

Computing by pulse-driven nanodevice arrays

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Abstract

In this paper, we simulate the mixed electronic and mechanical vibrational behaviour of Coulomb-coupled nanodevices subject to electromagnetic chirped pulses. The electronic states of the devices are approximated with a finite number of quantum states coupled to a classical vibration and to a heat bath, as well as subject to optical pumping. We show that mechanical vibrational states of the nuclei can be switched by suitable optical chirps and binary information can be loaded onto nanodevice chains. Our simple model indicates that the loss of coherence in the electronic states can be reconstructed by proper excitation of the nuclear vibration.

1. Introduction

Coulomb coupling has been proposed to substitute wired integration of nanodevices [1]. In a previous paper, we proposed a mixed quantum–classical dynamical model for the description of Coulomb-coupled nanodevice arrays. The electronic states of the devices have been approximated with a finite number of quantum states coupled to a classical vibration and to a heat bath, as well as subject to optical pumping [2].

Optically pumped finite quantum state nanodevice arrays have been suggested as potential cellular computers [2–4]; however, none of those included the role of nuclear vibrations. In a recent paper, we studied arrays of nanodevices with two electronic states including the effects of a one-dimensional nuclear vibration with two nuclear equilibrium states [5].

In this paper, we study the mixed electronic and mechanical behaviour of Coulomb-coupled nanodevices subject to electromagnetic pulses.

An important consequence of the nuclear switching is that the chirp frequency required to switch the molecule from ground state to excited state is different from the frequency needed to switch the molecule back to ground state.

Our simple model indicates that the loss of coherence in the electronic states can be reconstructed by proper excitation of the nuclear vibration. In this paper, we study the loss and reconstruction of coherence in the framework of our model.

2. Modelling of a two-electronic quantum-state nanodevice with one-dimensional mechanical vibration

In this model, we describe the behaviour of a single nanodevice with two electronic states and one degree of freedom of mechanical vibration. The environment is modelled by an ideal heat bath coupled to the nanodevice.

In the case of a molecule with two states, $|\Psi_1\rangle$, $|\Psi_2\rangle$, and one freedom of nuclear vibration, the energy levels and the Hamiltonian matrix \mathbf{H} will depend on R , the distance between the nuclei,

$$\mathbf{H} = \begin{bmatrix} E_1(R) & G(R) \\ G(R) & E_2(R) \end{bmatrix}. \quad (1)$$

The dependence can be characterized by the potential energy surfaces (PES). In the case of the simplest dissipation model the molecule is characterized by the following equations,

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

$$\frac{d}{dt} R(t) = \frac{1}{M} P(t) \quad (3)$$

$$\frac{d}{dt} P(t) = \langle \Psi | -\frac{\partial}{\partial R} (V_{\text{nm}} + V_{\text{en}}) | \Psi \rangle - \alpha P(t) \quad (4)$$

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

$$\Omega = \begin{bmatrix} 0 & -H_{22} + H_{11} & -j(H_{12}^* - H_{12}) \\ H_{22} - H_{11} & 0 & -H_{12} - H_{12}^* \\ j(H_{12}^* - H_{12}) & H_{12} + H_{12}^* & 0 \end{bmatrix} \quad (5)$$

the dissipation can be characterized by the temperature T , the electronic relaxation τ and the nuclear relaxation α . The distance between the nuclei is $R(t)$, the momentum of the nuclei is $P(t)$. V_{nn} and V_{en} are the nucleus–nucleus and electron–nucleus potential energies respectively. In equation (4) α characterizes the mechanical relaxation.

Equation (2) describes the electronic behaviour, equations (3) and (4) describe the nuclear dynamics of the molecule.

We studied applications of pulse-driven molecules such as the one-dimensional molecular chain, the majority gate, a two-dimensional molecular array for digital image processing and the universal replacement computer [6].

3. Coherence

In coherent electronic states the absolute value of the coherence vector is one. If it becomes smaller than one decoherence occurs.

First, we show that the Bloch matrix does not influence the absolute value of the coherence vector.

Using equation (2), the time derivative of the square of the length of the coherence vector can be described as

$$\frac{d|\vec{\lambda}|^2}{dt} = -\frac{1}{\tau_0}(\lambda_1^2 + \lambda_2^2 + \lambda_3^2) - \frac{1}{\tau_0}\lambda_3 \left(\lambda_3 - \tanh \frac{E_2 - E_1}{k_B T} \right). \quad (6)$$

As can be seen from equation (6), we cannot modify the length of the coherence vector through introducing a time-variant Hamiltonian by electromagnetic radiation, since the Bloch matrix is not present in equation (6). Only the changes of the energy difference can change the absolute value of the coherence vector.

Thus an electromagnetic chirp coupled only to the electronic states cannot control coherence. However, a chirp properly coupled to the mechanical vibration (to the nuclei), according to (6) changes the length of the coherence vector.

If an electric field $\mathbf{E}(t)$ acts on the molecule, the electronic Hamiltonian matrix of the perturbation can be calculated from the equation

$$\delta H_{ij} = \langle \Psi_i | -\mathbf{p}(t)\mathbf{E}(t) | \Psi_j \rangle \quad \text{for } i \neq j \quad \delta H_{ii} = 0 \quad (7)$$

where $\mathbf{p}(t)$ is the dipole moment of the device.

If we apply an electric field with a frequency close to $\Delta E/h$, where ΔE is the energy difference between the two states, the electronic quantum-mechanical state of the molecule will oscillate between the two eigenstates (Rabi oscillation). Note that the influence of the chirps appears only in the Hamiltonian, i.e. in the Ω matrix. In the absence of the dissipation the length of the coherence vector stays unity in time, the electronic state of the molecule remains coherent.

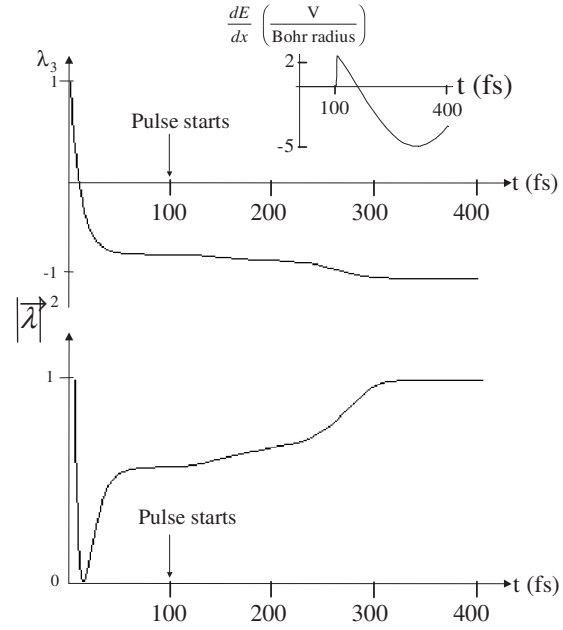


Figure 1. The upper plot describes the behaviour of λ_3 , the lower plot describes the square of the length of the coherence vector in time, when a time-varying electric field gradient is applied on the molecule. The applied pulse is shown in the inset.

If there is dissipation and the temperature of the thermal bath and the energy difference between the two states are not zero, then the coherence vector will converge in time to an equilibrium, where the length of the coherence vector becomes less than unity, thus decoherence occurs in the electronic states.

4. Coherence-restoration by chirp-generated nuclear vibration

In the case of our simple model, if we keep the temperature of the environment constant, the coherence can be restored only if we change the energy difference $E_2 - E_1$ between the two molecular states (see equation (6)). The energy difference depends on the distance R between the nuclei, thus it can be altered by vibrating the nuclei.

If an electric field is applied to the molecule, which does not change in space, we cannot vibrate the nuclei, since they have no dipole moment. However, it is possible to move the nuclei by the application of a time-varying electric field gradient, which interacts with the quadrupole moment of the nuclei. In this case equation (4) modifies to

$$\begin{aligned} \frac{d}{dt}P(t) &= \langle \Psi | -\frac{\partial}{\partial R} \left(V_{nn} + V_{en} + Q(R)\frac{dE(t)}{dx} \right) | \Psi \rangle \\ &= -\frac{\partial}{\partial R}V_{nn} + \langle \Psi | -\frac{\partial}{\partial R}V_{en} | \Psi \rangle - \frac{\partial Q(R)}{\partial R} \frac{dE(t)}{dx} \end{aligned} \quad (8)$$

where Q is the quadrupole moment of the nuclei.

If we apply a $dE(t)/dx$ electric field gradient with correct amplitude and frequency, the restoration of the coherence in the electronic states can be achieved as shown in figure 1.

At $t = 0$, $\lambda_3 = 1$, the nanodevice is in its excited state and the length of the coherence vector is unity, thus initially the

molecule is in a coherent state. As time evolves, coherence is gradually lost due to the dissipation. When the proper pulses are applied, the nanodevice goes to its ground state ($\lambda_3 = -1$), which is a coherent state, then it is driven to the coherent excited state.

5. Conclusions

Simulations show that

- mechanical vibrational states of the nuclei can be switched by suitable optical chirps,
- binary information can be loaded onto nanodevice chains, and
- the loss of coherence in the electronic states can be reconstructed by proper excitation of the nuclear vibration.

Simulations suggest that the decoherence caused by the environment cannot be restored by electromagnetic pulses coupled only to the electronic states; however, with the aid of a time-varying electric field-gradient coupled to the mechanical vibration of the device coherence can be restored.

Acknowledgments

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