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Phonon-mediated relaxation in doped quantum dot molecules

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Abstract. We study a single quantum dot molecule doped with one electron in the presence of electron-phonon coupling. Both diagonal and off-diagonal interactions representing real and virtual processes with acoustic phonons via deformation potential and piezoelectric coupling are taken into account. We employ a non-perturbative quantum kinetic theory and show that the phonon-mediated relaxation is dominated by an electron tunneling on a picosecond time scale. A dependence of the relaxation on the temperature and the strength of the tunneling coupling is analyzed.

1. Introduction
Coupled quantum dots (QDs) called quantum dot molecules (QDMs) have attracted much attention due to their proposed application in various quantum computation schemes. The two ground states of a single confined electron can be used as the logical qubit states and their electrical [1] and optical control [2, 3] have already been demonstrated. However, not only the electron-electron interaction [4] but also phonon-assisted relaxation [5, 6] can affect the coherent control to a large extent. In particular, the energy difference between the two electron ground states, which is of order of a few meV, can lead to both virtual pure dephasing processes [7, 8, 9] as well as efficient electron tunneling [10, 11].

In this contribution, a fully quantum kinetic description of the phonon-mediated relaxation in doped quantum dot molecules including non-Markovian effects is presented. It is shown that the coupling to the phonon reservoir in QDMs can lead to a fast electron tunneling on a picosecond timescale, which strongly affects the coherent electron evolution. We employ non-Markovian correlation expansion technique [12, 13] including up to three particle correlations. Both diagonal and usually neglected off-diagonal electron-phonon couplings representing virtual and real phonon-assisted processes are included. We study the temperature dependence of the phonon-mediated relaxation as well as the influence of the tunneling coupling strength.

2. Model system
We study a QDM doped with a single electron and consider the relaxation between the two energetically lowest states of the electron |1⟩ in the left and |2⟩ in the right quantum dot (see Fig. 1 with schematic plot of the energy levels in the QDM). The free Hamiltonian of the electron
reads

\[ H_c = \epsilon (|2\rangle\langle 2| - |1\rangle\langle 1|) + \Gamma (|1\rangle\langle 2| + |2\rangle\langle 1|). \] (1)

Here, \( \Gamma \) is the tunneling coupling between the QDs and \( 2\epsilon \) is the energy difference between the ground states in both QDs.

The equations of motion for the quantities of interest: electron occupation \( f_i(r) \) and microscopic quantum dynamics, which covers the memory effects in the non-Markovian regime.

We have numerically simulated the self-assembled GaAs QDs with the following parameters: \( \ell_1 = 4 \) nm, \( \ell_2 = 4.1 \) nm, and \( d = 6 \) nm, where \( \ell_i \) is the electron wave function size of the \( i \)-th QD, and the distance between the dots is \( d \). Here, \( \rho = 5360 \) kg/m\(^3\) is the crystal density, \( V \) is the normalization volume of the phonon modes, \( \alpha_i \) is the speed of sound (longitudinal \( v_L \) and two transverse \( v_T \) and \( v_P \)). The carrier-phonon interaction is described by the following Hamiltonian

\[ H_{\text{int}} = \sum_{i,j=1,2} \sum_{\mathbf{k},s} \left[ g_{ij,s}^{\text{M}}(\mathbf{k}) |i\rangle \langle j| b_{\mathbf{k},s}^{\dagger} + g_{ij,s}^{\text{M}}(\mathbf{k}) |j\rangle \langle i| b_{\mathbf{k},s}^{\dagger} \right]. \] (2)

The relevant coupling elements for the acoustic phonons coupled via both piezoelectric coupling and deformation potential read:

\[ g_{ij,s}^{\text{PE}}(\mathbf{k}) = -i \frac{\hbar}{2\rho v_L} M_s(\mathbf{k}) \int d^3 r \psi_i^*(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \psi_j(\mathbf{r}), \] (3)

\[ g_{ij,l}^{\text{DP}}(\mathbf{k}) = \frac{\hbar k}{2\rho v_L} D_e \int d^3 r \psi_i^*(\mathbf{r}) e^{i\mathbf{k} \cdot \mathbf{r}} \psi_j(\mathbf{r}) \] (4)

with Gaussian electron wave functions

\[ \psi_i(\mathbf{r}) = \frac{1}{\pi^{3/4} l_i^{3/2}} \exp \left( -\frac{\mathbf{r}^2}{2l_i^2} \right). \] (5)

We have numerically simulated the self-assembled GaAs QDs with the following parameters: \( \ell_1 = 4 \) nm, \( \ell_2 = 4.1 \) nm, and \( d = 6 \) nm, where \( \ell_i \) is the electron wave function size of the \( i \)-th QD, and the distance between the dots is \( d \). Here, \( \rho = 5360 \) kg/m\(^3\) is the crystal density, \( V \) is the normalization volume of the phonon modes, \( \alpha_i \) is the speed of sound (longitudinal \( v_L \) and two transverse \( v_T \) and \( v_P \)).

The dynamics of the electron confined in a QDM in the presence of electron-phonon interaction is studied by means of a second order correlation expansion method [12, 13], which is based on the assumption that correlations involving an increasing number of particles are of decreasing importance. This is a non-perturbative technique commonly used to describe the microscopic quantum dynamics, which covers the memory effects in the non-Markovian regime. The equations of motion for the quantities of interest: electron occupation \( f = \langle |2\rangle\langle 2| \) and

Figure 1. A schematic plot of two coupled quantum dots with two electron states \( |1\rangle \) and \( |2\rangle \) with the energy difference of \( \Delta \epsilon = 2\epsilon \). The dashed and curled arrows depict electron tunneling with simultaneous phonon emission.
coherence $p = \langle |1/2| \rangle$ are derived with the help of Heisenberg equation. The equations for the time evolution of the electron density and the coherence

$$
\dot{j} = \frac{2}{\hbar} \Gamma \text{Im}(p) - \frac{i}{\hbar} \sum_k g_{12}(k) \left[ s_k - s_k^{(+)*} + 2iB_k \text{Im}(p) \right] - \frac{i}{\hbar} \sum_k g_{12}^*(k) \left[ s_k^{(+)} - s_k^* + 2iB_k^* \text{Im}(p) \right]
$$

$$
\dot{p} = \frac{-i}{\hbar} 2cp - \frac{i}{\hbar} T(1 - 2f) - \frac{i}{\hbar} \sum_k g_{12}(k) [2t_k + (1 - 2f)B_k] - \frac{i}{\hbar} \sum_k g_{12}^*(k) [2t_k^* + (1 - 2f)B_k^*]
$$

$$
- \frac{i}{\hbar} \sum_k [g_{22}(k) - g_{11}(k)] (s_k + pB_k) - \frac{i}{\hbar} \sum_k [g_{22}^*(k) - g_{11}^*(k)] (s_k^{(+)} + pB_k^*)
$$

couple to each other, to $B_k = \langle b_k \rangle$, and to the phonon-assisted correlations: $s_k = \langle |1/2| b_k \rangle^{corr}$, $s_k^{(+)} = \langle |1/2| b_k^{(+)} \rangle^{corr}$, and $t_k = \langle |1/1| b_k \rangle^{corr}$. The factorization scheme has been used above with $\langle |1/2| b_k \rangle = \langle |1/2| b_k \rangle^{corr} + \langle |1/2| b_k \rangle^{corr}$, where the quantities have been decomposed into all possible lower-order factorizations. The next step is to derive the equations of motion for all the phonon-assisted correlation quantities, which will couple to three particle correlations, e.g. $\langle |1/2| b_{q,s} b_{k,s'} \rangle^{corr}$. These couple to up to four particle correlations, etc. Thus, in order to get a closed set of equations, one needs to truncate the hierarchy by neglecting higher order correlations. In the present paper, we included up to three particle correlations.

### 3. Phonon-induced relaxation

Initially, the electron is injected into a quantum dot with higher energy, $f = \langle |2/2| \rangle = 1$, where the injection time is much shorter than the reservoir response (all correlation terms can be initially set to zero). The time evolution of the occupation of the QD with higher energy in the presence of the phonon reservoir at three different temperatures is shown in Fig. 2. If the electron is not coupled to phonons (ideal evolution, solid black line in the inset of Fig. 2), it tunnels back and forth between the two QDs with a period determined by the tunneling coupling $\Gamma$ and the energy difference $\Delta \epsilon = 2\epsilon$ and is proportional to $\Gamma/(\Delta \epsilon)$. Using this parameter set with $\Delta \epsilon = 0.5$ meV and $\Gamma = 0.1$ meV, the electron mostly stays in the QD with higher energy since the tunneling coupling is too small to let the electron fully tunnel between the dots.

The dynamics of the electron is strongly affected if we include the electron-phonon interaction, which leads to the electron tunneling to the neighboring dot already on the picosecond time scale. At $T = 0$ K, only the emission processes are available, thus, the electron tunnels completely to the QD with lower energy. The probability of a phonon to be absorbed increases with temperatures, thus the final electron state shifts from the quantum dot with the lower energy towards an equal superposition of electron confined in the left $|1\rangle$ and right $|2\rangle$ QD. It results from the fact, that the probabilities of phonon absorption and emission are equal at high temperatures. Similarly, the damping gets stronger at higher temperatures, thus the oscillation amplitude decreases and the initial decay gets faster.

The fast relaxation processes result mainly from the direct electron tunneling assisted by phonons, which is described by the off-diagonal electron-phonon interaction. It can be seen in the inset of Fig. 2, where the time evolution of the QD occupation is modeled using only the diagonal part of the interaction Hamiltonian. In this case, the relaxation is considerably slower up to two orders of magnitude at all considered temperatures. Thus the proper description of the electron dynamics in a QDM should include the off-diagonal coupling to the phonon reservoir. We compared the results from the non-Markovian quantum kinetic model including up to two-phonon assisted processes to those with up to one phonon and we found out that the former leads only to a small correction. Thus, one can properly describe the electron dynamics by means of the first order correlation expansion technique.
Figure 2. The time evolution of the occupation of the QD with the higher energy at different temperatures with $\Delta \epsilon = 0.5$ meV, and $\Gamma = 0.1$ meV. Inset: The ideal electron evolution without coupling to phonons (black solid line) and the evolution including only the diagonal electron-phonon coupling.

Figure 3. The QD occupation probability as a function of time for four different tunneling couplings with the energy difference $\Delta \epsilon = 2$ meV and at the temperature of $T = 4$ K. Inset: The corresponding ideal evolution of the electron in a QD without electron-phonon interaction.

The phonon-mediated relaxation in quantum dot molecules depends on the parameters of the system, in particular on the strength of the tunneling coupling $\Gamma$ between the dots. In Fig. 3, we show the time evolution of the quantum dot occupation for four different values of the tunneling coupling and for considerably large energy difference, $\Delta \epsilon = 2$ meV. As one can see from the inset in Fig. 3 with ideal time evolution of the electron, the amplitude of the oscillations grows when the direct tunneling coupling is increased. For small values of the coupling, the phonon-induced relaxation is very fast, the electron tunnels to the neighboring dot within 20 ps. If the tunneling element grows, the relaxation slows down, however the increased oscillations in the case of large $\Gamma$ are damped by the phonon reservoir even at low temperature of $T = 4$K.

4. Conclusion
A full description of the electron dynamics in the presence of the electron-phonon coupling in a quantum dot molecule doped with a single electron has been presented. The two couplings to the relevant acoustic phonons via deformation potential and piezoelectric coupling with diagonal and off-diagonal interactions have been taken into account. It has been shown that the phonon-mediated relaxation is a fast process on a picosecond timescale strongly modifying the coherent evolution of the electron. It is dominated by the usually neglected off-diagonal electron-phonon coupling two orders of magnitude faster then the relaxation due to pure dephasing. We analyzed the dependence of the relaxation on the temperature as well as on the strength of the tunneling coupling. The presented results are important for nanoscience, in particular for quantum information processing and for the currently performed experiments in the area of quantum transport and optics of quantum dots.

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