On a Bloch type model with electron-phonon interactions: modeling and numerical simulations

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Bloch model for quantum dots

Quantum dot description

We use a conduction and valence electron description.

Due to the 3D confinement, energy levels in a quantum dot are quantized:
- conduction energy levels $(\epsilon_j^c)_{j\in\mathcal{I}^c}$,
- valence energy levels $(\epsilon_j^v)_{j\in\mathcal{I}^v}$.

To describe the time evolution of the energy level occupations, we define a global electron density matrix by

$$\rho = \begin{pmatrix} \rho^c & \rho^{cv} \\ \rho^{vc} & \rho^v \end{pmatrix} \quad (1)$$

where
- ρ^c and ρ^v are the conduction and valence densities. Their diagonal terms, called populations, are the occupation probabilities and their off-diagonal terms, called coherences, describe the intra-band transitions.
- ρ^{cv} and $\rho^{vc} = \rho^{cv^*}$ describe the inter-band transitions.

Maxwell-Bloch equations

The time evolution of ρ can be driven by a free electron Hamiltonian associated to electron level energies and the interaction with an electromagnetic wave. It is described by a Liouville type equation

$$i\hbar\partial_t\rho = [E_0 + \mathbf{E}\cdot\mathbf{M}, \rho], \quad (2)$$

where
- $[A, B]$ denotes the commutator $AB - BA$,
- $E_0 = \mathrm{diag}(\{\epsilon_j^c\}, \{\epsilon_j^v\})$,
- $\mathbf{M}$ is the dipolar moment matrix
  (expressed in terms of the wave functions associated to each level),
- $\mathbf{E}$ is a time-dependent electric field.

It can be coupled with Maxwell equations:

$$\partial_t\mathbf{E} = c^2 \operatorname{curl}\mathbf{B} - \mu_0 c^2 \mathbf{J}, \quad (3)$$
$$\partial_t\mathbf{B} = -\operatorname{curl}\mathbf{E}, \quad (4)$$

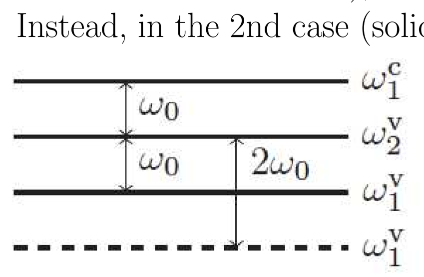
where $\mathbf{B}$ is the magnetic field. The coupling is expressed via the current density $\mathbf{J}$ given by

$$\mathbf{J} = n_a \operatorname{Tr}(\mathbf{M}\partial_t\rho)$$

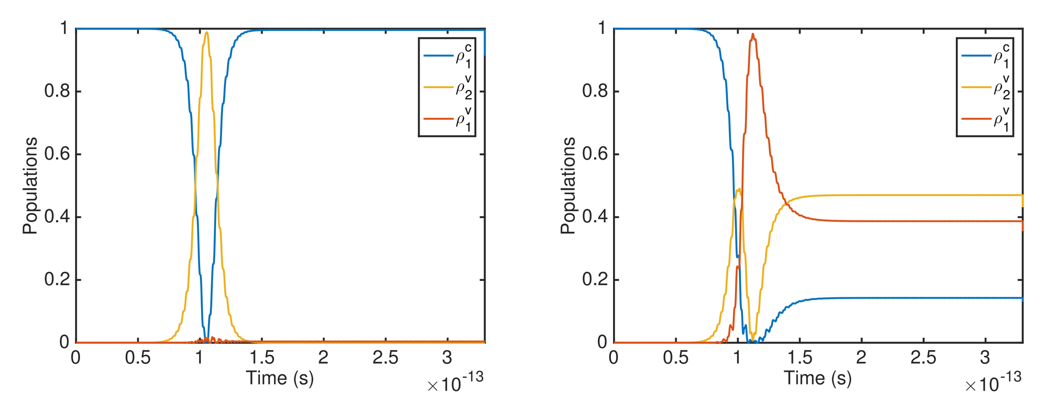
where n_a is the quantum dot volume density.

Self-Induced Transparency experiments

We consider two 3-level test cases with 1 conduction level and 2 valence levels. The energy between the conduction level and the first valence level is $\hbar\omega_0$. In the 1st case (dashed line on the scheme below), the transition between the 2 valence levels is $2\hbar\omega_0$. Instead, in the 2nd case (solid line), it is also $\hbar\omega_0$.



An electromagnetic pulse, whose center frequency is also ω_0, propagates through the dots. When the transition between the 2 valence levels is resonant with the field (right), the SIT phenomenon is destroyed. Instead, it suffices to get both valence levels far apart enough to recover the SIT.



Time evolution of populations (Left: $\epsilon_2^v - \epsilon_1^v = 2\hbar\omega_0$; Right: $\epsilon_2^v - \epsilon_1^v = \hbar\omega_0$).

Addition of electron–phonon interactions

Electron–phonon (e–ph) Hamiltonian

The starting point is to use field quantification to write an e–ph Hamiltonian.

Assumptions:
- e–ph interactions cannot lead the electron to change species:

$$H^{e-ph} = H^{c-ph} + H^{v-ph}.$$

- Only polar coupling to optical phonons is considered
  (leads to the fastest dynamics in low excitation regime).

The corresponding Fröhlich interaction Hamiltonian is given by

$$H^{c-ph} = \frac{1}{|\mathcal{B}|}\int_{\mathcal{B}} \sum_{\alpha,\alpha'\in\mathcal{I}^c} G^c_{\mathbf{q},\alpha,\alpha'}\, c^\dagger_\alpha \left(b_{\mathbf{q}} + b^\dagger_{-\mathbf{q}}\right) c_{\alpha'}\, \mathrm{d}\mathbf{q}, \quad (5)$$
$$H^{v-ph} = \frac{1}{|\mathcal{B}|}\int_{\mathcal{B}} \sum_{\alpha,\alpha'\in\mathcal{I}^v} G^v_{\mathbf{q},\alpha,\alpha'}\, v^\dagger_\alpha \left(b_{\mathbf{q}} + b^\dagger_{-\mathbf{q}}\right) v_{\alpha'}\, \mathrm{d}\mathbf{q}. \quad (6)$$

$c_j^\dagger$ and c_j (resp. $v_j^\dagger$ and v_j) are creation and annihilation operators for conduction (resp. valence) electrons and $b_{\mathbf{q}}^\dagger$ and $b_{\mathbf{q}}$ are those for phonons. The phonon mode $\mathbf{q}$ belongs to the Brillouin zone $\mathcal{B}$ of the underlying crystal.

For $e \in \{c, v\}$, $G^e_{\mathbf{q}}$ is a matrix whose coefficients are expressed in terms of the wave functions associated to each energy level:

$$G^e_{\mathbf{q},\alpha,\alpha'} = \mathcal{E}_{\mathbf{q}} \int \psi^{e*}_\alpha(\mathbf{r}) \exp(i\mathbf{q}\cdot\mathbf{r}) \psi^e_{\alpha'}(\mathbf{r})\, \mathrm{d}\mathbf{r}, \quad (7)$$

$\mathcal{E}_{\mathbf{q}}$ being the Fröhlich constant defined such that $G^{e*}_{\mathbf{q}} = G^e_{-\mathbf{q}}$.

Phonon-assisted densities

We introduce phonon-assisted density matrices

$$S_{\mathbf{q}} = \begin{pmatrix} S^{cc}_{\mathbf{q}} & S^{cv}_{\mathbf{q}} \\ S^{vc}_{\mathbf{q}} & S^{vv}_{\mathbf{q}} \end{pmatrix} \quad \text{where} \quad S^{ef}_{\mathbf{q},\alpha,\alpha'} = \left\langle f^\dagger_{\alpha'} b_{\mathbf{q}} e_\alpha \right\rangle, \quad e, f \in \{c, v\}. \quad (8)$$

Then, the time evolution of ρ due to e–ph interactions can be cast as

$$i\hbar\partial_t\rho|_{e-ph} = \frac{1}{|\mathcal{B}|}\int_{\mathcal{B}} [G_{\mathbf{q}}, S_{\mathbf{q}} + S^*_{-\mathbf{q}}]\mathrm{d}\mathbf{q} \equiv P(S), \quad (9)$$

where

$$G_{\mathbf{q}} = \begin{pmatrix} G^c_{\mathbf{q}} & 0 \\ 0 & G^v_{\mathbf{q}} \end{pmatrix} \text{ and } S = \{S_{\mathbf{q}},\ \mathbf{q}\in\mathcal{B}\}. \quad (10)$$

To close the system, we now look for the time evolution of $S_{\mathbf{q}}$, for each $\mathbf{q}\in\mathcal{B}$:
- making explicit the commutators between H^{e-ph} and the other Hamiltonians,
- using the Wick theorem to approximate the means involving four operators.

After computations, we obtain

$$i\hbar\partial_t S_{\mathbf{q}}|_{e-ph} = E_{\mathbf{q}} S_{\mathbf{q}} + \frac{1}{2}\{G^*_{\mathbf{q}}, \rho\} + (\frac{1}{2} + n_{\mathbf{q}})[G^*_{\mathbf{q}}, \rho] + C(\rho, G^*_{\mathbf{q}}) \equiv E_{\mathbf{q}} S_{\mathbf{q}} + Q_{\mathbf{q}}(\rho) \quad (11)$$

where
- $\{A, B\}$ denotes the skew-commutator $AB + BA$,
- $n_{\mathbf{q}}$ is the phonon density expressed in terms of the phonon energy $E_{\mathbf{q}}$
  by the Bose–Einstein statistics,
- $C(\rho, G^*_{\mathbf{q}})$ is a non-linear term expressed as

$$C(\rho, G^*_{\mathbf{q}}) = -\widetilde{\rho} G^*_{\mathbf{q}} \widetilde{\rho} + \mathrm{Tr}(G^*_{\mathbf{q}}\widetilde{\rho})\widetilde{\rho}$$

where $\widetilde{\rho} = \rho \begin{pmatrix} I^c & 0 \\ 0 & -I^v \end{pmatrix}$, $I^{c/v}$ being the conduction/valence identity matrices.

Final e–ph Bloch model

To summarize, the e-ph Bloch model consists in coupling an equation on ρ

$$i\hbar\partial_t\rho = [E_0 + \mathbf{E}\cdot\mathbf{M}, \rho] + P(S) \quad (12)$$

with a set of equations on phonon-assisted densities $S_{\mathbf{q}}$ (one for each $\mathbf{q}$)

$$i\hbar\partial_t S_{\mathbf{q}} = E_{\mathbf{q}} S_{\mathbf{q}} + [E_0 + \mathbf{E}\cdot\mathbf{M}, S_{\mathbf{q}}] + Q_{\mathbf{q}}(\rho). \quad (13)$$

Numerical issues and e–ph simulations

Discretization

We consider a collection of quantum dots scattered in a one dimensional space along the z direction.

We introduce a uniform discretization of phonon modes using $N_{\mathbf{q}}$ points and integrals over $\mathbf{q}$ are approximated by a simple quadrature formula.

$\Rightarrow$ We compute $N_{\mathbf{q}}$ densities $S_{\mathbf{q}}$ solving $N_{\mathbf{q}}$ independent equations (13).

A finite difference Yee scheme is used for Maxwell equations (3)-(4):

$$B^{n+\frac{1}{2}}_{y,j+\frac{1}{2}} = B^{n-\frac{1}{2}}_{y,j+\frac{1}{2}} - \frac{\delta t}{\delta z}(E^n_{x,j+1} - E^n_{x,j}), \quad (14)$$

$$E^{n+1}_{x,j} = E^n_{x,j} - c^2\frac{\delta t}{\delta z}(B^{n+\frac{1}{2}}_{y,j+\frac{1}{2}} - B^{n+\frac{1}{2}}_{y,j-\frac{1}{2}}) - \mu_0 c^2 \delta t J^{n+\frac{1}{2}}_{x,j}, \quad (15)$$

with $B^{-\frac{1}{2}}_{y,j+\frac{1}{2}} = 0$, $E^0_{x,j}$ given and $J^{n+\frac{1}{2}}_{x,j} = -\frac{in_a}{\hbar}Tr\Big(M_x\Big[E_0, \rho_j^{n+\frac{1}{2}}\Big] + M_x P(S_j^n)\Big)$.

Equations (12)-(13) are discretized on a staggered grid in time and each equation is solved using a Strang splitting procedure:

$$S^{n+1}_{\mathbf{q},j} = \mathcal{A}_3\Big(\frac{\delta t}{2}, E_{\mathbf{q}} I\Big)\mathcal{A}_2\Big(\frac{\delta t}{2}, E_0 + \frac{E^n_{x,j} + E^{n+1}_{x,j}}{2} M_x\Big) \quad (16)$$
$$\mathcal{A}_1\Big(\delta t, Q_{\mathbf{q}}(\rho_j^{n+\frac{1}{2}})\Big)\mathcal{A}_2\Big(\frac{\delta t}{2}, E_0 + \frac{E^n_{x,j} + E^{n+1}_{x,j}}{2} M_x\Big)\mathcal{A}_3\Big(\frac{\delta t}{2}, E_{\mathbf{q}} I\Big) S^n_{\mathbf{q},j},$$

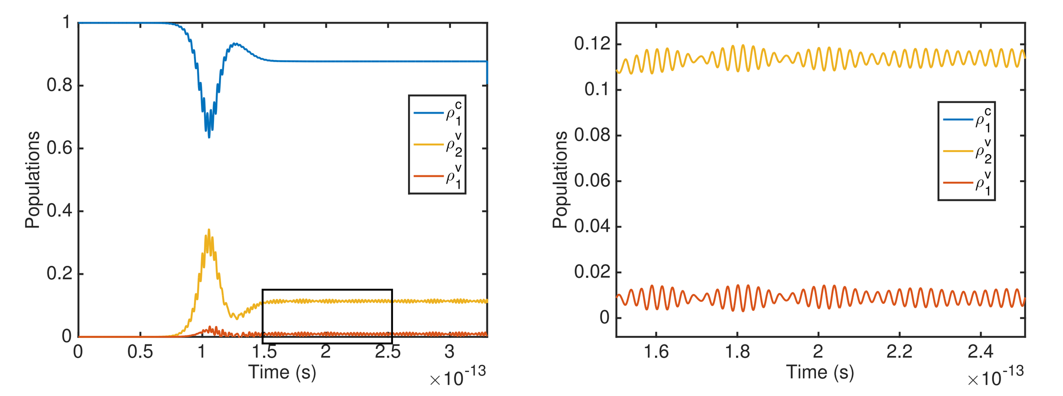
$$\rho_j^{n+\frac{3}{2}} = \mathcal{A}_2\Big(\frac{\delta t}{2}, E_0 + E^{n+1}_{x,j} M_x\Big)\mathcal{A}_1\Big(\delta t, P(S_j^{n+1})\Big)\mathcal{A}_2\Big(\frac{\delta t}{2}, E_0 + E^{n+1}_{x,j} M_x\Big)\rho_j^{n+\frac{1}{2}}, \quad (17)$$

initialized by $S^0_{\mathbf{q},j} = 0$ and $\rho_j^{\frac{1}{2}} = \mathcal{A}_2\Big(\frac{\delta t}{2}, E_0 + E^0_{x,j} M_x\Big)\rho^0_j$. In these expressions, $\mathcal{A}_1$, $\mathcal{A}_2$ and $\mathcal{A}_3$ are three semigroups defined by

$$\mathcal{A}_1(t, B)A = A - \frac{it}{\hbar}B, \quad \mathcal{A}_2(t, B)A = e^{-\frac{itB}{\hbar}} A e^{\frac{itB}{\hbar}} \quad \text{and} \quad \mathcal{A}_3(t, B)A = e^{-\frac{itB}{\hbar}} A.$$

Scattering term effects

We consider the 3-level test case with $\epsilon_1^c - \epsilon_2^v = \hbar\omega_0$ and $\epsilon_2^v - \epsilon_1^v = 2\hbar\omega_0$.



Time evolution of populations for $N_{\mathbf{q}} = 100$ (left) and zoom inside the rectangle (right).

e-ph interactions destroy the SIT phenomenon, even for valence levels far apart enough. In addition to a relaxation behavior, fast oscillations are generated for the two valence levels and persist after the electromagnetic pulse.

Conclusion / Perspective

To study the interaction of quantum dots with an electromagnetic field taking into account e-ph interactions, we proposed an efficient discretization for the coupling between the equation on ρ and the set of equations on $S_{\mathbf{q}}$.

In the future, we would like to take into account, via a kinetic equation, the quantum-well wetting layer into which the quantum dots are embedded.

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