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Recovering pure states in two-state quantum systems

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Abstract

In this work, we study the loss and recovery of pure states (i.e., coherence) in two-state molecules and quantum dots. The molecules of two electronic states and a one-dimensional nuclear vibration are modeled by a quantum–classical dynamical model. According to the simulations, pure states of a two-state molecule can be restored by the excitation of the nuclear vibration by a well-defined electromagnetic field. In the case of a quantum dot, pure states can be regained through the modulation of the energy levels through the application of a proper bias voltage on the dot.

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1. Introduction

Coulomb-coupled devices on the nanometer scale and quantum-dot arrays have been proposed for the realization of logic arrays used for computations [1–4]. In a previous study the modeling of molecules with two electronic states has been described [5]. Molecular arrays composed of such molecules are possible candidates for use in realizing nanoelectronic devices in the future such as the one-dimensional molecular chain and the majority gate [6].

These devices can work properly only if pure (coherent) quantum-mechanical states are maintained. Dissipation due to the environment will cause the system to evolve to a mixed state. In this paper we study the loss and revival of pure states in two-state molecules and in quantum dots.

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In Section 2, a simple model for the description of two-state quantum systems is introduced. The effect of the dissipation on the system is described.

In Section 3, the effect of electromagnetic pulses on molecules of two electronic states and a one-dimensional nuclear vibration is examined, and we study the effect of the confining voltages on the energy levels in a gate-confined quantum-dot structure.

Our model shows that it is possible to regain pure states in a two-state molecule if the vibrations of the nuclei are appropriately excited by a time-varying electric field gradient. Furthermore, we show that one can restore pure states for a quantum dot if one alters the energy levels of the dot by a well-defined potential. The modeling of this effect and the results of the simulations are discussed in Section 4.

2. A simple model of a quantum system with two electronic states

In this section we describe the behavior of a quantum system with two electronic states. The effect of the nuclear motion is taken into account in the case of a single molecule with two electronic states and a one-dimensional mechanical vibration.

The Hamiltonian matrix of a quantum system with two states, $|\Psi_1\rangle, |\Psi_2\rangle$, can be written in the form

$$\mathbf{H} = \begin{bmatrix} E_1 & G \\ G & E_2 \end{bmatrix} = \begin{bmatrix} H_{11} & H_{12} \\ H_{12}^* & H_{22} \end{bmatrix} \quad (1)$$

where E_1 and E_2 are the energy levels of the system in the ground and excited states respectively, G is the energy of tunneling between the two states.

A two-state system can be described by the equation

$$\hbar \frac{d\vec{\lambda}(t)}{dt} = \mathbf{\Omega}\vec{\lambda}(t) + \mathbf{R}\vec{\lambda}(t) + \vec{k} \quad (2)$$

where $\hbar = h/2\pi$, h is Planck's constant, $\vec{\lambda}(t) = [\lambda_1(t), \lambda_2(t), \lambda_3(t)]$ is the coherence vector, $\mathbf{\Omega}$ is the Bloch matrix,

$$\mathbf{\Omega} = \begin{bmatrix} 0 & -H_{22} + H_{11} & -j(H_{12}^* - H_{12}) \\ H_{22} - H_{11} & 0 & -H_{12} - H_{12}^* \\ j(H_{12}^* - H_{12}) & H_{12} + H_{12}^* & 0 \end{bmatrix}, \quad (3)$$

\mathbf{R} and \vec{k} are the damping matrix and damping vector characterizing the dissipation.

If we use the simplest dissipation model, Eq. (2) can be written in the form

$$\hbar \frac{d\vec{\lambda}(t)}{dt} = \mathbf{\Omega}\vec{\lambda}(t) - \frac{\hbar}{\tau} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{bmatrix} + \frac{\hbar}{\tau} \begin{bmatrix} 0 \\ 0 \\ 2 \tanh\left(\frac{\Delta E}{k_B T}\right) \end{bmatrix} \quad (4)$$

where k_B is Boltzmann's constant, T is the temperature of the environment and τ is the electronic relaxation.

In the case of a two-state molecule with a one-dimensional nuclear vibration the energy levels and the Hamiltonian matrix \mathbf{H} will depend on R , the distance between the nuclei:

$$\mathbf{H} = \begin{bmatrix} E_1(R) & G(R) \\ G(R) & E_2(R) \end{bmatrix}. \quad (5)$$

The dependence of the energy levels on the distance between the nuclei can be described by the potential energy surfaces (PES).

To describe the behavior of such molecules, we need to apply the equations

$$\frac{d}{dt}R(t) = \frac{1}{M}P(t) \tag{6}$$

$$\frac{d}{dt}P(t) = \langle \Psi | - \frac{\partial}{\partial R}(V_{nn} + V_{en}) | \Psi \rangle - \alpha P(t) \tag{7}$$

in addition to Eq. (4). $R(t)$ is the distance between the nuclei, $P(t)$ is the momentum of the nuclei, V_{nn} and V_{en} are the nucleus–nucleus and electron–nucleus potential energies respectively. In Eq. (7), α characterizes the mechanical relaxation.

In the absence of the dissipation, the length of the coherence vector stays as unity over time, and the electronic state of the molecule remains in a pure coherent state.

If there is dissipation and the temperature of the thermal bath and the energy difference between the two states are not zero, the coherence vector will converge over time to an equilibrium, where the length of the coherence vector becomes less than unity, and the system will evolve to a mixed state.

3. Regaining pure states in a two-state quantum system

Using Eq. (4) we get the formula which describes the behavior of the square of the length of the coherence vector over time:

$$\frac{d|\vec{\lambda}|^2}{dt} = -\frac{1}{\tau_0} \left(\lambda_1^2 + \lambda_2^2 + \lambda_3^2 \right) - \frac{1}{\tau_0} \lambda_3 \left(\lambda_3 - \tanh \frac{E_2 - E_1}{k_B T} \right). \tag{8}$$

From this equation, we can see that there are several effects which change the length of the coherence vector. Dissipation, modeled through a decay constant, reduces the length of the coherence vector. In particular, an initial pure state (with the length of the coherence vector equal to one) will decay into a mixed state (with a coherence vector of length less than one). Note that the above equation also contains a term (the last term, which depends on the energy difference $E_2 - E_1$), which allows an increase in the length of the coherence vector. In other words, a pure state can be obtained from a mixed state through appropriate modulation of the energy difference $E_2 - E_1$ in the two-state system.

In the case of a two-state molecule with a one-dimensional nuclear vibration we can modulate the energy difference between the two states by changing the distance between the nuclei of the molecule. This can be realized by the application of an electric field gradient to the molecule, which interacts with the quadrupole moment, Q , of the nuclei. In this case Eq. (7) modifies to

$$\begin{aligned} \frac{d}{dt}P(t) &= \langle \Psi | - \frac{\partial}{\partial R} \left(V_{nn} + V_{en} + Q(R) \frac{dE(t)}{dx} \right) | \Psi \rangle \\ &= -\frac{\partial}{\partial R} V_{nn} + \langle \Psi | - \frac{\partial}{\partial R} V_{en} | \Psi \rangle - \frac{\partial Q(R)}{\partial R} \frac{dE(t)}{dx}. \end{aligned} \tag{9}$$

In the case of a quantum dot we can change the energy difference between the two energy levels if we change the confining potential of the dot. The dependence of the energy

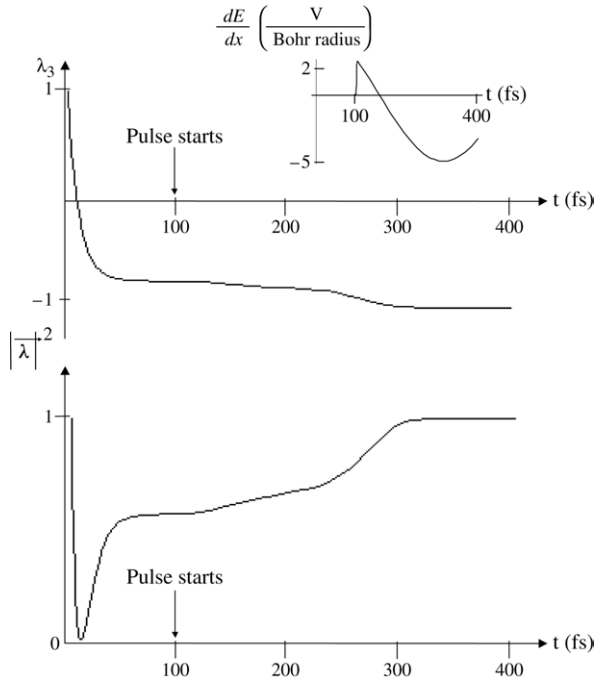


Fig. 1. The coherence vector dynamics for a two-state molecule with one degree of nuclear vibration. The applied electric field gradient is shown in the inset.

levels on the dimensions of the confining potential can be described by the formula

$$E = \frac{\hbar^2}{8m^*} \left(\frac{n_1^2}{L_x} + \frac{n_2^2}{L_y} + \frac{n_3^2}{L_z} \right) \quad (10)$$

where m^* is the effective mass of the electrons in the dot, L_x , L_y and L_z are the dimensions of the quantum dot.

4. Results and discussion

On the basis of the above model, we performed numerical simulations, and the results are shown in Figs. 1 and 2. For the case of a two-state molecule with a nuclear vibration, our model predicts that the length of the coherence vector can be modulated through an electric field gradient, which changes the energy difference. Fig. 1 shows both a loss of coherence due to dissipation and also an increase in the length of the coherence vector as an external field with the proper magnitude and duration is applied. Originally the molecule is in its pure excited state ($\lambda_3 = 1$), but due to the dissipation it decays into a mixed state as time passes. After we apply an appropriate electric field gradient, as shown in Fig. 1, the coherence vector can be restored to its pure ground state ($\lambda_3 = -1$).

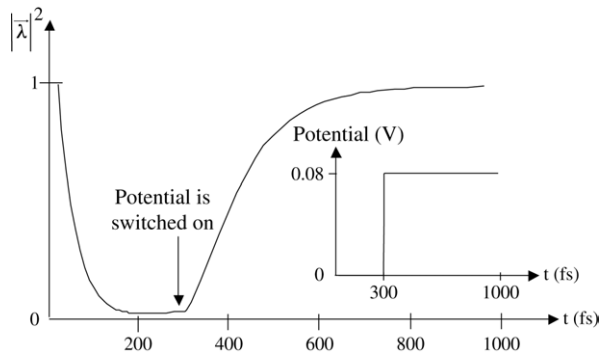


Fig. 2. The coherence vector dynamics for a gate-confined quantum dot. The applied voltage is shown in the inset.

To demonstrate the regaining of pure states in a quantum dot, we used the data on a gate-confined quantum-dot structure proposed in a previous paper [7]. In this case, an applied bias voltage can modulate the size of the quantum dot. Since the energy levels depend on the size of the quantum dot (see Eq. (10)), it is possible to modulate the length of the coherence vector through an applied bias voltage. Fig. 2 shows how this effect can be used to restore the length of the coherence vector to unity, and the quantum-dot system is transformed into a pure state.

5. Conclusions

In this paper, we study the loss and restoration of coherence (pure states) for two-state quantum systems. On the basis of our model for the dynamics of the coherence vector, we find that pure states can be regained from mixed states if appropriate external field pulses are applied. We showed the results of our model simulations for two examples, namely a two-state molecule coupled to nuclear vibrations and a gate-confined quantum dot.

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