TIME-DEPENDENT DESCRIPTION OF QUANTUM INTERFERENCE NANOTRANSISTOR

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Received 30 April 2012; accepted 05 May 2012

1. Introduction

Basic understanding of DC currents through nanoscale molecular junctions or nanojunctions (NJ) is provided by Landauer-Büttiker formalism [1]. A more general and very powerful approach is offered by non-equilibrium Green's functions formalism [2] which uses self-energies to account for effects of conductors (leads) attached to the NJ. In these approaches, a nanoscale system (which sets the bottom limit on the overall resistance) is described so that most important physical effects including the quantum ones are included. It is important to realise that the small system has open boundary conditions with electrons coming into and leaving out from the NJ. Temporal domain – i.e. description of time-dependence of induced electric current due to a general time-dependent bias and/or other perturbation – has been approached by time-dependent density-functional theory (TDDFT) [3]. The open boundary conditions however place a significant complication which makes this approach difficult.

In this contribution we use our original approach [4, 5, 6] to time-dependent quantum transport and demonstrate it on an atomistic model of quantum-interference effect transistor (QuIET). Proposed devices of this kind have ring shape and nanoscale size and have been proposed in Refs. [7, 8]. An atomistic ring structure – in simplest case a benzene molecule – is embedded between the source and drain leads. The basic principle of operation of such elements is the quantum interference effect between electron amplitudes propagating in the two ring branches. Nanoscale rings of this kind have been studied by several groups of authors in stationary regimes. The most important outcome of these studies is determination of which ring structures are insulating and which are conducting. Particularly simple and practical results have been provided in Ref. [9]. The authors have shown that rings consisting from an even number of atoms can be both conducting and insulating, depending on the mutual position of source and drain attachment sites (vertices). Explicit results for multibranch devices have been found in Ref. [10].

Major unique feature of our approach is its ability to perform explicit time-dependent simulations of electron propagation through systems with open boundary conditions. This is achieved by employment of stroboscopic wave packets [4, 5] which serve as an orthonormal basis set in which electron wavefunctions can be expanded. The method treats electrons either independently or it can include a mean-field interaction.

2. Studied model of the QuIET

Studied model of the QuIET and its attachment to an electric circuit are schematically shown on Fig. 1. It is a semi-quantitative model in which the source and the drain leads are assumed to consist of long conductive monoatomic wires. The central part is the ring. The ring itself is also built from the conducting monoatomic wire. Since we do not have any specific

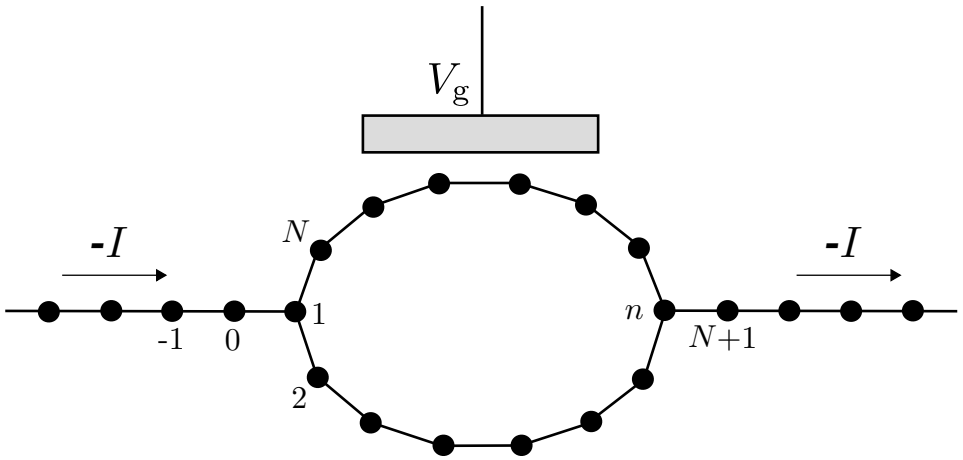

Fig. 1: *Schematic model of an atomistic ring structure in an electric circuit. In the upper part there is the gate electrode. Indexing scheme of individual atoms is shown.* N *denotes the total number of ring atoms and also the index of the atom next to the left (source) vertex site.* n *is the index of the right (drain) vertex site. In actual simulations we use rings having* $N = 20$ *atoms.* n *in the simulations is either 10 (normally insulating configuration) or 11 (normally conducting one). The arrows show the direction of the flow of electrons which is opposite to the conventional direction of electric current.*

reason to introduce unnecessary parameters into the studied model, we assume basic physical parameters (specified below) of the ring atoms to be the same as those of atoms in the leads. The atoms and their interactions are modelled by tight-binding (Hückel) approximation with single orbital per atom. Formal quantum-mechanical description is started defining the Hamiltonian which is

$$\hat{H}(t) = \hat{H}^{\mathrm{peri}} + \hat{H}^{\mathrm{ring}} + \hat{H}^{\mathrm{bias}} + \hat{H}^{\mathrm{gate}}(t) \tag{1}$$

with

$$\hat{H}^{\mathrm{peri}} = \sum_{l=-\infty}^{\infty} \epsilon\, a_l^\dagger a_l + \sum_{l=-\infty}^{\infty} t_{\mathrm{B}} (a_{l+1}^\dagger a_l + a_l^\dagger a_{l+1}) \tag{2}$$

being the periodic infinite chain (1-dimensional crystal or bulk) operator. Here ϵ is the bulk on-site energy and t_{B} is the tight-binding (TB) bulk hopping parameter which is assumed to be negative and its magnitude will be used as the energy unit. Index l runs over all lattice sites. $\hat{H}^{\mathrm{ring}}$ is a modification to the bulk Hamiltonian in order to include the ring system into the model. It has only the following non-vanishing matrix elements in the atomic orbital basis:

$$\begin{array}{rclcrcl} H^{\mathrm{ring}}_{N,N+1} & = & H^{\mathrm{ring}}_{N+1,N} & = & -t_{\mathrm{B}} & & \\ H^{\mathrm{ring}}_{1,N} & = & H^{\mathrm{ring}}_{N,1} & = & t_{\mathrm{B}} & . & \\ H^{\mathrm{ring}}_{n,N+1} & = & H^{\mathrm{ring}}_{N+1,n} & = & t_{\mathrm{B}} & & \end{array} \tag{3}$$

$\hat{H}^{\mathrm{bias}}$ describes effect of applied electric bias. Within the TB model it is simply a proper lifts of the on-site energies. The right-hand-side (drain) lead has its potential set to zero. The left-hand-side lead (source) has an electric bias U applied on. On the source side, the bias is represented by the uniform lift eU of on-site energies of all the atoms in the source lead (e being the magnitude of the electron charge). Impact of the bias on the ring requires special treatment. A fully quantitative approach would necessitate a self-consistent determination of $\hat{H}^{\mathrm{bias}}$. In our semi-quantitative model we have lifted energies of the ring atoms by half of the bias value as can be

seen from the following formula:

$$H_{l,l'}^{\rm bias} = \begin{cases} eU\ \delta_{l,l'}\ , & l \le 0 \quad \text{(in the left lead)} \\ \frac{1}{2}eU\ \delta_{l,l'}\ , & 1 \le l \le N \quad \text{(within the ring)} \\ 0\ , & \text{all other } l, l' \end{cases} . \tag{4}$$

Finally we have the contribution $\hat{H}^{\rm gate}(t) = e\hat{V}_{\rm g}(t)$ which describes an effect of a gate potential applied to the upper ring branch. As we wish to simulate an effect of a gate field switching on and off, $\hat{H}^{\rm gate}(t)$ is a time-dependent contribution. We could similarly use a time-dependent $\hat{H}^{\rm bias}$ (which is not the case in the present work though).

Devices of the kind described above are expected not to remain theoretical concepts. The basic building block – the ring – can be realized by employment of an aromatic molecule like benzene. (The hydrogen atoms bound to carbons need not be considered in a simplified theoretical description like that sketched above.) This would provide effectively a 6-atom ring. Larger rings can be formed for example using conducting polymers [7]. The leads can be attached via thiolate bonds (sulphur atoms). The gate potential is expected to be realized by an approaching STM tip in close vicinity of the ring.

Quantum dynamics of electrons in the whole system is described by Schrödinger equation (SchE)

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = \hat{H}(t)|\psi(t)\rangle\ . \tag{5}$$

using the independent-electron model. (A model mean field could also be used within out method). Wavefunction $\psi(t)$ of each electron is expanded in the unitarily propagating stroboscopic basis set [5]. Having the wavefunction available (after the SchE is solved) we can calculate electric current contribution of one electron. The total current is obtained by summing up the contributions from all electrons in the system. For details see Ref. [6]. The current is a spatially resolved. In stationary situations it would however loose its the spatial dependence far in the leads.

3. Results

A complete simulation leading to results presented below consists of several stages. (i) In the first stage we let evolve the system under the effect of a constant electric bias here chosen $U = 0.4\,|t_{\rm B}|/e$. During this time ($500\,\hbar/|t_{\rm B}|$) a quasistationary current is established (Fig. 1). (ii) At time $t_{\rm on} = 500$ units we turn on the gate potential with the exponential time dependence described below. (iii) At time $t_{\rm off} = 1000$ units we turn off the gate potential, again with an exponential temporal dependence. The overall time-dependence is described by

$$V_{\rm g}(t) = \begin{cases} 0, & t < t_{\rm on} \\ V_0\, e^{-s(t-t_{\rm on})}, & t_{\rm on} \le t \le t_{\rm off} \\ V_0\, \left[1 - e^{-s(t-t_{\rm on})}\right], & t > t_{\rm off} \end{cases} \tag{6}$$

where s is the gate switching speed. We use two finite values of s: 0.02 and 0.10 of $|t_{\rm B}|/\hbar$. In addition we simulate also an ideal rectangular gate switch on-off, which mathematically corresponds to an infinite value of the speed s. As for the gate field amplitude, we use $eV_0 = 0.51\,|t_{\rm B}|$ for the normally insulating ($n = 10$) ring and $eV_0 = 0.62\,|t_{\rm B}|$ for the normally conducting ($n = 11$) ring. These value maximise the switching effect for given ring structure as obtained from the stationary analysis using formulas derived in Ref. [10].

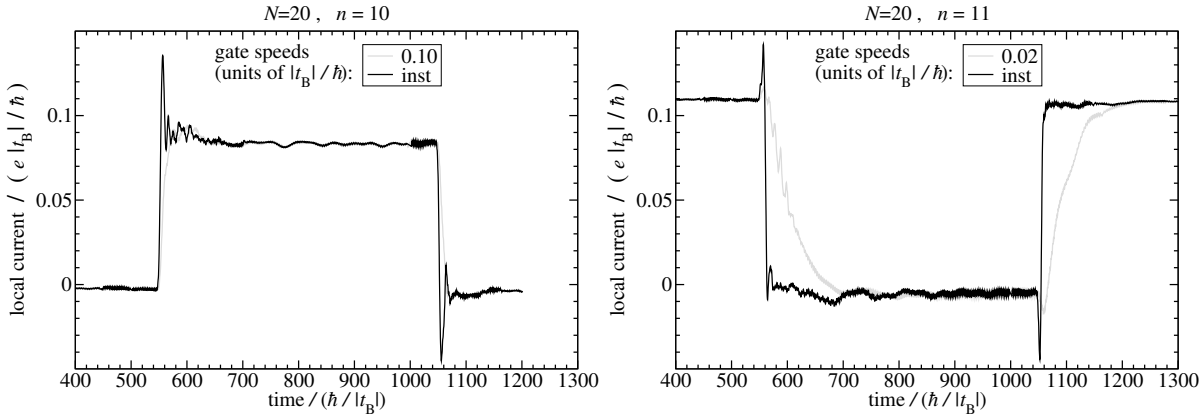

Fig. 2: *Electron currents through the two ring configurations response to gate operation. Electric bias is stationary and equal to* $U = 0.4\,|t_{\mathrm{B}}|/e$*. In the left panel (*$n = 10$*) we use the amplitude of the gate potential* $V_0 = 0.51\,|t_{\mathrm{B}}|/e$*. In the right panel (*$n = 11$*) we use* $V_0 = 0.62\,|t_{\mathrm{B}}|/e$*. See text for more details.*

As a main outcome from the simulations, we compute the electron current in the leads; it is a spatially resolved current and it has positive sign defined by the flow of electrons (i.e. not positive charge). It is computed from time-dependent wavefunctions of all electrons in the system. Despite the spatial dependence, main features of the current do not depend dramatically on chosen observation point, apart from a time delay due to finite propagation speed of electrons. The results are presented on Fig. 2. The left panel shows currents for the ring with $N = 20$ sites and the right lead attached to site $n = 10$. It is the case of normally insulating ring junction. There is no electric current for times $t < t_{\mathrm{on}}$, i.e. at normal conditions (gate field off) which is the result of destructive quantum interference between the electron amplitudes in the lower and upper ring branches. As soon as the gate potential is turned on we observe the formation of current through the device. Thanks to the interference as the principle of the operation, the response to the applied gate field is very fast. In our simplified model the characteristic times are on optical timescale. The limiting factor in real setups would be the speed of the gate switching mechanism which can not be arbitrarily fast. The response of the device to the applied gate field would not present a limiting factor to the device's overall performance.

Because the interference pattern depends on the lengths of the interfering paths, the situation differs when we use different drain vertex (site) while keeping the source fixed. Attaching the drain to site $n = 11$ makes the ring conducting under normal (non-gated) operation [9]. What is now the effect of the applied gate potential is shown on the right panel of Fig. 2. The potential now has its maximum $V_0 = 0.62\,|t_{\mathrm{B}}|/e$. We see the operation of the $n = 11$ device is quite complementary to the $n = 10$ ring.

The tiny rapid oscillations in the displayed plots result from the finite cutoff on the number of basis set functions; we use 2820 wavepackets forming our basis set [6]. The plots exhibit the oscillations even those have been in most part suppressed by a proper smoothing procedure.

4. Conclusion

In this contribution we have presented simulations of electron current response to applied gate potentials in a ring-shaped quantum interference device which has been proposed in

works [7, 8]. Such device could function like a current-switching quantum-interference transistor. We demonstrated capability of our approach to describe this kind of system keeping full quantum coherence in the description for extended periods of time. This have been achieved thanks to the unique feature of our method which allows for explicit simulations of small quantum subsystems with open boundary conditions. Further generalisation of the method is needed to reduce the number of basis set functions required to describe the system.

Acknowledgements
This work was supported by the Slovak Grant Agency for Science through Grants No. 2/0192/10 and 1/0632/10.

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