TWO MODELS OF QUANTUM BRIDGES CONNECTED WITH SEMICONDUCTORS OR METALS

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Abstract

It is proposed two models describing transport and absorption processes that occur in nanoscale fragments of electrical circuits, pulled adsorbed molecules, atomic or molecular chains connecting electrodes. Discrete chain model of a molecular bridge between metallic electrodes considers quantum jumps between atoms containing the chain. A potential approach is represented by three-dimensional Kronig-Penney model. The conductivity theory is developed in a supposition that the main contribution into the electron transfer belongs to non-equilibrium affinity populated states of the bridge. Current-voltage and thermodynamical characteristics are calculated for different cases. Explanations for experimentally obtained step-like dependencies in I-V characteristics and its asymmetry are made. The charging effect and Coulomb blockade effect are discussed. It is shown the essential role of transitions between different bridge’s charge states.
1 I. Introduction

Semiconductor wires, pulled linear molecules, point contact atomic chains connected with prepared metal or semiconductor surface are examples of quantum fragments embedded into electric circuits [1, 2, 3, 4, 5, 6, 7, 8]. These elements may play a role of main functional unites of the circuit sufficiently determining its properties. The most important property of such "bottle neck"-like fragments is that electronic structure depends strongly on small number of captured electrons is the subject of our investigation. Statistically quantum bridges are systems with alternating particles number determined by interaction with contacting reservoir. In recent paper [3] the conductivity of adsorbed bistertiothene molecule junction (fig.1) fabricated by suspended micro-bridges technique combined with mechanically controlled break method was studied experimentally. The results obtained have shown several interesting features including stepwise dependence of current-voltage characteristics and sometimes its asymmetry relatively the sign of applied voltage. An example of pure quantum circuit is represented in fig.2a. The role of short pulse voltage source can play a polar molecule embedded into the closed chain. Quantum voltage source polarization may be controlled by resonant external electromagnetic field switching the molecule into long lived triplet state. The current pulse arising is caused by the difference of dipole moments in ground and excited states. The stabilization of excited state may be implemented by means of voltage bias between ends of the molecule (fig.1). Transition process in excited state modifies affinity spectrum of the molecule that in turn influences on the electron transport through the molecular bridge. Our results show that the voltage applied modifies significantly the electronic structure of all kinds of bridges and leads to nonequilibrium redistribution of states population. The theory developed here for contact and transport phenomena in quantum bridges is based on the conception of mesoscopic system's charge states. Two approaches are discussed in the work for pulled quantum bridges: potential model and discrete chain model (DCM). Potential model proposed describes semiconductor quantum wire connecting semiconductor or metal electrodes is shown in figure 3. The model is based on exactly solved problem for terminated Kronig-Penney crystal. The DCM approach describing molecular or atomic bridges starts from initial (atomic) generalized affinity energy $E_i$ for external reservoir electron, chain geometry and intersite transfer matrix elements $V_i$ (fig.4). Index i represents the number of electrons left the chain, $E_i$ is the exited states band center for one-fold ionized molecule. Quantum bridge capturing or losing electrons in absorbing process or due to applied voltage changes weakly its charge states $M^{(i)}$ [3, 8]. General picture of charge state transitions for ionized quantum bridge contacting with metal surface is represented in the figure 3, where $\chi$ is electrode chemical potential, $I_1$ is the first ionization potential, $I_0$ is affinity energy. Pulled linear molecular chains adsorbed on prepared metal or semiconductor surface may be very interesting due to its physical properties and possible applications. Extremely large effective surface of these objects (Fig. 5) in case its density is sufficiently high makes them attractive as adsorbing elements for gaseous sensors. We have proposed in [3, 7] to use the forest of molecular chains directed by external electric field for adsorbing, storage and testing small concentration of gas molecules in surrounding medium. Adsorbed long molecular constructions are most compact and small contenders for conducting elements of quantum circuits, STM tips and neural networks.
Meanwhile many properties of 1D systems absorbed in electric field on a semiconductor or dielectric surface demand further theoretical investigations: the conductivity problem at low frequencies, chain-surface local states and states arising due to the capture of air molecules by the chain, electron energy spectrum in external field, mobility of electrons, affinity spectrum, chain topology, interaction with vibrational modes etc. In the paper we propose a theoretical consideration for some of these problems. Our DCM analysis is based on the electron Hamiltonian for a chain with N-sites. The conductivity of quantum bridges is investigated theoretically using obtained exact solutions for electron states of a linear chain in steady state electric field. It is taken into account quantum interaction between electronic subsystem and either metallic or semiconductor electrodes playing the role of electrons reservoirs. In the ground of theory proposed lies the supposition about main contribution of affinity states into the conductivity of point contacts both semiconductor wires and molecular or atomic junctions. Transfer matrix method was used out the framework of approximation of translation invariance and periodic boundary conditions. In nearest-neighbor approximation for chain atoms interaction and hopping probability the current-voltage characteristics are calculated at different temperatures and electronic structures of the chain. The Coulomb blockade effect is taken into account phenomenologically in a self-consisted procedure. It is represented the explanation of current-voltage asymmetry observed experimentally in [3]. It is shown the leading role of field modification of affinity spectrum for conductivity of molecular bridges. Irreversible states population and current Coulomb charging is calculated.

2 II. An adsorbed linear molecule in electric field.

We will describe the problem of field influence using secondary quantization Hamiltonian for a trapped electron in N-periodic linear chain (Fig.2b)

$$\hat{H}_0 = \sum_{k,j} \varepsilon_{kj} a^+_k a_j + \sum_{k,j,m,i} V_{km}^{ij} a^+_k a_{mi}$$

$$\varepsilon_{kj} = \varepsilon_{0j} + \varepsilon ekd + \varepsilon ed_l$$

where k numbers elementary cells, d marks distance between atoms along the chain, j numbers atoms in the elementary cell, $\varepsilon_j$ determine initial atomic affinity levels, the hermitian matrix $V_{nm}^{ij}$ describes interatomic electron transfer, $d_l$ is the length of absorption bonds on the left-hand side of linear molecule, $\varepsilon$ represents applied electric field. The matrix of Hamiltonian (1) will be wrote in nearest neighbour approximation for an adsorbed molecular chain like polyacetylene $R-(CH)_n-R$. In the model under consideration the transfer between elementary cells is possible through carbon atoms only; the amplitude of the process equals W, hopping amplitudes inside elementary cells equals V ( Q is its value for end atoms). Considering $U = \varepsilon (Nd-d+dl)$ as the whole voltage between chain ends we can obtain the energy dispersion equation

$$\left(\lambda, -\nu_l\right) \prod_{k=2}^{N-1} \hat{\Lambda}_k \left( \frac{\nu'_r}{\lambda'_r} \right) = 0$$
\[ \hat{\Lambda}_k = \begin{pmatrix} \mu_k & \nu_k \\ \lambda_k & 0 \end{pmatrix} \]

containing transfer matrix product instead of transfer matrix power. Here

\[ \mu_k = (\varepsilon_0 - E + \varepsilon ekd + \varepsilon ed_t)(\varepsilon_1 - E + \varepsilon ekd + \varepsilon ed_l) - V^2 \]

\[ \nu_k = -\lambda_k = W \cdot (\varepsilon_0 - E + \varepsilon ekd + \varepsilon ed_t) \]

\[ \nu'_r = (\varepsilon_0 - E + U - \varepsilon ed_r)((\varepsilon_0 - E + U - \varepsilon ed_r)(\varepsilon_1 - E + U - \varepsilon ed_r) - 2Q^2 \]

\[ \lambda'_r = -W \cdot (\varepsilon_0 - E + U - \varepsilon ed_r)^2 \] (4)

Using canonical transformation and the procedure described in [3] the equation (3) is transformed to convenient view obtained in absence of external field.

\[ e^{f_1}(\nu_r y_{22} - \lambda_r y_{21})(\nu_0 y_{11} - \nu_0 y_{12}) - e^{f_2}(\nu_r y_{12} - \lambda_r y_{11})(\nu_0 y_{21} - \nu_0 y_{22}) = 0 \] (5)

where \( f_1 \) and \( f_2 = -f_1 \) are eigenvalues of matrix \( \hat{F} \) in the power of exponent

\[ \hat{F} = Ln(\prod_k \hat{\Lambda}_k) \]

\[ \prod_{k=2}^{N-1} \hat{\Lambda}_k = \exp \left( \sum_k \left( \frac{\lambda_k^1 \ln \lambda_k^2 - \lambda_k^3 \ln \lambda_k^4}{\lambda_k^3 - \lambda_k^4} \ln \lambda_k^5 - \ln \lambda_k^6 \right) \right) \] (6)

Here \( \lambda_k^i = (\mu_k + (\mu_k^2 + 4\lambda_k \nu_k)^{1/2})/2 \) are eigenvalues of transfer matrix taking part in the product. The condition \( \mu_k^2 + 4\lambda_k \nu_k = 0 \) determines imagine boundary between extended band states and that localised due to the influence of extended field. As another matter for the states localization may serve structure defects including both ends of the chain. The calculations show that with the growth of electric field \( \varepsilon \) the extended states energy range is narrowed in directions from band edges to the middle. At the same time the band width increases to the value of applied voltage \( U \). The last extended states transforms to localized ones when \( U \) exceeds starting band width. The distribution of the electron density amplitudes along the chain is given by eigenvectors of the problem solved above. The model under consideration (DCM) allows to obtain analytical expressions for eigenvectors determined by coefficients \( C_{kj} \) of the canonical transformation

\[ a^+_s = \sum_{k,j} C_{kj}^+(s)a^+_{kj} \]

\[ a_s = \sum_{k,j} C_{kj}^+(s)a_{kj} \]

The summation is performed on chain cells \( k \) and on atoms \( j \) inside the elementary cell. Index \( s=1,2,...,N \) numbers in the work the electron affinity states. One can obtain the coefficients \( C_{ij} \) analytically using well known Kramer’s rule and revealing determinants corresponded to each variable.

\[ C_{k1} = d_{k-1} \cdot QV \prod_{i=k+1}^{N} (-\varepsilon_0, W) \] (7)
\[ C_{k2} = C_{k1} \frac{V}{E_s - \varepsilon_0} \]

\[ d_{k-1} = \frac{1}{\Theta_{k-3}} (e^{f_{k-3}}(\nu_r y_{22} - \lambda_r y_{21})(\lambda_0 y_{11} - \nu_0 y_{12}) - e^{-f_{k-3}}(\nu_r y_{12} - \lambda_r y_{11})(\lambda_0 y_{21} - \nu_0 y_{22})) \quad (8) \]

The determinants of k-order \( \Theta_k \) are determined by the left upper edge of the Hamiltonian dynamic matrix described in (1). Numerical calculations for electron density \( |C_{kj}(s, i)|^2 \) both with the account of field dependence in transfer matrix elements \( V \) and without that influence was performed in [5]. With the growth of applied voltage the standing probability waves \( |C_{kj}(s, i)|^2 \) become less symmetric (or anti-symmetric) respectively the center of the linear molecule. At the same time, the interatomic barriers begin to decrease at sufficiently great fields ( \( 10^9 \text{ V/m} \) ) that leads to repairing of the symmetry in electron density distribution.

### 3 III. Electronic specific heat of adsorbed molecules.

The contribution of affinity electrons captured by a free molecule into the specific heat \( C_{aff} \) is determined by expression

\[ C_{aff} = T^{-2} \sum_s [(E_s - E_1)^2 n_s(1 - n_s)] \quad (9) \]

where \( n_s = (\exp(\frac{E_s - E_1}{T}) + 1)^{-1} \), \( E_1 \) marks the lowest level that plays the role of system chemical potential. The temperature dependence of \( C_{aff} \) calculated by (9) in absence of electric field for a long 20-atomic chain is represented in fig.6, curve 1. Energy parameters of the chain were taken \( \varepsilon_0 = -4.3 \text{ eV}, V = 0.02 \text{ eV} \). In case of an adsorbed molecule its specific heat \( C_{aff} \) depends on affinity band position relatively the surface chemical potential. We suppose here that the latter coincides with band center \( \chi_1 = \varepsilon_0 \). In case all levels lying below \( \chi_1 \) the states are filling completely by left reservoir electrons. The curve 2 in fig.6 shows \( C_{aff} \) temperature dependence for molecules adsorbed in external electric field \( U = 0.5 \text{ V/molecule} \) on a gold surface \( \chi_1 = -4.3 \text{ eV} \) calculated by (9) at \( E_1 = \chi_1 \). We do not take into account the Coulomb blockade effect in specific heat calculations. It should be marked that external (negative) electric field is significant stabilizing factor, which allow linear molecule to contact with adsorbing surface by left or right end only. Field absence may cause the capture of a molecule by the surface due to attracting image forces with molecule following reconstruction. Negative electric field interacting with dipole momentum arising in chain due to its charging pulls molecule normally to the surface (fig.5). Opposite field direction vice versa overturn the molecule on adsorbing surface. Changing electric field may influence strongly on molecular strain and orientation that is on the effective volume of molecular forest. To compare we consider the same chain connecting two gold electrodes having different potentials. At room temperature \( T = 0.025 \text{ eV} \) calculations give falling \( C_{aff} \) dependence on applied voltage \( U \) (fig.5, curve 3). The maxims observed are well known thermodynamic Shottky anomalies.
4 IV. Semiconductor quantum wire in electric field.

To describe contact and transport phenomena in semiconductor quantum wires we used exactly solvable 3D Kronig-Penney model with open boundary conditions. The proposed potential model describing quantum bridge with sizes 20x20x100 elementary cells is based on exact solution for terminated 1D Kronig-Penney crystal with $\delta$-functional barriers (Dirac’comb potential) obtained in [14] without using of translation invariant approximation. One-dimensional model crystal contains N wells of width $a$, deep $U_0$ and opaque coefficient $\Omega$. As a result of superposition of the same potential in three dimensions it is obtained a separable 3D potential shown in fig.7. The summation of superposing combs creates suitable system of 3D wells and barriers inside the crystal volume but there arises simultaneously a potential $\Delta U(x, y, z)$ additional to crystal one. In different ranges $\Delta U(x, y, z)$ takes values $U_0$, $2U_0$ and combinations of $U_0$ and alternating barriers $\Omega$ (fig.7). The Hamiltonian of the problem may be represented as

$$\hat{H} = \hat{H}_0(x, y, z) - \Delta U(x, y, z),$$

where

$$\hat{H}_0(x, y, z) = \hat{H}_{ox} + \hat{H}_{oy} + \hat{H}_{oz}$$

where $H_0$ is separable part of entire Hamiltonian. The main idea of the method proposed is based on the fact that corrections to zero-order results are small because of wave function’s tails in additional ranges of $\Delta U(x, y, z)$ are asymptotically small for band states and to some extent for deep local states. Zero wave function is represented in a view of product

$$\tilde{\Psi}_0(x, y, z) = \tilde{\Psi}_{ox}(x)\tilde{\Psi}_{oy}(y)\tilde{\Psi}_{oz}(z)$$

where $\tilde{\Psi}_{ox}(x)$, $\tilde{\Psi}_{oy}(y)$, $\tilde{\Psi}_{oz}(z)$ are 1D solutions obtained exactly in [14]. Non-additive addition leads to asymptotically small corrections for band states. We have studied GaAs and AlGaAs quantum bridges between metallic electrodes using active computer designer of hierarchical structures (ACDHS) which allows to built and to calculate different potential well systems both periodical and hierarchical. Electric field modifies states of semiconductor quantum bridge similar to considered above molecular chains. Let we consider GaAs quantum bridge of length 199.15 Å connecting metallic electrodes in steady state electric field with intensity $\varepsilon$. The Kronig-Penney crystal parameters in case of GaAs satisfying to its affinity energy are $U_0=1.2278$ eV, $\Omega a = -0.215$, $a=5.69$ Å. Taking into account the GaAs band gap value $E_g=1.52$ eV we will consider voltage bias small enough to avoid interband transfer $\varepsilon L \ll E_g$, where L is the crystal length. Calculations by means of ACDHC give band structure, band position and distribution of electron density in different exited states. Figure 8a shows the system geometry and relative positions of energy bands in semiconductor wire and in metal. Figures 8b and 8c represent electron density distribution near the band bottom and top, respectively. The field applied manifests itself in states modification leading to electron density drive away from left-hand or right-hand shores.
5 V. Conductivity of quantum bridges.

Theoretical analyze of bridge conductivity is based mainly on two approaches. Landauer wave model [10, 11] interprets the molecular junction as a scattering center reflecting electronic waves moving from cathode. Electrical current is proportional either to transmission coefficient of the electronic wave near the Fermi energy of the electrode or to some integral of the transmission in a proper energy range [3, 10, 11]. Calculations of linear conductance in wave model give a more intensive current in comparison with experimental data [3, 10, 11]. As it was shown in [5] this effect is the consequence of both neglecting by spectrum field modification and by important role of molecular affinity charge states.

The kinetic (sequential) conductivity model [3, 12, 13] operates by a phenomenological transfer rate describing threefold tunneling processes of electron’s jumps between a cathode and a couple of molecular states. Though calculations of conductance in kinetic model for gold-bistertiothene-gold contact [3] gave a good agreement with the experiment as to the values order and reflects main features of current voltage dependencies, we suppose the theoretical grounds of the model leaves much to be desired due to the independent physical meaning of threefold processes. We will consider below the conductivity of molecular bridge in DCM. The bridge electron subsystem relation with the electrodes manifests itself in nonzero possibility amplitude of electron transfer onto the molecule. Respective addition to the Hamiltonian

\[
\hat{H}_{ad} = G_l \cdot (a_l^+ a_{10} + a_{10}^+ a_l) + G_r \cdot (a_r^+ a_{N,0} + a_{N,0}^+ a_r)
\]  

contains jump amplitudes \(G_{l,r}\) between metallic shores and end atoms of the chain. Indexes \(l,r\) correspond to left and right shores, respectively. In case of an adsorbed molecule (11) contains only one term. The model presented determines electronic structure of metallic electrodes by density of states

\[
g(\varepsilon_{r,l}) = \frac{4\pi H}{\hbar^3} (2m)^{3/2} \varepsilon_{r,l}^{1/2}
\]

where \(H\) is effective volume of the electrode contacting the molecule, \(m\) is electron effective mass, \(\varepsilon_{r,l} = E_{Frl} - \chi(r,l) + E_{sj} + U_{l,r}\) expresses the state energy \(E_{sj}\), measured from the beginning of electrode’s Fermi-stage with account of the bias value \(U_{l,r}\). \(E_{Frl}\) marks right or left Fermi-energy. Both chemical potential \(\chi_{x,l}\) and energy \(E_{sj}\) are measured respective to vacuum level accepted to be zero (Fig.4). Due to the field widening of the discrete energy band the affinity levels pass sequentially the active ranges near Fermi surfaces of both shores. Each pass corresponds to the current sharp increasing in I-V dependence. There is a current dependence on the density of states both left-hand and right-hand electrodes. This effect is significant one in case of semiconductor shores. Intrinsisic phonons (or vibrons) influence weakly on the electron transfer and non-equilibrium states population putting in a molecule with current [6]. The shores play the role of infinite thermodynamically balanced reservoirs of electrons. Equilibrium populations of baths’ electronic states are described by the Fermi distribution. In model under consideration the injected electron occupies either one of the affinity states \(E_{sj}\) or one of vibrational sublevels. The possibility rate of the process can be expressed in second order of perturbation theory using well known Fermi golden rule. We suppose the weak absorption contact plays the role of
a small parameter. We will consider the phononless contribution into the conductivity. Then one can obtain from the coinciding for left end and right end electronic currents through bridge’s sj- state the entire current $I$ through the junction

$$I = \frac{2\pi e}{h} \sum_{s,j} |G_{l,sj}|^2 |G_{r,sj}|^2 g_l(E_{sj} - \chi_l + E_{F_l} + U_l) \cdot g_r(E_{sj} - \chi_r + E_{F_r} + U_r) \cdot \frac{(N_l - N_r)}{(|G_{l,sj}|^2 g_l(E_{sj} - \chi_l + E_{F_l} + U_l) + |G_{r,sj}|^2 g_r(E_{sj} - \chi_r + E_{F_r} + U_r))} \cdot (N_l - N_r)}{(|G_{l,sj}|^2 g_l(E_{sj} - \chi_l + E_{F_l} + U_l) + |G_{r,sj}|^2 g_r(E_{sj} - \chi_r + E_{F_r} + U_r))}$$

(13)

where the summation is performed over all affinity states. The dimensional part of entire current

$$I_0 = \frac{e \cdot (2m)^{3/2} H G^2}{\pi h^4} \cdot (1eV)^{5/2}$$

(14)

where $G$ is the amplitude of the shore-bridge transfer, plays the role of a current unity. Numerical value $I_0$, in case all energies in (13) are measured in eV and the effective volume $H$ is taken in $A^3$, is equal to $10.41 x H G^2$ mkA. The expression obtained takes into account both the difference between materials of left and right electrodes and possible asymmetry of voltage connection in the circuit relatively the vacuum level. In the symmetric case $U_r = -U_l = U/2$, then in case of similar metallic electrodes the current-voltage characteristics is symmetric one relatively the applied voltage. In case the left electrode is earth then one should take in (13) $U_l = 0$ and $U_r = U$. Therefore, the I-V dependence has lost its symmetry relatively the sign of applied voltage. In experimental work [3] it was presented the examples both symmetric and asymmetric I-V characteristics of quantum junctions. Our calculations show that the current value vs voltage depends sufficiently on the distribution of electron densities near ends of the chain $|C_{sj}(l,0)|^2$ and $|C_{sj}(N,0)|^2$ in the standing wave as well as from the difference in metallic shores populations on the absolute energy level $E_{sj}$. The influence of square root energy dependence of state densities $g_l$ and $g_r$ manifests itself not so strongly. An essential fact for understanding the phenomenon of current going through a mesoscopic linear system is that that characteristic temperatures being of order $T \sim 0.02 - 0.03 eV$ are as a rule much less than the distances between levels of bridge affinity band. Therefore with growth of applied voltage $U$ the affinity levels one by one pass through the range near the Fermi surfaces $E_{F_l}$ and $E_{F_r}$ where the transfer become very effective. The entry of each new level into the active range accompanies by sharply increasing of current. The energy pauses between levels cause a plateau I-V dependence. The charging - entire charge trapped by chain has similar behaviour. Below we will analyze taking, for example, a simple chain, the nature of electron transfer through the molecular bridge connecting metal electrodes without taking into account the Coulomb blockade effect. The contact conditions may be so that the external electric field is negligible small at comparatively big voltages. It is the case when a pulled molecule connects the tips of fine electrodes and the drop of voltage occurs in vicinity of molecular ends. External electrical field doesn’t influences the molecular affinity states. The solid line in Fig. 9 shows calculated I-V characteristics for a chain with four starting affinity states at $E_0 = -4.0$ eV, $V = 0.2$ eV, $U_0 = 0.5$ eV, $E = 0.01 eV$ in case of gold electrodes. Dotted line shows the charging effect. One can see the characteristic tendency of fraction and semi-integer
charging the molecule under voltage as the matter of thermodynamically non-equilibrium states population. The almost exactly semi-integer chain’s charge arises at sufficiently low temperatures $T \approx V$, if the energy range $(\chi, \chi + U)$ contains an odd number of affinity states. States laying above the range are unoccupied ones $n_s = 0$, down states are filled completely $n_s = 1$. Immediate states marked in case of symmetric contacts molecule-electrodes have populations $n_s = 1/2$. An additional circumstance important for semi-integer charging effect is approximate equality for electrodes’ density of states $g_r$, $g_l$ (12) small bias $U$ under consideration. Many body character of the problem may be taken into account phenomenologically in a self-consisting procedure including general spectrum shift due to the charging and band widening. We have used for ground state energy $\varepsilon_i$ in $M^{(i)}$-state.

$$\varepsilon_i = \varepsilon_{i+1} + \varphi_i - 2V_{i+1} \exp(\varphi_i/\varphi_{i+1})$$  \hspace{1cm} (15)

Coulomb barrier potentials $\varphi_i$ are determined in a minimization procedure for many electron system of the proper state $M^{(i)}$. Starting from initial charge state $M^{(i)}$ we have for bridge’s many-body energy terms

$$X_1 = \varepsilon_1 - 2V_1 = E_v$$
$$X_0 = 2(\varepsilon_0 - 2V_0)$$
$$X_1 = 3(\varepsilon_{-1} - 2V_{-1})$$
$$X_2 = 4(\varepsilon_{-2} - 2V_{-2})$$  \hspace{1cm} (16)

where $E_v$ is absolute valence band top position of neutral molecule. Using (15) we obtain from (16) the ionization potentials of the chain under consideration

$$I_i = X_i - X_{i-1}$$

Calculations performed in DCM framework show a good agreement with experimental data for ionization potentials of carbon nanosystems and molecular wires I-V characteristics.

6 VI. Conclusion.

Quantum bridges under the current are parametric many-body systems having steady state non-equilibrium distribution. The number of electrons captured by the molecule’s affinity states from outside is controlled by external conditions that determine the molecule charge’s state described by own electronic structure. The discrete chain model considered as well as Kronig-Penney model belong to the number of simplest ones. Nevertheless it allow to take into account in an united formalism the main features of current carrying through the mesoscopic junctions. The cathode electrons at first occupy the system eigenstates and then they transit to anode. The model supposes existing an initial affinity level in each potential well. Due to the finite barriers width there arises a band of states in the system of potential wells. The band structure and its situation relatively the shores chemical potentials determines the current character in framework of given molecular charge’s state. Following charging creates a Coulomb barrier modifying the affinity spectrum. The electron spectrum of neutral molecule $M^0$ begin participate in conductivity in...
case of a single-ionized molecule. These states fills partially by an electron transited from the electrode. With the growth of applied voltage total population may exceed unity. In the case it is switch on the next affinity spectrum $M'$ and so on. In present work the Coulomb charging was taken into account phenomenologically. A more correct approach demands the resolution of a quantum many-body problem for discrete chain with alternative number of particles depending on voltage applied. Both models able to describe low-temperature electron transfer in metallic point contacts. The structures were investigated experimentally in [1, 15] for monoatomic wires between Au, Pt, Al, Nb, Pb, K Na electrodes. The transfer mechanism through affinity states leads also for such systems to stepwise conductance with both positive and negative step slopes. Our models give an other alternative to explain the vanishing of conductivity at sufficiently long distances between electrode’s tips. The matter may be laying in electronic structure transformation lifting due to the Coulomb blockade effect the bottom of conductivity band upper than Fermi level. Quantum fragments of electric circuit plays important role in single electron transistors and ratchets [16]. Though the linear models considered can’t be directly applied to such systems, one should mark the general equivalence between bridges and quantum dots possessing discrete spectrum and contacting with several electrodes.
Figure 1: BISTERTIOPHENE MOLECULE AS A QUANTUM FRAGMENT OF ELECTRIC CIRCUIT INVESTIGATED EXPERIMENTALLY IN [3]
Figure 2: A DIPOLE MOLECULE AS AN EMF SOURCE IN AN ELECTRIC CIRCUIT

a) Complete electric circuit with an inverse asymmetric molecule as voltage source activated by light. DP is the dipole momenta difference in ground and excited states. Zigzag show light causing dipole changing.

b) A model of hydrocarbon linear molecule. W is transfer amplitude between carbon atoms, V is the same inside the elementary cell; Q is the same for end cells.
Figure 3: SEMICONDUCTOR QUANTUM WIRE
a,c mark electrodes, b represents quantum wire, elementary cells are shown by lines.
Figure 4: A SCHEME OF QUANTUM BRIDGE CHARGE STATES
$M_i$ mark quantum bridge charge state with $i$ electrons left the bridge, $I_i$ corresponds to ionization energy of respective state.
Figure 5: THE FOREST OF LINEAR MOLECULES ADSORBED ON CONDUCTING SURFACE
Molecular chain forest on the substrate. Dark colour marks an absorbed gas molecule.
Figure 6: SPECIFIC HEAT TEMPERATURE DEPENDENCE OF A LINEAR CHAIN
Curves 1, 2 show specific heat for free molecule and for adsorbed molecule, respectively (lower axe). Curve 3 (upper axe) is calculated $C_{aff}$ for a molecular bridge under current.
Figure 7: POTENTIAL MODEL OF A QUANTUM WIRE CONNECTING METALLIC CONTACTS
The range 1 is additional potential at parallelepiped tops, range 2 is additional potential at ribs, intrinsic range 3 is semiconductor wire and range 4 represents metallic electrodes.
Figure 8: QUANTUM WIRE IN ELECTRIC FIELD
(a) chain of 35 GaAs potential wells at applied voltage $dU = 0.152 \text{ eV}$, $\chi$ is chemical potential of electrodes, $a = 5.69 \text{ Å}$, $\Omega a = -2.1337$, $U_0 = 1.2278 \text{ eV}$, dotted line marks the level of vacuum. (b, c) electron wave functions of the lower and upper exited states $s=3$, $s=35$ respectively.
Figure 9: A QUANTUM BRIDGE I-V CHARACTERISTICS

$E_0 = -4.0 \text{ eV}$, $V_0 = 0.2 \text{ eV}$, $U_0 = 0.08 \text{ eV}$. Solid line represents current-voltage dependence without charging for intermediate electronic band at $T=116 \text{ K}$; Dotted line shows trapped charge.
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