(\dagger)}$s and $b^{(\dagger)}$s denote the creation/destruction operators in the dots and leads. In H_1 the symbol t_c represents the coupling constant concerning the coupling of the dots to the leads, which should be small compared to the asymmetry energy. Note, that we have chosen a slightly asymmetric notation in order to highlight the physical model: For the actual calculation, H_1 is also expressed in the eigenstate basis of the dot.

For our Gedanken experiment, we assume that first the inter-dot coupling γ is large ($\gamma \gg \epsilon_{\mathrm{as}}, V$) such that the system relaxes into the ground state, which is a molecular superposition state of the form $|g\rangle = (|0,1\rangle - |1,0\rangle)/\sqrt{2}$. Then the gate voltage that controls the inter-dot coupling is switched to high values, so that the coupling is practically zero. After this, the system dephases and relaxes into a thermal mixture of the localized eigenstates of the new system.

Thus, in order to describe decoherence, we only have to consider the case $\gamma = 0$ K. This means, that H_0 is already diagonal, i.e. the states $|1,1\rangle$, $|1,0\rangle$, $|0,1\rangle$ and $|0,0\rangle$ are eigenstates of our system.

The decoherence is analyzed applying the well-established Bloch-Redfield theory, which is based on the Born approximation in the system-bath coupling. As we are in the Coulomb blockade regime, the rates evaluated from the original coupling Hamiltonian H_1 vanish in

that order. In order to treat cotunneling with this formalism, we perform a generalized Schrieffer-Wolf transformation [7, 8]. This transformation maps our original Hamiltonian H_1, which is zero in the computational basis but couples the computational states to the $|v_{0/2}\rangle$ onto a Hamiltonian which does *not* have this coupling to higher states but which has nonzero matrix elements in the computational basis. The new terms in the Hamiltonian describe the amplitude of transitions between the basis states via the intermediate states. We perform this transformation perturbatively up to second order, i.e. all processes involving at most *one* intermediate state are taken into account.

The new Hamiltomian H_I in our special case then can be written as

$$H_{I,++} = A(R\dagger, R, ++)\ b_m^{R\dagger} b_n^R + A(L, L\dagger, ++)\ b_l^L b_k^{L\dagger} \tag{4}$$

$$H_{I,--} = A(L\dagger, L, --)\ b_k^{L\dagger} b_l^L + A(R, R\dagger, --)\ b_n^R b_m^{R\dagger} \tag{5}$$

$$H_{I,+-} = A(R\dagger, L, +-)\ b_m^{R\dagger} b_l^L + A(L, R\dagger, +-)\ b_l^L b_m^{R\dagger} \tag{6}$$

$$H_{I,-+} = A(L\dagger, R, -+)\ b_k^{L\dagger} b_n^R + A(R, L\dagger, -+)\ b_n^R b_k^{L\dagger}. \tag{7}$$

The + and − signs are indizes for the states $|1,0\rangle$ resp. $|0,1\rangle$. We call the As Schrieffer-Wolff coefficients, they are calculated along the lines of [8] using mainly second order perturbation theory. For example, $A(R\dagger, R, ++)$ is

$$A(R\dagger, R, ++) = \frac{t_c^2}{2}\left[\frac{1}{\epsilon_m^R - (-\epsilon_{\rm as} + \epsilon_\beta)} - \frac{1}{\epsilon_n^R - (\epsilon_{\rm as} - \epsilon_\beta)}\right]. \tag{8}$$

We now use the Bloch-Redfield equations [9, 10]

$$\dot{\rho}_{nm}(t) = -i\omega_{nm}\rho_{nm} - \sum_{k,l} R_{nmkl}\rho_{kl}(t) \tag{9}$$

where R_{nmkl} are the elements of the Redfield tensor. These equations of motion for the reduced density matrix are obtained within Born approximation in the effective system-bath coupling, so after the Schrieffer-Wolff transformation, R is of order t_c^4. Let us remark that our perturbation theory naturally breaks down below the Kondo temperature, which can however be made arbitrarily small by lowering t_c through pinching off the contacts to the reservoirs.

The Bloch-Redfield equations are of Markovian form, however, by properly using the free time evolution of the system, they take into account all bath correlations which are relevant within the Born approximation [11].

The Redfield tensor has the form

$$R_{nmkl} = \delta_{lm} \sum_r \Gamma^{(+)}_{nrrk} + \delta_{nk} \sum_r \Gamma^{(-)}_{lrrm} - \Gamma^{(+)}_{lmnk} - \Gamma^{(-)}_{lmnk}. \tag{10}$$

The rates entering the Redfield tensor elements are given by the following Golden-Rule expressions

$$\Gamma^{(+)}_{lmnk} \;=\; \hbar^{-2} \int_0^\infty dt\; e^{-i\omega_{nk}t} \langle \tilde{H}_{I,lm}(t) \tilde{H}_{I,nk}(0) \rangle \tag{11}$$

$$\Gamma^{(-)}_{lmnk} \;=\; \hbar^{-2} \int_0^\infty dt\; e^{-i\omega_{lm}t} \langle \tilde{H}_{I,lm}(0) \tilde{H}_{I,nk}(t) \rangle \tag{12}$$

where H_I appears in the interaction representation (written as $\tilde{H}_I$). In our formalism, it is of crucial importance that the expectation values over H_I vanish, i.e. that the bath produces only noise. As a number of expectation values of H_I turns out to be finite, we tacitly replace H_I by $H_I - \langle H_I \rangle$ in eqs. (11) and (12) and use the finite expectation values to renormalize the diagonalized, unperturbed Hamiltonian $H_0 \to H_0 + \langle H_I \rangle$. In our case, the effect of this renormalization is of the order of 0.1 % of the original matrix elements of H_0.
After a straightforward calculation of the above Golden-Rule rates, one gets in the general case a (large) sum over terms with the generic form

$$\begin{aligned}
\Gamma^{(+)} \;=\; c \Bigg\{ & \frac{i\pi}{\epsilon_b - \epsilon_a \mp 2\epsilon_{\rm as}} [f_1(\epsilon_b \mp 2\epsilon_{\rm as})(1 - f_2(\epsilon_b)) - f_1(\epsilon_a)(1 - f_2(\epsilon_a \pm 2\epsilon_{\rm as}))] + \\
& + \frac{-n_1(\mu_2 \mp 2\epsilon_{\rm as})}{\epsilon_b - \epsilon_a \mp 2\epsilon_{\rm as}} \Bigg[\psi\left(\frac{1}{2} + \frac{i\beta}{2\pi}\left(\epsilon_b \mp 2\epsilon_{\rm as} - \mu_1\right)\right) - \psi\left(\frac{1}{2} + \frac{i\beta}{2\pi}\left(\epsilon_a - \mu_1\right)\right) - \\
& - \psi\left(\frac{1}{2} + \frac{i\beta}{2\pi}\left(\epsilon_b - \mu_2\right)\right) + \psi\left(\frac{1}{2} + \frac{i\beta}{2\pi}\left(\epsilon_a \pm 2\epsilon_{\rm as} - \mu_2\right)\right) \Bigg] \Bigg\}
\end{aligned} \tag{13}$$

$$\begin{aligned}
\Gamma^{(-)} \;=\; c \Bigg\{ & \frac{i\pi}{\epsilon_b - \epsilon_a \mp 2\epsilon_{\rm as}} [f_2(\epsilon_b)(1 - f_1(\epsilon_b \mp 2\epsilon_{\rm as})) - f_2(\epsilon_a \pm 2\epsilon_{\rm as})(1 - f_1(\epsilon_a))] + \\
& + \frac{-n_2(\mu_1 \pm 2\epsilon_{\rm as})}{\epsilon_b - \epsilon_a \mp 2\epsilon_{\rm as}} \Bigg[- \psi\left(\frac{1}{2} + \frac{i\beta}{2\pi}\left(\epsilon_b \mp 2\epsilon_{\rm as} - \mu_1\right)\right) + \psi\left(\frac{1}{2} + \frac{i\beta}{2\pi}\left(\epsilon_a - \mu_1\right)\right) + \\
& + \psi\left(\frac{1}{2} + \frac{i\beta}{2\pi}\left(\epsilon_b - \mu_2\right)\right) - \psi\left(\frac{1}{2} + \frac{i\beta}{2\pi}\left(\epsilon_a \pm 2\epsilon_{\rm as} - \mu_2\right)\right) \Bigg] \Bigg\}
\end{aligned} \tag{14}$$

where $c = \frac{t_c^4 \pi V^2 m_*^2}{4\hbar(2\pi\hbar^2)^2}$. One can express the coupling to the leads t_c by $t_c = \sqrt{\frac{g}{8\pi^2}} \cdot \frac{E_F}{n}$, where g is a conductance in terms of the quantum conductance, E_F is the Fermi energy of the leads and n is the number of electrons in the leads. Consequently, c is then changed to $c = \frac{t_c^2 g}{32\pi\hbar}$. The ϵ_a and ϵ_b are terms containing varying sums or differences of ϵ_β, ϵ_α and $\epsilon_{\rm as}$. Due to the

multitude of possibilities for virtual transitions, each element of the Redfield tensor contains a number of terms of this generic structure.

In the above equations, the terms containing the Fermi function $f(\epsilon)$ only play a role close to resonance and can be neglected in the Coulomb blockade [12]. The $n_{l/r}$'s represent Bose functions for the electron-hole pairs (excitons) that are generated during the virtual processes. The ψ's denote Digamma functions and hence diverge logarithmically at low temperatures.

By solving equation (9), one finds that the off-diagonal elements decay towards zero on a time scale τ_ϕ (dephasing time) whereas the diagonal density matrix elements equilibrate on a time scale τ_r (relaxation time).

Using the above expressions, we find the rates as

$$\Gamma_r \;=\; 2\;(\Gamma^{(+)}_{+--+} + \Gamma^{(+)}_{-++-}) \tag{15}$$

$$\Gamma_\phi \;=\; \frac{\Gamma_r}{2} + (\Gamma^{(+)}_{++++} + \Gamma^{(+)}_{----} - 2\Gamma^{(+)}_{++--}) \tag{16}$$

where

$$\Gamma^{(+)}_{+--+} \;=\; \Gamma^{(-)}_{+--+} = c\;(-n_r(\mu_l + 2\epsilon_{\rm as}))Z \tag{17}$$

$$\Gamma^{(+)}_{-++-} \;=\; \Gamma^{(-)}_{-++-} = c\;(-n_l(\mu_r - 2\epsilon_{\rm as}))Z \tag{18}$$

$$\Gamma^{(+)}_{++++} \;=\; \Gamma^{(-)}_{++++} = c\;\frac{1}{\beta}\;Y_1 \tag{19}$$

$$\Gamma^{(+)}_{----} \;=\; \Gamma^{(-)}_{----} = c\;\frac{1}{\beta}\;Y_{-1} \tag{20}$$

$$\Gamma^{(+)}_{++--} \;=\; \Gamma^{(-)}_{++--} = c\;\frac{1}{\beta}\;Y_{1,-1}. \tag{21}$$

Z is a function containing several ψ-functions (or logarithms). Y_1, Y_{-1} and $Y_{1,-1}$ are different functions of several ψ'-(Trigamma-) functions (or reciprocals), however, these functions only have a very weak temperature dependence. The most important part of the temperature dependence comes in through $\frac{1}{\beta}$ and in $n_{l/r}$ and is summarized in Figure 2. We find in Figure 2 that the temperature dependence is similar to the Spin-Boson case [13]. This can be confirmed by inspection of the formulas (17)-(21): For the relaxation rate, one has only Bose functions taken at the finite amount energy which is dissipated. In case of the dephasing rate, there are also terms that are proportional to T, which represent dephasing processes which do not change the energy of the qubit, i.e. cotunneling processes which originate and end in the same state. This explains the observed behaviour. Note, that in the Spin-Boson

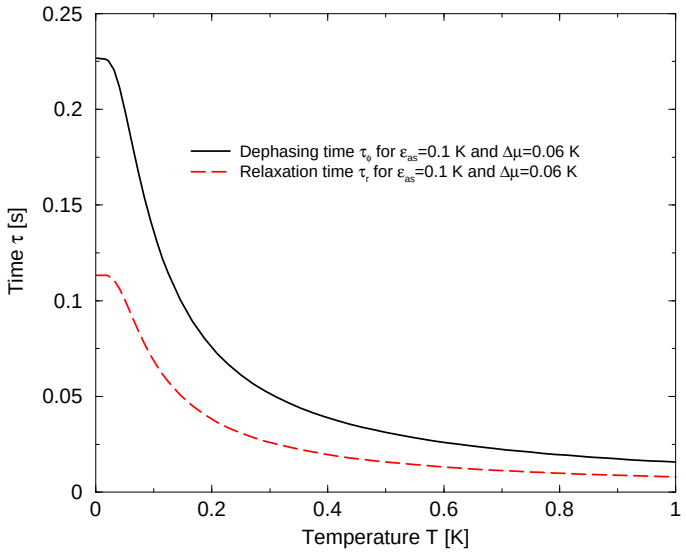

FIG. 2: Relaxation and dephasing time (τ_r and τ_ϕ) as a function of temperature T, with $\mu_l = 0.85$ K, $\mu_r = 0.91$ K, $\epsilon_{\rm as} = 0.1$ K, $\epsilon_\beta = 11$ K, $\epsilon_\alpha = 9$ K, $g = 0.1$, $V = 10^{-12}$ m^2, $E_F = 5$ meV and $n/V = 1.7 \cdot 10^{15}$ m^{-2}.

case, where there is only one lead, the situation corresponding to our Gedanken-experiment (no tunneling between the classical states) would correspond to pure dephasing, whereas in our system relaxation is always possible by extracting an electron on one side and adding one on the other side from the other lead.

The numerical values for the relaxation and dephasing times are comparedly huge, on the order of 100 milliseconds as compared to the experimentally measured times, which are in the order of nanoseconds. Other possibilities to explain the small decoherence time are phononic and/or photonic baths [14, 15, 16], or the influence of the whole electronic circuitry.

We analyzed relaxation and dephasing processes in a system of two laterally coupled quantum dots which is coupled to two electronic (i.e. fermionic) baths. We showed that even in the case of vanishing inter-dot coupling, the system's energy can relax, unlike in the Spin-Boson model. On top of that, the temperature dependence of the rates resembles that of the Spin-Boson model. We identify, that this originates in the fact that the cotunneling rates are mostly sensitive to the distribution function of excitons.

As a next step, the case where the inter-dot coupling γ has finite values will be considered

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